



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 08:11 AM EDT

PDB ID : 6VYA
Title : Crystal structure of NotF in complex with brevianamide F and DMSPP
Authors : Dan, Q.; Smith, J.L.
Deposited on : 2020-02-25
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

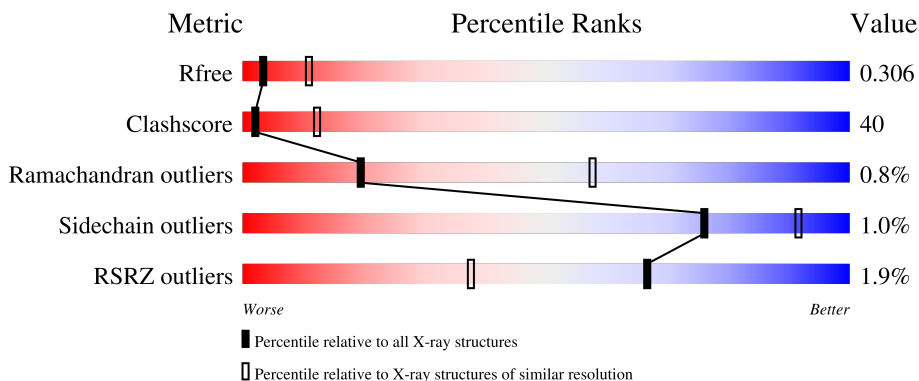
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	472	 37% 43% 18% 2%
1	B	472	 42% 39% 18% 2%
1	C	472	 38% 43% 18% 2%
1	D	472	 35% 45% 18% 2%
1	E	472	 36% 44% 18% 2%

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Mol	Chain	Length	Quality of chain			
1	F	472	%	36%	44%	18%
1	G	472	2%	38%	42%	18%
1	H	472	%	39%	42%	18%
1	I	472	2%	37%	44%	18%
1	J	472	3%	38%	42%	18%
1	K	472	%	37%	44%	18%
1	L	472	2%	38%	42%	18%
1	M	472	%	39%	42%	18%
1	N	472		39%	42%	18%
1	O	472	%	38%	43%	18%
1	P	472	%	38%	43%	18%
1	Q	472	%	38%	43%	18%
1	R	472	2%	37%	43%	18%
1	S	472	2%	39%	41%	18%
1	T	472	%	38%	42%	18%
1	U	472	2%	38%	42%	18%
1	V	472		38%	42%	18%
1	W	472	3%	37%	43%	18%
1	X	472	2%	38%	42%	18%

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
2	QRP	B	501	-	-	X	-
2	QRP	C	501	-	-	X	-
2	QRP	G	501	-	-	X	-
2	QRP	H	501	-	-	X	-
2	QRP	L	501	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	QRP	Q	501	-	-	X	-
2	QRP	R	501	-	-	X	-
2	QRP	X	501	-	-	X	-
3	DST	B	502	-	-	X	X
3	DST	F	502	-	-	X	-
3	DST	K	502	-	-	X	-
3	DST	M	502	-	-	X	-
3	DST	N	502	-	-	X	-
3	DST	O	502	-	-	X	-
3	DST	Q	502	-	-	X	-
3	DST	R	502	-	-	X	-
3	DST	T	502	-	-	X	-
3	DST	U	502	-	-	X	-
3	DST	V	502	-	-	X	-
3	DST	X	502	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 77376 atoms, of which 624 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Deoxybrevianamide E synthase notF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	387	3163	2059	528	569	7	0	0	0
1	A	387	3163	2059	528	569	7	0	0	0
1	V	387	3163	2059	528	569	7	0	0	0
1	E	387	3163	2059	528	569	7	0	0	0
1	G	387	3163	2059	528	569	7	0	0	0
1	B	387	3163	2059	528	569	7	0	0	0
1	D	387	3163	2059	528	569	7	0	0	0
1	F	387	3163	2059	528	569	7	0	0	0
1	H	387	3163	2059	528	569	7	0	0	0
1	I	387	3163	2059	528	569	7	0	0	0
1	J	387	3163	2059	528	569	7	0	0	0
1	K	387	3163	2059	528	569	7	0	0	0
1	L	387	3163	2059	528	569	7	0	0	0
1	M	387	3163	2059	528	569	7	0	0	0
1	N	387	3163	2059	528	569	7	0	0	0
1	O	387	3163	2059	528	569	7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	387	Total	C	N	O	S	0	0	0
			3163	2059	528	569	7			
1	Q	387	Total	C	N	O	S	0	0	0
			3163	2059	528	569	7			
1	R	387	Total	C	N	O	S	0	0	0
			3163	2059	528	569	7			
1	S	387	Total	C	N	O	S	0	0	0
			3163	2059	528	569	7			
1	T	387	Total	C	N	O	S	0	0	0
			3163	2059	528	569	7			
1	U	387	Total	C	N	O	S	0	0	0
			3163	2059	528	569	7			
1	W	387	Total	C	N	O	S	0	0	0
			3163	2059	528	569	7			
1	X	387	Total	C	N	O	S	0	0	0
			3163	2059	528	569	7			

There are 480 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP E0Y3X1
C	-18	GLY	-	expression tag	UNP E0Y3X1
C	-17	SER	-	expression tag	UNP E0Y3X1
C	-16	SER	-	expression tag	UNP E0Y3X1
C	-15	HIS	-	expression tag	UNP E0Y3X1
C	-14	HIS	-	expression tag	UNP E0Y3X1
C	-13	HIS	-	expression tag	UNP E0Y3X1
C	-12	HIS	-	expression tag	UNP E0Y3X1
C	-11	HIS	-	expression tag	UNP E0Y3X1
C	-10	HIS	-	expression tag	UNP E0Y3X1
C	-9	SER	-	expression tag	UNP E0Y3X1
C	-8	SER	-	expression tag	UNP E0Y3X1
C	-7	GLY	-	expression tag	UNP E0Y3X1
C	-6	LEU	-	expression tag	UNP E0Y3X1
C	-5	VAL	-	expression tag	UNP E0Y3X1
C	-4	PRO	-	expression tag	UNP E0Y3X1
C	-3	ARG	-	expression tag	UNP E0Y3X1
C	-2	GLY	-	expression tag	UNP E0Y3X1
C	-1	SER	-	expression tag	UNP E0Y3X1
C	0	HIS	-	expression tag	UNP E0Y3X1
A	-19	MET	-	initiating methionine	UNP E0Y3X1
A	-18	GLY	-	expression tag	UNP E0Y3X1
A	-17	SER	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	SER	-	expression tag	UNP E0Y3X1
A	-15	HIS	-	expression tag	UNP E0Y3X1
A	-14	HIS	-	expression tag	UNP E0Y3X1
A	-13	HIS	-	expression tag	UNP E0Y3X1
A	-12	HIS	-	expression tag	UNP E0Y3X1
A	-11	HIS	-	expression tag	UNP E0Y3X1
A	-10	HIS	-	expression tag	UNP E0Y3X1
A	-9	SER	-	expression tag	UNP E0Y3X1
A	-8	SER	-	expression tag	UNP E0Y3X1
A	-7	GLY	-	expression tag	UNP E0Y3X1
A	-6	LEU	-	expression tag	UNP E0Y3X1
A	-5	VAL	-	expression tag	UNP E0Y3X1
A	-4	PRO	-	expression tag	UNP E0Y3X1
A	-3	ARG	-	expression tag	UNP E0Y3X1
A	-2	GLY	-	expression tag	UNP E0Y3X1
A	-1	SER	-	expression tag	UNP E0Y3X1
A	0	HIS	-	expression tag	UNP E0Y3X1
V	-19	MET	-	initiating methionine	UNP E0Y3X1
V	-18	GLY	-	expression tag	UNP E0Y3X1
V	-17	SER	-	expression tag	UNP E0Y3X1
V	-16	SER	-	expression tag	UNP E0Y3X1
V	-15	HIS	-	expression tag	UNP E0Y3X1
V	-14	HIS	-	expression tag	UNP E0Y3X1
V	-13	HIS	-	expression tag	UNP E0Y3X1
V	-12	HIS	-	expression tag	UNP E0Y3X1
V	-11	HIS	-	expression tag	UNP E0Y3X1
V	-10	HIS	-	expression tag	UNP E0Y3X1
V	-9	SER	-	expression tag	UNP E0Y3X1
V	-8	SER	-	expression tag	UNP E0Y3X1
V	-7	GLY	-	expression tag	UNP E0Y3X1
V	-6	LEU	-	expression tag	UNP E0Y3X1
V	-5	VAL	-	expression tag	UNP E0Y3X1
V	-4	PRO	-	expression tag	UNP E0Y3X1
V	-3	ARG	-	expression tag	UNP E0Y3X1
V	-2	GLY	-	expression tag	UNP E0Y3X1
V	-1	SER	-	expression tag	UNP E0Y3X1
V	0	HIS	-	expression tag	UNP E0Y3X1
E	-19	MET	-	initiating methionine	UNP E0Y3X1
E	-18	GLY	-	expression tag	UNP E0Y3X1
E	-17	SER	-	expression tag	UNP E0Y3X1
E	-16	SER	-	expression tag	UNP E0Y3X1
E	-15	HIS	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	HIS	-	expression tag	UNP E0Y3X1
E	-13	HIS	-	expression tag	UNP E0Y3X1
E	-12	HIS	-	expression tag	UNP E0Y3X1
E	-11	HIS	-	expression tag	UNP E0Y3X1
E	-10	HIS	-	expression tag	UNP E0Y3X1
E	-9	SER	-	expression tag	UNP E0Y3X1
E	-8	SER	-	expression tag	UNP E0Y3X1
E	-7	GLY	-	expression tag	UNP E0Y3X1
E	-6	LEU	-	expression tag	UNP E0Y3X1
E	-5	VAL	-	expression tag	UNP E0Y3X1
E	-4	PRO	-	expression tag	UNP E0Y3X1
E	-3	ARG	-	expression tag	UNP E0Y3X1
E	-2	GLY	-	expression tag	UNP E0Y3X1
E	-1	SER	-	expression tag	UNP E0Y3X1
E	0	HIS	-	expression tag	UNP E0Y3X1
G	-19	MET	-	initiating methionine	UNP E0Y3X1
G	-18	GLY	-	expression tag	UNP E0Y3X1
G	-17	SER	-	expression tag	UNP E0Y3X1
G	-16	SER	-	expression tag	UNP E0Y3X1
G	-15	HIS	-	expression tag	UNP E0Y3X1
G	-14	HIS	-	expression tag	UNP E0Y3X1
G	-13	HIS	-	expression tag	UNP E0Y3X1
G	-12	HIS	-	expression tag	UNP E0Y3X1
G	-11	HIS	-	expression tag	UNP E0Y3X1
G	-10	HIS	-	expression tag	UNP E0Y3X1
G	-9	SER	-	expression tag	UNP E0Y3X1
G	-8	SER	-	expression tag	UNP E0Y3X1
G	-7	GLY	-	expression tag	UNP E0Y3X1
G	-6	LEU	-	expression tag	UNP E0Y3X1
G	-5	VAL	-	expression tag	UNP E0Y3X1
G	-4	PRO	-	expression tag	UNP E0Y3X1
G	-3	ARG	-	expression tag	UNP E0Y3X1
G	-2	GLY	-	expression tag	UNP E0Y3X1
G	-1	SER	-	expression tag	UNP E0Y3X1
G	0	HIS	-	expression tag	UNP E0Y3X1
B	-19	MET	-	initiating methionine	UNP E0Y3X1
B	-18	GLY	-	expression tag	UNP E0Y3X1
B	-17	SER	-	expression tag	UNP E0Y3X1
B	-16	SER	-	expression tag	UNP E0Y3X1
B	-15	HIS	-	expression tag	UNP E0Y3X1
B	-14	HIS	-	expression tag	UNP E0Y3X1
B	-13	HIS	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP E0Y3X1
B	-11	HIS	-	expression tag	UNP E0Y3X1
B	-10	HIS	-	expression tag	UNP E0Y3X1
B	-9	SER	-	expression tag	UNP E0Y3X1
B	-8	SER	-	expression tag	UNP E0Y3X1
B	-7	GLY	-	expression tag	UNP E0Y3X1
B	-6	LEU	-	expression tag	UNP E0Y3X1
B	-5	VAL	-	expression tag	UNP E0Y3X1
B	-4	PRO	-	expression tag	UNP E0Y3X1
B	-3	ARG	-	expression tag	UNP E0Y3X1
B	-2	GLY	-	expression tag	UNP E0Y3X1
B	-1	SER	-	expression tag	UNP E0Y3X1
B	0	HIS	-	expression tag	UNP E0Y3X1
D	-19	MET	-	initiating methionine	UNP E0Y3X1
D	-18	GLY	-	expression tag	UNP E0Y3X1
D	-17	SER	-	expression tag	UNP E0Y3X1
D	-16	SER	-	expression tag	UNP E0Y3X1
D	-15	HIS	-	expression tag	UNP E0Y3X1
D	-14	HIS	-	expression tag	UNP E0Y3X1
D	-13	HIS	-	expression tag	UNP E0Y3X1
D	-12	HIS	-	expression tag	UNP E0Y3X1
D	-11	HIS	-	expression tag	UNP E0Y3X1
D	-10	HIS	-	expression tag	UNP E0Y3X1
D	-9	SER	-	expression tag	UNP E0Y3X1
D	-8	SER	-	expression tag	UNP E0Y3X1
D	-7	GLY	-	expression tag	UNP E0Y3X1
D	-6	LEU	-	expression tag	UNP E0Y3X1
D	-5	VAL	-	expression tag	UNP E0Y3X1
D	-4	PRO	-	expression tag	UNP E0Y3X1
D	-3	ARG	-	expression tag	UNP E0Y3X1
D	-2	GLY	-	expression tag	UNP E0Y3X1
D	-1	SER	-	expression tag	UNP E0Y3X1
D	0	HIS	-	expression tag	UNP E0Y3X1
F	-19	MET	-	initiating methionine	UNP E0Y3X1
F	-18	GLY	-	expression tag	UNP E0Y3X1
F	-17	SER	-	expression tag	UNP E0Y3X1
F	-16	SER	-	expression tag	UNP E0Y3X1
F	-15	HIS	-	expression tag	UNP E0Y3X1
F	-14	HIS	-	expression tag	UNP E0Y3X1
F	-13	HIS	-	expression tag	UNP E0Y3X1
F	-12	HIS	-	expression tag	UNP E0Y3X1
F	-11	HIS	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	HIS	-	expression tag	UNP E0Y3X1
F	-9	SER	-	expression tag	UNP E0Y3X1
F	-8	SER	-	expression tag	UNP E0Y3X1
F	-7	GLY	-	expression tag	UNP E0Y3X1
F	-6	LEU	-	expression tag	UNP E0Y3X1
F	-5	VAL	-	expression tag	UNP E0Y3X1
F	-4	PRO	-	expression tag	UNP E0Y3X1
F	-3	ARG	-	expression tag	UNP E0Y3X1
F	-2	GLY	-	expression tag	UNP E0Y3X1
F	-1	SER	-	expression tag	UNP E0Y3X1
F	0	HIS	-	expression tag	UNP E0Y3X1
H	-19	MET	-	initiating methionine	UNP E0Y3X1
H	-18	GLY	-	expression tag	UNP E0Y3X1
H	-17	SER	-	expression tag	UNP E0Y3X1
H	-16	SER	-	expression tag	UNP E0Y3X1
H	-15	HIS	-	expression tag	UNP E0Y3X1
H	-14	HIS	-	expression tag	UNP E0Y3X1
H	-13	HIS	-	expression tag	UNP E0Y3X1
H	-12	HIS	-	expression tag	UNP E0Y3X1
H	-11	HIS	-	expression tag	UNP E0Y3X1
H	-10	HIS	-	expression tag	UNP E0Y3X1
H	-9	SER	-	expression tag	UNP E0Y3X1
H	-8	SER	-	expression tag	UNP E0Y3X1
H	-7	GLY	-	expression tag	UNP E0Y3X1
H	-6	LEU	-	expression tag	UNP E0Y3X1
H	-5	VAL	-	expression tag	UNP E0Y3X1
H	-4	PRO	-	expression tag	UNP E0Y3X1
H	-3	ARG	-	expression tag	UNP E0Y3X1
H	-2	GLY	-	expression tag	UNP E0Y3X1
H	-1	SER	-	expression tag	UNP E0Y3X1
H	0	HIS	-	expression tag	UNP E0Y3X1
I	-19	MET	-	initiating methionine	UNP E0Y3X1
I	-18	GLY	-	expression tag	UNP E0Y3X1
I	-17	SER	-	expression tag	UNP E0Y3X1
I	-16	SER	-	expression tag	UNP E0Y3X1
I	-15	HIS	-	expression tag	UNP E0Y3X1
I	-14	HIS	-	expression tag	UNP E0Y3X1
I	-13	HIS	-	expression tag	UNP E0Y3X1
I	-12	HIS	-	expression tag	UNP E0Y3X1
I	-11	HIS	-	expression tag	UNP E0Y3X1
I	-10	HIS	-	expression tag	UNP E0Y3X1
I	-9	SER	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-8	SER	-	expression tag	UNP E0Y3X1
I	-7	GLY	-	expression tag	UNP E0Y3X1
I	-6	LEU	-	expression tag	UNP E0Y3X1
I	-5	VAL	-	expression tag	UNP E0Y3X1
I	-4	PRO	-	expression tag	UNP E0Y3X1
I	-3	ARG	-	expression tag	UNP E0Y3X1
I	-2	GLY	-	expression tag	UNP E0Y3X1
I	-1	SER	-	expression tag	UNP E0Y3X1
I	0	HIS	-	expression tag	UNP E0Y3X1
J	-19	MET	-	initiating methionine	UNP E0Y3X1
J	-18	GLY	-	expression tag	UNP E0Y3X1
J	-17	SER	-	expression tag	UNP E0Y3X1
J	-16	SER	-	expression tag	UNP E0Y3X1
J	-15	HIS	-	expression tag	UNP E0Y3X1
J	-14	HIS	-	expression tag	UNP E0Y3X1
J	-13	HIS	-	expression tag	UNP E0Y3X1
J	-12	HIS	-	expression tag	UNP E0Y3X1
J	-11	HIS	-	expression tag	UNP E0Y3X1
J	-10	HIS	-	expression tag	UNP E0Y3X1
J	-9	SER	-	expression tag	UNP E0Y3X1
J	-8	SER	-	expression tag	UNP E0Y3X1
J	-7	GLY	-	expression tag	UNP E0Y3X1
J	-6	LEU	-	expression tag	UNP E0Y3X1
J	-5	VAL	-	expression tag	UNP E0Y3X1
J	-4	PRO	-	expression tag	UNP E0Y3X1
J	-3	ARG	-	expression tag	UNP E0Y3X1
J	-2	GLY	-	expression tag	UNP E0Y3X1
J	-1	SER	-	expression tag	UNP E0Y3X1
J	0	HIS	-	expression tag	UNP E0Y3X1
K	-19	MET	-	initiating methionine	UNP E0Y3X1
K	-18	GLY	-	expression tag	UNP E0Y3X1
K	-17	SER	-	expression tag	UNP E0Y3X1
K	-16	SER	-	expression tag	UNP E0Y3X1
K	-15	HIS	-	expression tag	UNP E0Y3X1
K	-14	HIS	-	expression tag	UNP E0Y3X1
K	-13	HIS	-	expression tag	UNP E0Y3X1
K	-12	HIS	-	expression tag	UNP E0Y3X1
K	-11	HIS	-	expression tag	UNP E0Y3X1
K	-10	HIS	-	expression tag	UNP E0Y3X1
K	-9	SER	-	expression tag	UNP E0Y3X1
K	-8	SER	-	expression tag	UNP E0Y3X1
K	-7	GLY	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	LEU	-	expression tag	UNP E0Y3X1
K	-5	VAL	-	expression tag	UNP E0Y3X1
K	-4	PRO	-	expression tag	UNP E0Y3X1
K	-3	ARG	-	expression tag	UNP E0Y3X1
K	-2	GLY	-	expression tag	UNP E0Y3X1
K	-1	SER	-	expression tag	UNP E0Y3X1
K	0	HIS	-	expression tag	UNP E0Y3X1
L	-19	MET	-	initiating methionine	UNP E0Y3X1
L	-18	GLY	-	expression tag	UNP E0Y3X1
L	-17	SER	-	expression tag	UNP E0Y3X1
L	-16	SER	-	expression tag	UNP E0Y3X1
L	-15	HIS	-	expression tag	UNP E0Y3X1
L	-14	HIS	-	expression tag	UNP E0Y3X1
L	-13	HIS	-	expression tag	UNP E0Y3X1
L	-12	HIS	-	expression tag	UNP E0Y3X1
L	-11	HIS	-	expression tag	UNP E0Y3X1
L	-10	HIS	-	expression tag	UNP E0Y3X1
L	-9	SER	-	expression tag	UNP E0Y3X1
L	-8	SER	-	expression tag	UNP E0Y3X1
L	-7	GLY	-	expression tag	UNP E0Y3X1
L	-6	LEU	-	expression tag	UNP E0Y3X1
L	-5	VAL	-	expression tag	UNP E0Y3X1
L	-4	PRO	-	expression tag	UNP E0Y3X1
L	-3	ARG	-	expression tag	UNP E0Y3X1
L	-2	GLY	-	expression tag	UNP E0Y3X1
L	-1	SER	-	expression tag	UNP E0Y3X1
L	0	HIS	-	expression tag	UNP E0Y3X1
M	-19	MET	-	initiating methionine	UNP E0Y3X1
M	-18	GLY	-	expression tag	UNP E0Y3X1
M	-17	SER	-	expression tag	UNP E0Y3X1
M	-16	SER	-	expression tag	UNP E0Y3X1
M	-15	HIS	-	expression tag	UNP E0Y3X1
M	-14	HIS	-	expression tag	UNP E0Y3X1
M	-13	HIS	-	expression tag	UNP E0Y3X1
M	-12	HIS	-	expression tag	UNP E0Y3X1
M	-11	HIS	-	expression tag	UNP E0Y3X1
M	-10	HIS	-	expression tag	UNP E0Y3X1
M	-9	SER	-	expression tag	UNP E0Y3X1
M	-8	SER	-	expression tag	UNP E0Y3X1
M	-7	GLY	-	expression tag	UNP E0Y3X1
M	-6	LEU	-	expression tag	UNP E0Y3X1
M	-5	VAL	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-4	PRO	-	expression tag	UNP E0Y3X1
M	-3	ARG	-	expression tag	UNP E0Y3X1
M	-2	GLY	-	expression tag	UNP E0Y3X1
M	-1	SER	-	expression tag	UNP E0Y3X1
M	0	HIS	-	expression tag	UNP E0Y3X1
N	-19	MET	-	initiating methionine	UNP E0Y3X1
N	-18	GLY	-	expression tag	UNP E0Y3X1
N	-17	SER	-	expression tag	UNP E0Y3X1
N	-16	SER	-	expression tag	UNP E0Y3X1
N	-15	HIS	-	expression tag	UNP E0Y3X1
N	-14	HIS	-	expression tag	UNP E0Y3X1
N	-13	HIS	-	expression tag	UNP E0Y3X1
N	-12	HIS	-	expression tag	UNP E0Y3X1
N	-11	HIS	-	expression tag	UNP E0Y3X1
N	-10	HIS	-	expression tag	UNP E0Y3X1
N	-9	SER	-	expression tag	UNP E0Y3X1
N	-8	SER	-	expression tag	UNP E0Y3X1
N	-7	GLY	-	expression tag	UNP E0Y3X1
N	-6	LEU	-	expression tag	UNP E0Y3X1
N	-5	VAL	-	expression tag	UNP E0Y3X1
N	-4	PRO	-	expression tag	UNP E0Y3X1
N	-3	ARG	-	expression tag	UNP E0Y3X1
N	-2	GLY	-	expression tag	UNP E0Y3X1
N	-1	SER	-	expression tag	UNP E0Y3X1
N	0	HIS	-	expression tag	UNP E0Y3X1
O	-19	MET	-	initiating methionine	UNP E0Y3X1
O	-18	GLY	-	expression tag	UNP E0Y3X1
O	-17	SER	-	expression tag	UNP E0Y3X1
O	-16	SER	-	expression tag	UNP E0Y3X1
O	-15	HIS	-	expression tag	UNP E0Y3X1
O	-14	HIS	-	expression tag	UNP E0Y3X1
O	-13	HIS	-	expression tag	UNP E0Y3X1
O	-12	HIS	-	expression tag	UNP E0Y3X1
O	-11	HIS	-	expression tag	UNP E0Y3X1
O	-10	HIS	-	expression tag	UNP E0Y3X1
O	-9	SER	-	expression tag	UNP E0Y3X1
O	-8	SER	-	expression tag	UNP E0Y3X1
O	-7	GLY	-	expression tag	UNP E0Y3X1
O	-6	LEU	-	expression tag	UNP E0Y3X1
O	-5	VAL	-	expression tag	UNP E0Y3X1
O	-4	PRO	-	expression tag	UNP E0Y3X1
O	-3	ARG	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	GLY	-	expression tag	UNP E0Y3X1
O	-1	SER	-	expression tag	UNP E0Y3X1
O	0	HIS	-	expression tag	UNP E0Y3X1
P	-19	MET	-	initiating methionine	UNP E0Y3X1
P	-18	GLY	-	expression tag	UNP E0Y3X1
P	-17	SER	-	expression tag	UNP E0Y3X1
P	-16	SER	-	expression tag	UNP E0Y3X1
P	-15	HIS	-	expression tag	UNP E0Y3X1
P	-14	HIS	-	expression tag	UNP E0Y3X1
P	-13	HIS	-	expression tag	UNP E0Y3X1
P	-12	HIS	-	expression tag	UNP E0Y3X1
P	-11	HIS	-	expression tag	UNP E0Y3X1
P	-10	HIS	-	expression tag	UNP E0Y3X1
P	-9	SER	-	expression tag	UNP E0Y3X1
P	-8	SER	-	expression tag	UNP E0Y3X1
P	-7	GLY	-	expression tag	UNP E0Y3X1
P	-6	LEU	-	expression tag	UNP E0Y3X1
P	-5	VAL	-	expression tag	UNP E0Y3X1
P	-4	PRO	-	expression tag	UNP E0Y3X1
P	-3	ARG	-	expression tag	UNP E0Y3X1
P	-2	GLY	-	expression tag	UNP E0Y3X1
P	-1	SER	-	expression tag	UNP E0Y3X1
P	0	HIS	-	expression tag	UNP E0Y3X1
Q	-19	MET	-	initiating methionine	UNP E0Y3X1
Q	-18	GLY	-	expression tag	UNP E0Y3X1
Q	-17	SER	-	expression tag	UNP E0Y3X1
Q	-16	SER	-	expression tag	UNP E0Y3X1
Q	-15	HIS	-	expression tag	UNP E0Y3X1
Q	-14	HIS	-	expression tag	UNP E0Y3X1
Q	-13	HIS	-	expression tag	UNP E0Y3X1
Q	-12	HIS	-	expression tag	UNP E0Y3X1
Q	-11	HIS	-	expression tag	UNP E0Y3X1
Q	-10	HIS	-	expression tag	UNP E0Y3X1
Q	-9	SER	-	expression tag	UNP E0Y3X1
Q	-8	SER	-	expression tag	UNP E0Y3X1
Q	-7	GLY	-	expression tag	UNP E0Y3X1
Q	-6	LEU	-	expression tag	UNP E0Y3X1
Q	-5	VAL	-	expression tag	UNP E0Y3X1
Q	-4	PRO	-	expression tag	UNP E0Y3X1
Q	-3	ARG	-	expression tag	UNP E0Y3X1
Q	-2	GLY	-	expression tag	UNP E0Y3X1
Q	-1	SER	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	HIS	-	expression tag	UNP E0Y3X1
R	-19	MET	-	initiating methionine	UNP E0Y3X1
R	-18	GLY	-	expression tag	UNP E0Y3X1
R	-17	SER	-	expression tag	UNP E0Y3X1
R	-16	SER	-	expression tag	UNP E0Y3X1
R	-15	HIS	-	expression tag	UNP E0Y3X1
R	-14	HIS	-	expression tag	UNP E0Y3X1
R	-13	HIS	-	expression tag	UNP E0Y3X1
R	-12	HIS	-	expression tag	UNP E0Y3X1
R	-11	HIS	-	expression tag	UNP E0Y3X1
R	-10	HIS	-	expression tag	UNP E0Y3X1
R	-9	SER	-	expression tag	UNP E0Y3X1
R	-8	SER	-	expression tag	UNP E0Y3X1
R	-7	GLY	-	expression tag	UNP E0Y3X1
R	-6	LEU	-	expression tag	UNP E0Y3X1
R	-5	VAL	-	expression tag	UNP E0Y3X1
R	-4	PRO	-	expression tag	UNP E0Y3X1
R	-3	ARG	-	expression tag	UNP E0Y3X1
R	-2	GLY	-	expression tag	UNP E0Y3X1
R	-1	SER	-	expression tag	UNP E0Y3X1
R	0	HIS	-	expression tag	UNP E0Y3X1
S	-19	MET	-	initiating methionine	UNP E0Y3X1
S	-18	GLY	-	expression tag	UNP E0Y3X1
S	-17	SER	-	expression tag	UNP E0Y3X1
S	-16	SER	-	expression tag	UNP E0Y3X1
S	-15	HIS	-	expression tag	UNP E0Y3X1
S	-14	HIS	-	expression tag	UNP E0Y3X1
S	-13	HIS	-	expression tag	UNP E0Y3X1
S	-12	HIS	-	expression tag	UNP E0Y3X1
S	-11	HIS	-	expression tag	UNP E0Y3X1
S	-10	HIS	-	expression tag	UNP E0Y3X1
S	-9	SER	-	expression tag	UNP E0Y3X1
S	-8	SER	-	expression tag	UNP E0Y3X1
S	-7	GLY	-	expression tag	UNP E0Y3X1
S	-6	LEU	-	expression tag	UNP E0Y3X1
S	-5	VAL	-	expression tag	UNP E0Y3X1
S	-4	PRO	-	expression tag	UNP E0Y3X1
S	-3	ARG	-	expression tag	UNP E0Y3X1
S	-2	GLY	-	expression tag	UNP E0Y3X1
S	-1	SER	-	expression tag	UNP E0Y3X1
S	0	HIS	-	expression tag	UNP E0Y3X1
T	-19	MET	-	initiating methionine	UNP E0Y3X1

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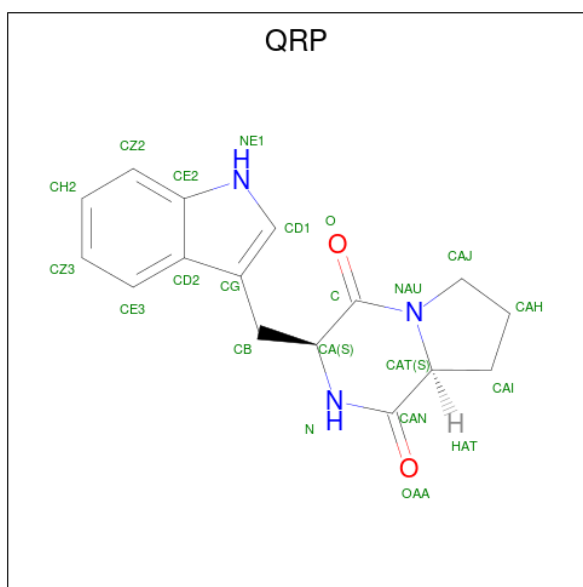
Chain	Residue	Modelled	Actual	Comment	Reference
T	-18	GLY	-	expression tag	UNP E0Y3X1
T	-17	SER	-	expression tag	UNP E0Y3X1
T	-16	SER	-	expression tag	UNP E0Y3X1
T	-15	HIS	-	expression tag	UNP E0Y3X1
T	-14	HIS	-	expression tag	UNP E0Y3X1
T	-13	HIS	-	expression tag	UNP E0Y3X1
T	-12	HIS	-	expression tag	UNP E0Y3X1
T	-11	HIS	-	expression tag	UNP E0Y3X1
T	-10	HIS	-	expression tag	UNP E0Y3X1
T	-9	SER	-	expression tag	UNP E0Y3X1
T	-8	SER	-	expression tag	UNP E0Y3X1
T	-7	GLY	-	expression tag	UNP E0Y3X1
T	-6	LEU	-	expression tag	UNP E0Y3X1
T	-5	VAL	-	expression tag	UNP E0Y3X1
T	-4	PRO	-	expression tag	UNP E0Y3X1
T	-3	ARG	-	expression tag	UNP E0Y3X1
T	-2	GLY	-	expression tag	UNP E0Y3X1
T	-1	SER	-	expression tag	UNP E0Y3X1
T	0	HIS	-	expression tag	UNP E0Y3X1
U	-19	MET	-	initiating methionine	UNP E0Y3X1
U	-18	GLY	-	expression tag	UNP E0Y3X1
U	-17	SER	-	expression tag	UNP E0Y3X1
U	-16	SER	-	expression tag	UNP E0Y3X1
U	-15	HIS	-	expression tag	UNP E0Y3X1
U	-14	HIS	-	expression tag	UNP E0Y3X1
U	-13	HIS	-	expression tag	UNP E0Y3X1
U	-12	HIS	-	expression tag	UNP E0Y3X1
U	-11	HIS	-	expression tag	UNP E0Y3X1
U	-10	HIS	-	expression tag	UNP E0Y3X1
U	-9	SER	-	expression tag	UNP E0Y3X1
U	-8	SER	-	expression tag	UNP E0Y3X1
U	-7	GLY	-	expression tag	UNP E0Y3X1
U	-6	LEU	-	expression tag	UNP E0Y3X1
U	-5	VAL	-	expression tag	UNP E0Y3X1
U	-4	PRO	-	expression tag	UNP E0Y3X1
U	-3	ARG	-	expression tag	UNP E0Y3X1
U	-2	GLY	-	expression tag	UNP E0Y3X1
U	-1	SER	-	expression tag	UNP E0Y3X1
U	0	HIS	-	expression tag	UNP E0Y3X1
W	-19	MET	-	initiating methionine	UNP E0Y3X1
W	-18	GLY	-	expression tag	UNP E0Y3X1
W	-17	SER	-	expression tag	UNP E0Y3X1

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Chain	Residue	Modelled	Actual	Comment	Reference
W	-16	SER	-	expression tag	UNP E0Y3X1
W	-15	HIS	-	expression tag	UNP E0Y3X1
W	-14	HIS	-	expression tag	UNP E0Y3X1
W	-13	HIS	-	expression tag	UNP E0Y3X1
W	-12	HIS	-	expression tag	UNP E0Y3X1
W	-11	HIS	-	expression tag	UNP E0Y3X1
W	-10	HIS	-	expression tag	UNP E0Y3X1
W	-9	SER	-	expression tag	UNP E0Y3X1
W	-8	SER	-	expression tag	UNP E0Y3X1
W	-7	GLY	-	expression tag	UNP E0Y3X1
W	-6	LEU	-	expression tag	UNP E0Y3X1
W	-5	VAL	-	expression tag	UNP E0Y3X1
W	-4	PRO	-	expression tag	UNP E0Y3X1
W	-3	ARG	-	expression tag	UNP E0Y3X1
W	-2	GLY	-	expression tag	UNP E0Y3X1
W	-1	SER	-	expression tag	UNP E0Y3X1
W	0	HIS	-	expression tag	UNP E0Y3X1
X	-19	MET	-	initiating methionine	UNP E0Y3X1
X	-18	GLY	-	expression tag	UNP E0Y3X1
X	-17	SER	-	expression tag	UNP E0Y3X1
X	-16	SER	-	expression tag	UNP E0Y3X1
X	-15	HIS	-	expression tag	UNP E0Y3X1
X	-14	HIS	-	expression tag	UNP E0Y3X1
X	-13	HIS	-	expression tag	UNP E0Y3X1
X	-12	HIS	-	expression tag	UNP E0Y3X1
X	-11	HIS	-	expression tag	UNP E0Y3X1
X	-10	HIS	-	expression tag	UNP E0Y3X1
X	-9	SER	-	expression tag	UNP E0Y3X1
X	-8	SER	-	expression tag	UNP E0Y3X1
X	-7	GLY	-	expression tag	UNP E0Y3X1
X	-6	LEU	-	expression tag	UNP E0Y3X1
X	-5	VAL	-	expression tag	UNP E0Y3X1
X	-4	PRO	-	expression tag	UNP E0Y3X1
X	-3	ARG	-	expression tag	UNP E0Y3X1
X	-2	GLY	-	expression tag	UNP E0Y3X1
X	-1	SER	-	expression tag	UNP E0Y3X1
X	0	HIS	-	expression tag	UNP E0Y3X1

- Molecule 2 is (3S,8aS)-3-(1H-indol-3-ylmethyl)hexahydropyrrolo[1,2-a]pyrazine-1,4-dione (three-letter code: QRP) (formula: C₁₆H₁₇N₃O₂) (labeled as "Ligand of Interest" by depositor).



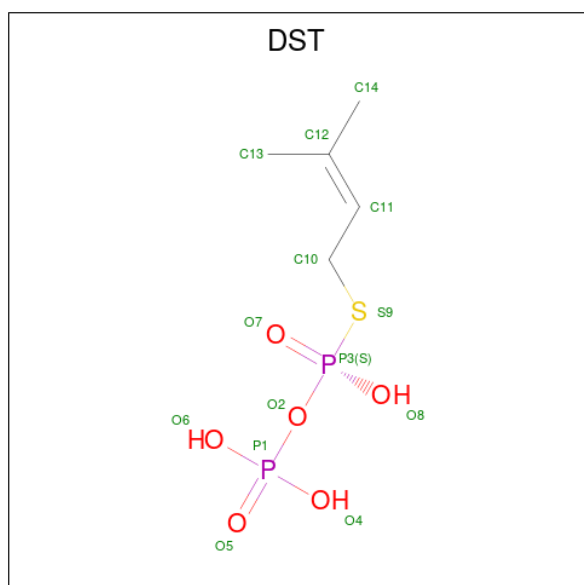
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	C	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	A	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	V	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	E	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	G	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	B	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	D	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	F	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	H	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	I	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	J	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	K	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	L	1	Total 38	C 16	H 17	N 3	O 2	0	0
2	M	1	Total 38	C 16	H 17	N 3	O 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	N	1	Total	C	H	N	O	0	0
			38	16	17	3	2		
2	O	1	Total	C	H	N	O	0	0
			38	16	17	3	2		
2	P	1	Total	C	H	N	O	0	0
			38	16	17	3	2		
2	Q	1	Total	C	H	N	O	0	0
			38	16	17	3	2		
2	R	1	Total	C	H	N	O	0	0
			38	16	17	3	2		
2	S	1	Total	C	H	N	O	0	0
			38	16	17	3	2		
2	T	1	Total	C	H	N	O	0	0
			38	16	17	3	2		
2	U	1	Total	C	H	N	O	0	0
			38	16	17	3	2		
2	W	1	Total	C	H	N	O	0	0
			38	16	17	3	2		
2	X	1	Total	C	H	N	O	0	0
			38	16	17	3	2		

- Molecule 3 is DIMETHYLALLYL S-THIOLODIPHOSPHATE (three-letter code: DST) (formula: $C_5H_{12}O_6P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	C	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		

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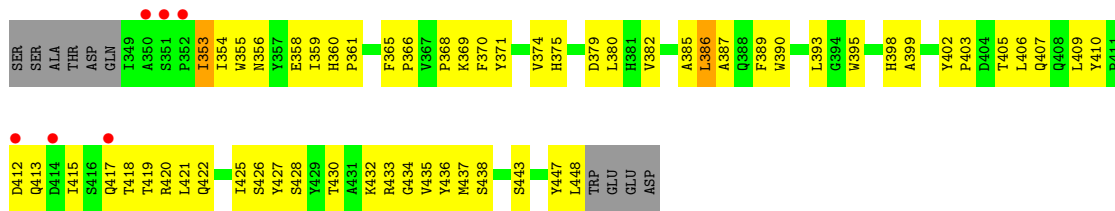
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	V	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	E	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	G	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	B	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	D	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	F	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	H	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	I	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	J	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	K	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	L	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	M	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	N	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	O	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	P	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	Q	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	R	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	S	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	T	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	U	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		

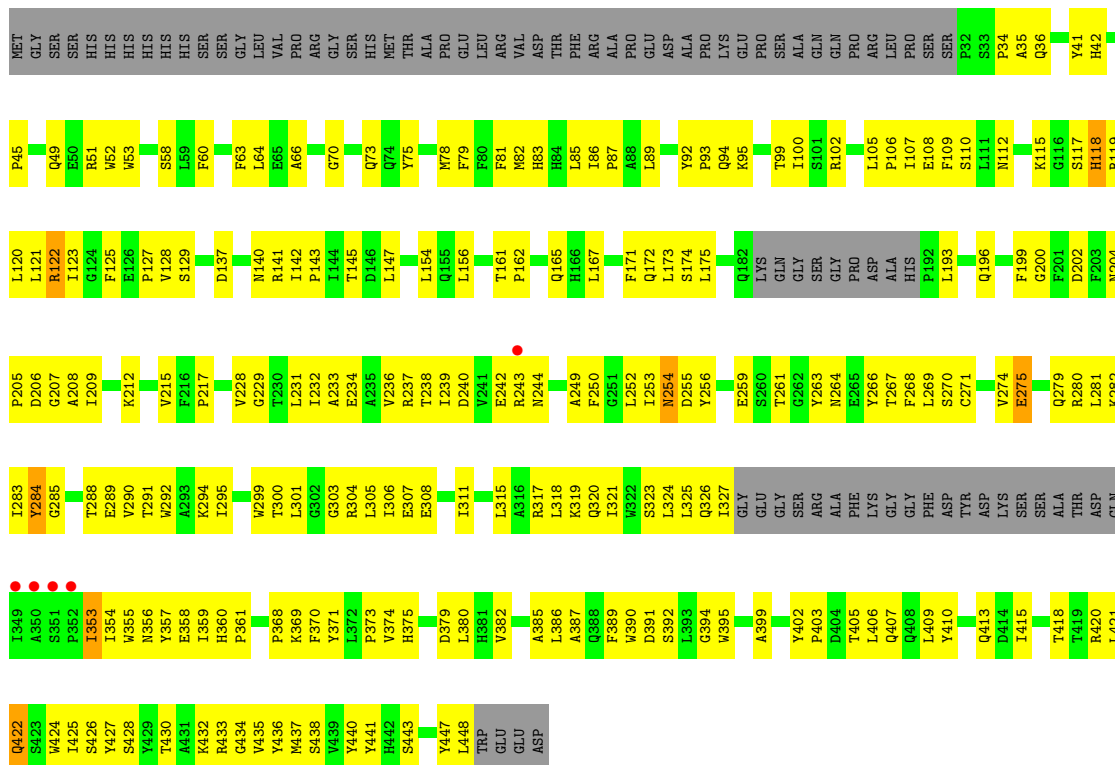
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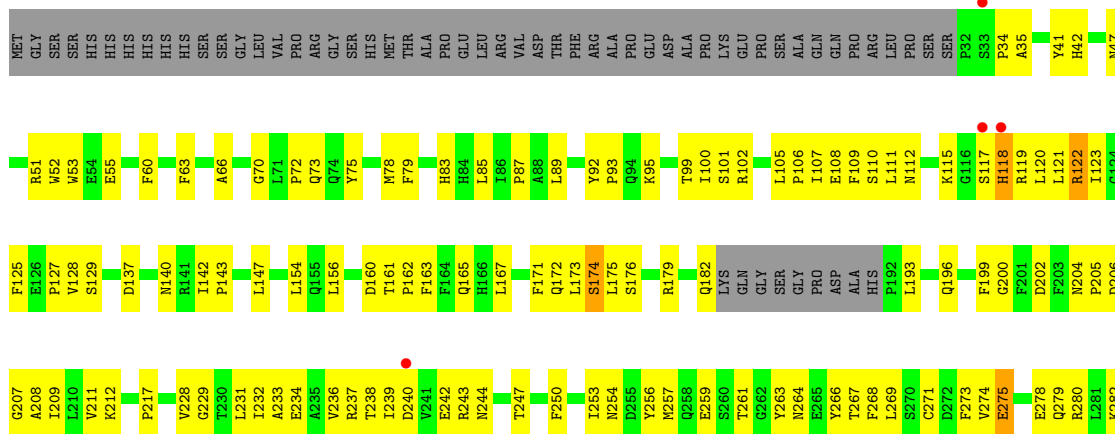
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	O	P			S
3	W	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		
3	X	1	Total	C	H	O	P	S	0	0
			23	5	9	6	2	1		

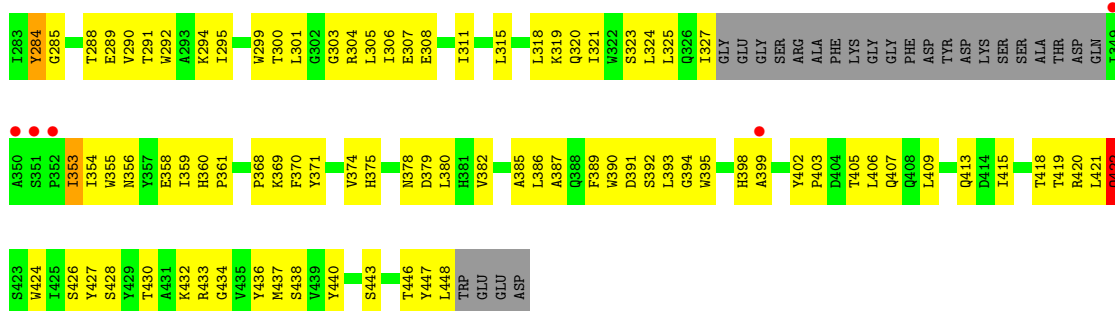


● Molecule 1: Deoxybrevianamide E synthase notF

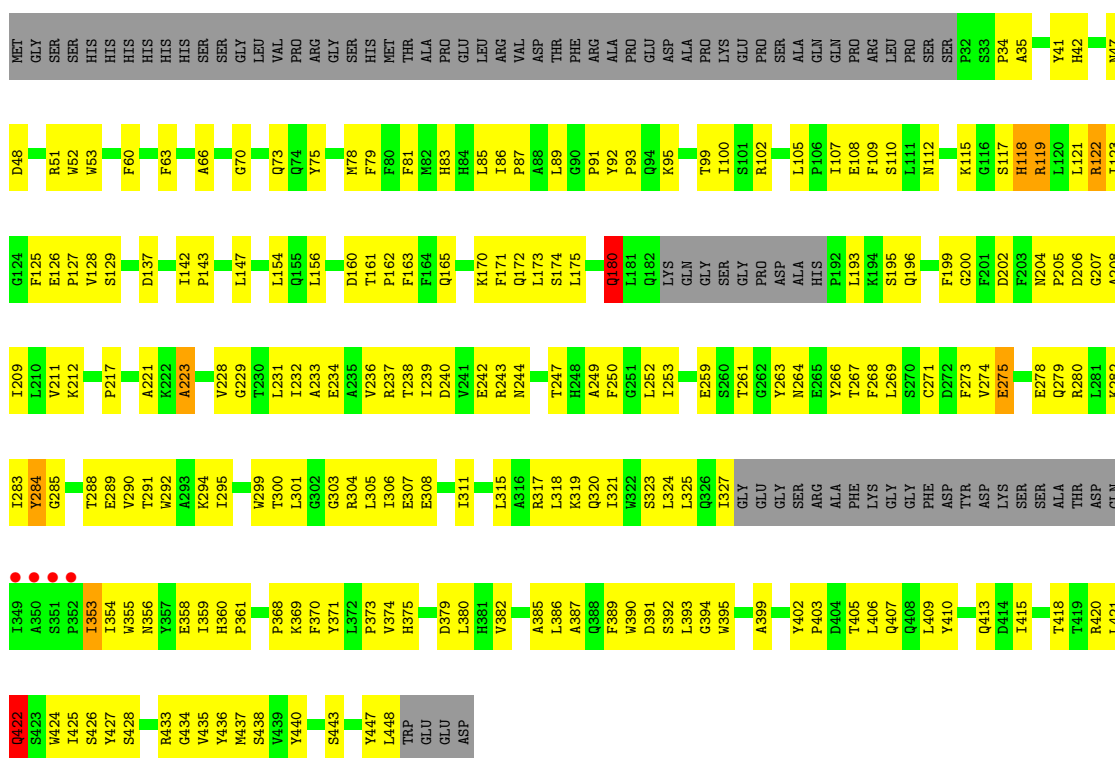


● Molecule 1: Deoxybrevianamide E synthase notF

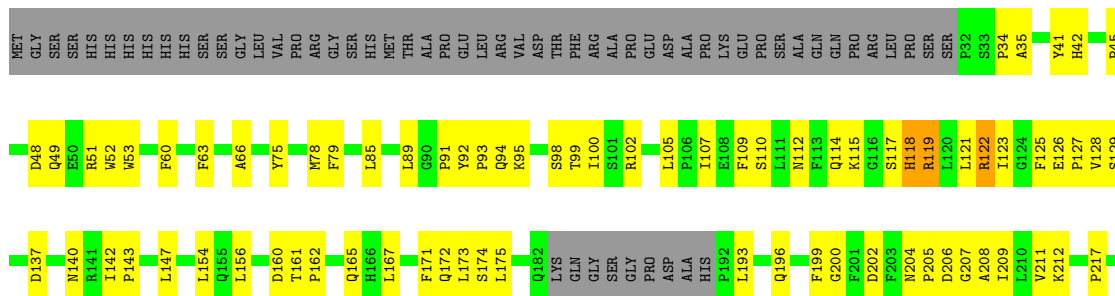


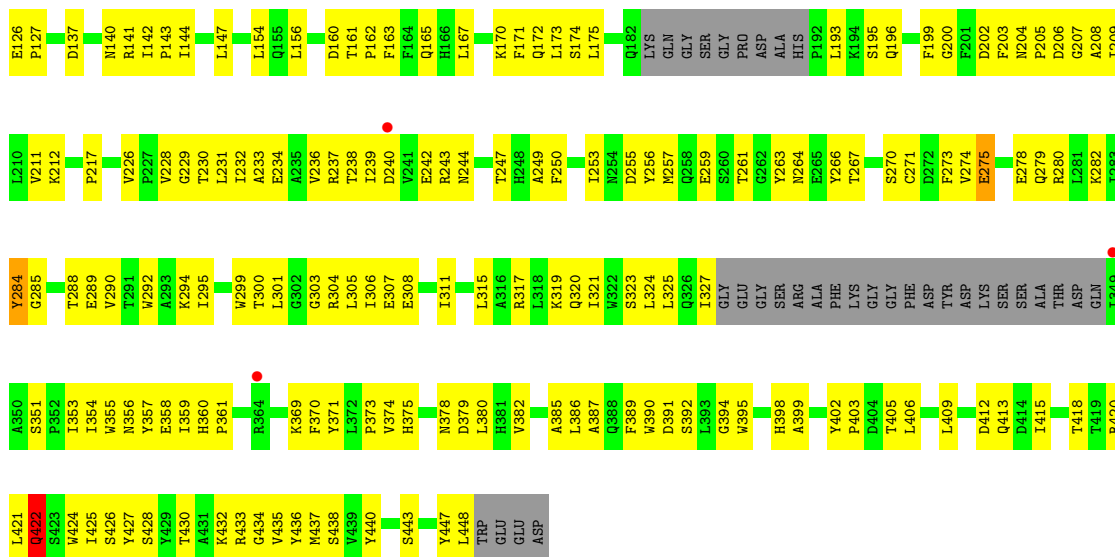


● Molecule 1: Deoxybrevianamide E synthase notF

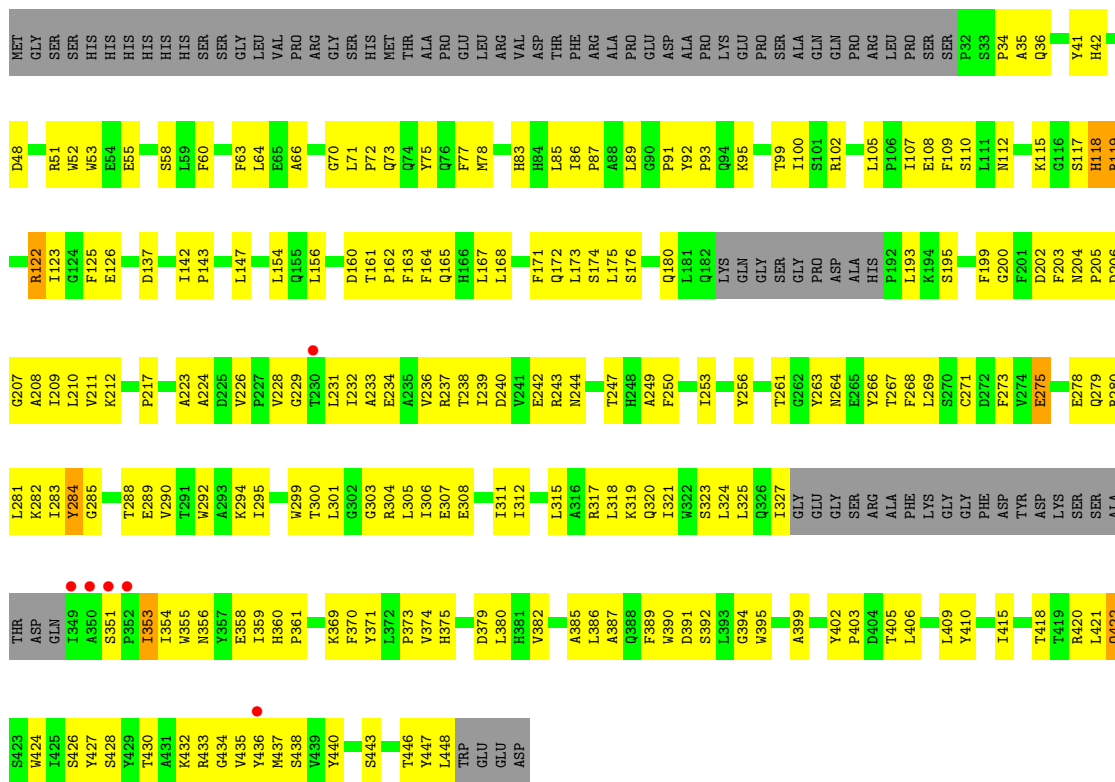


● Molecule 1: Deoxybrevianamide E synthase notF



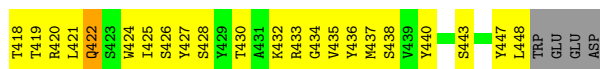


• Molecule 1: Deoxybrevianamide E synthase notF

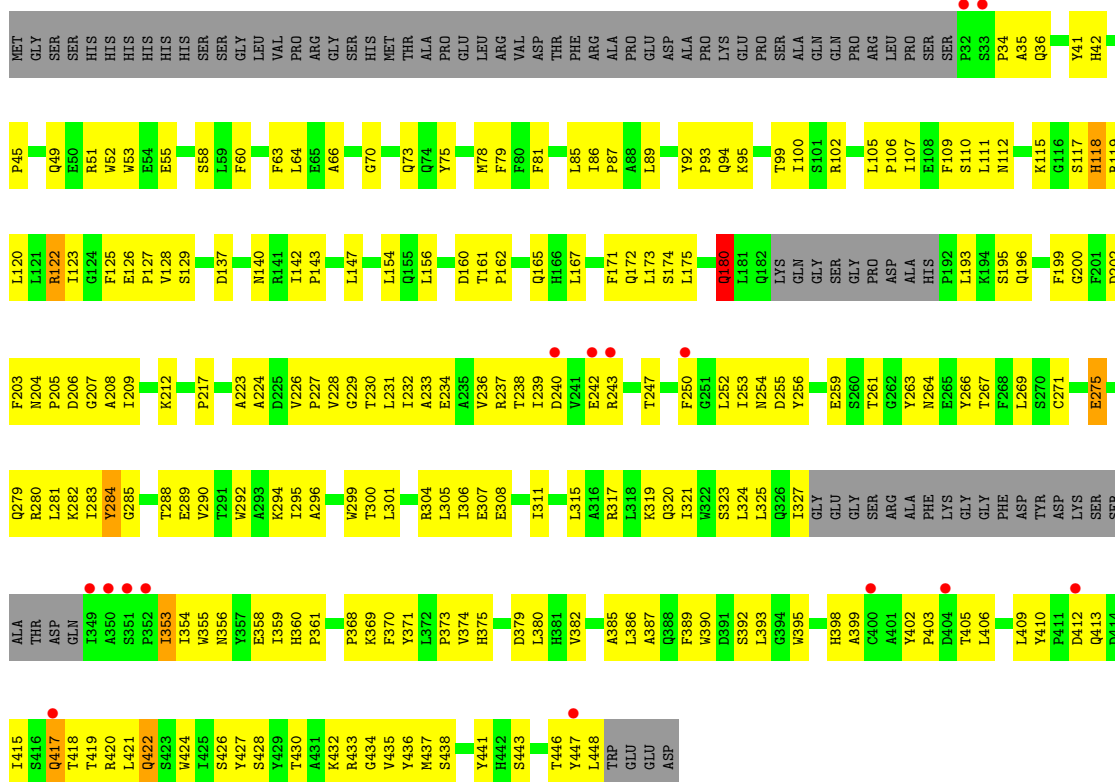


• Molecule 1: Deoxybrevianamide E synthase notF

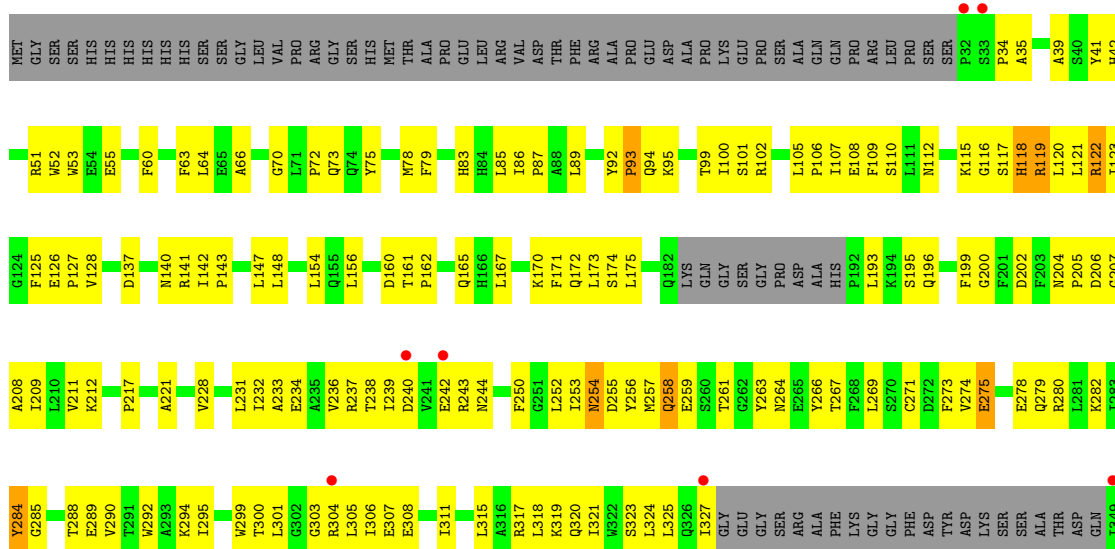


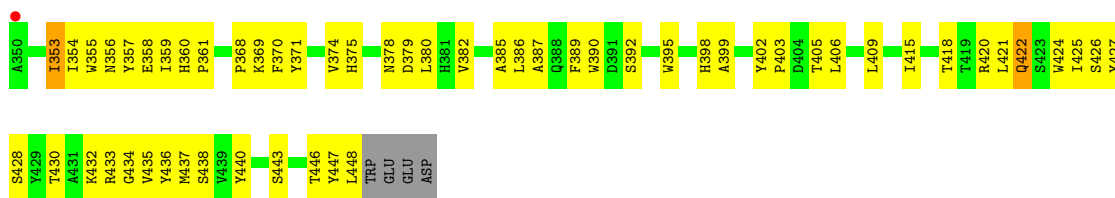


- Molecule 1: Deoxybrevianamide E synthase notF



- Molecule 1: Deoxybrevianamide E synthase notF





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	157.89Å 163.07Å 167.86Å 78.25° 65.05° 66.40°	Depositor
Resolution (Å)	49.13 – 3.00 49.13 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.13-3.00) 80.1 (49.13-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.40 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.265 , 0.308 0.270 , 0.306	Depositor DCC
R_{free} test set	1943 reflections (0.72%)	wwPDB-VP
Wilson B-factor (Å ²)	77.4	Xtrriage
Anisotropy	0.365	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	77376	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9482e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QRP, DST

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	3/3265 (0.1%)	0.64	5/4440 (0.1%)
1	B	0.50	5/3265 (0.2%)	0.64	8/4440 (0.2%)
1	C	0.46	1/3265 (0.0%)	0.61	3/4440 (0.1%)
1	D	0.41	0/3265	0.62	4/4440 (0.1%)
1	E	0.44	0/3265	0.61	3/4440 (0.1%)
1	F	0.43	1/3265 (0.0%)	0.67	8/4440 (0.2%)
1	G	0.51	5/3265 (0.2%)	0.70	13/4440 (0.3%)
1	H	0.50	1/3265 (0.0%)	0.64	3/4440 (0.1%)
1	I	0.46	3/3265 (0.1%)	0.61	6/4440 (0.1%)
1	J	0.55	6/3265 (0.2%)	0.66	10/4440 (0.2%)
1	K	0.39	1/3265 (0.0%)	0.59	3/4440 (0.1%)
1	L	0.42	1/3265 (0.0%)	0.62	4/4440 (0.1%)
1	M	0.50	5/3265 (0.2%)	0.64	7/4440 (0.2%)
1	N	0.49	4/3265 (0.1%)	0.63	6/4440 (0.1%)
1	O	0.43	0/3265	0.61	3/4440 (0.1%)
1	P	0.49	4/3265 (0.1%)	0.64	6/4440 (0.1%)
1	Q	0.44	0/3265	0.61	4/4440 (0.1%)
1	R	0.42	1/3265 (0.0%)	0.61	5/4440 (0.1%)
1	S	0.48	3/3265 (0.1%)	0.68	11/4440 (0.2%)
1	T	0.47	4/3265 (0.1%)	0.67	9/4440 (0.2%)
1	U	0.45	0/3265	0.61	4/4440 (0.1%)
1	V	0.47	3/3265 (0.1%)	0.62	4/4440 (0.1%)
1	W	0.43	0/3265	0.66	6/4440 (0.1%)
1	X	0.46	3/3265 (0.1%)	0.64	5/4440 (0.1%)
All	All	0.46	54/78360 (0.1%)	0.64	140/106560 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	D	0	2
1	E	0	2
1	F	0	1
1	G	0	2
1	H	0	1
1	I	0	2
1	J	0	4
1	L	0	2
1	M	0	2
1	N	0	1
1	O	0	1
1	P	0	2
1	R	0	1
1	S	0	3
1	T	0	3
1	V	0	1
1	W	0	2
All	All	0	36

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	320	GLN	CB-CG	10.92	1.82	1.52
1	S	320	GLN	CB-CG	10.00	1.79	1.52
1	I	320	GLN	CB-CG	9.30	1.77	1.52
1	V	254	ASN	CB-CG	8.36	1.70	1.51
1	J	254	ASN	CB-CG	8.24	1.70	1.51
1	N	254	ASN	CB-CG	8.23	1.70	1.51
1	B	422	GLN	CG-CD	8.21	1.70	1.51
1	M	180	GLN	CD-NE2	-7.91	1.13	1.32
1	J	320	GLN	CG-CD	7.90	1.69	1.51
1	T	422	GLN	CG-CD	7.50	1.68	1.51
1	G	320	GLN	CD-NE2	-7.35	1.14	1.32
1	A	258	GLN	CD-NE2	-7.31	1.14	1.32
1	P	422	GLN	CG-CD	7.30	1.67	1.51
1	J	320	GLN	CD-NE2	-7.20	1.14	1.32
1	X	258	GLN	CD-NE2	-7.17	1.15	1.32
1	B	320	GLN	CD-NE2	-7.11	1.15	1.32
1	T	422	GLN	CB-CG	6.99	1.71	1.52
1	B	422	GLN	CB-CG	6.66	1.70	1.52
1	P	422	GLN	CD-NE2	-6.42	1.16	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	422	GLN	CD-NE2	-6.40	1.16	1.32
1	P	422	GLN	CB-CG	6.28	1.69	1.52
1	B	422	GLN	CD-NE2	-6.12	1.17	1.32
1	T	95	LYS	CD-CE	6.04	1.66	1.51
1	R	196	GLN	CD-NE2	-5.91	1.18	1.32
1	X	95	LYS	CD-CE	5.90	1.66	1.51
1	N	196	GLN	CD-NE2	-5.88	1.18	1.32
1	G	320	GLN	CB-CG	5.84	1.68	1.52
1	V	422	GLN	CD-NE2	-5.80	1.18	1.32
1	I	254	ASN	CG-ND2	-5.68	1.18	1.32
1	B	320	GLN	CB-CG	5.68	1.67	1.52
1	M	422	GLN	CD-OE1	-5.66	1.11	1.24
1	K	422	GLN	CD-NE2	-5.64	1.18	1.32
1	A	180	GLN	CG-CD	5.63	1.64	1.51
1	G	196	GLN	CD-NE2	-5.58	1.18	1.32
1	C	422	GLN	CD-NE2	-5.49	1.19	1.32
1	M	422	GLN	CD-NE2	5.45	1.46	1.32
1	X	422	GLN	CD-NE2	-5.43	1.19	1.32
1	N	422	GLN	CD-NE2	-5.40	1.19	1.32
1	M	422	GLN	CG-CD	5.38	1.63	1.51
1	H	422	GLN	CD-NE2	-5.38	1.19	1.32
1	S	95	LYS	CD-CE	5.36	1.64	1.51
1	V	254	ASN	CG-ND2	-5.36	1.19	1.32
1	J	95	LYS	CD-CE	5.31	1.64	1.51
1	L	422	GLN	CD-NE2	-5.27	1.19	1.32
1	M	95	LYS	CD-CE	5.27	1.64	1.51
1	G	422	GLN	CD-NE2	-5.26	1.19	1.32
1	A	422	GLN	CD-NE2	-5.21	1.19	1.32
1	S	320	GLN	CG-CD	5.14	1.62	1.51
1	J	254	ASN	CG-ND2	-5.14	1.20	1.32
1	G	95	LYS	CD-CE	5.12	1.64	1.51
1	I	320	GLN	CG-CD	5.09	1.62	1.51
1	F	95	LYS	CD-CE	5.08	1.64	1.51
1	P	95	LYS	CD-CE	5.06	1.63	1.51
1	N	254	ASN	CG-ND2	-5.03	1.20	1.32

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	180	GLN	CA-CB-CG	-12.39	86.15	113.40
1	T	180	GLN	CG-CD-OE1	-11.44	98.72	121.60
1	F	180	GLN	CG-CD-OE1	-11.25	99.11	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	180	GLN	CG-CD-OE1	-10.53	100.54	121.60
1	H	95	LYS	CB-CG-CD	-10.38	84.62	111.60
1	G	180	GLN	CG-CD-OE1	-10.37	100.86	121.60
1	B	122	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	S	95	LYS	CB-CG-CD	-9.63	86.57	111.60
1	S	122	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	F	95	LYS	CB-CG-CD	-8.95	88.33	111.60
1	E	417	GLN	CG-CD-OE1	-8.81	103.97	121.60
1	S	417	GLN	CG-CD-OE1	-8.80	104.00	121.60
1	D	180	GLN	CA-CB-CG	-8.79	94.07	113.40
1	M	180	GLN	CA-CB-CG	-8.70	94.25	113.40
1	J	320	GLN	CG-CD-NE2	-8.63	95.97	116.70
1	L	95	LYS	CB-CG-CD	-8.57	89.31	111.60
1	P	95	LYS	CB-CG-CD	-8.57	89.30	111.60
1	J	95	LYS	CB-CG-CD	-8.53	89.41	111.60
1	C	122	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	M	95	LYS	CB-CG-CD	-8.44	89.66	111.60
1	W	417	GLN	CG-CD-OE1	-8.42	104.75	121.60
1	M	422	GLN	CG-CD-OE1	-8.31	104.98	121.60
1	G	95	LYS	CB-CG-CD	-8.27	90.11	111.60
1	Q	95	LYS	CB-CG-CD	-8.25	90.14	111.60
1	S	180	GLN	CB-CG-CD	8.19	132.90	111.60
1	F	180	GLN	CB-CG-CD	8.18	132.87	111.60
1	T	422	GLN	CA-CB-CG	-7.84	96.15	113.40
1	G	180	GLN	CB-CG-CD	7.84	131.98	111.60
1	P	422	GLN	CA-CB-CG	-7.76	96.32	113.40
1	K	422	GLN	N-CA-CB	-7.72	96.70	110.60
1	X	95	LYS	CB-CG-CD	-7.71	91.55	111.60
1	X	422	GLN	N-CA-CB	-7.69	96.75	110.60
1	W	95	LYS	CB-CG-CD	-7.64	91.74	111.60
1	O	95	LYS	CB-CG-CD	-7.54	92.00	111.60
1	B	422	GLN	CG-CD-NE2	-7.54	98.61	116.70
1	T	180	GLN	CB-CG-CD	7.52	131.16	111.60
1	T	422	GLN	CG-CD-NE2	-7.44	98.84	116.70
1	I	122	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	J	180	GLN	CG-CD-OE1	-7.37	106.87	121.60
1	P	422	GLN	CG-CD-NE2	-7.37	99.02	116.70
1	D	122	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	I	95	LYS	CB-CG-CD	-7.31	92.58	111.60
1	R	180	GLN	CG-CD-OE1	-7.19	107.22	121.60
1	X	122	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	M	122	ARG	NE-CZ-NH2	-7.11	116.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	95	LYS	CG-CD-CE	-7.10	90.60	111.90
1	U	95	LYS	CB-CG-CD	-7.08	93.19	111.60
1	F	180	GLN	CB-CA-C	6.96	124.32	110.40
1	S	95	LYS	CG-CD-CE	-6.94	91.07	111.90
1	R	422	GLN	N-CA-CB	-6.94	98.11	110.60
1	C	422	GLN	N-CA-CB	-6.93	98.12	110.60
1	X	95	LYS	CG-CD-CE	-6.92	91.15	111.90
1	T	42	HIS	CB-CG-ND1	-6.91	105.92	123.20
1	L	122	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	W	122	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	F	180	GLN	N-CA-CB	-6.86	98.25	110.60
1	N	122	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	D	122	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	N	422	GLN	N-CA-CB	-6.79	98.37	110.60
1	V	422	GLN	N-CA-CB	-6.78	98.39	110.60
1	W	422	GLN	N-CA-CB	-6.74	98.47	110.60
1	E	122	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	S	180	GLN	N-CA-CB	-6.72	98.51	110.60
1	S	180	GLN	CB-CA-C	6.68	123.76	110.40
1	B	398	HIS	N-CA-CB	-6.64	98.64	110.60
1	G	180	GLN	N-CA-CB	-6.57	98.77	110.60
1	B	422	GLN	CA-CB-CG	-6.57	98.96	113.40
1	B	122	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	422	GLN	CB-CA-C	6.42	123.25	110.40
1	A	122	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	R	122	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	O	122	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	R	196	GLN	CA-CB-CG	6.37	127.41	113.40
1	H	422	GLN	CB-CA-C	6.33	123.06	110.40
1	L	422	GLN	CB-CA-C	6.33	123.06	110.40
1	T	180	GLN	CB-CA-C	6.33	123.06	110.40
1	G	180	GLN	CB-CA-C	6.30	123.00	110.40
1	T	180	GLN	N-CA-CB	-6.27	99.31	110.60
1	T	122	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	U	422	GLN	CB-CA-C	6.23	122.86	110.40
1	G	422	GLN	CB-CA-C	6.23	122.86	110.40
1	J	320	GLN	CA-CB-CG	-6.22	99.71	113.40
1	J	122	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	Q	95	LYS	CG-CD-CE	-6.14	93.46	111.90
1	U	122	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	G	122	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	G	95	LYS	CG-CD-CE	-6.13	93.50	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	122	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	Q	422	GLN	CB-CA-C	6.08	122.57	110.40
1	D	180	GLN	CG-CD-OE1	-6.08	109.44	121.60
1	F	95	LYS	CG-CD-CE	-6.07	93.70	111.90
1	K	122	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	X	122	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	J	95	LYS	CG-CD-CE	-5.99	93.92	111.90
1	P	122	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	O	422	GLN	CB-CA-C	5.90	122.20	110.40
1	G	320	GLN	CB-CA-C	-5.86	98.67	110.40
1	S	122	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	L	95	LYS	CG-CD-CE	-5.85	94.34	111.90
1	M	95	LYS	CG-CD-CE	-5.84	94.39	111.90
1	S	320	GLN	CA-CB-CG	-5.82	100.61	113.40
1	A	180	GLN	CG-CD-OE1	-5.78	110.03	121.60
1	F	122	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	R	122	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	P	95	LYS	CG-CD-CE	-5.66	94.94	111.90
1	I	320	GLN	CA-CB-CG	-5.63	101.02	113.40
1	G	122	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	G	320	GLN	N-CA-CB	5.62	120.72	110.60
1	N	386	LEU	CA-CB-CG	5.60	128.19	115.30
1	F	386	LEU	CA-CB-CG	5.59	128.17	115.30
1	E	122	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	320	GLN	N-CA-CB	5.57	120.62	110.60
1	I	320	GLN	CG-CD-NE2	-5.52	103.46	116.70
1	W	180	GLN	CG-CD-OE1	-5.50	110.60	121.60
1	M	180	GLN	CG-CD-NE2	-5.47	103.58	116.70
1	N	122	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	M	223	ALA	CB-CA-C	-5.41	101.98	110.10
1	T	422	GLN	N-CA-CB	5.40	120.32	110.60
1	I	122	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	Q	122	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	P	422	GLN	N-CA-CB	5.32	120.18	110.60
1	B	320	GLN	CB-CA-C	-5.31	99.77	110.40
1	S	320	GLN	CG-CD-NE2	-5.31	103.95	116.70
1	I	422	GLN	CA-CB-CG	5.30	125.06	113.40
1	G	196	GLN	CA-CB-CG	5.29	125.04	113.40
1	B	422	GLN	N-CA-CB	5.25	120.05	110.60
1	V	254	ASN	CB-CG-ND2	-5.25	104.11	116.70
1	G	180	GLN	CA-CB-CG	-5.23	101.89	113.40
1	J	254	ASN	N-CA-CB	-5.22	101.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	N	196	GLN	CA-CB-CG	5.19	124.82	113.40
1	J	254	ASN	CB-CG-ND2	-5.19	104.25	116.70
1	C	122	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	N	254	ASN	CB-CG-ND2	-5.17	104.30	116.70
1	V	386	LEU	CA-CB-CG	5.11	127.06	115.30
1	J	386	LEU	CA-CB-CG	5.10	127.03	115.30
1	U	95	LYS	CG-CD-CE	-5.08	96.67	111.90
1	A	180	GLN	CB-CG-CD	-5.02	98.55	111.60
1	J	417	GLN	CA-CB-CG	5.01	124.42	113.40
1	V	122	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	GLN	Sidechain
1	A	422	GLN	Sidechain
1	B	398	HIS	Sidechain
1	B	422	GLN	Sidechain
1	D	180	GLN	Sidechain
1	D	398	HIS	Sidechain
1	E	398	HIS	Sidechain
1	E	417	GLN	Sidechain
1	F	180	GLN	Sidechain
1	G	180	GLN	Sidechain
1	G	398	HIS	Sidechain
1	H	422	GLN	Sidechain
1	I	320	GLN	Sidechain
1	I	398	HIS	Sidechain
1	J	180	GLN	Sidechain
1	J	254	ASN	Sidechain
1	J	320	GLN	Sidechain
1	J	398	HIS	Sidechain
1	L	398	HIS	Sidechain
1	L	422	GLN	Sidechain
1	M	180	GLN	Sidechain
1	M	422	GLN	Sidechain
1	N	254	ASN	Sidechain
1	O	398	HIS	Sidechain
1	P	398	HIS	Sidechain
1	P	422	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	R	180	GLN	Sidechain
1	S	180	GLN	Sidechain
1	S	320	GLN	Sidechain
1	S	417	GLN	Sidechain
1	T	180	GLN	Sidechain
1	T	42	HIS	Sidechain
1	T	422	GLN	Sidechain
1	V	254	ASN	Sidechain
1	W	180	GLN	Sidechain
1	W	417	GLN	Sidechain

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	3163	0	3054	267	0
1	B	3163	0	3054	252	0
1	C	3163	0	3054	254	0
1	D	3163	0	3055	269	0
1	E	3163	0	3054	265	0
1	F	3163	0	3054	264	0
1	G	3163	0	3054	250	0
1	H	3163	0	3054	265	0
1	I	3163	0	3054	274	0
1	J	3163	0	3054	251	0
1	K	3163	0	3055	283	0
1	L	3163	0	3054	256	0
1	M	3163	0	3055	259	0
1	N	3163	0	3054	256	0
1	O	3163	0	3055	266	0
1	P	3163	0	3054	260	0
1	Q	3163	0	3054	271	0
1	R	3163	0	3054	262	0
1	S	3163	0	3054	264	0
1	T	3163	0	3054	257	0
1	U	3163	0	3054	265	0
1	V	3163	0	3054	260	0
1	W	3163	0	3054	240	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	3163	0	3054	277	0
2	A	21	17	16	4	0
2	B	21	17	16	7	0
2	C	21	17	16	7	0
2	D	21	17	16	5	0
2	E	21	17	16	3	0
2	F	21	17	16	5	0
2	G	21	17	16	8	0
2	H	21	17	16	7	0
2	I	21	17	16	5	0
2	J	21	17	16	5	0
2	K	21	17	16	6	0
2	L	21	17	16	8	0
2	M	21	17	16	5	0
2	N	21	17	16	6	0
2	O	21	17	16	6	0
2	P	21	17	16	5	0
2	Q	21	17	16	9	0
2	R	21	17	16	7	0
2	S	21	17	16	6	0
2	T	21	17	16	6	0
2	U	21	17	16	5	0
2	V	21	17	16	5	0
2	W	21	17	16	4	0
2	X	21	17	16	7	0
3	A	14	9	10	5	0
3	B	14	9	10	7	0
3	C	14	9	10	4	0
3	D	14	9	10	5	0
3	E	14	9	10	3	0
3	F	14	9	10	6	0
3	G	14	9	10	5	0
3	H	14	9	10	5	0
3	I	14	9	10	5	0
3	J	14	9	10	5	0
3	K	14	9	10	7	0
3	L	14	9	10	5	0
3	M	14	9	10	9	0
3	N	14	9	10	6	0
3	O	14	9	10	6	0
3	P	14	9	10	5	0
3	Q	14	9	10	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	14	9	10	9	0
3	S	14	9	10	5	0
3	T	14	9	10	6	0
3	U	14	9	10	8	0
3	V	14	9	10	6	0
3	W	14	9	10	5	0
3	X	14	9	10	9	0
All	All	76752	624	73924	6046	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 40.

All (6046) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:320:GLN:CG	1:I:320:GLN:CB	1.77	1.59
1:S:320:GLN:CB	1:S:320:GLN:CG	1.79	1.57
1:J:320:GLN:CB	1:J:320:GLN:CG	1.82	1.52
1:I:110:SER:HB2	1:I:122:ARG:HB2	1.21	1.19
1:O:110:SER:HB2	1:O:122:ARG:HB2	1.20	1.19
1:G:110:SER:HB2	1:G:122:ARG:HB2	1.25	1.18
1:R:110:SER:HB2	1:R:122:ARG:HB2	1.22	1.16
1:X:110:SER:HB2	1:X:122:ARG:HB2	1.18	1.15
1:W:110:SER:HB2	1:W:122:ARG:HB2	1.17	1.14
1:C:110:SER:HB2	1:C:122:ARG:HB2	1.18	1.14
1:F:110:SER:HB2	1:F:122:ARG:HB2	1.15	1.14
1:W:35:ALA:HA	1:W:75:TYR:HE1	1.09	1.14
1:M:110:SER:HB2	1:M:122:ARG:HB2	1.26	1.13
1:V:110:SER:HB2	1:V:122:ARG:HB2	1.15	1.13
1:K:110:SER:HB2	1:K:122:ARG:HB2	1.14	1.13
1:P:110:SER:HB2	1:P:122:ARG:HB2	1.18	1.12
1:L:110:SER:HB2	1:L:122:ARG:HB2	1.22	1.12
1:O:35:ALA:HA	1:O:75:TYR:HE1	1.15	1.12
1:T:110:SER:HB2	1:T:122:ARG:HB2	1.16	1.11
1:U:110:SER:HB2	1:U:122:ARG:HB2	1.28	1.11
1:N:99:THR:HG23	1:N:193:LEU:HD23	1.33	1.11
1:B:110:SER:HB2	1:B:122:ARG:HB2	1.19	1.11
1:D:110:SER:HB2	1:D:122:ARG:HB2	1.20	1.10
1:E:110:SER:HB2	1:E:122:ARG:HB2	1.27	1.10
1:H:110:SER:HB2	1:H:122:ARG:HB2	1.20	1.10
1:N:110:SER:HB2	1:N:122:ARG:HB2	1.21	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:110:SER:HB2	1:S:122:ARG:HB2	1.19	1.10
1:C:390:TRP:HB2	1:C:399:ALA:HB2	1.31	1.09
1:C:99:THR:HG23	1:C:193:LEU:HD23	1.33	1.09
1:M:35:ALA:HA	1:M:75:TYR:HE1	1.17	1.09
1:N:390:TRP:HB2	1:N:399:ALA:HB2	1.35	1.08
1:J:110:SER:HB2	1:J:122:ARG:HB2	1.23	1.08
1:H:35:ALA:HA	1:H:75:TYR:HE1	1.19	1.07
1:E:35:ALA:HA	1:E:75:TYR:HE1	1.19	1.06
1:E:380:LEU:HB2	1:E:415:ILE:HG22	1.37	1.06
1:A:110:SER:HB2	1:A:122:ARG:HB2	1.17	1.06
1:P:390:TRP:HB2	1:P:399:ALA:HB2	1.35	1.06
1:X:35:ALA:HA	1:X:75:TYR:HE1	1.16	1.06
1:I:390:TRP:HB2	1:I:399:ALA:HB2	1.34	1.06
1:U:35:ALA:HA	1:U:75:TYR:HE1	1.17	1.05
1:Q:110:SER:HB2	1:Q:122:ARG:HB2	1.33	1.05
1:Q:165:GLN:HG3	1:S:172:GLN:HE22	1.15	1.05
1:J:35:ALA:HA	1:J:75:TYR:HE1	1.16	1.05
1:L:390:TRP:HB2	1:L:399:ALA:HB2	1.38	1.05
1:F:390:TRP:HB2	1:F:399:ALA:HB2	1.40	1.04
1:S:35:ALA:HA	1:S:75:TYR:HE1	1.17	1.04
1:S:420:ARG:HB2	1:S:447:TYR:HE1	1.20	1.04
1:V:35:ALA:HA	1:V:75:TYR:HE1	1.20	1.03
1:I:35:ALA:HA	1:I:75:TYR:HE1	1.24	1.03
1:F:99:THR:HG23	1:F:193:LEU:HD23	1.40	1.02
1:O:390:TRP:HB2	1:O:399:ALA:HB2	1.41	1.02
1:C:35:ALA:HA	1:C:75:TYR:HE1	1.26	1.01
1:G:35:ALA:HA	1:G:75:TYR:HE1	1.22	1.01
1:N:35:ALA:HA	1:N:75:TYR:HE1	1.20	1.01
1:R:99:THR:HG23	1:R:193:LEU:HD23	1.42	1.01
1:D:35:ALA:HA	1:D:75:TYR:HE1	1.22	1.01
1:T:390:TRP:HB2	1:T:399:ALA:HB2	1.41	1.01
1:F:35:ALA:HA	1:F:75:TYR:HE1	1.26	1.01
1:E:99:THR:HG23	1:E:193:LEU:HD23	1.41	1.00
1:G:390:TRP:HB2	1:G:399:ALA:HB2	1.36	1.00
1:B:35:ALA:HA	1:B:75:TYR:HE1	1.25	1.00
1:D:390:TRP:HB2	1:D:399:ALA:HB2	1.39	1.00
1:X:390:TRP:HB2	1:X:399:ALA:HB2	1.39	1.00
1:K:35:ALA:HA	1:K:75:TYR:HE1	1.26	1.00
1:R:390:TRP:HB2	1:R:399:ALA:HB2	1.40	1.00
1:K:420:ARG:HB2	1:K:447:TYR:HE1	1.26	1.00
1:L:99:THR:HG23	1:L:193:LEU:HD23	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:99:THR:HG23	1:V:193:LEU:HD23	1.44	1.00
1:K:420:ARG:HB2	1:K:447:TYR:CE1	1.97	1.00
1:C:420:ARG:HB2	1:C:447:TYR:HE1	1.27	0.99
1:P:99:THR:HG23	1:P:193:LEU:HD23	1.43	0.99
1:Q:35:ALA:HA	1:Q:75:TYR:HE1	1.22	0.99
1:W:35:ALA:HA	1:W:75:TYR:CE1	1.97	0.99
1:D:99:THR:HG23	1:D:193:LEU:HD23	1.41	0.99
1:X:35:ALA:HA	1:X:75:TYR:CE1	1.97	0.99
1:B:165:GLN:HG3	1:F:172:GLN:HE22	1.28	0.99
1:B:390:TRP:HB2	1:B:399:ALA:HB2	1.41	0.98
1:K:99:THR:HG23	1:K:193:LEU:HD23	1.44	0.98
1:M:165:GLN:HG3	1:O:172:GLN:HE22	1.25	0.98
1:A:165:GLN:HG3	1:E:172:GLN:HE22	1.28	0.98
1:B:116:GLY:H	1:B:398:HIS:CE1	1.81	0.98
1:D:380:LEU:HB2	1:D:415:ILE:HG22	1.45	0.98
1:S:420:ARG:HB2	1:S:447:TYR:CE1	1.98	0.97
1:V:390:TRP:HB2	1:V:399:ALA:HB2	1.42	0.97
1:D:374:VAL:HG13	1:D:382:VAL:HG21	1.46	0.97
1:H:420:ARG:HB2	1:H:447:TYR:HE1	1.29	0.97
1:C:420:ARG:HB2	1:C:447:TYR:CE1	1.99	0.97
1:J:172:GLN:HE22	1:L:165:GLN:HG3	1.30	0.97
1:U:172:GLN:HE22	1:W:165:GLN:HG3	1.30	0.97
1:I:420:ARG:HB2	1:I:447:TYR:HE1	1.30	0.97
1:K:390:TRP:HB2	1:K:399:ALA:HB2	1.45	0.97
1:R:35:ALA:HA	1:R:75:TYR:HE1	1.27	0.97
1:A:418:THR:HG21	1:A:421:LEU:HD12	1.46	0.96
1:F:420:ARG:HB2	1:F:447:TYR:CE1	2.00	0.96
1:K:428:SER:HB3	1:K:436:TYR:HB2	1.46	0.96
1:U:271:CYS:HB2	1:U:279:GLN:HE21	1.31	0.96
1:A:35:ALA:HA	1:A:75:TYR:HE1	1.28	0.96
1:O:420:ARG:HB2	1:O:447:TYR:HE1	1.29	0.96
1:M:35:ALA:HA	1:M:75:TYR:CE1	2.01	0.96
1:H:420:ARG:HB2	1:H:447:TYR:CE1	2.01	0.95
1:O:35:ALA:HA	1:O:75:TYR:CE1	2.01	0.95
1:W:420:ARG:HB2	1:W:447:TYR:CE1	2.01	0.95
1:X:420:ARG:HB2	1:X:447:TYR:CE1	2.01	0.95
1:J:75:TYR:HD2	1:K:75:TYR:HD2	1.09	0.95
1:W:420:ARG:HB2	1:W:447:TYR:HE1	1.28	0.95
1:F:420:ARG:HB2	1:F:447:TYR:HE1	1.32	0.95
1:G:420:ARG:HB2	1:G:447:TYR:CE1	2.01	0.95
1:W:390:TRP:HB2	1:W:399:ALA:HB2	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:420:ARG:HB2	1:N:447:TYR:HE1	1.32	0.95
1:T:99:THR:HG23	1:T:193:LEU:HD23	1.49	0.95
1:H:380:LEU:HB2	1:H:415:ILE:HG22	1.49	0.94
1:J:35:ALA:HA	1:J:75:TYR:CE1	2.02	0.94
1:U:420:ARG:HB2	1:U:447:TYR:CE1	2.01	0.94
1:S:35:ALA:HA	1:S:75:TYR:CE1	2.01	0.94
1:S:390:TRP:HB2	1:S:399:ALA:HB2	1.48	0.94
1:G:418:THR:HG21	1:G:421:LEU:HD12	1.49	0.94
1:O:420:ARG:HB2	1:O:447:TYR:CE1	2.02	0.94
1:V:172:GLN:HE22	1:X:165:GLN:HG3	1.30	0.94
1:P:35:ALA:HA	1:P:75:TYR:HE1	1.30	0.94
1:U:35:ALA:HA	1:U:75:TYR:CE1	2.03	0.94
1:A:99:THR:HG23	1:A:193:LEU:HD23	1.50	0.94
1:V:420:ARG:HB2	1:V:447:TYR:HE1	1.30	0.94
1:U:420:ARG:HB2	1:U:447:TYR:HE1	1.30	0.94
1:V:420:ARG:HB2	1:V:447:TYR:CE1	2.03	0.93
1:D:35:ALA:HA	1:D:75:TYR:CE1	2.04	0.93
1:L:271:CYS:HB2	1:L:279:GLN:HE21	1.32	0.93
1:E:35:ALA:HA	1:E:75:TYR:CE1	2.03	0.93
1:N:172:GLN:HE22	1:P:165:GLN:HG3	1.32	0.93
1:A:254:ASN:O	1:A:258:GLN:HG2	1.68	0.93
1:J:390:TRP:HB2	1:J:399:ALA:HB2	1.46	0.93
1:R:420:ARG:HB2	1:R:447:TYR:HE1	1.32	0.93
1:G:99:THR:HG23	1:G:193:LEU:HD23	1.47	0.93
1:D:172:GLN:HE22	1:H:165:GLN:HG3	1.31	0.93
1:I:428:SER:HB3	1:I:436:TYR:HB2	1.49	0.93
1:N:420:ARG:HB2	1:N:447:TYR:CE1	2.04	0.93
1:T:271:CYS:HB2	1:T:279:GLN:HE21	1.31	0.93
1:F:428:SER:HB3	1:F:436:TYR:HB2	1.51	0.93
1:K:228:VAL:HG12	1:K:232:ILE:HD11	1.47	0.93
1:Q:390:TRP:HB2	1:Q:399:ALA:HB2	1.48	0.93
1:E:271:CYS:HB2	1:E:279:GLN:HE21	1.34	0.93
1:I:420:ARG:HB2	1:I:447:TYR:CE1	2.02	0.93
1:X:420:ARG:HB2	1:X:447:TYR:HE1	1.33	0.93
1:C:172:GLN:HE22	1:G:165:GLN:HG3	1.31	0.93
1:T:228:VAL:HG12	1:T:232:ILE:HD11	1.49	0.92
1:D:75:TYR:HD2	1:F:75:TYR:HD2	1.14	0.92
1:J:380:LEU:HB2	1:J:415:ILE:HG22	1.50	0.92
1:B:420:ARG:HB2	1:B:447:TYR:CE1	2.02	0.92
1:X:99:THR:HG23	1:X:193:LEU:HD23	1.51	0.92
1:J:99:THR:HG23	1:J:193:LEU:HD23	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:ALA:HA	1:G:75:TYR:CE1	2.04	0.92
1:E:390:TRP:HB2	1:E:399:ALA:HB2	1.51	0.92
1:Q:99:THR:HG23	1:Q:193:LEU:HD23	1.50	0.92
1:G:420:ARG:HB2	1:G:447:TYR:HE1	1.33	0.92
1:B:116:GLY:N	1:B:398:HIS:HE1	1.67	0.91
1:T:420:ARG:HB2	1:T:447:TYR:CE1	2.06	0.91
1:P:35:ALA:HA	1:P:75:TYR:CE1	2.05	0.91
1:P:420:ARG:HB2	1:P:447:TYR:CE1	2.05	0.91
1:H:99:THR:HG23	1:H:193:LEU:HD23	1.52	0.91
1:P:428:SER:HB3	1:P:436:TYR:HB2	1.52	0.91
1:L:420:ARG:HB2	1:L:447:TYR:CE1	2.06	0.91
1:X:234:GLU:OE2	1:X:237:ARG:NH2	2.03	0.91
1:Q:242:GLU:O	1:Q:243:ARG:HG2	1.71	0.91
1:L:35:ALA:HA	1:L:75:TYR:HE1	1.32	0.90
1:M:420:ARG:HB2	1:M:447:TYR:CE1	2.05	0.90
1:J:402:TYR:HB3	1:J:403:PRO:HD3	1.53	0.90
1:M:242:GLU:O	1:M:243:ARG:HG2	1.71	0.90
1:V:35:ALA:HA	1:V:75:TYR:CE1	2.07	0.90
1:D:228:VAL:HG12	1:D:232:ILE:HD11	1.50	0.90
1:I:271:CYS:HB2	1:I:279:GLN:HE21	1.37	0.90
1:X:254:ASN:O	1:X:258:GLN:HG2	1.70	0.90
1:B:418:THR:HG21	1:B:421:LEU:HD12	1.52	0.90
1:U:242:GLU:O	1:U:243:ARG:HG2	1.71	0.90
1:V:242:GLU:O	1:V:243:ARG:HG2	1.72	0.90
1:C:35:ALA:HA	1:C:75:TYR:CE1	2.04	0.90
1:G:242:GLU:O	1:G:243:ARG:HG2	1.70	0.90
1:J:165:GLN:HG3	1:L:172:GLN:HE22	1.36	0.90
1:Q:402:TYR:HB3	1:Q:403:PRO:HD3	1.53	0.90
1:E:374:VAL:HG13	1:E:382:VAL:HG21	1.54	0.90
1:G:428:SER:HB3	1:G:436:TYR:HB2	1.52	0.90
1:A:242:GLU:O	1:A:243:ARG:HG2	1.71	0.90
1:N:242:GLU:O	1:N:243:ARG:HG2	1.72	0.90
1:U:99:THR:HG23	1:U:193:LEU:HD23	1.53	0.90
1:C:242:GLU:O	1:C:243:ARG:HG2	1.70	0.89
1:F:35:ALA:HA	1:F:75:TYR:CE1	2.06	0.89
1:A:380:LEU:HB2	1:A:415:ILE:HG22	1.54	0.89
1:I:165:GLN:HG3	1:K:172:GLN:HE22	1.37	0.89
1:J:420:ARG:HB2	1:J:447:TYR:CE1	2.06	0.89
1:O:371:TYR:OH	3:O:502:DST:O7	1.90	0.89
1:Q:35:ALA:HA	1:Q:75:TYR:CE1	2.08	0.89
1:T:380:LEU:HB2	1:T:415:ILE:HG22	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:242:GLU:O	1:K:243:ARG:HG2	1.71	0.89
1:N:35:ALA:HA	1:N:75:TYR:CE1	2.08	0.89
1:R:420:ARG:HB2	1:R:447:TYR:CE1	2.07	0.89
1:A:420:ARG:HB2	1:A:447:TYR:CE1	2.08	0.89
1:H:390:TRP:HB2	1:H:399:ALA:HB2	1.55	0.89
1:I:35:ALA:HA	1:I:75:TYR:CE1	2.08	0.89
1:M:420:ARG:HB2	1:M:447:TYR:HE1	1.35	0.89
1:R:242:GLU:O	1:R:243:ARG:HG2	1.73	0.89
1:M:99:THR:HG23	1:M:193:LEU:HD23	1.55	0.88
1:O:290:VAL:HG11	1:O:353:ILE:HG12	1.55	0.88
1:V:402:TYR:HB3	1:V:403:PRO:HD3	1.54	0.88
1:V:415:ILE:HA	1:V:418:THR:HG22	1.55	0.88
1:H:242:GLU:O	1:H:243:ARG:HG2	1.72	0.88
1:H:35:ALA:HA	1:H:75:TYR:CE1	2.07	0.88
1:S:380:LEU:HB2	1:S:415:ILE:HG22	1.55	0.88
1:W:99:THR:HG23	1:W:193:LEU:HD23	1.55	0.88
1:R:35:ALA:HA	1:R:75:TYR:CE1	2.08	0.88
1:N:402:TYR:HB3	1:N:403:PRO:HD3	1.55	0.88
1:X:242:GLU:O	1:X:243:ARG:HG2	1.72	0.88
1:B:420:ARG:HB2	1:B:447:TYR:HE1	1.34	0.88
1:M:390:TRP:HB2	1:M:399:ALA:HB2	1.55	0.88
1:Q:420:ARG:HB2	1:Q:447:TYR:CE1	2.08	0.88
1:U:165:GLN:HG3	1:W:172:GLN:HE22	1.39	0.88
1:W:380:LEU:HB2	1:W:415:ILE:HG22	1.55	0.88
1:E:282:LYS:HD2	1:E:356:ASN:HD21	1.39	0.88
1:H:428:SER:HB3	1:H:436:TYR:HB2	1.55	0.87
1:O:380:LEU:HB2	1:O:415:ILE:HG22	1.57	0.87
1:Q:75:TYR:HD2	1:T:75:TYR:HD2	1.20	0.87
1:U:390:TRP:HB2	1:U:399:ALA:HB2	1.54	0.87
1:I:242:GLU:O	1:I:243:ARG:HG2	1.73	0.87
1:O:228:VAL:HG12	1:O:232:ILE:HD11	1.54	0.87
1:K:35:ALA:HA	1:K:75:TYR:CE1	2.08	0.87
1:R:228:VAL:HG12	1:R:232:ILE:HD11	1.56	0.87
1:E:172:GLN:C	1:E:173:LEU:HD12	1.95	0.87
1:L:420:ARG:HB2	1:L:447:TYR:HE1	1.37	0.87
1:B:242:GLU:O	1:B:243:ARG:HG2	1.73	0.87
1:A:172:GLN:HE22	1:E:165:GLN:HG3	1.39	0.87
1:A:420:ARG:HB2	1:A:447:TYR:HE1	1.37	0.87
1:B:35:ALA:HA	1:B:75:TYR:CE1	2.10	0.87
1:T:242:GLU:O	1:T:243:ARG:HG2	1.74	0.87
1:J:242:GLU:O	1:J:243:ARG:HG2	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:420:ARG:HB2	1:J:447:TYR:HE1	1.37	0.87
1:L:242:GLU:O	1:L:243:ARG:HG2	1.74	0.87
1:P:234:GLU:OE2	1:P:237:ARG:NH2	2.07	0.87
1:E:308:GLU:HB2	1:E:311:ILE:HD13	1.56	0.86
1:S:228:VAL:HG12	1:S:232:ILE:HD11	1.55	0.86
1:J:172:GLN:C	1:J:173:LEU:HD12	1.95	0.86
1:L:380:LEU:HB2	1:L:415:ILE:HG22	1.55	0.86
1:N:415:ILE:HA	1:N:418:THR:HG22	1.58	0.86
1:O:242:GLU:O	1:O:243:ARG:HG2	1.74	0.86
1:S:172:GLN:C	1:S:173:LEU:HD12	1.95	0.86
1:A:264:ASN:O	1:A:267:THR:HG22	1.75	0.86
1:T:420:ARG:HB2	1:T:447:TYR:HE1	1.39	0.86
1:D:242:GLU:O	1:D:243:ARG:HG2	1.75	0.86
1:D:290:VAL:HG11	1:D:353:ILE:HG12	1.58	0.86
1:M:271:CYS:HB2	1:M:279:GLN:HE21	1.37	0.86
1:R:172:GLN:C	1:R:173:LEU:HD12	1.96	0.86
1:C:122:ARG:HG2	1:C:202:ASP:OD1	1.75	0.86
1:E:242:GLU:O	1:E:243:ARG:HG2	1.75	0.86
1:B:402:TYR:HB3	1:B:403:PRO:HD3	1.55	0.86
1:J:379:ASP:HB2	1:J:418:THR:HG23	1.56	0.86
1:B:374:VAL:HG13	1:B:382:VAL:HG21	1.58	0.86
1:F:242:GLU:O	1:F:243:ARG:HG2	1.74	0.86
1:P:402:TYR:HB3	1:P:403:PRO:HD3	1.57	0.86
1:C:406:LEU:HD12	1:C:415:ILE:CD1	2.05	0.85
1:M:75:TYR:HD2	1:P:75:TYR:HD2	1.21	0.85
1:M:180:GLN:HE21	1:M:223:ALA:HB2	1.41	0.85
1:C:428:SER:HB3	1:C:436:TYR:HB2	1.59	0.85
1:B:116:GLY:H	1:B:398:HIS:HE1	0.90	0.85
1:J:271:CYS:HB2	1:J:279:GLN:HE21	1.41	0.85
1:M:379:ASP:HB2	1:M:418:THR:HG23	1.58	0.85
1:P:242:GLU:O	1:P:243:ARG:HG2	1.74	0.85
1:S:242:GLU:O	1:S:243:ARG:HG2	1.74	0.85
1:W:242:GLU:O	1:W:243:ARG:HG2	1.75	0.85
1:Q:420:ARG:HB2	1:Q:447:TYR:HE1	1.38	0.85
1:G:380:LEU:HB2	1:G:415:ILE:HG22	1.58	0.85
1:O:99:THR:HG23	1:O:193:LEU:HD23	1.58	0.85
1:D:379:ASP:HB2	1:D:418:THR:HG23	1.56	0.85
1:J:308:GLU:HB2	1:J:311:ILE:HD13	1.57	0.85
1:E:420:ARG:HB2	1:E:447:TYR:HE1	1.41	0.85
1:G:271:CYS:HB2	1:G:279:GLN:HE21	1.40	0.85
1:H:402:TYR:HB3	1:H:403:PRO:HD3	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:75:TYR:HD2	1:X:75:TYR:HD2	1.24	0.85
1:E:402:TYR:HB3	1:E:403:PRO:HD3	1.58	0.84
1:H:271:CYS:HB2	1:H:279:GLN:HE21	1.40	0.84
1:I:75:TYR:HD2	1:L:75:TYR:HD2	1.23	0.84
1:O:173:LEU:HD13	1:O:196:GLN:HE22	1.41	0.84
1:I:418:THR:HG21	1:I:421:LEU:HD12	1.58	0.84
1:P:380:LEU:HB2	1:P:415:ILE:HG22	1.59	0.84
1:V:253:ILE:HD12	1:V:359:ILE:HD11	1.56	0.84
1:M:172:GLN:HE22	1:O:165:GLN:HG3	1.39	0.84
1:C:271:CYS:HB2	1:C:279:GLN:HE21	1.43	0.84
1:M:239:ILE:HD12	1:M:242:GLU:HG2	1.59	0.84
1:U:239:ILE:HD12	1:U:242:GLU:HG2	1.59	0.84
1:A:440:TYR:OH	3:A:502:DST:O7	1.93	0.84
1:O:402:TYR:HB3	1:O:403:PRO:HD3	1.59	0.84
1:F:228:VAL:HG12	1:F:232:ILE:HD11	1.59	0.84
1:P:172:GLN:C	1:P:173:LEU:HD12	1.98	0.84
1:D:420:ARG:HB2	1:D:447:TYR:CE1	2.11	0.84
1:L:228:VAL:HG12	1:L:232:ILE:HD11	1.56	0.84
1:B:172:GLN:C	1:B:173:LEU:HD12	1.99	0.84
1:B:271:CYS:HB2	1:B:279:GLN:HE21	1.42	0.84
1:D:420:ARG:HB2	1:D:447:TYR:HE1	1.42	0.84
1:P:420:ARG:HB2	1:P:447:TYR:HE1	1.39	0.84
1:A:35:ALA:HA	1:A:75:TYR:CE1	2.12	0.84
1:F:282:LYS:HD2	1:F:356:ASN:HD21	1.43	0.84
1:R:228:VAL:HG12	1:R:232:ILE:CD1	2.08	0.84
1:X:271:CYS:HB2	1:X:279:GLN:HE21	1.40	0.84
1:A:390:TRP:HB2	1:A:399:ALA:HB2	1.60	0.83
1:Q:122:ARG:HG2	1:Q:202:ASP:OD1	1.78	0.83
1:L:308:GLU:HB2	1:L:311:ILE:HD13	1.59	0.83
1:P:405:THR:O	1:P:409:LEU:HD13	1.77	0.83
1:C:75:TYR:HD2	1:E:75:TYR:HD2	1.23	0.83
1:G:285:GLY:HA3	1:G:355:TRP:CZ2	2.13	0.83
1:Q:428:SER:HB3	1:Q:436:TYR:HB2	1.59	0.83
1:B:75:TYR:HD2	1:H:75:TYR:HD2	1.21	0.83
1:L:264:ASN:O	1:L:267:THR:HG22	1.77	0.83
1:C:402:TYR:HB3	1:C:403:PRO:HD3	1.60	0.83
1:I:374:VAL:HG13	1:I:382:VAL:HG21	1.58	0.83
1:T:35:ALA:HA	1:T:75:TYR:HE1	1.41	0.83
1:T:228:VAL:HG12	1:T:232:ILE:CD1	2.08	0.83
1:M:122:ARG:HG2	1:M:202:ASP:OD1	1.78	0.83
1:N:75:TYR:HD2	1:O:75:TYR:HD2	1.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:172:GLN:HE22	1:S:165:GLN:HG3	1.41	0.83
1:W:271:CYS:HB2	1:W:279:GLN:HE21	1.43	0.83
1:X:172:GLN:C	1:X:173:LEU:HD12	1.98	0.83
1:R:402:TYR:HB3	1:R:403:PRO:HD3	1.60	0.83
1:S:173:LEU:HD13	1:S:196:GLN:HE22	1.43	0.83
1:F:280:ARG:HD2	1:F:358:GLU:OE2	1.78	0.83
1:K:354:ILE:HG21	3:K:502:DST:H132	1.61	0.83
1:M:264:ASN:O	1:M:267:THR:HG22	1.78	0.83
1:U:282:LYS:HD2	1:U:356:ASN:HD21	1.43	0.83
1:I:115:LYS:HE2	1:I:434:GLY:HA3	1.61	0.83
1:O:271:CYS:HB2	1:O:279:GLN:HE21	1.43	0.83
1:P:418:THR:HG21	1:P:421:LEU:HD12	1.59	0.83
1:I:320:GLN:CG	1:I:320:GLN:CA	2.56	0.82
1:H:264:ASN:O	1:H:267:THR:HG22	1.79	0.82
1:I:285:GLY:HA3	1:I:355:TRP:CZ2	2.14	0.82
1:P:271:CYS:HB2	1:P:279:GLN:HE21	1.43	0.82
1:S:290:VAL:HG11	1:S:353:ILE:HG12	1.60	0.82
1:A:172:GLN:C	1:A:173:LEU:HD12	1.99	0.82
1:D:172:GLN:C	1:D:173:LEU:HD12	2.00	0.82
1:D:271:CYS:HB2	1:D:279:GLN:HE21	1.44	0.82
1:W:402:TYR:HB3	1:W:403:PRO:HD3	1.60	0.82
1:V:112:ASN:HD22	1:V:122:ARG:HH21	1.28	0.82
1:G:259:GLU:OE2	1:G:304:ARG:NH1	2.11	0.82
1:M:428:SER:HB3	1:M:436:TYR:HB2	1.61	0.82
1:U:402:TYR:HB3	1:U:403:PRO:HD3	1.60	0.82
1:A:75:TYR:HD2	1:G:75:TYR:HD2	1.27	0.82
1:A:428:SER:HB3	1:A:436:TYR:HB2	1.62	0.82
1:V:75:TYR:HD2	1:W:75:TYR:HD2	1.27	0.82
1:E:420:ARG:HB2	1:E:447:TYR:CE1	2.13	0.82
1:D:308:GLU:HB2	1:D:311:ILE:HD13	1.61	0.82
1:I:380:LEU:HB2	1:I:415:ILE:HG22	1.59	0.82
1:X:228:VAL:HG12	1:X:232:ILE:HD11	1.60	0.82
1:X:415:ILE:HA	1:X:418:THR:HG22	1.61	0.82
1:A:271:CYS:HB2	1:A:279:GLN:HE21	1.43	0.82
1:G:172:GLN:C	1:G:173:LEU:HD12	2.00	0.82
1:K:271:CYS:HB2	1:K:279:GLN:HE21	1.45	0.82
1:R:165:GLN:HG3	1:T:172:GLN:HE22	1.42	0.82
1:E:379:ASP:HB2	1:E:418:THR:HG23	1.59	0.81
1:R:415:ILE:HA	1:R:418:THR:HG22	1.62	0.81
1:K:228:VAL:HG12	1:K:232:ILE:CD1	2.08	0.81
1:X:428:SER:HB3	1:X:436:TYR:HB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:228:VAL:HG12	1:I:232:ILE:HD11	1.62	0.81
1:J:320:GLN:CG	1:J:320:GLN:CA	2.58	0.81
1:V:380:LEU:HB2	1:V:415:ILE:HG22	1.62	0.81
1:Q:239:ILE:HD12	1:Q:242:GLU:HG2	1.61	0.81
1:R:115:LYS:HE2	1:R:434:GLY:HA3	1.60	0.81
1:S:320:GLN:CG	1:S:320:GLN:CA	2.57	0.81
1:G:228:VAL:HG12	1:G:232:ILE:HD11	1.63	0.81
1:I:228:VAL:HG12	1:I:232:ILE:CD1	2.10	0.81
1:S:99:THR:HG23	1:S:193:LEU:HD23	1.63	0.81
1:W:172:GLN:C	1:W:173:LEU:HD12	2.01	0.81
1:C:380:LEU:HB2	1:C:415:ILE:HG22	1.62	0.81
1:F:406:LEU:HD12	1:F:415:ILE:CD1	2.11	0.81
1:X:402:TYR:HB3	1:X:403:PRO:HD3	1.60	0.81
1:K:402:TYR:HB3	1:K:403:PRO:HD3	1.62	0.81
1:M:402:TYR:HB3	1:M:403:PRO:HD3	1.62	0.81
1:Q:271:CYS:HB2	1:Q:279:GLN:HE21	1.46	0.81
1:R:172:GLN:HE22	1:T:165:GLN:HG3	1.45	0.81
1:L:228:VAL:HG12	1:L:232:ILE:CD1	2.09	0.81
1:M:173:LEU:O	1:M:174:SER:OG	1.98	0.81
1:N:228:VAL:HG12	1:N:232:ILE:HD11	1.61	0.81
1:N:428:SER:HB3	1:N:436:TYR:HB2	1.62	0.81
1:W:308:GLU:HB2	1:W:311:ILE:HD13	1.61	0.81
1:B:234:GLU:OE2	1:B:237:ARG:NH2	2.13	0.81
1:O:374:VAL:HG13	1:O:382:VAL:HG21	1.64	0.81
1:X:122:ARG:HG2	1:X:202:ASP:OD1	1.81	0.81
1:A:171:PHE:CE1	1:A:217:PRO:HB3	2.16	0.80
1:P:228:VAL:HG12	1:P:232:ILE:HD11	1.63	0.80
1:L:171:PHE:CE1	1:L:217:PRO:HB3	2.16	0.80
1:M:380:LEU:HB2	1:M:415:ILE:HG22	1.62	0.80
1:D:280:ARG:HD2	1:D:358:GLU:OE2	1.80	0.80
1:O:234:GLU:O	1:O:238:THR:HG23	1.82	0.80
1:Q:115:LYS:HE2	1:Q:434:GLY:HA3	1.63	0.80
1:L:418:THR:HG21	1:L:421:LEU:HD12	1.61	0.80
1:T:172:GLN:C	1:T:173:LEU:HD12	2.02	0.80
1:F:122:ARG:HG2	1:F:202:ASP:OD1	1.82	0.80
1:P:259:GLU:OE2	1:P:304:ARG:NH1	2.14	0.80
1:X:115:LYS:HE2	1:X:434:GLY:HA3	1.63	0.80
1:R:115:LYS:CE	1:R:434:GLY:HA3	2.11	0.80
1:X:234:GLU:O	1:X:238:THR:HG23	1.82	0.80
1:B:395:TRP:HB3	1:B:398:HIS:ND1	1.96	0.80
1:L:428:SER:HB3	1:L:436:TYR:HB2	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:402:TYR:HB3	1:S:403:PRO:HD3	1.63	0.80
1:T:428:SER:HB3	1:T:436:TYR:HB2	1.61	0.80
1:E:387:ALA:HA	1:E:390:TRP:CD1	2.17	0.80
1:M:354:ILE:HG21	3:M:502:DST:H132	1.63	0.80
1:P:264:ASN:O	1:P:267:THR:HG22	1.81	0.80
1:P:280:ARG:HD2	1:P:358:GLU:OE2	1.81	0.80
1:E:292:TRP:HZ2	1:E:315:LEU:HD21	1.47	0.79
1:B:122:ARG:HG2	1:B:202:ASP:OD1	1.82	0.79
1:D:228:VAL:HG12	1:D:232:ILE:CD1	2.12	0.79
1:I:402:TYR:HB3	1:I:403:PRO:HD3	1.64	0.79
1:D:259:GLU:OE2	1:D:304:ARG:NH1	2.15	0.79
1:I:60:PHE:CE1	1:I:123:ILE:HD11	2.15	0.79
1:W:301:LEU:O	1:W:304:ARG:HG2	1.82	0.79
1:D:234:GLU:O	1:D:238:THR:HG23	1.82	0.79
1:F:259:GLU:OE2	1:F:304:ARG:NH1	2.14	0.79
1:C:280:ARG:HD2	1:C:358:GLU:OE2	1.83	0.79
1:I:60:PHE:HE1	1:I:123:ILE:HD11	1.48	0.79
1:I:99:THR:HG23	1:I:193:LEU:HD23	1.64	0.79
1:J:212:LYS:NZ	3:J:502:DST:O6	2.16	0.79
1:L:35:ALA:HA	1:L:75:TYR:CE1	2.16	0.79
1:M:292:TRP:CH2	1:M:319:LYS:HB2	2.18	0.79
1:O:285:GLY:HA3	1:O:355:TRP:CZ2	2.17	0.79
1:P:234:GLU:O	1:P:238:THR:HG23	1.82	0.79
1:X:264:ASN:O	1:X:267:THR:HG22	1.81	0.79
1:G:115:LYS:HE2	1:G:434:GLY:HA3	1.65	0.79
1:D:402:TYR:HB3	1:D:403:PRO:HD3	1.64	0.79
1:L:172:GLN:C	1:L:173:LEU:HD12	2.02	0.79
1:L:379:ASP:HB2	1:L:418:THR:HG23	1.64	0.79
1:S:301:LEU:O	1:S:304:ARG:HG2	1.83	0.79
1:W:259:GLU:OE2	1:W:304:ARG:NH1	2.16	0.79
1:O:253:ILE:HD12	1:O:359:ILE:HD11	1.63	0.79
1:Q:280:ARG:HD2	1:Q:358:GLU:OE2	1.82	0.79
1:T:35:ALA:HA	1:T:75:TYR:CE1	2.17	0.79
1:W:234:GLU:OE2	1:W:237:ARG:NH2	2.15	0.79
1:G:402:TYR:HB3	1:G:403:PRO:HD3	1.64	0.79
1:N:418:THR:HG21	1:N:421:LEU:HD12	1.63	0.79
1:O:228:VAL:HG12	1:O:232:ILE:CD1	2.13	0.79
1:C:234:GLU:OE2	1:C:237:ARG:NH2	2.16	0.79
1:K:308:GLU:HB2	1:K:311:ILE:HD13	1.63	0.79
1:V:165:GLN:HG3	1:X:172:GLN:HE22	1.45	0.79
1:R:354:ILE:HG21	3:R:502:DST:H132	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:GLU:O	1:G:238:THR:HG23	1.82	0.79
1:I:253:ILE:HD12	1:I:359:ILE:HD11	1.63	0.79
1:V:234:GLU:O	1:V:238:THR:HG23	1.83	0.78
1:D:112:ASN:HD22	1:D:122:ARG:HH21	1.31	0.78
1:K:379:ASP:HB2	1:K:418:THR:HG23	1.64	0.78
1:S:271:CYS:HB2	1:S:279:GLN:HE21	1.47	0.78
1:V:172:GLN:C	1:V:173:LEU:HD12	2.03	0.78
1:F:418:THR:HG21	1:F:421:LEU:HD12	1.63	0.78
1:K:234:GLU:OE2	1:K:237:ARG:NH2	2.16	0.78
1:K:380:LEU:HB2	1:K:415:ILE:HG22	1.64	0.78
1:S:418:THR:HG21	1:S:421:LEU:HD12	1.64	0.78
1:U:354:ILE:HG21	3:U:502:DST:H132	1.64	0.78
1:U:379:ASP:HB2	1:U:418:THR:HG23	1.64	0.78
1:G:122:ARG:HG2	1:G:202:ASP:OD1	1.83	0.78
1:I:239:ILE:HD12	1:I:242:GLU:HG2	1.63	0.78
1:J:290:VAL:HG11	1:J:353:ILE:HG12	1.63	0.78
1:D:234:GLU:OE2	1:D:237:ARG:NH2	2.15	0.78
1:I:264:ASN:O	1:I:267:THR:HG22	1.83	0.78
1:J:75:TYR:CD2	1:K:75:TYR:HD2	2.00	0.78
1:G:271:CYS:HB2	1:G:279:GLN:NE2	1.98	0.78
1:D:418:THR:HG21	1:D:421:LEU:HD12	1.65	0.78
1:F:115:LYS:HE2	1:F:434:GLY:HA3	1.66	0.78
1:H:306:ILE:HD12	1:H:307:GLU:HG3	1.64	0.78
1:U:172:GLN:C	1:U:173:LEU:HD12	2.03	0.78
1:U:228:VAL:HG12	1:U:232:ILE:HD11	1.63	0.78
1:H:228:VAL:HG12	1:H:232:ILE:CD1	2.13	0.78
1:K:280:ARG:HD2	1:K:358:GLU:OE2	1.83	0.78
1:J:75:TYR:HD2	1:K:75:TYR:CD2	1.97	0.78
1:N:172:GLN:C	1:N:173:LEU:HD12	2.04	0.78
1:Q:264:ASN:O	1:Q:267:THR:HG22	1.84	0.78
1:U:114:GLN:HE22	1:U:436:TYR:HD1	1.32	0.78
1:X:228:VAL:HG12	1:X:232:ILE:CD1	2.13	0.78
1:C:259:GLU:OE2	1:C:304:ARG:NH1	2.16	0.78
1:C:415:ILE:HA	1:C:418:THR:HG22	1.66	0.78
1:H:228:VAL:HG12	1:H:232:ILE:HD11	1.65	0.78
1:I:172:GLN:C	1:I:173:LEU:HD12	2.03	0.78
1:P:115:LYS:HE2	1:P:434:GLY:HA3	1.66	0.78
1:S:386:LEU:HD13	1:S:390:TRP:NE1	1.99	0.78
1:J:41:TYR:OH	1:K:208:ALA:HA	1.83	0.78
1:N:239:ILE:HD12	1:N:242:GLU:HG2	1.66	0.78
1:R:42:HIS:HB2	1:S:79:PHE:CE2	2.18	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:259:GLU:OE2	1:X:304:ARG:NH1	2.16	0.78
1:X:374:VAL:HG11	1:X:422:GLN:HG2	1.63	0.78
1:C:208:ALA:HA	1:E:41:TYR:OH	1.84	0.78
1:C:292:TRP:CH2	1:C:319:LYS:HB2	2.19	0.78
1:K:406:LEU:HD12	1:K:415:ILE:CD1	2.13	0.78
1:Q:112:ASN:HD22	1:Q:122:ARG:HH21	1.32	0.78
1:R:259:GLU:OE2	1:R:304:ARG:NH1	2.15	0.78
1:P:122:ARG:HG2	1:P:202:ASP:OD1	1.83	0.77
1:C:115:LYS:HE2	1:C:434:GLY:HA3	1.66	0.77
1:H:85:LEU:HB3	1:H:125:PHE:HE1	1.49	0.77
1:O:264:ASN:O	1:O:267:THR:HG22	1.84	0.77
1:F:228:VAL:HG12	1:F:232:ILE:CD1	2.13	0.77
1:T:405:THR:O	1:T:409:LEU:HD13	1.83	0.77
1:A:406:LEU:HD12	1:A:415:ILE:CD1	2.15	0.77
1:M:371:TYR:OH	3:M:502:DST:O7	2.02	0.77
1:Q:236:VAL:O	1:Q:239:ILE:HG22	1.84	0.77
1:U:387:ALA:HA	1:U:390:TRP:CD1	2.19	0.77
1:L:402:TYR:HB3	1:L:403:PRO:HD3	1.65	0.77
1:E:234:GLU:O	1:E:238:THR:HG23	1.84	0.77
1:K:105:LEU:HD12	1:K:107:ILE:H	1.48	0.77
1:O:115:LYS:HE2	1:O:434:GLY:HA3	1.67	0.77
1:A:114:GLN:HE22	1:A:436:TYR:HD1	1.32	0.77
1:G:239:ILE:HD12	1:G:242:GLU:HG2	1.65	0.77
1:I:172:GLN:HE22	1:K:165:GLN:HG3	1.48	0.77
1:K:292:TRP:CH2	1:K:319:LYS:HB2	2.19	0.77
1:O:172:GLN:C	1:O:173:LEU:HD12	2.05	0.77
1:T:171:PHE:CE1	1:T:217:PRO:HB3	2.20	0.77
1:T:402:TYR:HB3	1:T:403:PRO:HD3	1.67	0.77
1:G:228:VAL:HG12	1:G:232:ILE:CD1	2.15	0.77
1:M:433:ARG:HG3	1:M:436:TYR:OH	1.84	0.77
1:O:140:ASN:OD1	1:O:143:PRO:HG2	1.85	0.77
1:Q:282:LYS:HD2	1:Q:356:ASN:HD21	1.50	0.77
1:U:271:CYS:HB2	1:U:279:GLN:NE2	1.98	0.77
1:X:292:TRP:CH2	1:X:319:LYS:HB2	2.19	0.77
1:I:280:ARG:HD2	1:I:358:GLU:OE2	1.83	0.77
1:J:387:ALA:HA	1:J:390:TRP:CD1	2.19	0.77
1:L:271:CYS:HB2	1:L:279:GLN:NE2	2.00	0.77
1:D:264:ASN:O	1:D:267:THR:HG22	1.83	0.76
1:H:418:THR:HG21	1:H:421:LEU:HD12	1.66	0.76
1:I:321:ILE:HD11	1:I:389:PHE:CZ	2.20	0.76
1:R:75:TYR:HD2	1:S:75:TYR:HD2	1.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:228:VAL:HG12	1:S:232:ILE:CD1	2.15	0.76
1:T:285:GLY:HA3	1:T:355:TRP:CZ2	2.19	0.76
1:C:264:ASN:O	1:C:267:THR:HG22	1.85	0.76
1:J:374:VAL:HG13	1:J:382:VAL:HG21	1.67	0.76
1:D:415:ILE:HA	1:D:418:THR:HG22	1.67	0.76
1:Q:433:ARG:HG3	1:Q:436:TYR:OH	1.85	0.76
1:G:280:ARG:HD2	1:G:358:GLU:OE2	1.85	0.76
1:G:379:ASP:HB2	1:G:418:THR:HG23	1.68	0.76
1:C:171:PHE:CE1	1:C:217:PRO:HB3	2.21	0.76
1:K:112:ASN:HD22	1:K:122:ARG:HH21	1.32	0.76
1:K:418:THR:HG21	1:K:421:LEU:HD12	1.66	0.76
1:X:380:LEU:HB2	1:X:415:ILE:HG22	1.68	0.76
1:V:282:LYS:HE3	1:V:284:TYR:OH	1.85	0.76
1:B:428:SER:HB3	1:B:436:TYR:HB2	1.68	0.76
1:F:405:THR:O	1:F:409:LEU:HD13	1.86	0.76
1:I:259:GLU:OE2	1:I:304:ARG:NH1	2.17	0.76
1:N:165:GLN:HG3	1:P:172:GLN:HE22	1.49	0.76
1:C:285:GLY:HA3	1:C:355:TRP:CZ2	2.21	0.76
1:G:85:LEU:HB3	1:G:125:PHE:HE1	1.49	0.76
1:F:239:ILE:HD12	1:F:242:GLU:HG2	1.67	0.76
1:M:271:CYS:HB2	1:M:279:GLN:NE2	2.00	0.76
1:S:405:THR:O	1:S:409:LEU:HD13	1.86	0.76
1:H:172:GLN:C	1:H:173:LEU:HD12	2.06	0.76
1:P:239:ILE:HD12	1:P:242:GLU:HG2	1.68	0.76
1:R:256:TYR:CD2	1:R:301:LEU:HD12	2.20	0.76
1:W:321:ILE:CD1	1:W:437:MET:HE1	2.15	0.76
1:J:259:GLU:OE2	1:J:304:ARG:NH1	2.20	0.75
1:M:418:THR:HG21	1:M:421:LEU:HD12	1.68	0.75
1:W:405:THR:O	1:W:409:LEU:HD13	1.86	0.75
1:C:99:THR:HG23	1:C:193:LEU:CD2	2.14	0.75
1:J:234:GLU:O	1:J:238:THR:HG23	1.85	0.75
1:K:137:ASP:OD2	1:K:142:ILE:HG12	1.86	0.75
1:N:112:ASN:HD22	1:N:122:ARG:HH21	1.33	0.75
1:V:228:VAL:HG12	1:V:232:ILE:CD1	2.15	0.75
1:D:173:LEU:HD13	1:D:196:GLN:HE22	1.51	0.75
1:F:354:ILE:HG21	3:F:502:DST:H132	1.67	0.75
1:J:115:LYS:CE	1:J:434:GLY:HA3	2.17	0.75
1:J:264:ASN:O	1:J:267:THR:HG22	1.85	0.75
1:W:387:ALA:HA	1:W:390:TRP:CD1	2.22	0.75
1:K:172:GLN:C	1:K:173:LEU:HD12	2.06	0.75
1:P:112:ASN:HD22	1:P:122:ARG:HH21	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:354:ILE:HG21	3:T:502:DST:H132	1.68	0.75
1:U:264:ASN:O	1:U:267:THR:HG22	1.86	0.75
1:W:234:GLU:O	1:W:238:THR:HG23	1.85	0.75
1:V:264:ASN:O	1:V:267:THR:HG22	1.87	0.75
1:E:259:GLU:OE2	1:E:304:ARG:NH1	2.19	0.75
1:H:70:GLY:HA3	1:H:73:GLN:NE2	2.02	0.75
1:R:171:PHE:CE1	1:R:217:PRO:HB3	2.20	0.75
1:R:239:ILE:HD12	1:R:242:GLU:HG2	1.68	0.75
1:U:122:ARG:HG2	1:U:202:ASP:OD1	1.87	0.75
1:V:173:LEU:HD13	1:V:196:GLN:HE22	1.50	0.75
1:B:271:CYS:HB2	1:B:279:GLN:NE2	2.01	0.75
1:R:406:LEU:HD12	1:R:415:ILE:CD1	2.16	0.75
1:R:428:SER:HB3	1:R:436:TYR:HB2	1.69	0.75
1:K:60:PHE:CE1	1:K:123:ILE:HD11	2.22	0.75
1:M:299:TRP:CD1	1:M:311:ILE:HG23	2.21	0.75
1:S:234:GLU:O	1:S:238:THR:HG23	1.87	0.75
1:X:115:LYS:CE	1:X:434:GLY:HA3	2.17	0.75
1:E:406:LEU:HD12	1:E:415:ILE:CD1	2.17	0.75
1:D:75:TYR:HD2	1:F:75:TYR:CD2	2.03	0.75
1:X:236:VAL:O	1:X:239:ILE:HG22	1.87	0.75
1:E:428:SER:HB3	1:E:436:TYR:HB2	1.69	0.75
1:M:387:ALA:HA	1:M:390:TRP:CD1	2.22	0.75
1:T:264:ASN:O	1:T:267:THR:HG22	1.86	0.75
1:D:75:TYR:CD2	1:F:75:TYR:HD2	2.04	0.74
1:F:271:CYS:HB2	1:F:279:GLN:HE21	1.52	0.74
1:O:386:LEU:HD13	1:O:390:TRP:NE1	2.02	0.74
1:R:85:LEU:HB3	1:R:125:PHE:HE1	1.51	0.74
1:T:292:TRP:CH2	1:T:319:LYS:HB2	2.23	0.74
1:C:42:HIS:HB2	1:E:79:PHE:CE2	2.23	0.74
1:E:418:THR:HG21	1:E:421:LEU:HD12	1.68	0.74
1:B:173:LEU:HD13	1:B:196:GLN:HE22	1.52	0.74
1:B:280:ARG:HD2	1:B:358:GLU:OE2	1.87	0.74
1:J:115:LYS:HE2	1:J:434:GLY:HA3	1.69	0.74
1:O:115:LYS:CE	1:O:434:GLY:HA3	2.17	0.74
1:U:380:LEU:HB2	1:U:415:ILE:HG22	1.68	0.74
1:A:259:GLU:OE2	1:A:304:ARG:NH1	2.20	0.74
1:I:85:LEU:HB3	1:I:125:PHE:HE1	1.52	0.74
1:P:171:PHE:CE1	1:P:217:PRO:HB3	2.22	0.74
1:U:374:VAL:HG13	1:U:382:VAL:HG21	1.67	0.74
1:C:308:GLU:HB2	1:C:311:ILE:HD13	1.70	0.74
1:A:282:LYS:HD2	1:A:356:ASN:HD21	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:236:VAL:O	1:H:239:ILE:HG22	1.88	0.74
1:O:418:THR:HG21	1:O:421:LEU:HD12	1.70	0.74
1:U:234:GLU:O	1:U:238:THR:HG23	1.88	0.74
1:C:173:LEU:O	1:C:174:SER:OG	2.05	0.74
1:V:374:VAL:HG13	1:V:382:VAL:HG21	1.68	0.74
1:F:264:ASN:O	1:F:267:THR:HG22	1.88	0.74
1:N:208:ALA:HA	1:O:41:TYR:OH	1.88	0.74
1:N:374:VAL:HG13	1:N:382:VAL:HG21	1.68	0.74
1:Q:271:CYS:HB2	1:Q:279:GLN:NE2	2.02	0.74
1:L:236:VAL:O	1:L:239:ILE:HG22	1.88	0.74
1:O:282:LYS:HD2	1:O:356:ASN:HD21	1.51	0.74
1:R:418:THR:HG21	1:R:421:LEU:HD12	1.68	0.74
1:S:282:LYS:HD2	1:S:356:ASN:HD21	1.51	0.74
1:T:112:ASN:HD22	1:T:122:ARG:HH21	1.34	0.74
1:B:99:THR:HG23	1:B:193:LEU:HD23	1.70	0.74
1:I:208:ALA:HA	1:L:41:TYR:OH	1.87	0.74
1:R:271:CYS:HB2	1:R:279:GLN:HE21	1.53	0.74
1:X:171:PHE:CE1	1:X:217:PRO:HB3	2.22	0.74
1:A:387:ALA:HA	1:A:390:TRP:CD1	2.22	0.74
1:E:271:CYS:HB2	1:E:279:GLN:NE2	2.02	0.74
1:G:405:THR:O	1:G:409:LEU:HD13	1.88	0.74
1:H:171:PHE:CE1	1:H:217:PRO:HB3	2.23	0.74
1:O:308:GLU:HB2	1:O:311:ILE:HD13	1.68	0.74
1:S:234:GLU:OE2	1:S:237:ARG:NH2	2.20	0.74
1:U:418:THR:HG21	1:U:421:LEU:HD12	1.70	0.74
1:C:239:ILE:HD12	1:C:242:GLU:HG2	1.69	0.74
1:D:165:GLN:HG3	1:H:172:GLN:HE22	1.51	0.74
1:F:321:ILE:HD11	1:F:389:PHE:CZ	2.22	0.74
1:I:271:CYS:HB2	1:I:279:GLN:NE2	2.01	0.74
1:Q:243:ARG:NE	1:Q:243:ARG:HA	2.03	0.74
1:A:402:TYR:HB3	1:A:403:PRO:HD3	1.69	0.74
1:B:308:GLU:HB2	1:B:311:ILE:HD13	1.70	0.74
1:N:115:LYS:HE2	1:N:434:GLY:HA3	1.69	0.74
1:S:374:VAL:HG13	1:S:382:VAL:HG21	1.68	0.74
1:A:70:GLY:HA3	1:A:73:GLN:NE2	2.03	0.73
1:M:234:GLU:O	1:M:238:THR:HG23	1.88	0.73
1:M:280:ARG:HD2	1:M:358:GLU:OE2	1.88	0.73
1:N:115:LYS:CE	1:N:434:GLY:HA3	2.18	0.73
1:R:308:GLU:HB2	1:R:311:ILE:HD13	1.68	0.73
1:T:115:LYS:HE2	1:T:434:GLY:HA3	1.68	0.73
1:U:212:LYS:NZ	3:U:502:DST:O6	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASP:OD2	1:C:142:ILE:HG12	1.88	0.73
1:C:228:VAL:HG12	1:C:232:ILE:HD11	1.69	0.73
1:B:380:LEU:HB2	1:B:415:ILE:HG22	1.70	0.73
1:D:79:PHE:CE2	1:F:42:HIS:HB2	2.23	0.73
1:M:172:GLN:C	1:M:173:LEU:HD12	2.09	0.73
1:Q:292:TRP:CH2	1:Q:319:LYS:HB2	2.23	0.73
1:T:259:GLU:OE2	1:T:304:ARG:NH1	2.20	0.73
1:U:428:SER:HB3	1:U:436:TYR:HB2	1.71	0.73
1:F:320:GLN:HE22	1:F:392:SER:HB3	1.52	0.73
1:O:379:ASP:HB2	1:O:418:THR:HG23	1.71	0.73
1:S:115:LYS:HE2	1:S:434:GLY:HA3	1.71	0.73
1:W:290:VAL:HG11	1:W:353:ILE:HG12	1.69	0.73
1:M:282:LYS:HD2	1:M:356:ASN:HD21	1.53	0.73
1:T:271:CYS:HB2	1:T:279:GLN:NE2	2.03	0.73
1:C:115:LYS:CE	1:C:434:GLY:HA3	2.19	0.73
1:N:295:ILE:HG23	1:N:370:PHE:HE2	1.53	0.73
1:Q:165:GLN:CG	1:S:172:GLN:HE22	1.98	0.73
1:Q:228:VAL:HG12	1:Q:232:ILE:HD11	1.70	0.73
1:S:115:LYS:CE	1:S:434:GLY:HA3	2.18	0.73
1:T:280:ARG:HD2	1:T:358:GLU:OE2	1.89	0.73
1:X:280:ARG:HD2	1:X:358:GLU:OE2	1.87	0.73
1:F:234:GLU:O	1:F:238:THR:HG23	1.89	0.73
1:N:85:LEU:HB3	1:N:125:PHE:HE1	1.53	0.73
1:Q:380:LEU:HB2	1:Q:415:ILE:HG22	1.69	0.73
1:S:285:GLY:HA3	1:S:355:TRP:CZ2	2.22	0.73
1:U:173:LEU:O	1:U:174:SER:OG	2.04	0.73
1:G:264:ASN:O	1:G:267:THR:HG22	1.87	0.73
1:B:406:LEU:HD12	1:B:415:ILE:CD1	2.18	0.73
1:F:402:TYR:HB3	1:F:403:PRO:HD3	1.69	0.73
1:H:234:GLU:O	1:H:238:THR:HG23	1.87	0.73
1:K:374:VAL:HG11	1:K:422:GLN:HG2	1.70	0.73
1:F:380:LEU:HB2	1:F:415:ILE:HG22	1.69	0.73
1:O:173:LEU:O	1:O:174:SER:OG	2.04	0.73
1:E:112:ASN:HD22	1:E:122:ARG:HH21	1.34	0.73
1:D:239:ILE:HD12	1:D:242:GLU:HG2	1.70	0.73
1:N:323:SER:O	1:N:327:ILE:HB	1.89	0.73
1:R:282:LYS:HD2	1:R:356:ASN:HD21	1.53	0.73
1:U:292:TRP:CH2	1:U:319:LYS:HB2	2.24	0.73
1:A:234:GLU:O	1:A:238:THR:HG23	1.87	0.73
1:A:236:VAL:O	1:A:239:ILE:HG22	1.89	0.73
1:V:239:ILE:HD12	1:V:242:GLU:HG2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:VAL:HG12	1:E:232:ILE:HD11	1.69	0.73
1:G:171:PHE:CE1	1:G:217:PRO:HB3	2.24	0.73
1:B:171:PHE:CE1	1:B:217:PRO:HB3	2.24	0.73
1:K:60:PHE:HE1	1:K:123:ILE:HD11	1.53	0.73
1:N:234:GLU:O	1:N:238:THR:HG23	1.89	0.73
1:N:380:LEU:HB2	1:N:415:ILE:HG22	1.69	0.73
1:O:280:ARG:HD2	1:O:358:GLU:OE2	1.89	0.73
1:R:162:PRO:HG2	1:T:174:SER:HB3	1.71	0.73
1:T:440:TYR:OH	3:T:502:DST:O7	2.06	0.73
1:C:228:VAL:HG12	1:C:232:ILE:CD1	2.19	0.72
1:G:321:ILE:HD11	1:G:389:PHE:CZ	2.24	0.72
1:F:171:PHE:CE1	1:F:217:PRO:HB3	2.23	0.72
1:O:321:ILE:CD1	1:O:437:MET:HE2	2.18	0.72
1:C:321:ILE:HD11	1:C:389:PHE:CZ	2.25	0.72
1:G:406:LEU:HD12	1:G:415:ILE:CD1	2.19	0.72
1:B:115:LYS:HE2	1:B:434:GLY:HA3	1.69	0.72
1:H:285:GLY:HA3	1:H:355:TRP:CZ2	2.23	0.72
1:I:234:GLU:O	1:I:238:THR:HG23	1.89	0.72
1:J:282:LYS:HD2	1:J:356:ASN:HD21	1.54	0.72
1:U:259:GLU:OE2	1:U:304:ARG:NH1	2.22	0.72
1:A:228:VAL:HG12	1:A:232:ILE:CD1	2.19	0.72
1:H:386:LEU:HD13	1:H:390:TRP:NE1	2.04	0.72
1:N:390:TRP:CB	1:N:399:ALA:HB2	2.18	0.72
1:O:301:LEU:O	1:O:304:ARG:HG2	1.89	0.72
1:R:208:ALA:HA	1:S:41:TYR:OH	1.89	0.72
1:S:323:SER:O	1:S:327:ILE:HB	1.89	0.72
1:U:299:TRP:CD1	1:U:311:ILE:HG23	2.25	0.72
1:W:173:LEU:HD13	1:W:196:GLN:HE22	1.53	0.72
1:V:228:VAL:HG12	1:V:232:ILE:HD11	1.71	0.72
1:D:282:LYS:HD2	1:D:356:ASN:HD21	1.54	0.72
1:D:387:ALA:HA	1:D:390:TRP:CD1	2.24	0.72
1:T:234:GLU:O	1:T:238:THR:HG23	1.89	0.72
1:U:228:VAL:HG12	1:U:232:ILE:CD1	2.18	0.72
1:E:280:ARG:HD2	1:E:358:GLU:OE2	1.89	0.72
1:D:137:ASP:OD2	1:D:142:ILE:HG12	1.89	0.72
1:J:280:ARG:HD2	1:J:358:GLU:OE2	1.89	0.72
1:L:85:LEU:HB3	1:L:125:PHE:HE1	1.54	0.72
1:R:405:THR:O	1:R:409:LEU:HD13	1.88	0.72
1:S:112:ASN:HD22	1:S:122:ARG:HH21	1.38	0.72
1:S:253:ILE:HD12	1:S:359:ILE:HD11	1.70	0.72
1:C:51:ARG:HD3	1:C:92:TYR:CD2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:234:GLU:OE2	1:F:237:ARG:NH2	2.23	0.72
1:H:173:LEU:O	1:H:174:SER:OG	2.07	0.72
1:Q:173:LEU:O	1:Q:174:SER:OG	2.06	0.72
1:S:379:ASP:HB2	1:S:418:THR:HG23	1.70	0.72
1:A:315:LEU:O	1:A:315:LEU:HD23	1.90	0.72
1:M:105:LEU:HD12	1:M:107:ILE:H	1.54	0.72
1:P:390:TRP:CB	1:P:399:ALA:HB2	2.16	0.72
1:S:239:ILE:HD12	1:S:242:GLU:HG2	1.71	0.72
1:U:41:TYR:OH	1:X:208:ALA:HA	1.88	0.72
1:E:239:ILE:HD12	1:E:242:GLU:HG2	1.72	0.72
1:G:386:LEU:HD13	1:G:390:TRP:NE1	2.04	0.72
1:I:390:TRP:CB	1:I:399:ALA:HB2	2.18	0.72
1:K:239:ILE:HD12	1:K:242:GLU:HG2	1.71	0.72
1:N:406:LEU:HD12	1:N:415:ILE:CD1	2.20	0.72
1:E:173:LEU:HD13	1:E:196:GLN:HE22	1.53	0.72
1:G:115:LYS:CE	1:G:434:GLY:HA3	2.20	0.72
1:F:433:ARG:HG3	1:F:436:TYR:OH	1.89	0.72
1:H:161:THR:N	1:H:162:PRO:HD3	2.05	0.72
1:H:379:ASP:HB2	1:H:418:THR:HG23	1.69	0.72
1:K:290:VAL:HG11	1:K:353:ILE:HG12	1.70	0.72
1:O:105:LEU:HD12	1:O:107:ILE:H	1.54	0.72
1:X:323:SER:O	1:X:327:ILE:HB	1.89	0.72
1:A:110:SER:HB2	1:A:122:ARG:CB	2.10	0.72
1:V:162:PRO:HG2	1:X:174:SER:HB3	1.71	0.72
1:V:236:VAL:O	1:V:239:ILE:HG22	1.90	0.72
1:G:105:LEU:HD12	1:G:107:ILE:H	1.53	0.72
1:G:308:GLU:HB2	1:G:311:ILE:HD13	1.70	0.72
1:F:173:LEU:O	1:F:174:SER:OG	2.07	0.72
1:L:173:LEU:O	1:L:174:SER:OG	2.08	0.72
1:M:234:GLU:OE2	1:M:237:ARG:NH2	2.23	0.72
1:O:122:ARG:HG2	1:O:202:ASP:OD1	1.89	0.72
1:Q:172:GLN:C	1:Q:173:LEU:HD12	2.10	0.72
1:C:374:VAL:HG13	1:C:382:VAL:HG21	1.72	0.71
1:J:285:GLY:HA3	1:J:355:TRP:CZ2	2.25	0.71
1:P:406:LEU:HD12	1:P:415:ILE:CD1	2.19	0.71
1:S:308:GLU:HB2	1:S:311:ILE:HD13	1.72	0.71
1:S:428:SER:HB3	1:S:436:TYR:HB2	1.72	0.71
1:T:85:LEU:HB3	1:T:125:PHE:HE1	1.53	0.71
1:C:165:GLN:HG3	1:G:172:GLN:HE22	1.54	0.71
1:C:172:GLN:C	1:C:173:LEU:HD12	2.10	0.71
1:E:228:VAL:HG12	1:E:232:ILE:CD1	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:228:VAL:HG12	1:N:232:ILE:CD1	2.20	0.71
1:P:295:ILE:HG23	1:P:370:PHE:HE2	1.55	0.71
1:U:301:LEU:O	1:U:304:ARG:HG2	1.90	0.71
1:W:122:ARG:HG2	1:W:202:ASP:OD1	1.90	0.71
1:X:243:ARG:NE	1:X:243:ARG:HA	2.04	0.71
1:X:405:THR:O	1:X:409:LEU:HD13	1.90	0.71
1:K:122:ARG:HG2	1:K:202:ASP:OD1	1.90	0.71
1:N:280:ARG:HD2	1:N:358:GLU:OE2	1.90	0.71
1:K:115:LYS:HE2	1:K:434:GLY:HA3	1.70	0.71
1:N:147:LEU:HD23	1:N:199:PHE:CD2	2.26	0.71
1:O:239:ILE:HD12	1:O:242:GLU:HG2	1.72	0.71
1:Q:321:ILE:HD11	1:Q:389:PHE:CE2	2.24	0.71
1:W:374:VAL:HG13	1:W:382:VAL:HG21	1.72	0.71
1:C:354:ILE:HG21	3:C:502:DST:H132	1.72	0.71
1:O:387:ALA:HA	1:O:390:TRP:CD1	2.26	0.71
1:Q:354:ILE:HG21	3:Q:502:DST:H132	1.72	0.71
1:R:122:ARG:HG2	1:R:202:ASP:OD1	1.91	0.71
1:R:264:ASN:O	1:R:267:THR:HG22	1.91	0.71
1:W:243:ARG:NE	1:W:243:ARG:HA	2.04	0.71
1:W:418:THR:HG21	1:W:421:LEU:HD12	1.71	0.71
1:E:292:TRP:CZ2	1:E:315:LEU:HD21	2.25	0.71
1:G:374:VAL:HG13	1:G:382:VAL:HG21	1.72	0.71
1:B:115:LYS:CE	1:B:434:GLY:HA3	2.20	0.71
1:F:115:LYS:CE	1:F:434:GLY:HA3	2.21	0.71
1:H:66:ALA:HB2	1:H:409:LEU:HD11	1.71	0.71
1:I:115:LYS:CE	1:I:434:GLY:HA3	2.21	0.71
1:K:259:GLU:OE2	1:K:304:ARG:NH1	2.24	0.71
1:K:292:TRP:HE1	1:Q:306:ILE:HD13	1.55	0.71
1:V:85:LEU:HB3	1:V:125:PHE:HE1	1.55	0.71
1:V:428:SER:HB3	1:V:436:TYR:HB2	1.73	0.71
1:B:354:ILE:HG21	3:B:502:DST:H132	1.73	0.71
1:H:105:LEU:HD12	1:H:107:ILE:H	1.55	0.71
1:L:161:THR:N	1:L:162:PRO:HD3	2.06	0.71
1:M:228:VAL:HG12	1:M:232:ILE:HD11	1.71	0.71
1:N:374:VAL:HG11	1:N:422:GLN:HG2	1.72	0.71
1:O:256:TYR:CD2	1:O:301:LEU:HD12	2.25	0.71
1:Q:105:LEU:CD1	1:Q:107:ILE:HG22	2.20	0.71
1:V:115:LYS:HE2	1:V:434:GLY:HA3	1.71	0.71
1:D:301:LEU:O	1:D:304:ARG:HG2	1.90	0.71
1:M:243:ARG:HA	1:M:243:ARG:NE	2.05	0.71
1:N:253:ILE:HD12	1:N:359:ILE:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:115:LYS:HE2	1:W:434:GLY:HA3	1.73	0.71
1:X:239:ILE:HD12	1:X:242:GLU:HG2	1.73	0.71
1:C:234:GLU:O	1:C:238:THR:HG23	1.91	0.71
1:C:236:VAL:O	1:C:239:ILE:HG22	1.90	0.71
1:A:228:VAL:HG12	1:A:232:ILE:HD11	1.71	0.71
1:A:323:SER:O	1:A:327:ILE:HB	1.90	0.71
1:V:405:THR:O	1:V:409:LEU:HD13	1.89	0.71
1:K:70:GLY:HA3	1:K:73:GLN:NE2	2.06	0.71
1:L:234:GLU:O	1:L:238:THR:HG23	1.91	0.71
1:O:236:VAL:O	1:O:239:ILE:HG22	1.91	0.71
1:P:282:LYS:HE3	1:P:284:TYR:OH	1.90	0.71
1:R:415:ILE:HA	1:R:418:THR:CG2	2.19	0.71
1:T:243:ARG:NE	1:T:243:ARG:HA	2.06	0.71
1:C:290:VAL:HG23	1:C:294:LYS:CG	2.21	0.71
1:V:415:ILE:HA	1:V:418:THR:CG2	2.20	0.71
1:O:259:GLU:OE2	1:O:304:ARG:NH1	2.24	0.71
1:X:379:ASP:HB2	1:X:418:THR:HG23	1.71	0.71
1:C:390:TRP:CB	1:C:399:ALA:HB2	2.15	0.70
1:D:41:TYR:OH	1:F:208:ALA:HA	1.91	0.70
1:F:172:GLN:C	1:F:173:LEU:HD12	2.11	0.70
1:F:292:TRP:CH2	1:F:319:LYS:HB2	2.26	0.70
1:K:115:LYS:CE	1:K:434:GLY:HA3	2.20	0.70
1:R:374:VAL:HG11	1:R:422:GLN:HG2	1.73	0.70
1:X:415:ILE:HA	1:X:418:THR:CG2	2.21	0.70
1:V:259:GLU:OE2	1:V:304:ARG:NH1	2.24	0.70
1:L:105:LEU:HD12	1:L:107:ILE:H	1.55	0.70
1:O:405:THR:O	1:O:409:LEU:HD13	1.92	0.70
1:R:301:LEU:O	1:R:304:ARG:HG2	1.91	0.70
1:U:234:GLU:OE2	1:U:237:ARG:NH2	2.24	0.70
1:W:228:VAL:HG12	1:W:232:ILE:CD1	2.20	0.70
1:V:406:LEU:HD12	1:V:415:ILE:CD1	2.20	0.70
1:K:161:THR:N	1:K:162:PRO:HD3	2.05	0.70
1:M:75:TYR:HD2	1:P:75:TYR:CD2	2.07	0.70
1:N:405:THR:O	1:N:409:LEU:HD13	1.90	0.70
1:S:280:ARG:HD2	1:S:358:GLU:OE2	1.91	0.70
1:S:386:LEU:HD13	1:S:390:TRP:HE1	1.55	0.70
1:A:105:LEU:CD1	1:A:107:ILE:HG22	2.21	0.70
1:A:239:ILE:HD12	1:A:242:GLU:HG2	1.72	0.70
1:V:174:SER:HB3	1:X:162:PRO:HG2	1.74	0.70
1:M:228:VAL:HG12	1:M:232:ILE:CD1	2.21	0.70
1:P:253:ILE:HD12	1:P:359:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:415:ILE:HA	1:Q:418:THR:HG22	1.73	0.70
1:U:280:ARG:HD2	1:U:358:GLU:OE2	1.91	0.70
1:C:75:TYR:HD2	1:E:75:TYR:CD2	2.07	0.70
1:V:110:SER:HB2	1:V:122:ARG:CB	2.08	0.70
1:F:406:LEU:HD12	1:F:415:ILE:HD13	1.71	0.70
1:L:301:LEU:O	1:L:304:ARG:HG2	1.91	0.70
1:N:243:ARG:NE	1:N:243:ARG:HA	2.06	0.70
1:R:243:ARG:HA	1:R:243:ARG:NE	2.06	0.70
1:V:51:ARG:HD3	1:V:92:TYR:CD2	2.27	0.70
1:N:42:HIS:HB2	1:O:79:PHE:HE2	1.56	0.70
1:O:321:ILE:HD11	1:O:389:PHE:CE2	2.27	0.70
1:Q:418:THR:HG21	1:Q:421:LEU:HD12	1.72	0.70
1:T:236:VAL:O	1:T:239:ILE:HG22	1.90	0.70
1:U:243:ARG:HA	1:U:243:ARG:NE	2.05	0.70
1:U:306:ILE:HD12	1:U:307:GLU:N	2.06	0.70
1:W:282:LYS:HD2	1:W:356:ASN:HD21	1.56	0.70
1:W:285:GLY:HA3	1:W:355:TRP:CZ2	2.24	0.70
1:X:271:CYS:HB2	1:X:279:GLN:NE2	2.07	0.70
1:X:390:TRP:CB	1:X:399:ALA:HB2	2.17	0.70
1:C:415:ILE:HA	1:C:418:THR:CG2	2.22	0.70
1:H:323:SER:O	1:H:327:ILE:HB	1.91	0.70
1:J:292:TRP:CH2	1:J:319:LYS:HB2	2.26	0.70
1:N:415:ILE:HA	1:N:418:THR:CG2	2.20	0.70
1:P:285:GLY:HA3	1:P:355:TRP:CZ2	2.26	0.70
1:R:236:VAL:O	1:R:239:ILE:HG22	1.92	0.70
1:W:239:ILE:HD12	1:W:242:GLU:HG2	1.72	0.70
1:V:115:LYS:CE	1:V:434:GLY:HA3	2.21	0.70
1:B:243:ARG:HA	1:B:243:ARG:NE	2.07	0.70
1:L:99:THR:HG23	1:L:193:LEU:CD2	2.21	0.70
1:N:137:ASP:OD2	1:N:142:ILE:HG12	1.91	0.70
1:D:406:LEU:HD12	1:D:415:ILE:CD1	2.22	0.70
1:F:236:VAL:O	1:F:239:ILE:HG22	1.90	0.70
1:F:290:VAL:HG23	1:F:294:LYS:CG	2.21	0.70
1:H:243:ARG:NE	1:H:243:ARG:HA	2.06	0.70
1:Q:387:ALA:HA	1:Q:390:TRP:CD1	2.27	0.70
1:U:315:LEU:HD23	1:U:315:LEU:O	1.92	0.70
1:W:115:LYS:CE	1:W:434:GLY:HA3	2.22	0.70
1:E:290:VAL:HG11	1:E:353:ILE:HG12	1.73	0.70
1:J:228:VAL:HG12	1:J:232:ILE:CD1	2.21	0.70
1:L:354:ILE:HG21	3:L:502:DST:H132	1.72	0.70
1:P:147:LEU:HD23	1:P:199:PHE:CD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:369:LYS:NZ	3:R:502:DST:O4	2.24	0.70
1:T:122:ARG:HG2	1:T:202:ASP:OD1	1.91	0.70
1:U:115:LYS:HE2	1:U:434:GLY:HA3	1.73	0.70
1:U:415:ILE:HA	1:U:418:THR:HG22	1.74	0.70
1:A:243:ARG:NE	1:A:243:ARG:HA	2.06	0.69
1:I:66:ALA:HB2	1:I:409:LEU:HD11	1.74	0.69
1:L:243:ARG:NE	1:L:243:ARG:HA	2.05	0.69
1:P:292:TRP:CH2	1:P:319:LYS:HB2	2.27	0.69
1:W:167:LEU:HD23	1:W:269:LEU:HD23	1.73	0.69
1:G:323:SER:O	1:G:327:ILE:HB	1.91	0.69
1:B:228:VAL:HG12	1:B:232:ILE:CD1	2.23	0.69
1:I:379:ASP:HB2	1:I:418:THR:HG23	1.74	0.69
1:J:171:PHE:CE1	1:J:217:PRO:HB3	2.28	0.69
1:J:236:VAL:O	1:J:239:ILE:HG22	1.92	0.69
1:J:290:VAL:HG23	1:J:294:LYS:CG	2.22	0.69
1:K:290:VAL:HG23	1:K:294:LYS:CG	2.23	0.69
1:M:374:VAL:HG13	1:M:382:VAL:HG21	1.74	0.69
1:O:271:CYS:HB2	1:O:279:GLN:NE2	2.06	0.69
1:R:380:LEU:HB2	1:R:415:ILE:HG22	1.73	0.69
1:U:253:ILE:HD12	1:U:359:ILE:HD11	1.74	0.69
1:P:243:ARG:NE	1:P:243:ARG:HA	2.07	0.69
1:P:290:VAL:HG11	1:P:353:ILE:HG12	1.74	0.69
1:Q:115:LYS:CE	1:Q:434:GLY:HA3	2.22	0.69
1:Q:379:ASP:HB2	1:Q:418:THR:HG23	1.73	0.69
1:W:173:LEU:O	1:W:174:SER:OG	2.04	0.69
1:W:292:TRP:CH2	1:W:319:LYS:HB2	2.27	0.69
1:G:301:LEU:O	1:G:304:ARG:HG2	1.93	0.69
1:D:115:LYS:HE2	1:D:434:GLY:HA3	1.74	0.69
1:N:42:HIS:HB2	1:O:79:PHE:CE2	2.26	0.69
1:O:428:SER:HB3	1:O:436:TYR:HB2	1.73	0.69
1:S:236:VAL:O	1:S:239:ILE:HG22	1.92	0.69
1:S:271:CYS:HB2	1:S:279:GLN:NE2	2.07	0.69
1:T:239:ILE:HD12	1:T:242:GLU:HG2	1.74	0.69
1:X:418:THR:HG21	1:X:421:LEU:HD12	1.74	0.69
1:C:387:ALA:HA	1:C:390:TRP:CD1	2.28	0.69
1:V:323:SER:O	1:V:327:ILE:HB	1.93	0.69
1:V:418:THR:HG21	1:V:421:LEU:HD12	1.73	0.69
1:G:430:THR:HG22	1:G:432:LYS:H	1.58	0.69
1:F:321:ILE:HG22	1:F:325:LEU:HD23	1.74	0.69
1:H:433:ARG:HG3	1:H:436:TYR:OH	1.93	0.69
1:L:70:GLY:HA3	1:L:73:GLN:NE2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:41:TYR:OH	1:P:208:ALA:HA	1.91	0.69
1:U:292:TRP:CZ2	1:U:319:LYS:HB2	2.27	0.69
1:V:208:ALA:HA	1:W:41:TYR:OH	1.92	0.69
1:E:405:THR:O	1:E:409:LEU:HD13	1.92	0.69
1:D:85:LEU:HB3	1:D:125:PHE:HE1	1.56	0.69
1:I:236:VAL:O	1:I:239:ILE:HG22	1.91	0.69
1:J:271:CYS:HB2	1:J:279:GLN:NE2	2.06	0.69
1:L:387:ALA:HA	1:L:390:TRP:CD1	2.27	0.69
1:N:234:GLU:OE2	1:N:237:ARG:NH2	2.24	0.69
1:P:147:LEU:HD23	1:P:199:PHE:HD2	1.58	0.69
1:P:271:CYS:HB2	1:P:279:GLN:NE2	2.08	0.69
1:Q:85:LEU:HB3	1:Q:125:PHE:HE1	1.56	0.69
1:Q:228:VAL:HG12	1:Q:232:ILE:CD1	2.23	0.69
1:T:323:SER:O	1:T:327:ILE:HB	1.92	0.69
1:X:406:LEU:HD12	1:X:415:ILE:CD1	2.22	0.69
1:V:243:ARG:NE	1:V:243:ARG:HA	2.07	0.69
1:V:301:LEU:O	1:V:304:ARG:HG2	1.92	0.69
1:V:354:ILE:HG21	3:V:502:DST:H132	1.74	0.69
1:D:321:ILE:CD1	1:D:437:MET:HE1	2.22	0.69
1:N:285:GLY:HA3	1:N:355:TRP:CZ2	2.28	0.69
1:Q:299:TRP:CD1	1:Q:311:ILE:HG23	2.27	0.69
1:R:390:TRP:CB	1:R:399:ALA:HB2	2.21	0.69
1:C:243:ARG:NE	1:C:243:ARG:HA	2.07	0.69
1:C:323:SER:O	1:C:327:ILE:HB	1.92	0.69
1:B:228:VAL:HG12	1:B:232:ILE:HD11	1.75	0.69
1:H:305:LEU:CD1	1:H:311:ILE:HG12	2.22	0.69
1:I:406:LEU:HD12	1:I:415:ILE:CD1	2.22	0.69
1:J:173:LEU:HD13	1:J:196:GLN:HE22	1.57	0.69
1:J:405:THR:O	1:J:409:LEU:HD13	1.91	0.69
1:K:234:GLU:O	1:K:238:THR:HG23	1.93	0.69
1:N:171:PHE:CE1	1:N:217:PRO:HB3	2.28	0.69
1:R:42:HIS:HB2	1:S:79:PHE:HE2	1.55	0.69
1:C:282:LYS:HD2	1:C:356:ASN:HD21	1.57	0.69
1:C:301:LEU:O	1:C:304:ARG:HG2	1.92	0.69
1:F:379:ASP:HB2	1:F:418:THR:HG23	1.73	0.69
1:F:415:ILE:HA	1:F:418:THR:HG22	1.73	0.69
1:K:415:ILE:HA	1:K:418:THR:HG22	1.75	0.69
1:Q:374:VAL:HG13	1:Q:382:VAL:HG21	1.75	0.69
1:S:264:ASN:O	1:S:267:THR:HG22	1.93	0.69
1:V:290:VAL:HG23	1:V:294:LYS:CG	2.23	0.69
1:G:70:GLY:HA3	1:G:73:GLN:NE2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:LEU:HD13	1:F:196:GLN:HE22	1.58	0.69
1:F:290:VAL:HG11	1:F:353:ILE:HG12	1.74	0.69
1:O:243:ARG:HA	1:O:243:ARG:NE	2.07	0.69
1:P:236:VAL:O	1:P:239:ILE:HG22	1.91	0.69
1:W:415:ILE:HA	1:W:418:THR:HG22	1.75	0.69
1:A:379:ASP:HB2	1:A:418:THR:HG23	1.73	0.68
1:A:386:LEU:HD13	1:A:390:TRP:NE1	2.08	0.68
1:A:387:ALA:HA	1:A:390:TRP:HD1	1.57	0.68
1:B:239:ILE:HD12	1:B:242:GLU:HG2	1.75	0.68
1:F:374:VAL:HG13	1:F:382:VAL:HG21	1.75	0.68
1:J:112:ASN:HD22	1:J:122:ARG:HH21	1.41	0.68
1:L:282:LYS:HD2	1:L:356:ASN:HD21	1.59	0.68
1:R:323:SER:O	1:R:327:ILE:HB	1.93	0.68
1:U:371:TYR:OH	3:U:502:DST:O7	2.05	0.68
1:V:60:PHE:HE1	1:V:123:ILE:HD11	1.59	0.68
1:F:115:LYS:HG2	1:F:395:TRP:HE1	1.58	0.68
1:P:173:LEU:HD13	1:P:196:GLN:HE22	1.58	0.68
1:R:234:GLU:OE2	1:R:237:ARG:NH2	2.25	0.68
1:R:321:ILE:HG22	1:R:325:LEU:HD23	1.75	0.68
1:S:243:ARG:NE	1:S:243:ARG:HA	2.06	0.68
1:U:51:ARG:HD3	1:U:92:TYR:CD2	2.27	0.68
1:G:379:ASP:OD2	1:G:421:LEU:HB2	1.92	0.68
1:H:85:LEU:HB3	1:H:125:PHE:CE1	2.28	0.68
1:H:98:SER:OG	1:H:126:GLU:OE1	2.05	0.68
1:I:292:TRP:CH2	1:I:319:LYS:HB2	2.28	0.68
1:P:228:VAL:HG12	1:P:232:ILE:CD1	2.22	0.68
1:U:63:PHE:HE2	1:U:109:PHE:HB2	1.57	0.68
1:U:236:VAL:O	1:U:239:ILE:HG22	1.93	0.68
1:C:379:ASP:HB2	1:C:418:THR:HG23	1.74	0.68
1:V:321:ILE:HD11	1:V:389:PHE:CZ	2.27	0.68
1:B:259:GLU:OE2	1:B:304:ARG:NH1	2.26	0.68
1:D:161:THR:N	1:D:162:PRO:HD3	2.08	0.68
1:H:239:ILE:HD12	1:H:242:GLU:HG2	1.74	0.68
1:K:374:VAL:HG13	1:K:382:VAL:HG21	1.74	0.68
1:M:301:LEU:O	1:M:304:ARG:HG2	1.94	0.68
1:N:282:LYS:HD2	1:N:356:ASN:HD21	1.57	0.68
1:T:282:LYS:HE3	1:T:284:TYR:OH	1.93	0.68
1:A:208:ALA:HA	1:G:41:TYR:OH	1.92	0.68
1:E:264:ASN:O	1:E:267:THR:HG22	1.93	0.68
1:B:115:LYS:HE2	1:B:435:VAL:H	1.57	0.68
1:I:63:PHE:HE2	1:I:109:PHE:HB2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:323:SER:O	1:L:327:ILE:HB	1.93	0.68
1:L:406:LEU:HD12	1:L:415:ILE:CD1	2.23	0.68
1:P:60:PHE:CE1	1:P:123:ILE:HD11	2.28	0.68
1:Q:160:ASP:OD2	1:S:174:SER:HB2	1.94	0.68
1:U:323:SER:O	1:U:327:ILE:HB	1.94	0.68
1:W:236:VAL:O	1:W:239:ILE:HG22	1.93	0.68
1:B:415:ILE:HA	1:B:418:THR:HG22	1.75	0.68
1:F:288:THR:HG23	1:F:289:GLU:H	1.59	0.68
1:H:105:LEU:CD1	1:H:107:ILE:HG22	2.22	0.68
1:I:171:PHE:CE1	1:I:217:PRO:HB3	2.29	0.68
1:K:323:SER:O	1:K:327:ILE:HB	1.93	0.68
1:M:382:VAL:O	1:M:386:LEU:HB2	1.93	0.68
1:N:236:VAL:O	1:N:239:ILE:HG22	1.93	0.68
1:O:323:SER:O	1:O:327:ILE:HB	1.93	0.68
1:R:137:ASP:OD2	1:R:142:ILE:HG12	1.94	0.68
1:W:323:SER:O	1:W:327:ILE:HB	1.93	0.68
1:W:428:SER:HB3	1:W:436:TYR:HB2	1.74	0.68
1:W:433:ARG:HG3	1:W:436:TYR:OH	1.94	0.68
1:C:75:TYR:CD2	1:E:75:TYR:HD2	2.09	0.68
1:V:292:TRP:HZ2	1:V:315:LEU:HD21	1.59	0.68
1:E:236:VAL:O	1:E:239:ILE:HG22	1.92	0.68
1:B:172:GLN:HE22	1:F:165:GLN:HG3	1.59	0.68
1:B:236:VAL:O	1:B:239:ILE:HG22	1.92	0.68
1:H:306:ILE:HD12	1:H:307:GLU:N	2.08	0.68
1:L:280:ARG:HD2	1:L:358:GLU:OE2	1.94	0.68
1:U:433:ARG:HG3	1:U:436:TYR:OH	1.93	0.68
1:V:308:GLU:HB2	1:V:311:ILE:HD13	1.75	0.68
1:D:243:ARG:NE	1:D:243:ARG:HA	2.06	0.68
1:F:212:LYS:NZ	3:F:502:DST:O6	2.27	0.68
1:I:290:VAL:HG23	1:I:294:LYS:CG	2.24	0.68
1:K:51:ARG:HD3	1:K:92:TYR:CD2	2.28	0.68
1:K:173:LEU:O	1:K:174:SER:OG	2.11	0.68
1:N:271:CYS:HB2	1:N:279:GLN:HE21	1.58	0.68
1:N:301:LEU:O	1:N:304:ARG:HG2	1.93	0.68
1:R:51:ARG:HD3	1:R:92:TYR:CD2	2.29	0.68
1:X:290:VAL:HG11	1:X:353:ILE:HG12	1.76	0.68
1:A:112:ASN:HD22	1:A:122:ARG:HH21	1.42	0.68
1:A:402:TYR:O	1:A:405:THR:N	2.27	0.68
1:D:42:HIS:HB2	1:F:79:PHE:CE2	2.29	0.68
1:D:236:VAL:O	1:D:239:ILE:HG22	1.92	0.68
1:H:253:ILE:HD12	1:H:359:ILE:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:390:TRP:CB	1:V:399:ALA:HB2	2.22	0.68
1:F:176:SER:O	1:F:180:GLN:HB2	1.93	0.68
1:H:271:CYS:HB2	1:H:279:GLN:NE2	2.08	0.68
1:H:301:LEU:O	1:H:304:ARG:HG2	1.94	0.68
1:I:415:ILE:HA	1:I:418:THR:HG22	1.76	0.68
1:L:285:GLY:HA3	1:L:355:TRP:CZ2	2.29	0.68
1:P:315:LEU:HD23	1:P:315:LEU:O	1.93	0.68
1:A:374:VAL:HG13	1:A:382:VAL:HG21	1.76	0.67
1:B:234:GLU:O	1:B:238:THR:HG23	1.93	0.67
1:F:200:GLY:N	1:F:212:LYS:O	2.25	0.67
1:I:356:ASN:HB3	1:I:369:LYS:HB3	1.76	0.67
1:K:236:VAL:O	1:K:239:ILE:HG22	1.94	0.67
1:L:112:ASN:HD22	1:L:122:ARG:HH21	1.42	0.67
1:L:212:LYS:NZ	3:L:502:DST:O4	2.27	0.67
1:S:415:ILE:HA	1:S:418:THR:HG22	1.75	0.67
1:A:180:GLN:NE2	1:A:223:ALA:HA	2.09	0.67
1:F:51:ARG:HD3	1:F:92:TYR:CD2	2.30	0.67
1:I:70:GLY:HA3	1:I:73:GLN:NE2	2.10	0.67
1:L:66:ALA:HB2	1:L:409:LEU:HD11	1.76	0.67
1:L:239:ILE:HD12	1:L:242:GLU:HG2	1.75	0.67
1:M:137:ASP:OD2	1:M:142:ILE:HG12	1.94	0.67
1:P:85:LEU:HB3	1:P:125:PHE:HE1	1.59	0.67
1:P:387:ALA:HA	1:P:390:TRP:CD1	2.29	0.67
1:Q:70:GLY:HA3	1:Q:73:GLN:NE2	2.09	0.67
1:Q:165:GLN:HG3	1:S:172:GLN:NE2	2.00	0.67
1:S:173:LEU:O	1:S:174:SER:OG	2.07	0.67
1:E:387:ALA:HA	1:E:390:TRP:HD1	1.57	0.67
1:D:115:LYS:CE	1:D:434:GLY:HA3	2.24	0.67
1:F:99:THR:HG23	1:F:193:LEU:CD2	2.22	0.67
1:J:208:ALA:HA	1:K:41:TYR:OH	1.94	0.67
1:K:301:LEU:O	1:K:304:ARG:HG2	1.93	0.67
1:K:382:VAL:O	1:K:386:LEU:HB2	1.94	0.67
1:P:173:LEU:O	1:P:174:SER:OG	2.08	0.67
1:P:306:ILE:HD12	1:P:307:GLU:N	2.09	0.67
1:Q:239:ILE:HD12	1:Q:242:GLU:CG	2.24	0.67
1:C:85:LEU:HB3	1:C:125:PHE:HE1	1.60	0.67
1:V:321:ILE:CD1	1:V:437:MET:HE1	2.25	0.67
1:B:70:GLY:HA3	1:B:73:GLN:NE2	2.09	0.67
1:S:105:LEU:HD12	1:S:107:ILE:H	1.59	0.67
1:E:269:LEU:CD1	1:E:283:ILE:HG13	2.25	0.67
1:E:301:LEU:O	1:E:304:ARG:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:GLY:HA3	1:B:355:TRP:CZ2	2.29	0.67
1:L:211:VAL:HG12	1:L:273:PHE:CD2	2.29	0.67
1:M:142:ILE:HB	1:M:143:PRO:HD3	1.76	0.67
1:N:264:ASN:O	1:N:267:THR:HG22	1.94	0.67
1:O:234:GLU:OE2	1:O:237:ARG:NH2	2.27	0.67
1:C:406:LEU:HD12	1:C:415:ILE:HD13	1.77	0.67
1:B:161:THR:N	1:B:162:PRO:HD3	2.09	0.67
1:B:264:ASN:O	1:B:267:THR:HG22	1.93	0.67
1:F:270:SER:HB3	1:F:282:LYS:HB2	1.77	0.67
1:H:406:LEU:HD12	1:H:415:ILE:CD1	2.24	0.67
1:K:282:LYS:HD2	1:K:356:ASN:HD21	1.59	0.67
1:U:387:ALA:HA	1:U:390:TRP:HD1	1.58	0.67
1:X:142:ILE:HB	1:X:143:PRO:HD3	1.76	0.67
1:A:173:LEU:HD13	1:A:196:GLN:HE22	1.60	0.67
1:I:122:ARG:HG2	1:I:202:ASP:OD1	1.94	0.67
1:I:142:ILE:HB	1:I:143:PRO:HD3	1.76	0.67
1:I:386:LEU:HD13	1:I:390:TRP:NE1	2.10	0.67
1:K:285:GLY:HA3	1:K:355:TRP:CZ2	2.29	0.67
1:N:85:LEU:HD22	1:N:125:PHE:CE1	2.29	0.67
1:Q:301:LEU:O	1:Q:304:ARG:HG2	1.95	0.67
1:R:234:GLU:O	1:R:238:THR:HG23	1.94	0.67
1:R:292:TRP:CH2	1:R:319:LYS:HB2	2.28	0.67
1:X:354:ILE:HG21	3:X:502:DST:H132	1.76	0.67
1:F:243:ARG:NE	1:F:243:ARG:HA	2.08	0.67
1:H:212:LYS:NZ	3:H:502:DST:O4	2.27	0.67
1:H:387:ALA:HA	1:H:390:TRP:CD1	2.29	0.67
1:M:415:ILE:HA	1:M:418:THR:HG22	1.76	0.67
1:N:290:VAL:HG23	1:N:294:LYS:CG	2.25	0.67
1:P:379:ASP:HB2	1:P:418:THR:HG23	1.75	0.67
1:Q:305:LEU:CD1	1:Q:311:ILE:HG12	2.25	0.67
1:W:271:CYS:HB2	1:W:279:GLN:NE2	2.09	0.67
1:C:382:VAL:O	1:C:386:LEU:HB2	1.95	0.67
1:A:280:ARG:HD2	1:A:358:GLU:OE2	1.94	0.67
1:E:63:PHE:CE2	1:E:109:PHE:HB2	2.30	0.67
1:G:315:LEU:HD23	1:G:315:LEU:O	1.95	0.67
1:H:51:ARG:HD3	1:H:92:TYR:CD2	2.30	0.67
1:M:321:ILE:HD11	1:M:389:PHE:CE2	2.30	0.67
1:Q:323:SER:O	1:Q:327:ILE:HB	1.95	0.67
1:R:374:VAL:HG13	1:R:382:VAL:HG21	1.75	0.67
1:S:292:TRP:CH2	1:S:319:LYS:HB2	2.29	0.67
1:A:292:TRP:HZ2	1:A:315:LEU:HD21	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:161:THR:N	1:V:162:PRO:HD3	2.09	0.67
1:E:115:LYS:CE	1:E:434:GLY:HA3	2.25	0.67
1:B:406:LEU:HD12	1:B:415:ILE:HD13	1.76	0.67
1:J:418:THR:HG21	1:J:421:LEU:HD12	1.77	0.67
1:K:140:ASN:OD1	1:K:143:PRO:HG2	1.95	0.67
1:N:51:ARG:HD3	1:N:92:TYR:CD2	2.30	0.67
1:N:295:ILE:HG23	1:N:370:PHE:CE2	2.30	0.67
1:Q:285:GLY:HA3	1:Q:355:TRP:CZ2	2.30	0.67
1:S:406:LEU:HD12	1:S:415:ILE:CD1	2.25	0.67
1:T:234:GLU:OE2	1:T:237:ARG:NH2	2.28	0.67
1:T:387:ALA:HA	1:T:390:TRP:CD1	2.30	0.67
1:W:171:PHE:CE1	1:W:217:PRO:HB3	2.30	0.67
1:A:167:LEU:HD23	1:A:269:LEU:HD23	1.77	0.66
1:P:308:GLU:HB2	1:P:311:ILE:HD13	1.77	0.66
1:Q:433:ARG:HG3	1:Q:436:TYR:CZ	2.30	0.66
1:T:379:ASP:HB2	1:T:418:THR:HG23	1.76	0.66
1:U:70:GLY:HA3	1:U:73:GLN:NE2	2.09	0.66
1:W:280:ARG:HD2	1:W:358:GLU:OE2	1.95	0.66
1:X:282:LYS:HE3	1:X:284:TYR:OH	1.95	0.66
1:X:295:ILE:HG23	1:X:370:PHE:HE2	1.60	0.66
1:E:243:ARG:HA	1:E:243:ARG:NE	2.07	0.66
1:E:321:ILE:HG22	1:E:325:LEU:HD23	1.77	0.66
1:D:292:TRP:HZ2	1:D:315:LEU:HD21	1.60	0.66
1:D:321:ILE:HD11	1:D:437:MET:HE1	1.77	0.66
1:H:256:TYR:CD2	1:H:301:LEU:HD12	2.29	0.66
1:K:85:LEU:HB3	1:K:125:PHE:HE1	1.61	0.66
1:R:290:VAL:HG23	1:R:294:LYS:CG	2.25	0.66
1:S:387:ALA:HA	1:S:390:TRP:CD1	2.31	0.66
1:G:236:VAL:O	1:G:239:ILE:HG22	1.94	0.66
1:B:75:TYR:HD2	1:H:75:TYR:CD2	2.09	0.66
1:J:85:LEU:HB3	1:J:125:PHE:HE1	1.60	0.66
1:L:105:LEU:CD1	1:L:107:ILE:HG22	2.24	0.66
1:P:290:VAL:HG23	1:P:294:LYS:CG	2.25	0.66
1:Q:41:TYR:OH	1:T:208:ALA:HA	1.96	0.66
1:W:386:LEU:HD13	1:W:390:TRP:NE1	2.09	0.66
1:V:173:LEU:O	1:V:174:SER:OG	2.12	0.66
1:E:115:LYS:HE2	1:E:434:GLY:HA3	1.77	0.66
1:I:232:ILE:O	1:I:236:VAL:HG23	1.96	0.66
1:J:243:ARG:HA	1:J:243:ARG:NE	2.08	0.66
1:K:387:ALA:HA	1:K:390:TRP:CD1	2.31	0.66
1:V:200:GLY:N	1:V:212:LYS:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:THR:N	1:F:162:PRO:HD3	2.10	0.66
1:K:229:GLY:HA3	1:K:263:TYR:CE2	2.31	0.66
1:K:256:TYR:CD2	1:K:301:LEU:HD12	2.30	0.66
1:M:321:ILE:HG22	1:M:325:LEU:HD23	1.77	0.66
1:A:204:ASN:HB2	1:A:205:PRO:HD2	1.78	0.66
1:B:290:VAL:HG11	1:B:353:ILE:HG12	1.77	0.66
1:D:200:GLY:N	1:D:212:LYS:O	2.29	0.66
1:D:271:CYS:HB2	1:D:279:GLN:NE2	2.09	0.66
1:T:301:LEU:O	1:T:304:ARG:HG2	1.95	0.66
1:C:110:SER:HB2	1:C:122:ARG:CB	2.11	0.66
1:A:99:THR:HG23	1:A:193:LEU:CD2	2.25	0.66
1:A:292:TRP:CH2	1:A:319:LYS:HB2	2.30	0.66
1:V:292:TRP:CH2	1:V:319:LYS:HB2	2.31	0.66
1:K:405:THR:O	1:K:409:LEU:HD13	1.95	0.66
1:M:92:TYR:HB3	1:M:93:PRO:HD3	1.76	0.66
1:M:147:LEU:HD23	1:M:199:PHE:CD2	2.30	0.66
1:N:200:GLY:N	1:N:212:LYS:O	2.29	0.66
1:P:323:SER:O	1:P:327:ILE:HB	1.96	0.66
1:C:42:HIS:HB2	1:E:79:PHE:HE2	1.61	0.66
1:V:282:LYS:HD2	1:V:356:ASN:HD21	1.61	0.66
1:K:243:ARG:NE	1:K:243:ARG:HA	2.09	0.66
1:P:415:ILE:HA	1:P:418:THR:HG22	1.78	0.66
1:Q:234:GLU:O	1:Q:238:THR:HG23	1.96	0.66
1:R:63:PHE:CE1	1:R:409:LEU:HD23	2.31	0.66
1:R:321:ILE:HD11	1:R:389:PHE:CZ	2.30	0.66
1:U:382:VAL:O	1:U:386:LEU:HB2	1.95	0.66
1:W:85:LEU:HB3	1:W:125:PHE:HE1	1.59	0.66
1:A:321:ILE:HG22	1:A:325:LEU:HD23	1.78	0.66
1:G:51:ARG:HD3	1:G:92:TYR:CD2	2.31	0.66
1:B:292:TRP:CH2	1:B:319:LYS:HB2	2.31	0.66
1:B:433:ARG:HG3	1:B:436:TYR:OH	1.95	0.66
1:D:51:ARG:HD3	1:D:92:TYR:CD2	2.30	0.66
1:Q:374:VAL:HG11	1:Q:422:GLN:HG3	1.78	0.66
1:R:110:SER:O	1:R:121:LEU:HD12	1.96	0.66
1:R:292:TRP:HZ2	1:R:315:LEU:HD21	1.61	0.66
1:U:79:PHE:CE2	1:X:42:HIS:HB2	2.31	0.66
1:A:292:TRP:CZ2	1:A:315:LEU:HD21	2.31	0.66
1:V:280:ARG:HD2	1:V:358:GLU:OE2	1.96	0.66
1:B:60:PHE:HE1	1:B:123:ILE:HD11	1.61	0.66
1:F:308:GLU:HB2	1:F:311:ILE:HD13	1.78	0.66
1:N:147:LEU:HD23	1:N:199:PHE:HD2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:112:ASN:HD22	1:O:122:ARG:HH21	1.44	0.66
1:P:379:ASP:OD1	1:P:422:GLN:HG3	1.96	0.66
1:Q:389:PHE:HE2	1:Q:437:MET:HE3	1.60	0.66
1:R:295:ILE:HG23	1:R:370:PHE:CE2	2.31	0.66
1:X:374:VAL:HG13	1:X:382:VAL:HG21	1.78	0.66
1:D:321:ILE:HD11	1:D:389:PHE:CZ	2.32	0.65
1:O:292:TRP:HZ2	1:O:315:LEU:HD21	1.61	0.65
1:P:51:ARG:HD3	1:P:92:TYR:CD2	2.31	0.65
1:P:301:LEU:O	1:P:304:ARG:HG2	1.95	0.65
1:B:387:ALA:HA	1:B:390:TRP:CD1	2.30	0.65
1:I:406:LEU:HD12	1:I:415:ILE:HD13	1.78	0.65
1:J:228:VAL:HG12	1:J:232:ILE:HD11	1.78	0.65
1:M:315:LEU:HD23	1:M:315:LEU:O	1.95	0.65
1:O:92:TYR:HB3	1:O:93:PRO:HD3	1.78	0.65
1:T:45:PRO:HD2	1:T:49:GLN:OE1	1.96	0.65
1:U:105:LEU:HD12	1:U:107:ILE:H	1.61	0.65
1:D:354:ILE:HG21	3:D:502:DST:H132	1.78	0.65
1:I:405:THR:O	1:I:409:LEU:HD13	1.95	0.65
1:R:406:LEU:HD12	1:R:415:ILE:HD13	1.76	0.65
1:W:290:VAL:HG23	1:W:294:LYS:CG	2.26	0.65
1:L:370:PHE:O	1:L:426:SER:HA	1.96	0.65
1:O:433:ARG:HG3	1:O:436:TYR:OH	1.96	0.65
1:P:386:LEU:HD13	1:P:390:TRP:NE1	2.12	0.65
1:T:200:GLY:N	1:T:212:LYS:O	2.29	0.65
1:T:290:VAL:HG23	1:T:294:LYS:CG	2.26	0.65
1:X:253:ILE:HD12	1:X:359:ILE:HD11	1.78	0.65
1:C:115:LYS:HG2	1:C:395:TRP:HE1	1.61	0.65
1:B:173:LEU:O	1:B:174:SER:OG	2.11	0.65
1:J:42:HIS:HB2	1:K:79:PHE:CE2	2.31	0.65
1:W:161:THR:N	1:W:162:PRO:HD3	2.12	0.65
1:X:70:GLY:HA3	1:X:73:GLN:NE2	2.11	0.65
1:V:122:ARG:HG2	1:V:202:ASP:OD1	1.96	0.65
1:V:290:VAL:HG11	1:V:353:ILE:HG12	1.78	0.65
1:D:180:GLN:HE21	1:D:223:ALA:HB2	1.62	0.65
1:K:85:LEU:HB3	1:K:125:PHE:CE1	2.32	0.65
1:N:204:ASN:HB2	1:N:205:PRO:HD2	1.77	0.65
1:O:85:LEU:HB3	1:O:125:PHE:HE1	1.62	0.65
1:Q:308:GLU:HB2	1:Q:311:ILE:HD13	1.78	0.65
1:R:295:ILE:HG23	1:R:370:PHE:HE2	1.61	0.65
1:A:301:LEU:O	1:A:304:ARG:HG2	1.96	0.65
1:E:204:ASN:HB2	1:E:205:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:CD1	1:B:107:ILE:HG22	2.27	0.65
1:B:165:GLN:HG3	1:F:172:GLN:NE2	2.07	0.65
1:D:120:LEU:HD21	1:D:205:PRO:HD3	1.79	0.65
1:H:60:PHE:CE1	1:H:123:ILE:HD11	2.32	0.65
1:H:382:VAL:O	1:H:386:LEU:HB2	1.97	0.65
1:J:160:ASP:OD2	1:L:174:SER:HB2	1.97	0.65
1:N:389:PHE:CE2	1:N:437:MET:HE1	2.31	0.65
1:Q:208:ALA:HA	1:T:41:TYR:OH	1.96	0.65
1:R:92:TYR:HB3	1:R:93:PRO:HD3	1.79	0.65
1:U:406:LEU:HD12	1:U:415:ILE:CD1	2.27	0.65
1:X:308:GLU:HB2	1:X:311:ILE:HD13	1.78	0.65
1:C:92:TYR:HB3	1:C:93:PRO:HD3	1.78	0.65
1:E:92:TYR:HB3	1:E:93:PRO:HD3	1.78	0.65
1:E:229:GLY:HA3	1:E:263:TYR:CE2	2.31	0.65
1:G:239:ILE:CD1	1:G:242:GLU:HG2	2.26	0.65
1:D:126:GLU:OE2	1:D:195:SER:HB2	1.97	0.65
1:H:433:ARG:HG3	1:H:436:TYR:CZ	2.32	0.65
1:I:239:ILE:CD1	1:I:242:GLU:HG2	2.27	0.65
1:T:292:TRP:CZ2	1:T:319:LYS:HB2	2.31	0.65
1:T:386:LEU:HD13	1:T:390:TRP:NE1	2.11	0.65
1:T:406:LEU:HD12	1:T:415:ILE:CD1	2.27	0.65
1:W:406:LEU:HD12	1:W:415:ILE:CD1	2.27	0.65
1:V:137:ASP:OD2	1:V:142:ILE:HG12	1.96	0.65
1:V:295:ILE:HG23	1:V:370:PHE:HE2	1.61	0.65
1:B:41:TYR:OH	1:H:208:ALA:HA	1.97	0.65
1:D:433:ARG:HG3	1:D:436:TYR:OH	1.97	0.65
1:I:137:ASP:OD2	1:I:142:ILE:HG12	1.97	0.65
1:S:92:TYR:HB3	1:S:93:PRO:HD3	1.79	0.65
1:T:83:HIS:O	1:T:87:PRO:HG2	1.97	0.65
1:T:390:TRP:CB	1:T:399:ALA:HB2	2.24	0.65
1:T:418:THR:HG21	1:T:421:LEU:HD12	1.79	0.65
1:G:415:ILE:HA	1:G:418:THR:HG22	1.78	0.65
1:D:256:TYR:CD2	1:D:301:LEU:HD12	2.31	0.65
1:F:63:PHE:CE1	1:F:409:LEU:HD23	2.32	0.65
1:J:386:LEU:HD13	1:J:390:TRP:NE1	2.11	0.65
1:N:288:THR:HG23	1:N:289:GLU:H	1.62	0.65
1:N:320:GLN:HE22	1:N:392:SER:HB3	1.61	0.65
1:G:356:ASN:HB3	1:G:369:LYS:HB3	1.79	0.64
1:F:390:TRP:CB	1:F:399:ALA:HB2	2.22	0.64
1:I:299:TRP:CD1	1:I:311:ILE:HG23	2.33	0.64
1:I:308:GLU:HB2	1:I:311:ILE:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:45:PRO:HD2	1:K:49:GLN:OE1	1.96	0.64
1:L:122:ARG:HG2	1:L:202:ASP:OD1	1.97	0.64
1:O:66:ALA:HB2	1:O:409:LEU:HD11	1.79	0.64
1:Q:42:HIS:HB2	1:T:79:PHE:CE2	2.32	0.64
1:R:204:ASN:HB2	1:R:205:PRO:HD2	1.77	0.64
1:X:292:TRP:CZ2	1:X:319:LYS:HB2	2.32	0.64
1:E:60:PHE:CE2	1:E:64:LEU:HD11	2.32	0.64
1:E:85:LEU:HB3	1:E:125:PHE:HE1	1.62	0.64
1:E:321:ILE:HD11	1:E:389:PHE:CZ	2.33	0.64
1:G:63:PHE:CE1	1:G:409:LEU:HD23	2.32	0.64
1:G:243:ARG:HA	1:G:243:ARG:NE	2.12	0.64
1:I:256:TYR:CD2	1:I:301:LEU:HD12	2.31	0.64
1:L:204:ASN:HB2	1:L:205:PRO:HD2	1.78	0.64
1:C:105:LEU:HD12	1:C:107:ILE:H	1.61	0.64
1:G:92:TYR:HB3	1:G:93:PRO:HD3	1.80	0.64
1:B:379:ASP:HB2	1:B:418:THR:HG23	1.80	0.64
1:B:405:THR:O	1:B:409:LEU:HD13	1.96	0.64
1:D:92:TYR:HB3	1:D:93:PRO:HD3	1.79	0.64
1:I:323:SER:O	1:I:327:ILE:HB	1.96	0.64
1:I:433:ARG:HG3	1:I:436:TYR:OH	1.97	0.64
1:L:290:VAL:HG11	1:L:353:ILE:HG12	1.79	0.64
1:M:292:TRP:CZ2	1:M:319:LYS:HB2	2.32	0.64
1:N:239:ILE:CD1	1:N:242:GLU:HG2	2.27	0.64
1:O:167:LEU:HD23	1:O:269:LEU:HD23	1.77	0.64
1:R:280:ARG:HD2	1:R:358:GLU:OE2	1.96	0.64
1:S:204:ASN:HB2	1:S:205:PRO:HD2	1.80	0.64
1:W:92:TYR:HB3	1:W:93:PRO:HD3	1.78	0.64
1:X:85:LEU:HB3	1:X:125:PHE:HE1	1.62	0.64
1:X:321:ILE:HG22	1:X:325:LEU:HD23	1.79	0.64
1:A:161:THR:N	1:A:162:PRO:HD3	2.13	0.64
1:A:271:CYS:HB2	1:A:279:GLN:NE2	2.12	0.64
1:V:320:GLN:HE22	1:V:392:SER:HB3	1.62	0.64
1:B:323:SER:O	1:B:327:ILE:HB	1.98	0.64
1:F:306:ILE:HD12	1:F:307:GLU:N	2.12	0.64
1:J:323:SER:O	1:J:327:ILE:HB	1.97	0.64
1:P:115:LYS:CE	1:P:434:GLY:HA3	2.26	0.64
1:T:369:LYS:HA	1:T:427:TYR:O	1.97	0.64
1:F:285:GLY:HA3	1:F:355:TRP:CZ2	2.31	0.64
1:F:387:ALA:HA	1:F:390:TRP:CD1	2.33	0.64
1:H:92:TYR:HB3	1:H:93:PRO:HD3	1.80	0.64
1:I:212:LYS:NZ	3:I:502:DST:O4	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:TRP:CE3	1:K:89:LEU:HD13	2.32	0.64
1:K:127:PRO:HG3	1:K:147:LEU:CD2	2.26	0.64
1:N:386:LEU:HD13	1:N:390:TRP:NE1	2.11	0.64
1:O:406:LEU:HD12	1:O:415:ILE:CD1	2.28	0.64
1:P:171:PHE:HE1	1:P:231:LEU:HD13	1.61	0.64
1:Q:92:TYR:HB3	1:Q:93:PRO:HD3	1.78	0.64
1:T:378:ASN:O	1:T:382:VAL:HG23	1.97	0.64
1:X:406:LEU:HD12	1:X:415:ILE:HD13	1.79	0.64
1:B:52:TRP:CE3	1:B:89:LEU:HD13	2.32	0.64
1:B:105:LEU:HD12	1:B:107:ILE:H	1.63	0.64
1:K:115:LYS:HE2	1:K:435:VAL:H	1.63	0.64
1:M:63:PHE:HE2	1:M:109:PHE:HB2	1.61	0.64
1:O:374:VAL:HG11	1:O:422:GLN:HG3	1.80	0.64
1:P:70:GLY:HA3	1:P:73:GLN:NE2	2.11	0.64
1:Q:288:THR:HG23	1:Q:289:GLU:H	1.61	0.64
1:U:115:LYS:HG2	1:U:395:TRP:NE1	2.12	0.64
1:W:433:ARG:HG3	1:W:436:TYR:CZ	2.31	0.64
1:E:433:ARG:HG3	1:E:436:TYR:OH	1.98	0.64
1:B:315:LEU:HD23	1:B:315:LEU:O	1.98	0.64
1:I:301:LEU:O	1:I:304:ARG:HG2	1.98	0.64
1:I:360:HIS:ND1	1:I:361:PRO:HD2	2.13	0.64
1:N:321:ILE:HG22	1:N:325:LEU:HD23	1.79	0.64
1:Q:321:ILE:HG22	1:Q:325:LEU:HD23	1.80	0.64
1:R:253:ILE:HD12	1:R:359:ILE:HD11	1.80	0.64
1:R:290:VAL:HG11	1:R:353:ILE:HG12	1.80	0.64
1:A:92:TYR:HB3	1:A:93:PRO:HD3	1.78	0.64
1:A:305:LEU:CD1	1:A:311:ILE:HG12	2.28	0.64
1:H:386:LEU:HD13	1:H:390:TRP:HE1	1.61	0.64
1:N:79:PHE:CE2	1:O:42:HIS:HB2	2.33	0.64
1:Q:292:TRP:CZ2	1:Q:319:LYS:HB2	2.33	0.64
1:U:406:LEU:HD12	1:U:415:ILE:HD13	1.79	0.64
1:X:105:LEU:HD12	1:X:107:ILE:H	1.61	0.64
1:A:275:GLU:HB2	1:E:175:LEU:HD21	1.79	0.64
1:B:60:PHE:CE1	1:B:123:ILE:HD11	2.33	0.64
1:D:204:ASN:HB2	1:D:205:PRO:HD2	1.80	0.64
1:H:204:ASN:HB2	1:H:205:PRO:HD2	1.80	0.64
1:H:299:TRP:CD1	1:H:311:ILE:HG23	2.33	0.64
1:N:92:TYR:HB3	1:N:93:PRO:HD3	1.80	0.64
1:Q:204:ASN:HB2	1:Q:205:PRO:HD2	1.78	0.64
1:T:110:SER:HB2	1:T:122:ARG:CB	2.11	0.64
1:U:98:SER:OG	1:U:126:GLU:OE1	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:228:VAL:HG12	1:W:232:ILE:HD11	1.78	0.64
1:X:212:LYS:NZ	3:X:502:DST:O5	2.29	0.64
1:X:321:ILE:HD11	1:X:389:PHE:CZ	2.33	0.64
1:C:173:LEU:HD13	1:C:196:GLN:HE22	1.63	0.64
1:A:285:GLY:HA3	1:A:355:TRP:CZ2	2.33	0.64
1:V:285:GLY:HA3	1:V:355:TRP:CZ2	2.32	0.64
1:I:105:LEU:HD12	1:I:107:ILE:H	1.62	0.64
1:I:211:VAL:HG12	1:I:273:PHE:CD2	2.33	0.64
1:L:306:ILE:HD12	1:L:307:GLU:N	2.13	0.64
1:M:239:ILE:CD1	1:M:242:GLU:HG2	2.28	0.64
1:Q:321:ILE:HD11	1:Q:389:PHE:CZ	2.33	0.64
1:U:386:LEU:HD13	1:U:390:TRP:NE1	2.13	0.64
1:W:112:ASN:HD22	1:W:122:ARG:HH21	1.45	0.64
1:W:320:GLN:HE22	1:W:392:SER:HB3	1.61	0.64
1:C:321:ILE:HG22	1:C:325:LEU:HD23	1.79	0.63
1:V:60:PHE:CE1	1:V:123:ILE:HD11	2.33	0.63
1:H:280:ARG:HD2	1:H:358:GLU:OE2	1.98	0.63
1:I:92:TYR:HB3	1:I:93:PRO:HD3	1.79	0.63
1:N:406:LEU:HD12	1:N:415:ILE:HD13	1.80	0.63
1:O:115:LYS:HG2	1:O:395:TRP:NE1	2.12	0.63
1:O:173:LEU:HD13	1:O:196:GLN:NE2	2.12	0.63
1:R:374:VAL:HG11	1:R:382:VAL:HG11	1.80	0.63
1:S:212:LYS:NZ	3:S:502:DST:O6	2.31	0.63
1:W:264:ASN:O	1:W:267:THR:HG22	1.98	0.63
1:I:243:ARG:NE	1:I:243:ARG:HA	2.13	0.63
1:I:382:VAL:O	1:I:386:LEU:HB2	1.98	0.63
1:J:301:LEU:O	1:J:304:ARG:HG2	1.98	0.63
1:K:306:ILE:HD12	1:K:307:GLU:N	2.12	0.63
1:L:115:LYS:HG2	1:L:395:TRP:HE1	1.62	0.63
1:U:285:GLY:HA3	1:U:355:TRP:CZ2	2.33	0.63
1:X:301:LEU:O	1:X:304:ARG:HG2	1.97	0.63
1:V:321:ILE:HD11	1:V:437:MET:HE1	1.80	0.63
1:H:99:THR:HG23	1:H:193:LEU:CD2	2.28	0.63
1:J:256:TYR:CD2	1:J:301:LEU:HD12	2.32	0.63
1:L:386:LEU:HD13	1:L:390:TRP:NE1	2.13	0.63
1:T:63:PHE:CE2	1:T:109:PHE:HB2	2.33	0.63
1:X:92:TYR:HB3	1:X:93:PRO:HD3	1.80	0.63
1:C:161:THR:N	1:C:162:PRO:HD3	2.13	0.63
1:C:292:TRP:HZ2	1:C:315:LEU:HD21	1.64	0.63
1:E:389:PHE:HE2	1:E:437:MET:HE1	1.63	0.63
1:B:374:VAL:HG11	1:B:382:VAL:HG11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:115:LYS:HG2	1:L:395:TRP:NE1	2.11	0.63
1:M:42:HIS:HB2	1:P:79:PHE:CE2	2.34	0.63
1:O:167:LEU:O	1:O:171:PHE:HD2	1.81	0.63
1:S:161:THR:N	1:S:162:PRO:HD3	2.13	0.63
1:S:167:LEU:HD23	1:S:269:LEU:HD23	1.80	0.63
1:S:256:TYR:CD2	1:S:301:LEU:HD12	2.33	0.63
1:T:115:LYS:CE	1:T:434:GLY:HA3	2.28	0.63
1:U:239:ILE:CD1	1:U:242:GLU:HG2	2.29	0.63
1:U:379:ASP:OD2	1:U:421:LEU:HB2	1.98	0.63
1:G:173:LEU:O	1:G:174:SER:OG	2.15	0.63
1:B:299:TRP:CD1	1:B:311:ILE:HG23	2.33	0.63
1:F:92:TYR:HB3	1:F:93:PRO:HD3	1.81	0.63
1:L:60:PHE:CE1	1:L:123:ILE:HD11	2.33	0.63
1:M:85:LEU:HB3	1:M:125:PHE:HE1	1.63	0.63
1:M:323:SER:O	1:M:327:ILE:HB	1.98	0.63
1:O:386:LEU:HD13	1:O:390:TRP:HE1	1.64	0.63
1:Q:390:TRP:CB	1:Q:399:ALA:HB2	2.27	0.63
1:S:85:LEU:HB3	1:S:125:PHE:HE1	1.64	0.63
1:S:137:ASP:OD2	1:S:142:ILE:HG12	1.99	0.63
1:S:171:PHE:CE1	1:S:217:PRO:HB3	2.33	0.63
1:U:42:HIS:HB2	1:X:79:PHE:CE2	2.34	0.63
1:W:387:ALA:HA	1:W:390:TRP:HD1	1.62	0.63
1:B:290:VAL:HG23	1:B:294:LYS:CG	2.29	0.63
1:I:63:PHE:CE2	1:I:109:PHE:HB2	2.34	0.63
1:L:92:TYR:HB3	1:L:93:PRO:HD3	1.79	0.63
1:P:212:LYS:NZ	3:P:502:DST:O5	2.32	0.63
1:T:51:ARG:HD3	1:T:92:TYR:CD2	2.33	0.63
1:T:142:ILE:HB	1:T:143:PRO:HD3	1.81	0.63
1:A:306:ILE:HD12	1:A:307:GLU:N	2.14	0.63
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.14	0.63
1:F:161:THR:N	1:F:162:PRO:CD	2.62	0.63
1:F:323:SER:O	1:F:327:ILE:HB	1.98	0.63
1:H:52:TRP:CE3	1:H:89:LEU:HD13	2.33	0.63
1:I:105:LEU:CD1	1:I:107:ILE:HG22	2.29	0.63
1:K:292:TRP:CZ2	1:K:319:LYS:HB2	2.32	0.63
1:K:320:GLN:HB2	1:Q:312:ILE:CG2	2.29	0.63
1:M:115:LYS:HG2	1:M:395:TRP:NE1	2.13	0.63
1:O:440:TYR:OH	3:O:502:DST:O8	2.16	0.63
1:R:288:THR:HG23	1:R:289:GLU:H	1.63	0.63
1:T:161:THR:N	1:T:162:PRO:HD3	2.14	0.63
1:U:321:ILE:HD11	1:U:389:PHE:CZ	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:295:ILE:HG23	1:V:370:PHE:CE2	2.34	0.63
1:V:321:ILE:HG22	1:V:325:LEU:HD23	1.80	0.63
1:B:92:TYR:HB3	1:B:93:PRO:HD3	1.81	0.63
1:D:142:ILE:HB	1:D:143:PRO:HD3	1.81	0.63
1:H:266:TYR:CD1	2:H:501:QRP:HAHA	2.33	0.63
1:N:115:LYS:HE2	1:N:435:VAL:H	1.63	0.63
1:Q:105:LEU:HD12	1:Q:107:ILE:H	1.64	0.63
1:T:305:LEU:CD1	1:T:311:ILE:HG12	2.29	0.63
1:U:85:LEU:HB3	1:U:125:PHE:HE1	1.63	0.63
1:C:405:THR:O	1:C:409:LEU:HD13	1.98	0.63
1:A:180:GLN:NE2	1:A:223:ALA:HB2	2.13	0.63
1:V:356:ASN:HB3	1:V:369:LYS:HB3	1.81	0.63
1:E:315:LEU:HD23	1:E:315:LEU:O	1.99	0.63
1:D:292:TRP:CH2	1:D:319:LYS:HB2	2.34	0.63
1:D:415:ILE:HA	1:D:418:THR:CG2	2.28	0.63
1:D:428:SER:HB3	1:D:436:TYR:HB2	1.81	0.63
1:I:288:THR:HG23	1:I:289:GLU:H	1.64	0.63
1:J:200:GLY:N	1:J:212:LYS:O	2.31	0.63
1:J:387:ALA:HA	1:J:390:TRP:HD1	1.63	0.63
1:K:271:CYS:HB2	1:K:279:GLN:NE2	2.13	0.63
1:T:282:LYS:HD2	1:T:356:ASN:HD21	1.62	0.63
1:X:204:ASN:HB2	1:X:205:PRO:HD2	1.81	0.63
1:C:200:GLY:N	1:C:212:LYS:O	2.31	0.62
1:C:271:CYS:HB2	1:C:279:GLN:NE2	2.13	0.62
1:V:239:ILE:CD1	1:V:242:GLU:HG2	2.29	0.62
1:G:292:TRP:CZ2	1:G:315:LEU:HD21	2.33	0.62
1:G:386:LEU:HD13	1:G:390:TRP:HE1	1.62	0.62
1:I:305:LEU:CD1	1:I:311:ILE:HG12	2.29	0.62
1:J:269:LEU:CD1	1:J:283:ILE:HG13	2.29	0.62
1:K:389:PHE:HE2	1:K:437:MET:HE3	1.64	0.62
1:K:406:LEU:HD12	1:K:415:ILE:HD13	1.81	0.62
1:M:180:GLN:NE2	1:M:223:ALA:HB2	2.14	0.62
1:W:390:TRP:CB	1:W:399:ALA:HB2	2.28	0.62
1:C:320:GLN:HE22	1:C:392:SER:HB3	1.64	0.62
1:E:406:LEU:HD12	1:E:415:ILE:HD13	1.79	0.62
1:B:85:LEU:HB3	1:B:125:PHE:HE1	1.63	0.62
1:B:301:LEU:O	1:B:304:ARG:HG2	1.98	0.62
1:D:406:LEU:HD12	1:D:415:ILE:HD13	1.79	0.62
1:T:204:ASN:HB2	1:T:205:PRO:HD2	1.81	0.62
1:W:321:ILE:HD11	1:W:389:PHE:CZ	2.34	0.62
1:B:386:LEU:HD13	1:B:390:TRP:NE1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:315:LEU:O	1:H:315:LEU:HD23	1.99	0.62
1:K:204:ASN:HB2	1:K:205:PRO:HD2	1.82	0.62
1:M:204:ASN:HB2	1:M:205:PRO:HD2	1.80	0.62
1:N:173:LEU:O	1:N:174:SER:OG	2.14	0.62
1:P:295:ILE:HG23	1:P:370:PHE:CE2	2.34	0.62
1:R:285:GLY:HA3	1:R:355:TRP:CZ2	2.34	0.62
1:T:360:HIS:ND1	1:T:361:PRO:HD2	2.14	0.62
1:U:92:TYR:HB3	1:U:93:PRO:HD3	1.80	0.62
1:U:239:ILE:HD12	1:U:242:GLU:CG	2.28	0.62
1:W:212:LYS:NZ	3:W:502:DST:O6	2.33	0.62
1:C:70:GLY:HA3	1:C:73:GLN:NE2	2.14	0.62
1:G:89:LEU:HD22	1:G:106:PRO:HG2	1.80	0.62
1:B:415:ILE:HA	1:B:418:THR:CG2	2.29	0.62
1:D:212:LYS:NZ	3:D:502:DST:O6	2.32	0.62
1:F:433:ARG:HG3	1:F:436:TYR:CZ	2.33	0.62
1:H:292:TRP:HZ2	1:H:315:LEU:HD21	1.65	0.62
1:J:204:ASN:HB2	1:J:205:PRO:HD2	1.81	0.62
1:K:228:VAL:O	1:K:232:ILE:HG13	2.00	0.62
1:M:308:GLU:HB2	1:M:311:ILE:HD13	1.82	0.62
1:S:354:ILE:HG21	3:S:502:DST:H132	1.80	0.62
1:T:290:VAL:HG11	1:T:353:ILE:HG12	1.81	0.62
1:U:170:LYS:NZ	1:U:238:THR:HG21	2.13	0.62
1:C:288:THR:HG23	1:C:289:GLU:H	1.64	0.62
1:C:433:ARG:HG3	1:C:436:TYR:OH	2.00	0.62
1:V:386:LEU:HD13	1:V:390:TRP:NE1	2.14	0.62
1:F:115:LYS:HG2	1:F:395:TRP:NE1	2.14	0.62
1:I:41:TYR:OH	1:L:208:ALA:HA	1.99	0.62
1:M:239:ILE:HA	1:M:242:GLU:HB3	1.82	0.62
1:O:105:LEU:CD1	1:O:107:ILE:HG22	2.30	0.62
1:Q:161:THR:N	1:Q:162:PRO:HD3	2.14	0.62
1:T:266:TYR:CD1	2:T:501:QRP:HAHA	2.35	0.62
1:T:379:ASP:OD1	1:T:422:GLN:HG3	2.00	0.62
1:X:299:TRP:CD1	1:X:311:ILE:HG23	2.35	0.62
1:G:387:ALA:HA	1:G:390:TRP:CD1	2.34	0.62
1:D:292:TRP:CZ2	1:D:315:LEU:HD21	2.35	0.62
1:L:266:TYR:CD1	2:L:501:QRP:HAHA	2.35	0.62
1:N:162:PRO:HG2	1:P:174:SER:HB3	1.82	0.62
1:N:354:ILE:HG21	3:N:502:DST:H132	1.82	0.62
1:T:308:GLU:HB2	1:T:311:ILE:HD13	1.82	0.62
1:W:379:ASP:HB2	1:W:418:THR:HG23	1.82	0.62
1:A:180:GLN:HE21	1:A:223:ALA:CB	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:288:THR:HG23	1:V:289:GLU:H	1.65	0.62
1:E:171:PHE:CE1	1:E:217:PRO:HB3	2.34	0.62
1:D:79:PHE:HE2	1:F:42:HIS:HB2	1.64	0.62
1:F:256:TYR:CD2	1:F:301:LEU:HD12	2.35	0.62
1:I:321:ILE:HD11	1:I:389:PHE:CE2	2.34	0.62
1:J:115:LYS:HE2	1:J:435:VAL:H	1.63	0.62
1:J:406:LEU:HD12	1:J:415:ILE:HD13	1.81	0.62
1:K:321:ILE:HD11	1:K:389:PHE:CZ	2.35	0.62
1:M:406:LEU:HD12	1:M:415:ILE:CD1	2.30	0.62
1:N:290:VAL:HG11	1:N:353:ILE:HG12	1.80	0.62
1:O:321:ILE:HG22	1:O:325:LEU:HD23	1.81	0.62
1:Q:256:TYR:CD2	1:Q:301:LEU:HD12	2.34	0.62
1:R:142:ILE:HB	1:R:143:PRO:HD3	1.81	0.62
1:U:204:ASN:HB2	1:U:205:PRO:HD2	1.81	0.62
1:C:418:THR:HG21	1:C:421:LEU:HD12	1.81	0.62
1:G:137:ASP:OD2	1:G:142:ILE:HG12	2.00	0.62
1:G:433:ARG:HG3	1:G:436:TYR:OH	2.00	0.62
1:D:288:THR:HG23	1:D:289:GLU:H	1.64	0.62
1:J:173:LEU:O	1:J:174:SER:OG	2.09	0.62
1:L:288:THR:HG23	1:L:289:GLU:H	1.63	0.62
1:M:239:ILE:HD12	1:M:242:GLU:CG	2.29	0.62
1:O:360:HIS:ND1	1:O:361:PRO:HD2	2.14	0.62
1:P:92:TYR:HB3	1:P:93:PRO:HD3	1.82	0.62
1:P:354:ILE:HG21	3:P:502:DST:H132	1.82	0.62
1:Q:206:ASP:OD1	1:Q:207:GLY:N	2.32	0.62
1:R:269:LEU:CD1	1:R:283:ILE:HG13	2.30	0.62
1:W:292:TRP:CZ2	1:W:319:LYS:HB2	2.34	0.62
1:X:261:THR:O	1:X:261:THR:HG22	2.00	0.62
1:V:315:LEU:O	1:V:315:LEU:HD23	2.00	0.62
1:G:305:LEU:CD1	1:G:311:ILE:HG12	2.30	0.62
1:D:173:LEU:HD13	1:D:196:GLN:NE2	2.14	0.62
1:K:115:LYS:HG2	1:K:395:TRP:HE1	1.65	0.62
1:K:321:ILE:CD1	1:K:437:MET:HE1	2.30	0.62
1:M:406:LEU:HD12	1:M:415:ILE:HD13	1.81	0.62
1:S:167:LEU:O	1:S:171:PHE:HD2	1.83	0.62
1:S:176:SER:O	1:S:180:GLN:HB2	1.99	0.62
1:A:180:GLN:NE2	1:A:223:ALA:CA	2.63	0.62
1:V:271:CYS:HB2	1:V:279:GLN:HE21	1.65	0.62
1:B:42:HIS:HB2	1:H:79:PHE:CE2	2.34	0.62
1:B:75:TYR:CD2	1:H:75:TYR:HD2	2.12	0.62
1:B:161:THR:N	1:B:162:PRO:CD	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:LEU:CD1	1:D:107:ILE:HG22	2.30	0.62
1:J:161:THR:N	1:J:162:PRO:HD3	2.15	0.62
1:O:292:TRP:CH2	1:O:319:LYS:HB2	2.35	0.62
1:O:415:ILE:HA	1:O:418:THR:HG22	1.81	0.62
1:P:292:TRP:CZ2	1:P:319:LYS:HB2	2.35	0.62
1:T:321:ILE:HD11	1:T:389:PHE:CZ	2.35	0.62
1:E:70:GLY:HA3	1:E:73:GLN:NE2	2.15	0.61
1:E:430:THR:HG22	1:E:432:LYS:H	1.64	0.61
1:B:174:SER:HB3	1:F:162:PRO:HG2	1.82	0.61
1:H:374:VAL:HG13	1:H:382:VAL:HG21	1.82	0.61
1:Q:161:THR:N	1:Q:162:PRO:CD	2.63	0.61
1:Q:321:ILE:CD1	1:Q:437:MET:HE1	2.30	0.61
1:R:79:PHE:CE2	1:S:42:HIS:HB2	2.35	0.61
1:R:239:ILE:CD1	1:R:242:GLU:HG2	2.30	0.61
1:S:389:PHE:CE2	1:S:437:MET:HE1	2.34	0.61
1:U:285:GLY:O	1:U:354:ILE:HG23	2.00	0.61
1:U:369:LYS:HA	1:U:427:TYR:O	2.00	0.61
1:A:424:TRP:HB2	1:A:440:TYR:CD2	2.35	0.61
1:G:60:PHE:CE1	1:G:123:ILE:HD11	2.35	0.61
1:G:85:LEU:HB3	1:G:125:PHE:CE1	2.35	0.61
1:D:60:PHE:CE1	1:D:123:ILE:HD11	2.36	0.61
1:J:211:VAL:HG12	1:J:273:PHE:CD2	2.34	0.61
1:L:433:ARG:HG3	1:L:436:TYR:OH	2.00	0.61
1:R:161:THR:N	1:R:162:PRO:CD	2.63	0.61
1:R:255:ASP:O	1:R:259:GLU:HG3	2.00	0.61
1:T:92:TYR:HB3	1:T:93:PRO:HD3	1.82	0.61
1:T:147:LEU:HD23	1:T:199:PHE:HD2	1.65	0.61
1:T:173:LEU:O	1:T:174:SER:OG	2.15	0.61
1:X:374:VAL:HG11	1:X:382:VAL:HG11	1.82	0.61
1:X:386:LEU:HD13	1:X:390:TRP:NE1	2.15	0.61
1:A:137:ASP:OD2	1:A:142:ILE:HG12	2.00	0.61
1:V:92:TYR:HB3	1:V:93:PRO:HD3	1.83	0.61
1:E:127:PRO:HG3	1:E:147:LEU:HD23	1.83	0.61
1:E:212:LYS:NZ	3:E:502:DST:O6	2.33	0.61
1:E:292:TRP:CH2	1:E:319:LYS:HB2	2.34	0.61
1:B:379:ASP:OD2	1:B:421:LEU:HB2	1.99	0.61
1:F:127:PRO:HG3	1:F:147:LEU:CD2	2.30	0.61
1:H:387:ALA:HA	1:H:390:TRP:HD1	1.63	0.61
1:M:306:ILE:HD12	1:M:307:GLU:N	2.14	0.61
1:O:115:LYS:HG2	1:O:395:TRP:HE1	1.65	0.61
1:O:127:PRO:HG3	1:O:147:LEU:CD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:161:THR:N	1:O:162:PRO:HD3	2.15	0.61
1:O:239:ILE:CD1	1:O:242:GLU:HG2	2.29	0.61
1:P:161:THR:N	1:P:162:PRO:HD3	2.15	0.61
1:R:292:TRP:CZ2	1:R:315:LEU:HD21	2.35	0.61
1:U:405:THR:O	1:U:409:LEU:HD13	2.00	0.61
1:W:63:PHE:CE1	1:W:409:LEU:HD23	2.35	0.61
1:X:112:ASN:HD22	1:X:122:ARG:HH21	1.46	0.61
1:X:290:VAL:HG23	1:X:294:LYS:CG	2.30	0.61
1:D:70:GLY:HA3	1:D:73:GLN:NE2	2.14	0.61
1:D:221:ALA:HB2	1:D:231:LEU:HD21	1.81	0.61
1:F:204:ASN:HB2	1:F:205:PRO:HD2	1.83	0.61
1:H:269:LEU:CD1	1:H:283:ILE:HG13	2.30	0.61
1:H:292:TRP:CZ2	1:H:315:LEU:HD21	2.36	0.61
1:K:115:LYS:HG2	1:K:395:TRP:NE1	2.15	0.61
1:K:200:GLY:N	1:K:212:LYS:O	2.32	0.61
1:L:161:THR:N	1:L:162:PRO:CD	2.64	0.61
1:M:160:ASP:OD2	1:O:174:SER:HB2	2.00	0.61
1:O:288:THR:HG23	1:O:289:GLU:H	1.63	0.61
1:R:315:LEU:HD23	1:R:315:LEU:O	2.01	0.61
1:U:60:PHE:CE2	1:U:64:LEU:HD11	2.36	0.61
1:C:292:TRP:CZ2	1:C:315:LEU:HD21	2.35	0.61
1:V:275:GLU:CD	1:X:175:LEU:HD11	2.21	0.61
1:B:51:ARG:HD3	1:B:92:TYR:CD2	2.35	0.61
1:F:120:LEU:HD21	1:F:205:PRO:HD3	1.81	0.61
1:H:282:LYS:HD2	1:H:356:ASN:HD21	1.66	0.61
1:H:426:SER:O	1:H:437:MET:HG3	2.00	0.61
1:I:112:ASN:HD22	1:I:122:ARG:HH21	1.45	0.61
1:J:63:PHE:CE2	1:J:109:PHE:HB2	2.36	0.61
1:K:92:TYR:HB3	1:K:93:PRO:HD3	1.81	0.61
1:M:369:LYS:NZ	3:M:502:DST:O4	2.33	0.61
1:O:387:ALA:HA	1:O:390:TRP:HD1	1.63	0.61
1:S:66:ALA:HB2	1:S:409:LEU:HD11	1.82	0.61
1:U:290:VAL:HG11	1:U:353:ILE:HG12	1.81	0.61
1:U:433:ARG:HG3	1:U:436:TYR:CZ	2.36	0.61
1:W:321:ILE:HD13	1:W:437:MET:HE1	1.82	0.61
1:C:295:ILE:HG23	1:C:370:PHE:HE2	1.65	0.61
1:C:406:LEU:HD12	1:C:415:ILE:HD11	1.82	0.61
1:A:105:LEU:HD12	1:A:107:ILE:H	1.66	0.61
1:A:115:LYS:HG2	1:A:395:TRP:NE1	2.14	0.61
1:V:292:TRP:CZ2	1:V:315:LEU:HD21	2.36	0.61
1:H:211:VAL:HG12	1:H:273:PHE:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:LEU:HD21	1:I:205:PRO:HD3	1.81	0.61
1:I:161:THR:N	1:I:162:PRO:HD3	2.14	0.61
1:K:105:LEU:CD1	1:K:107:ILE:HG22	2.31	0.61
1:N:161:THR:N	1:N:162:PRO:HD3	2.15	0.61
1:N:321:ILE:HD11	1:N:389:PHE:CZ	2.36	0.61
1:O:433:ARG:HG3	1:O:436:TYR:CZ	2.34	0.61
1:Q:440:TYR:OH	3:Q:502:DST:O8	2.13	0.61
1:T:147:LEU:HD23	1:T:199:PHE:CD2	2.34	0.61
1:W:374:VAL:HG11	1:W:422:GLN:HG2	1.82	0.61
1:X:167:LEU:O	1:X:171:PHE:HD2	1.83	0.61
1:X:285:GLY:HA3	1:X:355:TRP:CZ2	2.36	0.61
1:C:360:HIS:ND1	1:C:361:PRO:HD2	2.16	0.61
1:A:176:SER:O	1:A:180:GLN:HG2	2.01	0.61
1:H:115:LYS:HE2	1:H:434:GLY:HA3	1.81	0.61
1:H:402:TYR:O	1:H:405:THR:N	2.33	0.61
1:J:41:TYR:HH	1:K:208:ALA:HA	1.66	0.61
1:K:228:VAL:CG1	1:K:232:ILE:HD11	2.26	0.61
1:L:324:LEU:HB3	1:L:385:ALA:HB1	1.83	0.61
1:M:387:ALA:HA	1:M:390:TRP:HD1	1.63	0.61
1:O:306:ILE:HD12	1:O:307:GLU:N	2.16	0.61
1:R:112:ASN:HD22	1:R:122:ARG:HH21	1.48	0.61
1:R:115:LYS:HG2	1:R:395:TRP:HE1	1.65	0.61
1:T:306:ILE:HD12	1:T:307:GLU:N	2.15	0.61
1:U:115:LYS:CE	1:U:434:GLY:HA3	2.31	0.61
1:X:306:ILE:HD12	1:X:307:GLU:N	2.16	0.61
1:A:85:LEU:HB3	1:A:125:PHE:HE1	1.66	0.61
1:A:228:VAL:HG11	1:A:267:THR:HG23	1.82	0.61
1:F:290:VAL:HG23	1:F:294:LYS:HG2	1.82	0.61
1:N:105:LEU:HD12	1:N:107:ILE:H	1.65	0.61
1:N:174:SER:HB3	1:P:162:PRO:HG2	1.81	0.61
1:Q:405:THR:O	1:Q:409:LEU:HD13	1.99	0.61
1:R:211:VAL:HG12	1:R:273:PHE:CD2	2.35	0.61
1:S:387:ALA:HA	1:S:390:TRP:HD1	1.66	0.61
1:U:374:VAL:HG11	1:U:422:GLN:HG3	1.82	0.61
1:X:116:GLY:HA2	1:X:398:HIS:NE2	2.14	0.61
1:A:307:GLU:OE1	1:I:364:ARG:NH1	2.22	0.61
1:V:374:VAL:HG11	1:V:382:VAL:HG11	1.82	0.61
1:F:321:ILE:HG22	1:F:325:LEU:CD2	2.31	0.61
1:H:161:THR:N	1:H:162:PRO:CD	2.64	0.61
1:J:406:LEU:HD12	1:J:415:ILE:CD1	2.31	0.61
1:L:160:ASP:HB3	1:L:162:PRO:CD	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:236:VAL:O	1:M:239:ILE:HG22	2.01	0.61
1:N:208:ALA:HA	1:O:41:TYR:HH	1.64	0.61
1:R:105:LEU:HD12	1:R:107:ILE:H	1.64	0.61
1:R:306:ILE:HD12	1:R:307:GLU:N	2.16	0.61
1:X:161:THR:N	1:X:162:PRO:HD3	2.15	0.61
1:X:256:TYR:CD2	1:X:301:LEU:HD12	2.36	0.61
1:X:382:VAL:O	1:X:386:LEU:HB2	2.01	0.61
1:C:161:THR:N	1:C:162:PRO:CD	2.64	0.61
1:V:51:ARG:HB3	1:V:92:TYR:CG	2.36	0.61
1:G:382:VAL:O	1:G:386:LEU:HB2	2.00	0.61
1:H:112:ASN:HD22	1:H:122:ARG:HH21	1.48	0.61
1:H:321:ILE:HG22	1:H:325:LEU:HD23	1.82	0.61
1:I:266:TYR:HD1	2:I:501:QRP:HAHA	1.66	0.61
1:I:282:LYS:HD2	1:I:356:ASN:HD21	1.66	0.61
1:J:122:ARG:HG2	1:J:202:ASP:OD1	2.01	0.61
1:J:229:GLY:HA3	1:J:263:TYR:CE2	2.35	0.61
1:L:85:LEU:HB3	1:L:125:PHE:CE1	2.33	0.61
1:M:112:ASN:HD22	1:M:122:ARG:HH21	1.49	0.61
1:Q:306:ILE:HD12	1:Q:307:GLU:N	2.16	0.61
1:R:63:PHE:HE2	1:R:109:PHE:HB2	1.63	0.61
1:U:173:LEU:HD13	1:U:196:GLN:HE22	1.66	0.61
1:X:295:ILE:HG23	1:X:370:PHE:CE2	2.36	0.61
1:V:41:TYR:OH	1:W:208:ALA:HA	2.01	0.60
1:B:288:THR:HG23	1:B:289:GLU:H	1.64	0.60
1:B:356:ASN:HB3	1:B:369:LYS:HB3	1.83	0.60
1:I:204:ASN:HB2	1:I:205:PRO:HD2	1.83	0.60
1:N:41:TYR:CZ	1:O:209:ILE:HD12	2.36	0.60
1:P:99:THR:HG23	1:P:193:LEU:CD2	2.26	0.60
1:Q:370:PHE:O	1:Q:426:SER:HA	2.01	0.60
1:R:261:THR:O	1:R:261:THR:HG22	2.01	0.60
1:W:239:ILE:CD1	1:W:242:GLU:HG2	2.30	0.60
1:A:290:VAL:HG11	1:A:353:ILE:HG12	1.83	0.60
1:E:161:THR:N	1:E:162:PRO:HD3	2.16	0.60
1:D:239:ILE:CD1	1:D:242:GLU:HG2	2.31	0.60
1:J:41:TYR:CZ	1:K:209:ILE:HD12	2.36	0.60
1:J:239:ILE:HD12	1:J:242:GLU:HG2	1.81	0.60
1:J:318:LEU:HD12	1:J:427:TYR:CD2	2.36	0.60
1:J:415:ILE:HA	1:J:418:THR:HG22	1.81	0.60
1:K:95:LYS:NZ	1:L:47:ASN:HD22	1.99	0.60
1:K:161:THR:N	1:K:162:PRO:CD	2.63	0.60
1:K:212:LYS:NZ	3:K:502:DST:O6	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:374:VAL:HG13	1:L:382:VAL:HG21	1.82	0.60
1:P:387:ALA:HA	1:P:390:TRP:HD1	1.66	0.60
1:S:127:PRO:HG3	1:S:147:LEU:CD2	2.31	0.60
1:A:42:HIS:HB2	1:G:79:PHE:CE2	2.37	0.60
1:E:386:LEU:HD13	1:E:390:TRP:NE1	2.17	0.60
1:G:282:LYS:HE3	1:G:284:TYR:OH	2.00	0.60
1:F:167:LEU:HD23	1:F:269:LEU:HD23	1.84	0.60
1:M:321:ILE:HD11	1:M:389:PHE:CZ	2.36	0.60
1:O:161:THR:N	1:O:162:PRO:CD	2.64	0.60
1:Q:160:ASP:HB3	1:Q:162:PRO:HD2	1.83	0.60
1:Q:290:VAL:HG11	1:Q:353:ILE:HG12	1.83	0.60
1:R:212:LYS:NZ	3:R:502:DST:O5	2.33	0.60
1:S:299:TRP:CD1	1:S:311:ILE:HG23	2.36	0.60
1:U:415:ILE:HA	1:U:418:THR:CG2	2.31	0.60
1:G:167:LEU:O	1:G:171:PHE:HD2	1.84	0.60
1:B:63:PHE:CE1	1:B:409:LEU:HD23	2.36	0.60
1:D:161:THR:N	1:D:162:PRO:CD	2.64	0.60
1:L:292:TRP:CH2	1:L:319:LYS:HB2	2.36	0.60
1:M:75:TYR:CD2	1:P:75:TYR:HD2	2.11	0.60
1:M:212:LYS:NZ	3:M:502:DST:O6	2.34	0.60
1:M:433:ARG:HG3	1:M:436:TYR:CZ	2.37	0.60
1:N:356:ASN:HB3	1:N:369:LYS:HB3	1.82	0.60
1:O:51:ARG:HD3	1:O:92:TYR:CD2	2.36	0.60
1:R:386:LEU:HD13	1:R:390:TRP:NE1	2.17	0.60
1:X:370:PHE:O	1:X:426:SER:HA	2.02	0.60
1:V:275:GLU:HB2	1:X:175:LEU:HD21	1.82	0.60
1:E:206:ASP:OD1	1:E:207:GLY:N	2.34	0.60
1:B:261:THR:O	1:B:261:THR:HG22	2.01	0.60
1:B:305:LEU:CD1	1:B:311:ILE:HG12	2.32	0.60
1:B:374:VAL:CG1	1:B:382:VAL:HG21	2.31	0.60
1:L:390:TRP:CB	1:L:399:ALA:HB2	2.24	0.60
1:L:415:ILE:HA	1:L:418:THR:HG22	1.82	0.60
1:M:305:LEU:CD1	1:M:311:ILE:HG12	2.31	0.60
1:N:292:TRP:CH2	1:N:319:LYS:HB2	2.35	0.60
1:P:110:SER:HB2	1:P:122:ARG:CB	2.13	0.60
1:Q:63:PHE:CE1	1:Q:409:LEU:HD23	2.36	0.60
1:S:390:TRP:CB	1:S:399:ALA:HB2	2.28	0.60
1:V:171:PHE:CE1	1:V:217:PRO:HB3	2.36	0.60
1:J:92:TYR:HB3	1:J:93:PRO:HD3	1.83	0.60
1:K:321:ILE:HD11	1:K:389:PHE:CE2	2.36	0.60
1:L:315:LEU:O	1:L:315:LEU:HD23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:LYS:HE2	1:M:434:GLY:HA3	1.82	0.60
1:P:200:GLY:N	1:P:212:LYS:O	2.30	0.60
1:T:211:VAL:HG12	1:T:273:PHE:CD2	2.36	0.60
1:T:228:VAL:CG1	1:T:232:ILE:HD11	2.27	0.60
1:U:63:PHE:CE2	1:U:109:PHE:HB2	2.35	0.60
1:U:305:LEU:HD12	1:U:311:ILE:CD1	2.31	0.60
1:X:356:ASN:HB3	1:X:369:LYS:HB3	1.84	0.60
1:A:266:TYR:CD1	2:A:501:QRP:HAHA	2.37	0.60
1:A:406:LEU:HD12	1:A:415:ILE:HD13	1.81	0.60
1:G:390:TRP:CB	1:G:399:ALA:HB2	2.20	0.60
1:F:147:LEU:HD23	1:F:199:PHE:CD2	2.37	0.60
1:M:79:PHE:CE2	1:P:42:HIS:HB2	2.37	0.60
1:N:306:ILE:HD12	1:N:307:GLU:N	2.16	0.60
1:O:389:PHE:HE2	1:O:437:MET:HE1	1.65	0.60
1:P:390:TRP:HB2	1:P:399:ALA:CB	2.23	0.60
1:Q:369:LYS:HA	1:Q:427:TYR:O	2.02	0.60
1:R:387:ALA:HA	1:R:390:TRP:CD1	2.36	0.60
1:T:85:LEU:HB3	1:T:125:PHE:CE1	2.34	0.60
1:X:387:ALA:HA	1:X:390:TRP:CD1	2.37	0.60
1:C:105:LEU:CD1	1:C:107:ILE:HG22	2.30	0.60
1:A:288:THR:HG23	1:A:289:GLU:H	1.66	0.60
1:A:292:TRP:CZ2	1:A:319:LYS:HB2	2.36	0.60
1:V:105:LEU:HD12	1:V:107:ILE:H	1.67	0.60
1:I:63:PHE:CE1	1:I:409:LEU:HD23	2.36	0.60
1:K:264:ASN:O	1:K:267:THR:HG22	2.01	0.60
1:L:356:ASN:HB3	1:L:369:LYS:HB3	1.84	0.60
1:P:63:PHE:CE1	1:P:409:LEU:HD23	2.37	0.60
1:U:373:PRO:HG3	1:U:424:TRP:CZ3	2.37	0.60
1:C:275:GLU:HB2	1:G:175:LEU:HD21	1.84	0.60
1:C:306:ILE:HD12	1:C:307:GLU:N	2.16	0.60
1:E:305:LEU:HD12	1:E:311:ILE:HD11	1.84	0.60
1:G:306:ILE:HD12	1:G:307:GLU:N	2.17	0.60
1:G:418:THR:OG1	1:G:421:LEU:HG	2.02	0.60
1:D:369:LYS:NZ	3:D:502:DST:O4	2.35	0.60
1:D:390:TRP:CB	1:D:399:ALA:HB2	2.25	0.60
1:H:122:ARG:HG2	1:H:202:ASP:OD1	2.02	0.60
1:I:290:VAL:HG11	1:I:353:ILE:HG12	1.82	0.60
1:L:256:TYR:CD2	1:L:301:LEU:HD12	2.36	0.60
1:Q:430:THR:HG22	1:Q:432:LYS:H	1.66	0.60
1:R:206:ASP:OD1	1:R:207:GLY:N	2.35	0.60
1:W:253:ILE:HD12	1:W:359:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:306:ILE:HD12	1:W:307:GLU:N	2.17	0.60
1:X:115:LYS:HE2	1:X:435:VAL:H	1.67	0.60
2:X:501:QRP:CD1	3:X:502:DST:H142	2.32	0.60
1:C:167:LEU:HD23	1:C:269:LEU:HD23	1.84	0.60
1:C:391:ASP:O	1:C:394:GLY:N	2.35	0.60
1:A:180:GLN:HE21	1:A:223:ALA:HB2	1.65	0.60
1:A:299:TRP:CD1	1:A:311:ILE:HG23	2.36	0.60
1:G:142:ILE:HB	1:G:143:PRO:HD3	1.83	0.60
1:G:290:VAL:HG11	1:G:353:ILE:HG12	1.83	0.60
1:D:127:PRO:HG3	1:D:147:LEU:HD23	1.84	0.60
1:F:356:ASN:HB3	1:F:369:LYS:HB3	1.84	0.60
1:I:51:ARG:HB3	1:I:92:TYR:CG	2.37	0.60
1:I:387:ALA:HA	1:I:390:TRP:CD1	2.36	0.60
1:K:171:PHE:CE1	1:K:217:PRO:HB3	2.37	0.60
1:L:228:VAL:CG1	1:L:232:ILE:HD11	2.29	0.60
1:L:305:LEU:CD1	1:L:311:ILE:HG12	2.31	0.60
1:M:51:ARG:HD3	1:M:92:TYR:CD2	2.37	0.60
1:M:299:TRP:NE1	1:M:311:ILE:HG23	2.17	0.60
1:N:391:ASP:O	1:N:394:GLY:N	2.34	0.60
1:P:321:ILE:HD11	1:P:389:PHE:CZ	2.37	0.60
1:Q:406:LEU:HD12	1:Q:415:ILE:CD1	2.31	0.60
1:S:386:LEU:CD1	1:S:390:TRP:HE1	2.15	0.60
1:T:415:ILE:HA	1:T:418:THR:HG22	1.84	0.60
1:U:41:TYR:CZ	1:X:209:ILE:HD12	2.37	0.60
1:X:321:ILE:CD1	1:X:437:MET:HE1	2.31	0.60
1:C:448:LEU:HD12	1:C:448:LEU:N	2.16	0.59
1:A:433:ARG:HG3	1:A:436:TYR:OH	2.02	0.59
1:E:63:PHE:HE2	1:E:109:PHE:HB2	1.66	0.59
1:E:415:ILE:HA	1:E:418:THR:HG22	1.83	0.59
1:F:269:LEU:CD1	1:F:283:ILE:HG13	2.32	0.59
1:I:51:ARG:HD3	1:I:92:TYR:CD2	2.37	0.59
1:N:292:TRP:HZ2	1:N:315:LEU:HD21	1.66	0.59
1:P:299:TRP:CD1	1:P:311:ILE:HG23	2.37	0.59
1:R:161:THR:H	1:R:162:PRO:HD3	1.67	0.59
1:R:174:SER:HB3	1:T:162:PRO:HG2	1.83	0.59
1:G:63:PHE:HE2	1:G:109:PHE:HB2	1.67	0.59
1:B:66:ALA:HB2	1:B:409:LEU:HD11	1.84	0.59
1:B:110:SER:O	1:B:121:LEU:HD12	2.00	0.59
1:D:110:SER:HB2	1:D:122:ARG:CB	2.14	0.59
1:U:171:PHE:CE1	1:U:217:PRO:HB3	2.37	0.59
1:X:60:PHE:CE1	1:X:123:ILE:HD11	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:63:PHE:CE1	1:X:409:LEU:HD23	2.37	0.59
1:X:288:THR:HG23	1:X:289:GLU:H	1.66	0.59
1:E:173:LEU:O	1:E:174:SER:OG	2.13	0.59
1:G:406:LEU:HD12	1:G:415:ILE:HD13	1.83	0.59
1:D:209:ILE:HD12	1:F:41:TYR:CZ	2.38	0.59
1:F:386:LEU:HD13	1:F:390:TRP:NE1	2.17	0.59
2:H:501:QRP:CD1	3:H:502:DST:H142	2.33	0.59
1:I:318:LEU:HD12	1:I:427:TYR:CD2	2.37	0.59
1:J:290:VAL:HG23	1:J:294:LYS:HG2	1.83	0.59
1:L:52:TRP:CE3	1:L:89:LEU:HD13	2.37	0.59
1:N:239:ILE:HD12	1:N:242:GLU:CG	2.32	0.59
1:O:115:LYS:HE2	1:O:435:VAL:H	1.66	0.59
1:Q:239:ILE:HA	1:Q:242:GLU:HB3	1.84	0.59
1:Q:318:LEU:HD12	1:Q:427:TYR:CD2	2.37	0.59
1:R:115:LYS:HE2	1:R:435:VAL:H	1.66	0.59
1:R:228:VAL:CG1	1:R:232:ILE:HD11	2.30	0.59
1:T:256:TYR:CD2	1:T:301:LEU:HD12	2.37	0.59
1:U:63:PHE:CE1	1:U:409:LEU:HD23	2.36	0.59
1:W:229:GLY:HA3	1:W:263:TYR:CE2	2.37	0.59
1:V:98:SER:OG	1:V:126:GLU:OE1	2.04	0.59
1:G:266:TYR:HD1	2:G:501:QRP:HAHA	1.68	0.59
1:B:161:THR:H	1:B:162:PRO:HD3	1.67	0.59
1:B:354:ILE:HB	1:B:371:TYR:HB2	1.85	0.59
1:F:137:ASP:OD2	1:F:142:ILE:HG12	2.03	0.59
1:H:60:PHE:HE1	1:H:123:ILE:HD11	1.67	0.59
1:H:228:VAL:CG1	1:H:232:ILE:HD11	2.32	0.59
1:I:167:LEU:O	1:I:171:PHE:HD2	1.85	0.59
1:I:239:ILE:HD12	1:I:242:GLU:CG	2.31	0.59
1:K:426:SER:OG	1:K:438:SER:HB2	2.02	0.59
1:M:170:LYS:NZ	1:M:238:THR:HG21	2.18	0.59
1:M:208:ALA:HA	1:P:41:TYR:OH	2.01	0.59
1:O:161:THR:H	1:O:162:PRO:HD3	1.68	0.59
1:R:160:ASP:HB3	1:R:162:PRO:HD2	1.83	0.59
1:S:60:PHE:CE1	1:S:123:ILE:HD11	2.37	0.59
1:T:105:LEU:HD12	1:T:107:ILE:H	1.67	0.59
1:U:370:PHE:O	1:U:426:SER:HA	2.02	0.59
1:U:426:SER:O	1:U:437:MET:HG3	2.02	0.59
1:A:66:ALA:HB2	1:A:409:LEU:HD11	1.83	0.59
1:G:63:PHE:CE2	1:G:109:PHE:HB2	2.37	0.59
1:G:374:VAL:HG11	1:G:422:GLN:HG3	1.84	0.59
1:G:387:ALA:HA	1:G:390:TRP:HD1	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:295:ILE:HG23	1:H:370:PHE:HE2	1.67	0.59
1:I:72:PRO:HA	1:L:75:TYR:HE2	1.67	0.59
1:I:116:GLY:HA2	1:I:398:HIS:NE2	2.18	0.59
1:J:356:ASN:HB3	1:J:369:LYS:HB3	1.84	0.59
1:K:142:ILE:HB	1:K:143:PRO:HD3	1.84	0.59
1:L:60:PHE:HE1	1:L:123:ILE:HD11	1.67	0.59
1:O:430:THR:HG22	1:O:432:LYS:H	1.68	0.59
1:P:142:ILE:HB	1:P:143:PRO:HD3	1.83	0.59
1:R:305:LEU:HD23	1:R:305:LEU:H	1.66	0.59
1:S:60:PHE:HE1	1:S:123:ILE:HD11	1.67	0.59
1:S:379:ASP:OD2	1:S:421:LEU:HB2	2.03	0.59
1:S:433:ARG:HG3	1:S:436:TYR:OH	2.01	0.59
1:C:386:LEU:HD13	1:C:390:TRP:NE1	2.17	0.59
1:A:41:TYR:OH	1:G:208:ALA:HA	2.03	0.59
1:E:239:ILE:CD1	1:E:242:GLU:HG2	2.31	0.59
1:E:306:ILE:HG21	1:O:303:GLY:HA3	1.84	0.59
1:D:321:ILE:HG22	1:D:325:LEU:HD23	1.83	0.59
1:J:282:LYS:HE3	1:J:284:TYR:OH	2.02	0.59
1:J:292:TRP:HZ2	1:J:315:LEU:HD21	1.66	0.59
1:M:147:LEU:HD23	1:M:199:PHE:HD2	1.67	0.59
1:P:321:ILE:HG22	1:P:325:LEU:HD23	1.85	0.59
1:Q:228:VAL:HG11	1:Q:267:THR:HG23	1.84	0.59
1:T:370:PHE:O	1:T:426:SER:HA	2.02	0.59
1:U:208:ALA:HA	1:X:41:TYR:OH	2.02	0.59
1:X:170:LYS:NZ	1:X:238:THR:HG21	2.17	0.59
1:A:63:PHE:CE1	1:A:409:LEU:HD23	2.37	0.59
1:B:433:ARG:HG3	1:B:436:TYR:CZ	2.38	0.59
1:D:115:LYS:HG2	1:D:395:TRP:NE1	2.17	0.59
1:D:175:LEU:HD21	1:H:275:GLU:HB2	1.83	0.59
1:D:253:ILE:HD12	1:D:359:ILE:HD11	1.83	0.59
1:J:51:ARG:HD3	1:J:92:TYR:CD2	2.38	0.59
1:J:137:ASP:OD2	1:J:142:ILE:HG12	2.02	0.59
1:M:285:GLY:HA3	1:M:355:TRP:CZ2	2.37	0.59
1:O:321:ILE:HD11	1:O:389:PHE:CZ	2.37	0.59
1:P:374:VAL:HG13	1:P:382:VAL:HG21	1.84	0.59
1:Q:288:THR:HG23	1:Q:289:GLU:N	2.18	0.59
1:S:60:PHE:HD1	1:S:109:PHE:CE1	2.20	0.59
1:S:115:LYS:HE2	1:S:435:VAL:H	1.65	0.59
1:V:306:ILE:HD12	1:V:307:GLU:N	2.17	0.59
1:E:51:ARG:HD3	1:E:92:TYR:CD2	2.37	0.59
1:E:402:TYR:O	1:E:405:THR:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:LEU:HD23	1:F:199:PHE:HD2	1.67	0.59
1:H:70:GLY:HA3	1:H:73:GLN:HE22	1.67	0.59
1:I:234:GLU:OE2	1:I:237:ARG:NH2	2.35	0.59
1:J:321:ILE:HD11	1:J:389:PHE:CE2	2.37	0.59
1:J:321:ILE:HD11	1:J:389:PHE:CZ	2.36	0.59
1:K:386:LEU:HD13	1:K:390:TRP:NE1	2.17	0.59
1:G:229:GLY:HA3	1:G:263:TYR:CE2	2.38	0.59
1:B:321:ILE:HG22	1:B:325:LEU:HD23	1.85	0.59
1:F:161:THR:H	1:F:162:PRO:HD3	1.67	0.59
1:I:161:THR:N	1:I:162:PRO:CD	2.66	0.59
1:K:63:PHE:CE2	1:K:109:PHE:HB2	2.38	0.59
1:Q:382:VAL:O	1:Q:386:LEU:HB2	2.03	0.59
1:S:211:VAL:HG12	1:S:273:PHE:CD2	2.38	0.59
1:S:321:ILE:HD11	1:S:389:PHE:CE2	2.38	0.59
1:T:161:THR:N	1:T:162:PRO:CD	2.65	0.59
1:U:66:ALA:HB2	1:U:409:LEU:HD11	1.84	0.59
1:A:239:ILE:CD1	1:A:242:GLU:HG2	2.32	0.59
1:E:256:TYR:CD2	1:E:301:LEU:HD12	2.38	0.59
1:D:228:VAL:CG1	1:D:232:ILE:HD11	2.29	0.59
1:F:301:LEU:O	1:F:304:ARG:HG2	2.02	0.59
1:H:60:PHE:CE2	1:H:64:LEU:HD11	2.38	0.59
1:K:290:VAL:HG23	1:K:294:LYS:HG2	1.83	0.59
1:K:305:LEU:H	1:K:305:LEU:HD23	1.66	0.59
1:N:374:VAL:HG11	1:N:382:VAL:HG11	1.85	0.59
1:R:63:PHE:CE2	1:R:109:PHE:HB2	2.37	0.59
1:T:299:TRP:CD1	1:T:311:ILE:HG23	2.38	0.59
1:T:321:ILE:HG22	1:T:325:LEU:HD23	1.84	0.59
1:W:81:PHE:CE2	1:W:86:ILE:HD11	2.38	0.59
1:W:261:THR:HG22	1:W:261:THR:O	2.02	0.59
1:X:161:THR:N	1:X:162:PRO:CD	2.65	0.59
1:A:174:SER:HB2	1:E:160:ASP:OD2	2.03	0.58
1:A:206:ASP:OD1	1:A:207:GLY:N	2.35	0.58
1:A:379:ASP:OD2	1:A:421:LEU:HB2	2.02	0.58
1:F:239:ILE:CD1	1:F:242:GLU:HG2	2.32	0.58
1:H:259:GLU:OE2	1:H:304:ARG:NH1	2.36	0.58
1:H:321:ILE:HD11	1:H:389:PHE:CZ	2.38	0.58
1:K:70:GLY:HA3	1:K:73:GLN:HE22	1.66	0.58
1:L:250:PHE:O	1:L:253:ILE:N	2.36	0.58
1:P:204:ASN:HB2	1:P:205:PRO:HD2	1.85	0.58
1:P:282:LYS:HD2	1:P:356:ASN:HD21	1.67	0.58
1:Q:42:HIS:HB2	1:T:79:PHE:HE2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:105:LEU:CD1	1:R:107:ILE:HG22	2.33	0.58
1:C:115:LYS:HG2	1:C:395:TRP:NE1	2.19	0.58
1:V:161:THR:N	1:V:162:PRO:CD	2.66	0.58
1:E:140:ASN:OD1	1:E:143:PRO:HG2	2.02	0.58
1:G:261:THR:HG22	1:G:261:THR:O	2.03	0.58
1:B:282:LYS:HE3	1:B:284:TYR:OH	2.02	0.58
1:F:105:LEU:HD12	1:F:107:ILE:H	1.68	0.58
1:H:282:LYS:HE3	1:H:284:TYR:OH	2.03	0.58
1:N:321:ILE:HG22	1:N:325:LEU:CD2	2.33	0.58
1:O:390:TRP:CB	1:O:399:ALA:HB2	2.25	0.58
1:P:60:PHE:HE1	1:P:123:ILE:HD11	1.67	0.58
1:Q:60:PHE:CE1	1:Q:123:ILE:HD11	2.38	0.58
1:S:81:PHE:CE2	1:S:86:ILE:HD11	2.38	0.58
1:U:239:ILE:HA	1:U:242:GLU:HB3	1.85	0.58
1:C:261:THR:O	1:C:261:THR:HG22	2.03	0.58
1:A:253:ILE:HD12	1:A:359:ILE:HD11	1.85	0.58
1:V:406:LEU:HD12	1:V:415:ILE:HD13	1.85	0.58
1:G:112:ASN:HD22	1:G:122:ARG:HH21	1.48	0.58
1:B:204:ASN:HB2	1:B:205:PRO:HD2	1.85	0.58
1:D:85:LEU:HB3	1:D:125:PHE:CE1	2.37	0.58
1:D:174:SER:HB2	1:H:160:ASP:OD2	2.03	0.58
1:F:318:LEU:HD12	1:F:427:TYR:CD2	2.37	0.58
1:H:239:ILE:CD1	1:H:242:GLU:HG2	2.33	0.58
1:P:290:VAL:HG23	1:P:294:LYS:HG2	1.85	0.58
1:S:63:PHE:CE2	1:S:109:PHE:HB2	2.38	0.58
1:S:161:THR:N	1:S:162:PRO:CD	2.66	0.58
1:U:41:TYR:HH	1:X:208:ALA:HA	1.67	0.58
1:W:52:TRP:CE3	1:W:89:LEU:HD13	2.37	0.58
1:W:161:THR:N	1:W:162:PRO:CD	2.66	0.58
1:C:255:ASP:O	1:C:259:GLU:HG3	2.03	0.58
1:A:295:ILE:HG23	1:A:370:PHE:HE2	1.69	0.58
1:A:405:THR:O	1:A:409:LEU:HD13	2.02	0.58
1:V:115:LYS:HE2	1:V:435:VAL:H	1.67	0.58
1:E:105:LEU:HD12	1:E:107:ILE:H	1.68	0.58
1:G:99:THR:HG23	1:G:193:LEU:CD2	2.29	0.58
1:G:239:ILE:HD12	1:G:242:GLU:CG	2.31	0.58
1:D:41:TYR:CZ	1:F:209:ILE:HD12	2.39	0.58
1:I:410:TYR:CD1	1:I:421:LEU:HD22	2.39	0.58
1:K:369:LYS:NZ	3:K:502:DST:O4	2.36	0.58
1:L:321:ILE:HG22	1:L:325:LEU:HD23	1.85	0.58
1:M:290:VAL:HG11	1:M:353:ILE:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:311:ILE:H	1:M:311:ILE:HD12	1.68	0.58
1:U:161:THR:N	1:U:162:PRO:HD3	2.17	0.58
1:U:320:GLN:HE22	1:U:392:SER:HB3	1.69	0.58
1:W:171:PHE:HE1	1:W:231:LEU:HD13	1.67	0.58
1:W:204:ASN:HB2	1:W:205:PRO:HD2	1.85	0.58
1:C:167:LEU:O	1:C:171:PHE:HD2	1.85	0.58
1:C:356:ASN:HB3	1:C:369:LYS:HB3	1.85	0.58
1:E:324:LEU:HB3	1:E:385:ALA:HB1	1.86	0.58
1:G:321:ILE:HG22	1:G:325:LEU:HD23	1.86	0.58
1:G:430:THR:HG22	1:G:432:LYS:N	2.18	0.58
1:D:174:SER:HB3	1:H:162:PRO:HG2	1.84	0.58
1:D:386:LEU:HD13	1:D:390:TRP:NE1	2.18	0.58
1:I:42:HIS:HB2	1:L:79:PHE:CE2	2.38	0.58
1:O:292:TRP:CZ2	1:O:315:LEU:HD21	2.38	0.58
1:P:288:THR:HG23	1:P:289:GLU:H	1.68	0.58
1:Q:234:GLU:OE2	1:Q:237:ARG:NH2	2.36	0.58
1:U:160:ASP:OD2	1:W:174:SER:HB2	2.03	0.58
1:U:256:TYR:CD2	1:U:301:LEU:HD12	2.38	0.58
1:U:424:TRP:HB2	1:U:440:TYR:CD2	2.38	0.58
1:A:51:ARG:HD3	1:A:92:TYR:CD2	2.38	0.58
1:A:308:GLU:HB2	1:A:311:ILE:HD13	1.85	0.58
1:G:108:GLU:HA	1:G:443:SER:CB	2.33	0.58
1:D:208:ALA:HA	1:F:41:TYR:OH	2.04	0.58
1:F:85:LEU:HB3	1:F:125:PHE:HE1	1.69	0.58
1:F:428:SER:HB3	1:F:436:TYR:CB	2.32	0.58
1:H:126:GLU:OE2	1:H:195:SER:HB2	2.03	0.58
1:K:321:ILE:HG22	1:K:325:LEU:HD23	1.86	0.58
1:M:66:ALA:HB2	1:M:409:LEU:HD11	1.85	0.58
1:P:83:HIS:O	1:P:87:PRO:HG2	2.04	0.58
1:U:75:TYR:HD2	1:X:75:TYR:CD2	2.15	0.58
1:U:390:TRP:CB	1:U:399:ALA:HB2	2.32	0.58
1:W:288:THR:HG23	1:W:289:GLU:H	1.66	0.58
1:X:211:VAL:HG12	1:X:273:PHE:CD2	2.38	0.58
1:C:162:PRO:HG2	1:G:174:SER:HB3	1.85	0.58
1:A:115:LYS:HG2	1:A:395:TRP:HE1	1.68	0.58
1:V:85:LEU:HD22	1:V:125:PHE:CE1	2.38	0.58
1:V:370:PHE:O	1:V:426:SER:HA	2.04	0.58
1:V:440:TYR:OH	3:V:502:DST:O7	2.18	0.58
1:G:292:TRP:CH2	1:G:319:LYS:HB2	2.39	0.58
1:D:360:HIS:ND1	1:D:361:PRO:HD2	2.18	0.58
1:D:405:THR:O	1:D:409:LEU:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:360:HIS:ND1	1:H:361:PRO:HD2	2.19	0.58
1:O:204:ASN:HB2	1:O:205:PRO:HD2	1.86	0.58
1:Q:115:LYS:HG2	1:Q:395:TRP:NE1	2.18	0.58
1:Q:174:SER:HB2	1:S:160:ASP:OD2	2.03	0.58
1:T:261:THR:HG22	1:T:261:THR:O	2.04	0.58
1:C:204:ASN:HB2	1:C:205:PRO:HD2	1.85	0.58
1:C:270:SER:HB3	1:C:282:LYS:HB2	1.86	0.58
1:C:374:VAL:HG11	1:C:422:GLN:HG2	1.85	0.58
1:A:307:GLU:OE1	1:I:364:ARG:HD2	2.03	0.58
1:V:85:LEU:HB3	1:V:125:PHE:CE1	2.37	0.58
1:G:266:TYR:CD1	2:G:501:QRP:HAHA	2.39	0.58
1:F:426:SER:OG	1:F:438:SER:HB2	2.03	0.58
1:M:41:TYR:CZ	1:P:209:ILE:HD12	2.38	0.58
1:M:161:THR:N	1:M:162:PRO:HD3	2.18	0.58
1:M:320:GLN:HE22	1:M:392:SER:HB3	1.68	0.58
1:O:228:VAL:CG1	1:O:232:ILE:HD11	2.31	0.58
1:P:428:SER:HB3	1:P:436:TYR:CB	2.32	0.58
1:Q:85:LEU:HB3	1:Q:125:PHE:CE1	2.38	0.58
1:T:288:THR:HG23	1:T:289:GLU:H	1.68	0.58
1:W:321:ILE:HD11	1:W:389:PHE:CE2	2.38	0.58
1:C:318:LEU:HD12	1:C:427:TYR:CD2	2.38	0.58
1:A:161:THR:N	1:A:162:PRO:CD	2.67	0.58
1:E:288:THR:HG23	1:E:289:GLU:H	1.68	0.58
1:G:227:PRO:O	1:G:230:THR:OG1	2.19	0.58
1:G:292:TRP:HZ2	1:G:315:LEU:HD21	1.69	0.58
1:B:142:ILE:HB	1:B:143:PRO:HD3	1.86	0.58
1:B:173:LEU:HD13	1:B:196:GLN:NE2	2.19	0.58
1:B:237:ARG:HA	1:B:240:ASP:OD2	2.03	0.58
1:I:200:GLY:N	1:I:212:LYS:O	2.37	0.58
1:N:105:LEU:CD1	1:N:107:ILE:HG22	2.33	0.58
1:N:305:LEU:HD23	1:N:305:LEU:H	1.68	0.58
1:Q:161:THR:H	1:Q:162:PRO:HD3	1.69	0.58
1:R:85:LEU:HD22	1:R:125:PHE:CE1	2.39	0.58
1:R:161:THR:N	1:R:162:PRO:HD3	2.19	0.58
1:R:173:LEU:HD12	1:R:173:LEU:N	2.17	0.58
1:W:140:ASN:OD1	1:W:143:PRO:HG2	2.03	0.58
1:X:52:TRP:CE3	1:X:89:LEU:HD13	2.39	0.58
1:X:390:TRP:HB2	1:X:399:ALA:CB	2.25	0.58
1:C:239:ILE:HD12	1:C:242:GLU:CG	2.34	0.58
1:V:42:HIS:HB2	1:W:79:PHE:HE2	1.67	0.58
1:V:142:ILE:HB	1:V:143:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:261:THR:O	1:V:261:THR:HG22	2.03	0.58
1:D:167:LEU:O	1:D:171:PHE:HD2	1.86	0.58
1:I:162:PRO:HG2	1:K:174:SER:HB3	1.86	0.58
1:M:171:PHE:CE1	1:M:217:PRO:HB3	2.39	0.58
1:N:161:THR:N	1:N:162:PRO:CD	2.67	0.58
1:O:321:ILE:HD13	1:O:437:MET:HE2	1.86	0.58
1:P:206:ASP:OD1	1:P:207:GLY:N	2.37	0.58
1:P:305:LEU:CD1	1:P:311:ILE:HG12	2.34	0.58
1:S:288:THR:HG23	1:S:289:GLU:H	1.67	0.58
1:S:360:HIS:ND1	1:S:361:PRO:HD2	2.19	0.58
1:W:66:ALA:HB2	1:W:409:LEU:HD11	1.85	0.58
1:X:147:LEU:HD23	1:X:199:PHE:HD2	1.68	0.58
1:C:161:THR:H	1:C:162:PRO:HD3	1.69	0.57
1:A:212:LYS:NZ	3:A:502:DST:O4	2.37	0.57
1:E:398:HIS:H	1:E:398:HIS:CD2	2.22	0.57
1:G:299:TRP:CD1	1:G:311:ILE:HG23	2.39	0.57
1:G:415:ILE:HA	1:G:418:THR:CG2	2.34	0.57
1:D:395:TRP:HB3	1:D:398:HIS:HD2	1.68	0.57
1:F:83:HIS:O	1:F:87:PRO:HG2	2.04	0.57
1:F:89:LEU:HD22	1:F:106:PRO:HG2	1.86	0.57
1:I:228:VAL:CG1	1:I:232:ILE:HD11	2.33	0.57
1:L:303:GLY:O	1:L:306:ILE:HG13	2.04	0.57
1:N:261:THR:O	1:N:261:THR:HG22	2.04	0.57
1:O:171:PHE:CE1	1:O:217:PRO:HB3	2.38	0.57
1:P:105:LEU:HD12	1:P:107:ILE:H	1.69	0.57
1:P:382:VAL:O	1:P:386:LEU:HB2	2.04	0.57
1:Q:70:GLY:HA3	1:Q:73:GLN:HE22	1.68	0.57
1:S:115:LYS:HG2	1:S:395:TRP:NE1	2.19	0.57
1:S:127:PRO:HG3	1:S:147:LEU:HD23	1.86	0.57
1:W:256:TYR:CD2	1:W:301:LEU:HD12	2.39	0.57
1:V:387:ALA:HA	1:V:390:TRP:CD1	2.38	0.57
1:D:45:PRO:HD2	1:D:49:GLN:OE1	2.04	0.57
1:H:306:ILE:CD1	1:H:307:GLU:HG3	2.33	0.57
1:I:415:ILE:HA	1:I:418:THR:CG2	2.33	0.57
1:I:426:SER:O	1:I:437:MET:HG3	2.04	0.57
1:J:79:PHE:CE2	1:K:42:HIS:HB2	2.39	0.57
1:N:206:ASP:OD1	1:N:207:GLY:N	2.37	0.57
1:P:85:LEU:HB3	1:P:125:PHE:CE1	2.38	0.57
1:P:161:THR:N	1:P:162:PRO:CD	2.66	0.57
1:W:356:ASN:HB3	1:W:369:LYS:HB3	1.85	0.57
1:C:290:VAL:HG23	1:C:294:LYS:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:THR:N	1:E:162:PRO:CD	2.67	0.57
1:G:161:THR:N	1:G:162:PRO:HD3	2.19	0.57
1:G:288:THR:HG23	1:G:289:GLU:H	1.68	0.57
1:F:420:ARG:HB2	1:F:447:TYR:CZ	2.39	0.57
1:J:354:ILE:HG21	3:J:502:DST:H132	1.86	0.57
1:L:63:PHE:CE2	1:L:109:PHE:HB2	2.39	0.57
1:M:266:TYR:CD1	2:M:501:QRP:HAHA	2.39	0.57
1:S:226:VAL:HG12	1:S:230:THR:OG1	2.05	0.57
1:U:321:ILE:HD11	1:U:389:PHE:CE2	2.39	0.57
1:C:211:VAL:HG12	1:C:273:PHE:CD2	2.39	0.57
1:C:324:LEU:O	1:C:327:ILE:HG22	2.05	0.57
1:A:115:LYS:HE2	1:A:434:GLY:HA3	1.85	0.57
1:B:41:TYR:CZ	1:H:209:ILE:HD12	2.39	0.57
1:D:323:SER:O	1:D:327:ILE:HB	2.04	0.57
1:H:266:TYR:HD1	2:H:501:QRP:HAHA	1.69	0.57
1:I:48:ASP:CG	1:I:91:PRO:HA	2.24	0.57
1:K:282:LYS:HE3	1:K:284:TYR:OH	2.04	0.57
1:K:288:THR:HG23	1:K:289:GLU:H	1.69	0.57
1:L:63:PHE:CE1	1:L:409:LEU:HD23	2.39	0.57
1:L:374:VAL:HG11	1:L:422:GLN:HG3	1.86	0.57
1:N:63:PHE:CE2	1:N:109:PHE:HB2	2.40	0.57
1:P:173:LEU:HD13	1:P:196:GLN:NE2	2.19	0.57
1:P:426:SER:OG	1:P:438:SER:HB2	2.04	0.57
1:S:173:LEU:HD13	1:S:196:GLN:NE2	2.17	0.57
1:T:161:THR:H	1:T:162:PRO:HD3	1.70	0.57
1:T:290:VAL:HG23	1:T:294:LYS:HG2	1.87	0.57
1:T:430:THR:HG22	1:T:432:LYS:H	1.69	0.57
1:W:105:LEU:CD1	1:W:107:ILE:HG22	2.34	0.57
1:A:154:LEU:HB3	1:A:156:LEU:CD1	2.34	0.57
1:A:282:LYS:HE3	1:A:284:TYR:OH	2.04	0.57
1:A:354:ILE:HG21	3:A:502:DST:H132	1.87	0.57
1:E:305:LEU:CD1	1:E:311:ILE:HG12	2.34	0.57
1:G:311:ILE:H	1:G:311:ILE:HD12	1.70	0.57
1:B:282:LYS:HD2	1:B:356:ASN:HD21	1.68	0.57
1:B:395:TRP:HB3	1:B:398:HIS:CG	2.39	0.57
1:D:275:GLU:HB2	1:H:175:LEU:HD21	1.86	0.57
1:H:278:GLU:N	1:H:278:GLU:OE1	2.36	0.57
1:I:173:LEU:HD13	1:I:196:GLN:HE22	1.70	0.57
1:I:398:HIS:CD2	1:I:398:HIS:H	2.22	0.57
1:J:292:TRP:CZ2	1:J:315:LEU:HD21	2.39	0.57
1:K:420:ARG:HB2	1:K:447:TYR:CZ	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:288:THR:HG23	1:N:289:GLU:N	2.19	0.57
1:P:137:ASP:OD2	1:P:142:ILE:HG12	2.05	0.57
1:R:382:VAL:O	1:R:386:LEU:HB2	2.04	0.57
1:S:173:LEU:CD1	1:S:196:GLN:HE22	2.14	0.57
1:S:266:TYR:CD1	2:S:501:QRP:HAHA	2.39	0.57
1:X:83:HIS:O	1:X:87:PRO:HG2	2.04	0.57
1:C:299:TRP:CD1	1:C:311:ILE:HG23	2.40	0.57
1:D:387:ALA:HA	1:D:390:TRP:HD1	1.70	0.57
1:F:320:GLN:HE22	1:F:392:SER:CB	2.17	0.57
1:I:292:TRP:CZ2	1:I:315:LEU:HD21	2.39	0.57
1:J:174:SER:HB2	1:L:160:ASP:OD2	2.05	0.57
1:K:269:LEU:HD12	1:K:282:LYS:O	2.04	0.57
1:N:269:LEU:CD1	1:N:283:ILE:HG13	2.34	0.57
1:O:171:PHE:HE1	1:O:231:LEU:HD13	1.68	0.57
1:R:320:GLN:HE22	1:R:392:SER:HB3	1.68	0.57
1:R:369:LYS:HA	1:R:427:TYR:O	2.04	0.57
1:S:317:ARG:HB2	1:S:427:TYR:OH	2.04	0.57
1:S:321:ILE:HD11	1:S:389:PHE:CZ	2.39	0.57
1:U:303:GLY:O	1:U:306:ILE:HG13	2.03	0.57
1:C:85:LEU:HD22	1:C:125:PHE:CE1	2.40	0.57
1:A:110:SER:O	1:A:121:LEU:HD12	2.05	0.57
1:E:306:ILE:HD12	1:E:307:GLU:N	2.20	0.57
1:E:382:VAL:O	1:E:386:LEU:HB2	2.05	0.57
1:I:250:PHE:O	1:I:253:ILE:N	2.38	0.57
1:J:305:LEU:HD23	1:J:305:LEU:H	1.69	0.57
1:L:228:VAL:O	1:L:232:ILE:HG13	2.04	0.57
1:L:387:ALA:HA	1:L:390:TRP:HD1	1.68	0.57
1:M:63:PHE:CE2	1:M:109:PHE:HB2	2.39	0.57
1:M:415:ILE:HA	1:M:418:THR:CG2	2.34	0.57
1:O:299:TRP:CD1	1:O:311:ILE:HG23	2.39	0.57
1:P:63:PHE:CE2	1:P:109:PHE:HB2	2.40	0.57
1:T:63:PHE:HE2	1:T:109:PHE:HB2	1.69	0.57
1:U:83:HIS:O	1:U:87:PRO:HG2	2.05	0.57
1:U:147:LEU:HD23	1:U:199:PHE:HD2	1.69	0.57
1:W:127:PRO:HG3	1:W:147:LEU:CD2	2.35	0.57
1:X:239:ILE:CD1	1:X:242:GLU:HG2	2.34	0.57
1:C:239:ILE:CD1	1:C:242:GLU:HG2	2.34	0.57
1:C:407:GLN:NE2	1:C:413:GLN:O	2.30	0.57
1:E:173:LEU:HD13	1:E:196:GLN:NE2	2.19	0.57
1:D:112:ASN:ND2	1:D:122:ARG:HH21	2.00	0.57
1:H:142:ILE:HB	1:H:143:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:418:THR:OG1	1:K:421:LEU:HG	2.04	0.57
1:M:370:PHE:O	1:M:426:SER:HA	2.04	0.57
1:N:318:LEU:HD12	1:N:427:TYR:CD2	2.39	0.57
1:N:321:ILE:O	1:N:325:LEU:HD23	2.03	0.57
1:P:360:HIS:ND1	1:P:361:PRO:HD2	2.20	0.57
1:S:239:ILE:CD1	1:S:242:GLU:HG2	2.34	0.57
1:U:115:LYS:HG2	1:U:395:TRP:HE1	1.67	0.57
1:U:305:LEU:CD1	1:U:311:ILE:HG12	2.35	0.57
1:W:389:PHE:HE2	1:W:437:MET:HE3	1.69	0.57
1:A:180:GLN:NE2	1:A:223:ALA:CB	2.68	0.57
1:D:369:LYS:HA	1:D:427:TYR:O	2.05	0.57
1:H:83:HIS:O	1:H:87:PRO:HG2	2.05	0.57
1:H:110:SER:HB2	1:H:122:ARG:CB	2.14	0.57
1:I:282:LYS:HE3	1:I:284:TYR:OH	2.05	0.57
1:J:288:THR:HG23	1:J:289:GLU:H	1.69	0.57
1:O:305:LEU:HD23	1:O:305:LEU:H	1.69	0.57
1:R:115:LYS:HG2	1:R:395:TRP:NE1	2.20	0.57
1:C:275:GLU:CD	1:G:175:LEU:HD11	2.24	0.57
1:A:370:PHE:O	1:A:426:SER:HA	2.04	0.57
1:V:173:LEU:HD13	1:V:196:GLN:NE2	2.20	0.57
1:E:389:PHE:CE2	1:E:437:MET:HE1	2.40	0.57
1:G:354:ILE:HB	1:G:371:TYR:HB2	1.87	0.57
1:M:161:THR:N	1:M:162:PRO:CD	2.68	0.57
1:Q:154:LEU:HB3	1:Q:156:LEU:CD1	2.35	0.57
1:Q:305:LEU:HD12	1:Q:311:ILE:CD1	2.35	0.57
1:T:212:LYS:NZ	3:T:502:DST:O5	2.38	0.57
1:U:51:ARG:HB3	1:U:92:TYR:CG	2.39	0.57
1:X:108:GLU:HA	1:X:443:SER:CB	2.35	0.57
1:X:161:THR:H	1:X:162:PRO:HD3	1.70	0.57
1:A:52:TRP:CE3	1:A:89:LEU:HD13	2.40	0.56
1:V:42:HIS:HB2	1:W:79:PHE:CE2	2.39	0.56
1:I:261:THR:HG22	1:I:261:THR:O	2.05	0.56
1:I:321:ILE:HG22	1:I:325:LEU:HD23	1.87	0.56
1:J:321:ILE:HG22	1:J:325:LEU:HD23	1.87	0.56
1:N:379:ASP:HB2	1:N:418:THR:HG23	1.86	0.56
1:Q:162:PRO:HA	1:S:172:GLN:OE1	2.05	0.56
1:R:115:LYS:HA	1:R:395:TRP:CE2	2.39	0.56
1:R:221:ALA:HB2	1:R:231:LEU:HD21	1.87	0.56
1:S:51:ARG:HD3	1:S:92:TYR:CD2	2.40	0.56
1:W:142:ILE:HB	1:W:143:PRO:HD3	1.87	0.56
1:X:389:PHE:HE2	1:X:437:MET:HE3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:TYR:CD2	1:C:301:LEU:HD12	2.40	0.56
1:A:142:ILE:HB	1:A:143:PRO:HD3	1.87	0.56
1:V:95:LYS:NZ	1:U:47:ASN:HD22	2.02	0.56
1:V:172:GLN:NE2	1:X:165:GLN:HG3	2.11	0.56
1:G:161:THR:N	1:G:162:PRO:CD	2.68	0.56
1:J:105:LEU:HD12	1:J:107:ILE:H	1.70	0.56
1:K:320:GLN:HB2	1:Q:312:ILE:HG21	1.85	0.56
1:L:311:ILE:H	1:L:311:ILE:HD12	1.69	0.56
1:N:85:LEU:HB3	1:N:125:PHE:CE1	2.38	0.56
1:N:115:LYS:HG2	1:N:395:TRP:NE1	2.20	0.56
1:O:285:GLY:O	1:O:354:ILE:HG23	2.04	0.56
1:V:115:LYS:HG2	1:V:395:TRP:NE1	2.19	0.56
1:V:204:ASN:HB2	1:V:205:PRO:HD2	1.85	0.56
1:G:204:ASN:HB2	1:G:205:PRO:HD2	1.88	0.56
1:G:234:GLU:OE2	1:G:237:ARG:NH2	2.38	0.56
1:G:354:ILE:HG21	3:G:502:DST:H132	1.88	0.56
1:B:100:ILE:O	2:B:501:QRP:CD1	2.54	0.56
1:B:292:TRP:CZ2	1:B:315:LEU:HD21	2.40	0.56
1:D:266:TYR:CD1	2:D:501:QRP:HAHA	2.40	0.56
1:D:269:LEU:CD1	1:D:283:ILE:HG13	2.36	0.56
1:F:112:ASN:HD22	1:F:122:ARG:HH21	1.53	0.56
1:F:261:THR:HG22	1:F:261:THR:O	2.06	0.56
1:H:261:THR:O	1:H:261:THR:HG22	2.05	0.56
1:H:305:LEU:HD12	1:H:311:ILE:CD1	2.35	0.56
1:J:234:GLU:OE2	1:J:237:ARG:NH2	2.38	0.56
1:J:303:GLY:O	1:J:306:ILE:HG13	2.05	0.56
1:K:115:LYS:HE2	1:K:435:VAL:N	2.21	0.56
1:K:370:PHE:O	1:K:426:SER:HA	2.05	0.56
1:M:52:TRP:CE3	1:M:89:LEU:HD13	2.40	0.56
1:M:162:PRO:HA	1:O:172:GLN:OE1	2.06	0.56
1:M:288:THR:HG23	1:M:289:GLU:H	1.70	0.56
1:N:115:LYS:HG2	1:N:395:TRP:HE1	1.70	0.56
1:O:266:TYR:CD1	2:O:501:QRP:HAHA	2.41	0.56
1:P:70:GLY:HA3	1:P:73:GLN:HE22	1.69	0.56
1:P:261:THR:O	1:P:261:THR:HG22	2.05	0.56
1:Q:386:LEU:HD13	1:Q:390:TRP:NE1	2.21	0.56
1:R:288:THR:HG23	1:R:289:GLU:N	2.19	0.56
1:R:292:TRP:CZ2	1:R:319:LYS:HB2	2.40	0.56
1:S:261:THR:O	1:S:261:THR:HG22	2.04	0.56
1:S:269:LEU:CD1	1:S:283:ILE:HG13	2.36	0.56
1:U:147:LEU:HD23	1:U:199:PHE:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:60:PHE:HE1	1:X:123:ILE:HD11	1.69	0.56
1:X:85:LEU:HB3	1:X:125:PHE:CE1	2.40	0.56
1:X:127:PRO:HG3	1:X:147:LEU:HD23	1.87	0.56
1:X:420:ARG:HB2	1:X:447:TYR:CZ	2.40	0.56
1:A:211:VAL:HG12	1:A:273:PHE:CD2	2.40	0.56
1:A:430:THR:HG22	1:A:432:LYS:H	1.70	0.56
1:E:167:LEU:O	1:E:171:PHE:HD2	1.89	0.56
1:E:323:SER:O	1:E:327:ILE:HB	2.05	0.56
1:G:176:SER:O	1:G:180:GLN:HB2	2.06	0.56
1:B:60:PHE:CE2	1:B:64:LEU:HD11	2.40	0.56
1:B:300:THR:O	1:B:305:LEU:HD23	2.06	0.56
1:B:321:ILE:HD11	1:B:389:PHE:CZ	2.40	0.56
1:F:66:ALA:HB2	1:F:409:LEU:HD11	1.87	0.56
1:I:430:THR:HG22	1:I:432:LYS:H	1.71	0.56
1:J:261:THR:O	1:J:261:THR:HG22	2.05	0.56
1:J:275:GLU:HG3	1:J:278:GLU:OE1	2.06	0.56
1:J:278:GLU:OE1	1:J:278:GLU:N	2.37	0.56
1:J:324:LEU:HB3	1:J:385:ALA:HB1	1.88	0.56
1:L:402:TYR:O	1:L:405:THR:N	2.39	0.56
1:M:115:LYS:HG2	1:M:395:TRP:HE1	1.68	0.56
1:N:282:LYS:HE3	1:N:284:TYR:OH	2.05	0.56
1:P:161:THR:H	1:P:162:PRO:HD3	1.71	0.56
1:P:378:ASN:O	1:P:382:VAL:HG23	2.05	0.56
1:P:406:LEU:HD12	1:P:415:ILE:HD13	1.85	0.56
1:T:433:ARG:HG3	1:T:436:TYR:OH	2.05	0.56
1:U:142:ILE:HB	1:U:143:PRO:HD3	1.88	0.56
1:U:288:THR:HG23	1:U:289:GLU:H	1.69	0.56
1:U:426:SER:OG	1:U:438:SER:HB2	2.05	0.56
1:C:321:ILE:HG22	1:C:325:LEU:CD2	2.36	0.56
1:A:415:ILE:HA	1:A:418:THR:HG22	1.86	0.56
1:F:127:PRO:HG3	1:F:147:LEU:HD23	1.88	0.56
1:F:211:VAL:HG12	1:F:273:PHE:CD2	2.41	0.56
1:F:415:ILE:HA	1:F:418:THR:CG2	2.35	0.56
1:N:98:SER:OG	1:N:126:GLU:OE1	2.10	0.56
1:Q:387:ALA:HA	1:Q:390:TRP:HD1	1.69	0.56
1:X:99:THR:HG23	1:X:193:LEU:CD2	2.28	0.56
1:A:162:PRO:HG2	1:E:174:SER:HB3	1.87	0.56
1:V:305:LEU:HD23	1:V:305:LEU:H	1.69	0.56
1:E:142:ILE:HB	1:E:143:PRO:HD3	1.87	0.56
1:D:162:PRO:HG2	1:H:174:SER:HB3	1.87	0.56
1:I:227:PRO:O	1:I:230:THR:OG1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:228:VAL:HG11	1:I:267:THR:CG2	2.36	0.56
1:I:266:TYR:CD1	2:I:501:QRP:HAHA	2.41	0.56
1:O:120:LEU:HD21	1:O:205:PRO:HD3	1.87	0.56
1:P:448:LEU:HD12	1:P:448:LEU:N	2.21	0.56
1:Q:239:ILE:CD1	1:Q:242:GLU:HG2	2.34	0.56
1:R:208:ALA:HA	1:S:41:TYR:HH	1.71	0.56
1:S:63:PHE:HE2	1:S:109:PHE:HB2	1.71	0.56
1:U:60:PHE:CE1	1:U:123:ILE:HD11	2.40	0.56
1:X:315:LEU:HD23	1:X:315:LEU:O	2.05	0.56
1:C:206:ASP:OD1	1:C:207:GLY:N	2.38	0.56
1:A:239:ILE:HD12	1:A:242:GLU:CG	2.36	0.56
1:B:420:ARG:HB2	1:B:447:TYR:CZ	2.41	0.56
1:D:115:LYS:HG2	1:D:395:TRP:HE1	1.70	0.56
1:J:161:THR:N	1:J:162:PRO:CD	2.68	0.56
1:K:415:ILE:HA	1:K:418:THR:CG2	2.36	0.56
1:K:428:SER:HB3	1:K:436:TYR:CB	2.27	0.56
1:L:292:TRP:CZ2	1:L:319:LYS:HB2	2.40	0.56
1:P:374:VAL:HG11	1:P:382:VAL:HG11	1.88	0.56
1:P:402:TYR:O	1:P:405:THR:N	2.39	0.56
1:Q:137:ASP:OD2	1:Q:142:ILE:HG12	2.06	0.56
1:S:433:ARG:HG3	1:S:436:TYR:CZ	2.41	0.56
1:U:266:TYR:CD1	2:U:501:QRP:HAHA	2.40	0.56
1:U:290:VAL:HG21	1:U:298:MET:HE1	1.88	0.56
1:W:115:LYS:HG2	1:W:395:TRP:HE1	1.71	0.56
1:F:160:ASP:HB3	1:F:162:PRO:HD2	1.88	0.56
1:F:255:ASP:O	1:F:259:GLU:HG3	2.05	0.56
1:I:161:THR:H	1:I:162:PRO:HD3	1.71	0.56
1:I:228:VAL:HG11	1:I:267:THR:HG23	1.86	0.56
1:L:282:LYS:HE3	1:L:284:TYR:OH	2.05	0.56
1:N:63:PHE:HE2	1:N:109:PHE:HB2	1.71	0.56
1:N:161:THR:H	1:N:162:PRO:HD3	1.71	0.56
1:N:212:LYS:NZ	3:N:502:DST:O5	2.39	0.56
1:P:63:PHE:HE2	1:P:109:PHE:HB2	1.70	0.56
1:P:171:PHE:CE1	1:P:231:LEU:HD13	2.41	0.56
1:P:303:GLY:O	1:P:306:ILE:HG13	2.05	0.56
1:R:229:GLY:HA3	1:R:263:TYR:CE2	2.41	0.56
2:R:501:QRP:CD1	3:R:502:DST:H142	2.36	0.56
1:W:51:ARG:HD3	1:W:92:TYR:CD2	2.41	0.56
1:V:115:LYS:HG2	1:V:395:TRP:HE1	1.70	0.56
1:V:374:VAL:HG11	1:V:422:GLN:HG2	1.87	0.56
1:B:382:VAL:O	1:B:386:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:VAL:CG1	1:F:232:ILE:HD11	2.34	0.56
1:H:154:LEU:HB3	1:H:156:LEU:CD1	2.36	0.56
1:H:237:ARG:HA	1:H:240:ASP:OD2	2.06	0.56
1:I:221:ALA:HB2	1:I:231:LEU:HD21	1.87	0.56
1:I:288:THR:HG23	1:I:289:GLU:N	2.21	0.56
1:K:127:PRO:HG3	1:K:147:LEU:HD22	1.87	0.56
1:K:167:LEU:O	1:K:171:PHE:HD2	1.89	0.56
1:L:354:ILE:HB	1:L:371:TYR:HB2	1.87	0.56
1:N:122:ARG:HG2	1:N:202:ASP:OD1	2.05	0.56
1:P:266:TYR:CD1	2:P:501:QRP:HAHA	2.41	0.56
1:C:288:THR:HG23	1:C:289:GLU:N	2.21	0.56
1:E:261:THR:O	1:E:261:THR:HG22	2.05	0.56
1:B:200:GLY:N	1:B:212:LYS:O	2.37	0.56
1:D:288:THR:HG23	1:D:289:GLU:N	2.21	0.56
1:F:253:ILE:HD12	1:F:359:ILE:HD11	1.88	0.56
1:F:266:TYR:CD1	2:F:501:QRP:HAHA	2.41	0.56
1:F:391:ASP:O	1:F:394:GLY:N	2.39	0.56
1:M:126:GLU:OE2	1:M:195:SER:HB2	2.06	0.56
1:M:426:SER:OG	1:M:438:SER:HB2	2.06	0.56
1:N:321:ILE:HD11	1:N:389:PHE:CE2	2.41	0.56
1:O:200:GLY:N	1:O:212:LYS:O	2.36	0.56
1:S:370:PHE:O	1:S:426:SER:HA	2.06	0.56
1:T:63:PHE:CE1	1:T:409:LEU:HD23	2.41	0.56
1:U:261:THR:O	1:U:261:THR:HG22	2.05	0.56
1:G:300:THR:O	1:G:305:LEU:HD23	2.06	0.55
1:B:212:LYS:NZ	3:B:502:DST:O4	2.39	0.55
1:K:161:THR:H	1:K:162:PRO:HD3	1.70	0.55
1:N:228:VAL:O	1:N:232:ILE:HG13	2.05	0.55
1:O:154:LEU:HB2	1:O:156:LEU:HD13	1.88	0.55
1:Q:147:LEU:HD23	1:Q:199:PHE:CD2	2.41	0.55
1:S:259:GLU:OE2	1:S:304:ARG:NH1	2.40	0.55
1:U:161:THR:N	1:U:162:PRO:CD	2.69	0.55
1:W:137:ASP:OD2	1:W:142:ILE:HG12	2.06	0.55
1:A:433:ARG:HG3	1:A:436:TYR:CZ	2.41	0.55
1:G:51:ARG:HB3	1:G:92:TYR:CG	2.41	0.55
1:G:360:HIS:ND1	1:G:361:PRO:HD2	2.22	0.55
1:B:379:ASP:OD1	1:B:422:GLN:HG3	2.06	0.55
1:D:175:LEU:HD11	1:H:275:GLU:CD	2.26	0.55
1:H:137:ASP:OD2	1:H:142:ILE:HG12	2.06	0.55
1:K:239:ILE:HD12	1:K:242:GLU:CG	2.36	0.55
1:M:42:HIS:HB2	1:P:79:PHE:HE2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:390:TRP:CB	1:M:399:ALA:HB2	2.34	0.55
1:N:167:LEU:O	1:N:171:PHE:HD2	1.88	0.55
1:P:211:VAL:HG12	1:P:273:PHE:CD2	2.41	0.55
1:S:305:LEU:H	1:S:305:LEU:HD23	1.71	0.55
1:S:410:TYR:OH	1:S:441:TYR:HB3	2.07	0.55
1:T:295:ILE:HG23	1:T:370:PHE:HE2	1.72	0.55
1:C:79:PHE:CE2	1:E:42:HIS:HB2	2.40	0.55
1:C:290:VAL:HG11	1:C:353:ILE:HG12	1.87	0.55
1:A:261:THR:HG22	1:A:261:THR:O	2.06	0.55
1:V:234:GLU:OE2	1:V:237:ARG:NH2	2.39	0.55
1:V:288:THR:HG23	1:V:289:GLU:N	2.21	0.55
1:E:380:LEU:HB2	1:E:415:ILE:CG2	2.24	0.55
1:D:299:TRP:CD1	1:D:311:ILE:HG23	2.41	0.55
1:F:105:LEU:CD1	1:F:107:ILE:HG22	2.36	0.55
1:H:147:LEU:HD23	1:H:199:PHE:CD2	2.41	0.55
1:J:81:PHE:CE2	1:J:86:ILE:HD11	2.40	0.55
1:K:321:ILE:HD11	1:K:437:MET:HE1	1.88	0.55
1:L:239:ILE:CD1	1:L:242:GLU:HG2	2.36	0.55
1:L:321:ILE:HD11	1:L:389:PHE:CZ	2.42	0.55
1:Q:426:SER:O	1:Q:437:MET:HG3	2.06	0.55
1:S:142:ILE:HB	1:S:143:PRO:HD3	1.89	0.55
1:S:430:THR:HG22	1:S:432:LYS:H	1.72	0.55
1:X:193:LEU:N	1:X:193:LEU:HD12	2.21	0.55
1:C:387:ALA:HA	1:C:390:TRP:HD1	1.68	0.55
1:E:239:ILE:HD12	1:E:242:GLU:CG	2.36	0.55
1:E:253:ILE:HD12	1:E:359:ILE:HD11	1.87	0.55
1:G:161:THR:H	1:G:162:PRO:HD3	1.70	0.55
1:B:321:ILE:CD1	1:B:437:MET:HE1	2.36	0.55
1:B:387:ALA:HA	1:B:390:TRP:HD1	1.70	0.55
1:D:42:HIS:HB2	1:F:79:PHE:HE2	1.70	0.55
1:F:167:LEU:O	1:F:171:PHE:HD2	1.88	0.55
1:H:288:THR:HG23	1:H:289:GLU:H	1.69	0.55
1:H:415:ILE:HA	1:H:418:THR:HG22	1.88	0.55
1:L:51:ARG:HD3	1:L:92:TYR:CD2	2.42	0.55
1:T:84:HIS:NE2	1:T:154:LEU:HD11	2.21	0.55
1:X:360:HIS:ND1	1:X:361:PRO:HD2	2.22	0.55
1:V:105:LEU:CD1	1:V:107:ILE:HG22	2.36	0.55
1:V:239:ILE:HD12	1:V:242:GLU:CG	2.36	0.55
1:B:167:LEU:O	1:B:171:PHE:HD2	1.90	0.55
1:D:275:GLU:HG3	1:D:278:GLU:OE1	2.06	0.55
1:F:448:LEU:HD12	1:F:448:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:433:ARG:HG3	1:J:436:TYR:OH	2.06	0.55
1:L:115:LYS:HE2	1:L:434:GLY:HA3	1.87	0.55
1:O:282:LYS:HE3	1:O:284:TYR:OH	2.06	0.55
1:W:321:ILE:HD11	1:W:437:MET:HE1	1.87	0.55
1:W:321:ILE:HG22	1:W:325:LEU:HD23	1.89	0.55
1:X:51:ARG:HD3	1:X:92:TYR:CD2	2.41	0.55
1:V:430:THR:HG22	1:V:432:LYS:H	1.71	0.55
1:B:299:TRP:NE1	1:B:311:ILE:HG23	2.22	0.55
1:D:374:VAL:CG1	1:D:382:VAL:HG21	2.28	0.55
1:D:382:VAL:O	1:D:386:LEU:HB2	2.06	0.55
1:F:271:CYS:HB2	1:F:279:GLN:NE2	2.22	0.55
1:F:370:PHE:O	1:F:426:SER:HA	2.07	0.55
1:I:389:PHE:HE2	1:I:437:MET:HE3	1.70	0.55
1:I:390:TRP:HB2	1:I:399:ALA:CB	2.24	0.55
1:O:154:LEU:HB3	1:O:156:LEU:CD1	2.37	0.55
1:O:354:ILE:HG21	3:O:502:DST:H132	1.89	0.55
1:P:84:HIS:NE2	1:P:154:LEU:HD11	2.21	0.55
1:S:171:PHE:HE1	1:S:231:LEU:HD13	1.71	0.55
1:X:266:TYR:CD1	2:X:501:QRP:HAHA	2.42	0.55
1:A:51:ARG:HB3	1:A:92:TYR:CG	2.42	0.55
1:A:85:LEU:HD22	1:A:125:PHE:CE1	2.41	0.55
1:A:288:THR:HG23	1:A:289:GLU:N	2.22	0.55
1:V:290:VAL:HG23	1:V:294:LYS:HG2	1.88	0.55
1:E:356:ASN:HB3	1:E:369:LYS:HB3	1.87	0.55
1:D:147:LEU:HD23	1:D:199:PHE:HD2	1.71	0.55
1:H:147:LEU:HD23	1:H:199:PHE:HD2	1.72	0.55
1:K:390:TRP:CB	1:K:399:ALA:HB2	2.28	0.55
1:L:228:VAL:HG11	1:L:267:THR:HG23	1.89	0.55
1:M:81:PHE:CE2	1:M:86:ILE:HD11	2.41	0.55
1:O:407:GLN:OE1	1:O:415:ILE:HG13	2.07	0.55
1:S:70:GLY:HA3	1:S:73:GLN:NE2	2.21	0.55
1:S:415:ILE:HA	1:S:418:THR:CG2	2.36	0.55
1:T:180:GLN:HE21	1:T:180:GLN:HA	1.71	0.55
1:T:180:GLN:HA	1:T:180:GLN:NE2	2.22	0.55
1:T:233:ALA:HA	1:T:250:PHE:CE2	2.41	0.55
1:T:387:ALA:HA	1:T:390:TRP:HD1	1.72	0.55
1:C:51:ARG:HB3	1:C:92:TYR:CG	2.40	0.55
1:A:285:GLY:O	1:A:354:ILE:HG23	2.05	0.55
1:V:253:ILE:CD1	1:V:359:ILE:HD11	2.33	0.55
1:G:206:ASP:OD1	1:G:207:GLY:N	2.39	0.55
1:F:140:ASN:OD1	1:F:143:PRO:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:324:LEU:HB3	1:I:385:ALA:HB1	1.88	0.55
1:J:402:TYR:O	1:J:405:THR:N	2.40	0.55
1:L:229:GLY:HA3	1:L:263:TYR:CE2	2.42	0.55
1:M:70:GLY:HA3	1:M:73:GLN:NE2	2.22	0.55
1:Q:51:ARG:HD3	1:Q:92:TYR:CD2	2.42	0.55
1:Q:229:GLY:HA3	1:Q:263:TYR:CE2	2.42	0.55
1:Q:261:THR:HG22	1:Q:261:THR:O	2.07	0.55
1:Q:360:HIS:ND1	1:Q:361:PRO:HD2	2.22	0.55
1:R:374:VAL:CG1	1:R:382:VAL:HG11	2.36	0.55
1:W:154:LEU:HB2	1:W:156:LEU:HD13	1.88	0.55
1:W:227:PRO:O	1:W:230:THR:OG1	2.24	0.55
1:V:70:GLY:HA3	1:V:73:GLN:NE2	2.21	0.55
1:V:256:TYR:CD2	1:V:301:LEU:HD12	2.41	0.55
1:V:360:HIS:ND1	1:V:361:PRO:HD2	2.21	0.55
1:G:66:ALA:HB2	1:G:409:LEU:HD11	1.89	0.55
1:I:160:ASP:HB3	1:I:162:PRO:HD2	1.89	0.55
1:J:360:HIS:ND1	1:J:361:PRO:HD2	2.21	0.55
1:J:428:SER:HB3	1:J:436:TYR:HB2	1.88	0.55
1:K:95:LYS:HZ1	1:L:47:ASN:HD22	1.53	0.55
1:L:51:ARG:HB3	1:L:92:TYR:CG	2.42	0.55
1:L:206:ASP:OD1	1:L:207:GLY:N	2.39	0.55
1:N:115:LYS:HE2	1:N:435:VAL:N	2.22	0.55
1:Q:180:GLN:NE2	1:Q:223:ALA:HB2	2.22	0.55
1:S:206:ASP:OD1	1:S:207:GLY:N	2.40	0.55
1:T:60:PHE:CE2	1:T:64:LEU:HD11	2.42	0.55
1:W:115:LYS:HE2	1:W:435:VAL:H	1.70	0.55
1:W:285:GLY:O	1:W:354:ILE:HG23	2.07	0.55
1:X:200:GLY:N	1:X:212:LYS:O	2.37	0.55
1:A:237:ARG:HA	1:A:240:ASP:OD2	2.08	0.55
1:E:115:LYS:HG2	1:E:395:TRP:NE1	2.21	0.55
1:B:42:HIS:HB2	1:H:79:PHE:HE2	1.72	0.55
1:B:208:ALA:HA	1:H:41:TYR:OH	2.06	0.55
1:J:306:ILE:HD12	1:J:307:GLU:N	2.22	0.55
1:K:173:LEU:HD13	1:K:196:GLN:HE22	1.71	0.55
1:K:288:THR:HG23	1:K:289:GLU:N	2.21	0.55
1:M:105:LEU:CD1	1:M:107:ILE:HG22	2.37	0.55
1:M:171:PHE:HE1	1:M:231:LEU:HD13	1.72	0.55
1:N:371:TYR:OH	3:N:502:DST:O8	2.16	0.55
1:P:160:ASP:HB3	1:P:162:PRO:HD2	1.89	0.55
1:Q:126:GLU:OE2	1:Q:195:SER:HB2	2.07	0.55
1:S:402:TYR:O	1:S:405:THR:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:406:LEU:HD12	1:T:415:ILE:HD13	1.88	0.55
1:X:369:LYS:HA	1:X:427:TYR:O	2.06	0.55
1:G:250:PHE:O	1:G:253:ILE:N	2.39	0.54
1:B:266:TYR:CD1	2:B:501:QRP:HAHA	2.42	0.54
1:B:306:ILE:HD12	1:B:307:GLU:N	2.22	0.54
1:F:206:ASP:OD1	1:F:207:GLY:N	2.39	0.54
1:I:75:TYR:HE2	1:L:72:PRO:HA	1.72	0.54
1:L:100:ILE:O	2:L:501:QRP:CD1	2.55	0.54
1:O:173:LEU:HD12	1:O:173:LEU:N	2.22	0.54
1:P:301:LEU:HD13	1:P:357:TYR:CE1	2.42	0.54
1:U:81:PHE:CE2	1:U:86:ILE:HD11	2.42	0.54
1:C:370:PHE:O	1:C:426:SER:HA	2.07	0.54
1:A:75:TYR:HD2	1:G:75:TYR:CD2	2.17	0.54
1:A:79:PHE:CE2	1:G:42:HIS:HB2	2.42	0.54
1:A:209:ILE:HD12	1:G:41:TYR:CZ	2.43	0.54
1:E:126:GLU:OE2	1:E:195:SER:HB2	2.06	0.54
1:G:84:HIS:NE2	1:G:154:LEU:HD11	2.21	0.54
1:B:390:TRP:CB	1:B:399:ALA:HB2	2.27	0.54
1:B:395:TRP:HB3	1:B:398:HIS:HD1	1.70	0.54
1:D:228:VAL:O	1:D:232:ILE:HG13	2.07	0.54
1:F:110:SER:HB2	1:F:122:ARG:CB	2.10	0.54
1:F:239:ILE:HD12	1:F:242:GLU:CG	2.36	0.54
1:F:324:LEU:O	1:F:327:ILE:HG22	2.07	0.54
1:H:160:ASP:HB3	1:H:162:PRO:CD	2.37	0.54
1:I:75:TYR:HD2	1:L:75:TYR:CD2	2.15	0.54
1:K:295:ILE:HG23	1:K:370:PHE:HE2	1.73	0.54
1:Q:63:PHE:HE2	1:Q:109:PHE:HB2	1.72	0.54
1:R:239:ILE:HD12	1:R:242:GLU:CG	2.37	0.54
1:T:60:PHE:CE1	1:T:123:ILE:HD11	2.42	0.54
1:X:282:LYS:HD2	1:X:356:ASN:HD21	1.71	0.54
1:A:83:HIS:O	1:A:87:PRO:HG2	2.08	0.54
1:V:359:ILE:O	1:V:359:ILE:HG22	2.07	0.54
1:G:420:ARG:HB2	1:G:447:TYR:CZ	2.39	0.54
1:B:239:ILE:CD1	1:B:242:GLU:HG2	2.36	0.54
1:B:369:LYS:HA	1:B:427:TYR:O	2.07	0.54
1:B:430:THR:HG22	1:B:432:LYS:H	1.72	0.54
1:F:288:THR:HG23	1:F:289:GLU:N	2.23	0.54
1:M:115:LYS:CE	1:M:434:GLY:HA3	2.37	0.54
1:P:239:ILE:HD12	1:P:242:GLU:CG	2.36	0.54
1:P:433:ARG:HG3	1:P:436:TYR:OH	2.06	0.54
1:Q:389:PHE:CE2	1:Q:437:MET:HE3	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:300:THR:HA	1:T:305:LEU:HD21	1.90	0.54
1:W:173:LEU:HD13	1:W:196:GLN:NE2	2.22	0.54
1:X:160:ASP:HB3	1:X:162:PRO:HD2	1.88	0.54
1:C:402:TYR:O	1:C:405:THR:N	2.41	0.54
1:E:266:TYR:CD1	2:E:501:QRP:HAHA	2.42	0.54
1:E:359:ILE:HG22	1:E:359:ILE:O	2.07	0.54
1:G:60:PHE:HE1	1:G:123:ILE:HD11	1.72	0.54
1:F:60:PHE:CE1	1:F:123:ILE:HD11	2.42	0.54
1:F:292:TRP:CZ2	1:F:319:LYS:HB2	2.41	0.54
1:J:426:SER:O	1:J:437:MET:HG3	2.06	0.54
1:K:324:LEU:O	1:K:327:ILE:HG22	2.08	0.54
1:L:154:LEU:HB3	1:L:156:LEU:CD1	2.37	0.54
1:L:173:LEU:HD13	1:L:196:GLN:HE22	1.73	0.54
1:L:288:THR:HG23	1:L:289:GLU:N	2.22	0.54
1:N:321:ILE:HD11	1:N:437:MET:HE1	1.89	0.54
1:O:369:LYS:HA	1:O:427:TYR:O	2.08	0.54
1:P:100:ILE:O	2:P:501:QRP:CD1	2.54	0.54
1:P:288:THR:HG23	1:P:289:GLU:N	2.23	0.54
1:P:311:ILE:HD12	1:P:311:ILE:H	1.72	0.54
1:S:292:TRP:HZ2	1:S:315:LEU:HD21	1.71	0.54
1:U:105:LEU:CD1	1:U:107:ILE:HG22	2.38	0.54
1:W:85:LEU:HB3	1:W:125:PHE:CE1	2.43	0.54
1:W:115:LYS:HG2	1:W:395:TRP:NE1	2.21	0.54
1:C:100:ILE:O	2:C:501:QRP:CD1	2.55	0.54
1:C:282:LYS:HE3	1:C:284:TYR:OH	2.07	0.54
1:A:173:LEU:O	1:A:174:SER:OG	2.10	0.54
1:A:321:ILE:HG22	1:A:325:LEU:CD2	2.36	0.54
1:G:83:HIS:O	1:G:87:PRO:HG2	2.07	0.54
1:G:237:ARG:HA	1:G:240:ASP:OD2	2.07	0.54
1:G:369:LYS:HA	1:G:427:TYR:O	2.07	0.54
1:D:305:LEU:HD23	1:D:305:LEU:H	1.71	0.54
1:J:173:LEU:HD13	1:J:196:GLN:NE2	2.22	0.54
1:K:373:PRO:HG3	1:K:424:TRP:CZ3	2.42	0.54
1:L:379:ASP:OD2	1:L:421:LEU:HB2	2.06	0.54
1:R:108:GLU:HA	1:R:443:SER:OG	2.07	0.54
1:T:209:ILE:C	1:T:210:LEU:HD12	2.28	0.54
1:X:305:LEU:CD1	1:X:311:ILE:HG12	2.38	0.54
1:A:386:LEU:HD13	1:A:390:TRP:HE1	1.73	0.54
1:V:140:ASN:OD1	1:V:143:PRO:HG2	2.08	0.54
1:E:137:ASP:OD2	1:E:142:ILE:HG12	2.07	0.54
1:B:206:ASP:OD1	1:B:207:GLY:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:115:LYS:HG2	1:I:395:TRP:HE1	1.73	0.54
1:L:85:LEU:HD22	1:L:125:PHE:CD1	2.43	0.54
1:L:405:THR:O	1:L:409:LEU:HD13	2.06	0.54
1:N:209:ILE:HD12	1:O:41:TYR:CZ	2.42	0.54
1:N:266:TYR:HD1	2:N:501:QRP:HAHA	1.73	0.54
1:R:321:ILE:HD11	1:R:389:PHE:CE2	2.42	0.54
1:S:354:ILE:HB	1:S:371:TYR:HB2	1.90	0.54
1:T:89:LEU:HD22	1:T:106:PRO:HG2	1.88	0.54
1:X:171:PHE:CE1	1:X:231:LEU:HD13	2.43	0.54
1:X:418:THR:OG1	1:X:421:LEU:HG	2.08	0.54
1:C:115:LYS:HE2	1:C:435:VAL:H	1.72	0.54
1:C:285:GLY:O	1:C:354:ILE:HG23	2.07	0.54
1:E:303:GLY:O	1:E:306:ILE:HG13	2.07	0.54
1:B:255:ASP:O	1:B:259:GLU:HG3	2.08	0.54
2:B:501:QRP:HB	3:B:502:DST:C13	2.38	0.54
1:D:116:GLY:HA2	1:D:398:HIS:NE2	2.21	0.54
1:I:275:GLU:OE1	1:K:175:LEU:HD11	2.07	0.54
1:K:120:LEU:HD21	1:K:205:PRO:HD3	1.90	0.54
1:K:239:ILE:CD1	1:K:242:GLU:HG2	2.37	0.54
1:N:324:LEU:O	1:N:327:ILE:HG22	2.08	0.54
1:P:66:ALA:HB2	1:P:409:LEU:HD11	1.88	0.54
1:P:430:THR:HG22	1:P:432:LYS:H	1.70	0.54
1:Q:415:ILE:HA	1:Q:418:THR:CG2	2.36	0.54
1:S:172:GLN:CA	1:S:173:LEU:HD12	2.37	0.54
1:U:290:VAL:HG23	1:U:294:LYS:CG	2.37	0.54
1:U:373:PRO:HG3	1:U:424:TRP:HZ3	1.73	0.54
1:X:288:THR:HG23	1:X:289:GLU:N	2.23	0.54
1:C:369:LYS:O	1:C:370:PHE:HD1	1.91	0.54
1:C:410:TYR:CD1	1:C:421:LEU:HD22	2.43	0.54
1:A:232:ILE:O	1:A:236:VAL:HG23	2.08	0.54
1:V:41:TYR:CZ	1:W:209:ILE:HD12	2.42	0.54
1:V:224:ALA:O	1:V:226:VAL:HG23	2.07	0.54
1:B:288:THR:HG23	1:B:289:GLU:N	2.23	0.54
1:B:290:VAL:HG23	1:B:294:LYS:HG2	1.88	0.54
1:D:171:PHE:CE1	1:D:217:PRO:HB3	2.42	0.54
1:D:315:LEU:O	1:D:315:LEU:HD23	2.08	0.54
1:H:154:LEU:CB	1:H:156:LEU:HD13	2.38	0.54
1:I:63:PHE:HB3	1:I:121:LEU:HD13	1.90	0.54
1:K:99:THR:HG23	1:K:193:LEU:CD2	2.28	0.54
1:L:407:GLN:NE2	1:L:413:GLN:O	2.35	0.54
1:Q:175:LEU:HD11	1:S:275:GLU:CD	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:402:TYR:CB	1:Q:403:PRO:HD3	2.34	0.54
1:S:239:ILE:HD12	1:S:242:GLU:CG	2.37	0.54
1:T:173:LEU:HD13	1:T:196:GLN:HE22	1.72	0.54
1:T:229:GLY:HA3	1:T:263:TYR:CE2	2.43	0.54
1:X:321:ILE:HD11	1:X:389:PHE:CE2	2.43	0.54
1:X:420:ARG:HH12	1:X:448:LEU:HB2	1.72	0.54
1:C:321:ILE:CD1	1:C:437:MET:HE1	2.38	0.54
1:A:85:LEU:HB3	1:A:125:PHE:CE1	2.43	0.54
1:E:127:PRO:HG3	1:E:147:LEU:CD2	2.38	0.54
1:D:430:THR:HG22	1:D:432:LYS:H	1.72	0.54
1:F:231:LEU:HD12	1:F:232:ILE:N	2.23	0.54
1:H:250:PHE:O	1:H:253:ILE:N	2.41	0.54
1:I:174:SER:HB3	1:K:162:PRO:HG2	1.90	0.54
1:I:306:ILE:HD12	1:I:307:GLU:N	2.23	0.54
1:M:369:LYS:HA	1:M:427:TYR:O	2.07	0.54
1:P:420:ARG:HB2	1:P:447:TYR:CZ	2.42	0.54
1:S:382:VAL:O	1:S:386:LEU:HB2	2.08	0.54
1:T:228:VAL:O	1:T:232:ILE:HG13	2.08	0.54
1:T:239:ILE:HD12	1:T:242:GLU:CG	2.38	0.54
1:T:288:THR:HG23	1:T:289:GLU:N	2.23	0.54
1:X:303:GLY:O	1:X:306:ILE:HG13	2.08	0.54
1:A:160:ASP:OD2	1:E:174:SER:HB2	2.08	0.54
1:A:163:PHE:CD2	1:A:279:GLN:NE2	2.76	0.54
1:A:228:VAL:CG1	1:A:232:ILE:HD11	2.37	0.54
1:V:321:ILE:HG12	1:V:389:PHE:CD1	2.43	0.54
1:E:305:LEU:HD23	1:E:305:LEU:H	1.71	0.54
1:E:426:SER:OG	1:E:438:SER:HB2	2.07	0.54
1:G:390:TRP:HB2	1:G:399:ALA:CB	2.26	0.54
1:B:89:LEU:HD22	1:B:106:PRO:HG2	1.90	0.54
1:D:86:ILE:HB	1:D:87:PRO:HD3	1.91	0.54
1:F:360:HIS:ND1	1:F:361:PRO:HD2	2.23	0.54
1:H:228:VAL:O	1:H:232:ILE:HG13	2.07	0.54
1:K:117:SER:O	1:K:118:HIS:HB3	2.07	0.54
1:M:321:ILE:CD1	1:M:437:MET:HE2	2.38	0.54
1:M:360:HIS:ND1	1:M:361:PRO:HD2	2.23	0.54
1:O:370:PHE:O	1:O:426:SER:HA	2.08	0.54
1:P:239:ILE:CD1	1:P:242:GLU:HG2	2.37	0.54
1:Q:99:THR:HG23	1:Q:193:LEU:CD2	2.32	0.54
1:T:127:PRO:HD2	1:T:144:ILE:HD13	1.90	0.54
1:W:290:VAL:HG23	1:W:294:LYS:HG2	1.90	0.54
1:A:55:GLU:OE2	1:A:446:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PHE:CE1	1:A:123:ILE:HD11	2.42	0.53
1:D:266:TYR:HD1	2:D:501:QRP:HAHA	1.73	0.53
1:H:321:ILE:CD1	1:H:437:MET:HE1	2.37	0.53
1:I:100:ILE:O	2:I:501:QRP:CD1	2.56	0.53
1:J:433:ARG:HG3	1:J:436:TYR:CZ	2.42	0.53
1:L:292:TRP:CZ2	1:L:315:LEU:HD21	2.43	0.53
1:L:292:TRP:HZ2	1:L:315:LEU:HD21	1.73	0.53
1:M:261:THR:O	1:M:261:THR:HG22	2.08	0.53
1:O:160:ASP:HB3	1:O:162:PRO:HD2	1.90	0.53
1:Q:174:SER:HB3	1:S:162:PRO:HG2	1.90	0.53
1:R:371:TYR:OH	3:R:502:DST:O8	2.09	0.53
1:X:321:ILE:HG22	1:X:325:LEU:CD2	2.37	0.53
1:E:319:LYS:HE3	1:O:309:PRO:CB	2.38	0.53
1:D:426:SER:OG	1:D:438:SER:HB2	2.08	0.53
1:F:212:LYS:HZ3	3:F:502:DST:P1	2.31	0.53
1:H:227:PRO:O	1:H:230:THR:OG1	2.25	0.53
1:I:290:VAL:HG23	1:I:294:LYS:HG2	1.88	0.53
1:J:299:TRP:CD1	1:J:311:ILE:HG23	2.43	0.53
1:J:370:PHE:O	1:J:426:SER:HA	2.08	0.53
1:L:239:ILE:HD12	1:L:242:GLU:CG	2.38	0.53
1:O:212:LYS:NZ	3:O:502:DST:O6	2.42	0.53
1:O:315:LEU:HD23	1:O:315:LEU:O	2.08	0.53
1:R:448:LEU:N	1:R:448:LEU:HD12	2.23	0.53
1:T:374:VAL:HG13	1:T:382:VAL:HG21	1.89	0.53
1:T:433:ARG:HG3	1:T:436:TYR:CZ	2.44	0.53
1:U:85:LEU:HD22	1:U:125:PHE:CE1	2.43	0.53
1:U:211:VAL:HG12	1:U:273:PHE:CD2	2.43	0.53
1:U:308:GLU:HB2	1:U:311:ILE:HD13	1.89	0.53
1:W:373:PRO:HG3	1:W:424:TRP:CZ3	2.43	0.53
1:X:66:ALA:HB2	1:X:409:LEU:HD11	1.88	0.53
1:X:127:PRO:HG3	1:X:147:LEU:CD2	2.38	0.53
1:V:379:ASP:HB2	1:V:418:THR:HG23	1.89	0.53
1:G:200:GLY:N	1:G:212:LYS:O	2.39	0.53
1:H:370:PHE:O	1:H:426:SER:HA	2.08	0.53
1:N:324:LEU:HB3	1:N:385:ALA:HB1	1.90	0.53
1:Q:410:TYR:CD1	1:Q:421:LEU:HD22	2.43	0.53
1:T:108:GLU:HA	1:T:443:SER:OG	2.08	0.53
1:U:108:GLU:HA	1:U:443:SER:CB	2.39	0.53
1:C:420:ARG:HB2	1:C:447:TYR:CZ	2.43	0.53
1:E:154:LEU:HB3	1:E:156:LEU:CD1	2.37	0.53
1:J:51:ARG:HB3	1:J:92:TYR:CG	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:420:ARG:HB2	1:J:447:TYR:CZ	2.44	0.53
1:L:433:ARG:HG3	1:L:436:TYR:CZ	2.43	0.53
1:N:224:ALA:O	1:N:226:VAL:HG23	2.08	0.53
1:O:81:PHE:CE2	1:O:86:ILE:HD11	2.44	0.53
1:O:126:GLU:OE2	1:O:195:SER:HB2	2.09	0.53
1:Q:311:ILE:H	1:Q:311:ILE:HD12	1.73	0.53
1:Q:406:LEU:HD12	1:Q:415:ILE:HD13	1.89	0.53
1:S:321:ILE:HD11	1:S:437:MET:HE1	1.91	0.53
1:C:315:LEU:O	1:C:315:LEU:HD23	2.08	0.53
1:A:167:LEU:O	1:A:171:PHE:HD2	1.90	0.53
1:V:321:ILE:HG22	1:V:325:LEU:CD2	2.38	0.53
1:E:116:GLY:HA2	1:E:398:HIS:NE2	2.22	0.53
1:B:250:PHE:O	1:B:253:ILE:N	2.41	0.53
1:D:173:LEU:O	1:D:174:SER:OG	2.14	0.53
1:J:174:SER:HB3	1:L:162:PRO:HG2	1.89	0.53
1:K:320:GLN:HE22	1:K:392:SER:HB3	1.73	0.53
1:K:448:LEU:HD12	1:K:448:LEU:N	2.22	0.53
1:L:406:LEU:HD12	1:L:415:ILE:HD13	1.90	0.53
1:M:324:LEU:HB3	1:M:385:ALA:HB1	1.89	0.53
1:N:285:GLY:O	1:N:354:ILE:HG23	2.08	0.53
1:N:373:PRO:HG3	1:N:424:TRP:CZ3	2.44	0.53
1:T:110:SER:O	1:T:121:LEU:HD12	2.07	0.53
1:U:42:HIS:HB2	1:X:79:PHE:HE2	1.72	0.53
1:U:321:ILE:HG22	1:U:325:LEU:HD23	1.90	0.53
1:W:161:THR:H	1:W:162:PRO:HD3	1.71	0.53
1:C:60:PHE:CE1	1:C:123:ILE:HD11	2.44	0.53
1:C:321:ILE:HD11	1:C:389:PHE:CE2	2.44	0.53
1:A:161:THR:H	1:A:162:PRO:HD3	1.73	0.53
1:V:63:PHE:CE2	1:V:109:PHE:HB2	2.44	0.53
1:B:137:ASP:OD2	1:B:142:ILE:HG12	2.08	0.53
1:D:147:LEU:HD23	1:D:199:PHE:CD2	2.43	0.53
1:F:63:PHE:CE2	1:F:109:PHE:HB2	2.44	0.53
1:H:239:ILE:HD12	1:H:242:GLU:CG	2.39	0.53
1:J:110:SER:HB2	1:J:122:ARG:CB	2.16	0.53
1:L:430:THR:HG22	1:L:432:LYS:H	1.73	0.53
1:M:249:ALA:HB3	1:M:359:ILE:HG23	1.91	0.53
1:N:290:VAL:HG23	1:N:294:LYS:HG2	1.89	0.53
1:O:386:LEU:CD1	1:O:390:TRP:HE1	2.21	0.53
1:Q:75:TYR:HD2	1:T:75:TYR:CD2	2.12	0.53
1:T:420:ARG:HB2	1:T:447:TYR:CZ	2.42	0.53
1:C:115:LYS:HA	1:C:395:TRP:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:226:VAL:HG12	1:V:230:THR:OG1	2.08	0.53
1:E:115:LYS:HG2	1:E:395:TRP:HE1	1.74	0.53
1:B:70:GLY:HA3	1:B:73:GLN:HE22	1.73	0.53
1:H:318:LEU:HD23	1:H:318:LEU:O	2.08	0.53
1:L:115:LYS:HG2	1:L:395:TRP:CZ2	2.44	0.53
1:L:160:ASP:HB3	1:L:162:PRO:HD2	1.90	0.53
1:N:292:TRP:CZ2	1:N:315:LEU:HD21	2.44	0.53
1:P:84:HIS:CE1	1:P:154:LEU:HD11	2.44	0.53
1:Q:85:LEU:HD22	1:Q:125:PHE:CE1	2.44	0.53
1:R:356:ASN:HB3	1:R:369:LYS:HB3	1.89	0.53
1:T:239:ILE:CD1	1:T:242:GLU:HG2	2.37	0.53
1:U:305:LEU:HD12	1:U:311:ILE:HD11	1.90	0.53
1:W:127:PRO:HG3	1:W:147:LEU:HD23	1.91	0.53
1:C:305:LEU:H	1:C:305:LEU:HD23	1.72	0.53
1:E:85:LEU:HB3	1:E:125:PHE:CE1	2.43	0.53
1:G:256:TYR:CD2	1:G:301:LEU:HD12	2.44	0.53
1:F:295:ILE:HG23	1:F:370:PHE:HE2	1.73	0.53
1:H:237:ARG:O	1:H:240:ASP:HB2	2.08	0.53
1:I:83:HIS:O	1:I:87:PRO:HG2	2.08	0.53
1:K:127:PRO:HG3	1:K:147:LEU:HD23	1.90	0.53
1:M:379:ASP:OD2	1:M:421:LEU:HB2	2.09	0.53
1:N:160:ASP:HB3	1:N:162:PRO:HD2	1.90	0.53
1:O:206:ASP:OD1	1:O:207:GLY:N	2.42	0.53
1:P:60:PHE:CE2	1:P:64:LEU:HD11	2.44	0.53
1:P:115:LYS:HG2	1:P:395:TRP:NE1	2.24	0.53
1:Q:424:TRP:HB2	1:Q:440:TYR:CD2	2.44	0.53
1:T:320:GLN:HE22	1:T:392:SER:HB3	1.74	0.53
1:U:115:LYS:HE2	1:U:435:VAL:H	1.74	0.53
1:W:292:TRP:CZ2	1:W:315:LEU:HD21	2.44	0.53
1:V:448:LEU:HD12	1:V:448:LEU:N	2.24	0.53
1:B:266:TYR:HD1	2:B:501:QRP:HAHA	1.74	0.53
1:F:142:ILE:HB	1:F:143:PRO:HD3	1.91	0.53
1:F:324:LEU:HB3	1:F:385:ALA:HB1	1.91	0.53
1:I:300:THR:HA	1:I:305:LEU:HD21	1.90	0.53
2:I:501:QRP:HB	3:I:502:DST:C13	2.39	0.53
1:J:42:HIS:HB2	1:K:79:PHE:HE2	1.72	0.53
1:J:231:LEU:HD12	1:J:232:ILE:N	2.24	0.53
1:J:427:TYR:HD1	1:J:437:MET:HE2	1.74	0.53
1:P:379:ASP:HB3	1:P:422:GLN:HE21	1.74	0.53
1:Q:448:LEU:HD12	1:Q:448:LEU:N	2.24	0.53
1:S:63:PHE:CE1	1:S:409:LEU:HD23	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:305:LEU:CD1	1:S:311:ILE:HG12	2.38	0.53
1:T:36:GLN:OE1	1:T:58:SER:HA	2.08	0.53
1:T:84:HIS:CE1	1:T:154:LEU:HD11	2.44	0.53
1:T:167:LEU:O	1:T:171:PHE:HD2	1.92	0.53
1:V:317:ARG:HB2	1:V:427:TYR:OH	2.09	0.53
1:D:105:LEU:HD12	1:D:107:ILE:H	1.74	0.53
1:D:127:PRO:HG3	1:D:147:LEU:CD2	2.39	0.53
1:D:268:PHE:CZ	1:D:284:TYR:CD2	2.96	0.53
1:F:317:ARG:HB2	1:F:427:TYR:OH	2.09	0.53
1:J:390:TRP:CB	1:J:399:ALA:HB2	2.30	0.53
1:K:390:TRP:O	1:K:394:GLY:N	2.42	0.53
1:L:420:ARG:HB2	1:L:447:TYR:CZ	2.44	0.53
1:N:41:TYR:OH	1:O:208:ALA:HA	2.09	0.53
1:N:275:GLU:OE1	1:P:175:LEU:HD11	2.09	0.53
1:O:321:ILE:HD11	1:O:437:MET:HE2	1.90	0.53
1:O:415:ILE:HA	1:O:418:THR:CG2	2.39	0.53
1:Q:266:TYR:CD1	2:Q:501:QRP:HAHA	2.43	0.53
1:S:161:THR:H	1:S:162:PRO:HD3	1.73	0.53
1:S:315:LEU:O	1:S:315:LEU:HD23	2.08	0.53
1:U:70:GLY:HA3	1:U:73:GLN:HE22	1.73	0.53
1:W:305:LEU:HD23	1:W:305:LEU:H	1.74	0.53
1:C:229:GLY:HA3	1:C:263:TYR:CE2	2.44	0.52
1:C:295:ILE:HG23	1:C:370:PHE:CE2	2.44	0.52
1:E:160:ASP:HB3	1:E:162:PRO:HD2	1.90	0.52
1:G:386:LEU:CD1	1:G:390:TRP:HE1	2.20	0.52
1:B:116:GLY:N	1:B:398:HIS:CE1	2.57	0.52
1:D:239:ILE:HD12	1:D:242:GLU:CG	2.37	0.52
1:F:127:PRO:HD2	1:F:144:ILE:HD13	1.91	0.52
1:F:292:TRP:HZ2	1:F:315:LEU:HD21	1.75	0.52
1:J:266:TYR:CD1	2:J:501:QRP:HAHA	2.44	0.52
1:L:115:LYS:HG2	1:L:395:TRP:CE2	2.44	0.52
1:L:137:ASP:OD2	1:L:142:ILE:HG12	2.10	0.52
1:L:147:LEU:HD23	1:L:199:PHE:HD2	1.74	0.52
1:Q:147:LEU:HD23	1:Q:199:PHE:HD2	1.73	0.52
1:T:374:VAL:HG11	1:T:382:VAL:HG11	1.91	0.52
1:U:448:LEU:N	1:U:448:LEU:HD12	2.24	0.52
1:W:266:TYR:CD1	2:W:501:QRP:HAHA	2.44	0.52
1:X:105:LEU:CD1	1:X:107:ILE:HG22	2.39	0.52
1:X:115:LYS:HE2	1:X:434:GLY:CA	2.36	0.52
1:C:433:ARG:HG3	1:C:436:TYR:CZ	2.44	0.52
1:E:430:THR:HG22	1:E:432:LYS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:LYS:HG2	1:H:395:TRP:NE1	2.24	0.52
1:K:402:TYR:O	1:K:405:THR:N	2.42	0.52
1:L:115:LYS:HA	1:L:395:TRP:CE2	2.44	0.52
1:M:108:GLU:HA	1:M:443:SER:OG	2.10	0.52
1:O:147:LEU:HD23	1:O:199:PHE:HD2	1.74	0.52
1:O:171:PHE:CE1	1:O:231:LEU:HD13	2.43	0.52
1:O:317:ARG:HB2	1:O:427:TYR:OH	2.08	0.52
1:Q:142:ILE:HB	1:Q:143:PRO:HD3	1.91	0.52
1:R:172:GLN:CA	1:R:173:LEU:HD12	2.40	0.52
1:T:100:ILE:O	2:T:501:QRP:CD1	2.56	0.52
1:U:200:GLY:N	1:U:212:LYS:O	2.41	0.52
1:W:382:VAL:O	1:W:386:LEU:HB2	2.09	0.52
1:X:318:LEU:HD12	1:X:427:TYR:CD2	2.44	0.52
1:C:142:ILE:HB	1:C:143:PRO:HD3	1.90	0.52
1:C:231:LEU:HD12	1:C:232:ILE:N	2.25	0.52
1:A:353:ILE:O	1:A:353:ILE:HG13	2.10	0.52
1:V:147:LEU:HD23	1:V:199:PHE:HD2	1.75	0.52
1:V:167:LEU:O	1:V:171:PHE:HD2	1.92	0.52
1:V:266:TYR:HD1	2:V:501:QRP:HAHA	1.74	0.52
1:E:319:LYS:HE3	1:O:309:PRO:HB2	1.90	0.52
1:F:60:PHE:HE1	1:F:123:ILE:HD11	1.74	0.52
1:F:305:LEU:HD23	1:F:305:LEU:H	1.73	0.52
1:I:315:LEU:O	1:I:315:LEU:HD23	2.09	0.52
1:I:320:GLN:CB	1:I:320:GLN:CD	2.73	0.52
1:L:173:LEU:HD12	1:L:173:LEU:N	2.24	0.52
1:L:424:TRP:HB2	1:L:440:TYR:CD2	2.45	0.52
1:N:266:TYR:CD1	2:N:501:QRP:HAHA	2.45	0.52
1:S:406:LEU:HD12	1:S:415:ILE:HD13	1.90	0.52
1:T:266:TYR:HD1	2:T:501:QRP:HAHA	1.72	0.52
1:U:402:TYR:O	1:U:405:THR:N	2.42	0.52
1:W:105:LEU:HD12	1:W:107:ILE:H	1.74	0.52
1:W:200:GLY:N	1:W:212:LYS:O	2.39	0.52
1:C:212:LYS:NZ	3:C:502:DST:O6	2.43	0.52
1:A:256:TYR:CD2	1:A:301:LEU:HD12	2.45	0.52
1:A:278:GLU:OE1	1:A:278:GLU:N	2.42	0.52
1:E:173:LEU:HD12	1:E:173:LEU:N	2.24	0.52
1:E:354:ILE:HG21	3:E:502:DST:H132	1.92	0.52
1:B:110:SER:HB2	1:B:122:ARG:CB	2.14	0.52
1:B:126:GLU:OE2	1:B:195:SER:HB2	2.10	0.52
1:H:353:ILE:HG13	1:H:353:ILE:O	2.09	0.52
1:I:108:GLU:HA	1:I:443:SER:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:206:ASP:OD1	1:I:207:GLY:N	2.43	0.52
1:I:285:GLY:O	1:I:354:ILE:HG23	2.10	0.52
1:J:120:LEU:HD21	1:J:205:PRO:HD3	1.90	0.52
1:J:359:ILE:HG22	1:J:359:ILE:O	2.09	0.52
1:J:430:THR:HG22	1:J:432:LYS:H	1.74	0.52
1:M:85:LEU:HB3	1:M:125:PHE:CE1	2.43	0.52
1:N:387:ALA:HA	1:N:390:TRP:CD1	2.44	0.52
1:O:239:ILE:HD12	1:O:242:GLU:CG	2.38	0.52
1:O:288:THR:HG23	1:O:289:GLU:N	2.24	0.52
1:P:256:TYR:CD2	1:P:301:LEU:HD12	2.45	0.52
1:R:389:PHE:CE2	1:R:437:MET:HE1	2.44	0.52
1:S:115:LYS:HG2	1:S:395:TRP:CE2	2.45	0.52
1:S:306:ILE:HD12	1:S:307:GLU:N	2.25	0.52
1:W:402:TYR:O	1:W:405:THR:N	2.43	0.52
1:C:428:SER:HB3	1:C:436:TYR:CB	2.37	0.52
1:V:232:ILE:O	1:V:236:VAL:HG23	2.08	0.52
1:V:275:GLU:OE1	1:X:175:LEU:HD11	2.10	0.52
1:E:172:GLN:CA	1:E:173:LEU:HD12	2.40	0.52
1:E:266:TYR:HD1	2:E:501:QRP:HAHA	1.74	0.52
1:E:386:LEU:HD13	1:E:390:TRP:CE2	2.45	0.52
1:B:308:GLU:HB2	1:B:311:ILE:CD1	2.39	0.52
1:F:305:LEU:HD12	1:F:311:ILE:CD1	2.39	0.52
1:I:175:LEU:HD11	1:K:275:GLU:CD	2.29	0.52
1:I:305:LEU:HD23	1:I:305:LEU:H	1.74	0.52
1:J:142:ILE:HB	1:J:143:PRO:HD3	1.92	0.52
1:J:402:TYR:CB	1:J:403:PRO:HD3	2.35	0.52
1:K:52:TRP:CE2	1:K:89:LEU:HB3	2.45	0.52
1:L:120:LEU:HD21	1:L:205:PRO:HD3	1.90	0.52
1:M:288:THR:HG23	1:M:289:GLU:N	2.24	0.52
1:N:63:PHE:CE1	1:N:409:LEU:HD23	2.45	0.52
1:P:228:VAL:HG11	1:P:267:THR:HG23	1.92	0.52
1:P:229:GLY:HA3	1:P:263:TYR:CE2	2.44	0.52
1:R:290:VAL:HG23	1:R:294:LYS:HG2	1.92	0.52
1:S:173:LEU:HD12	1:S:173:LEU:N	2.23	0.52
1:T:315:LEU:O	1:T:315:LEU:HD23	2.08	0.52
1:W:167:LEU:O	1:W:171:PHE:HD2	1.91	0.52
1:W:315:LEU:HD23	1:W:315:LEU:O	2.10	0.52
1:C:233:ALA:HA	1:C:250:PHE:CE2	2.44	0.52
1:A:122:ARG:HG2	1:A:202:ASP:OD1	2.10	0.52
1:A:275:GLU:CD	1:E:175:LEU:HD11	2.29	0.52
1:G:115:LYS:HG2	1:G:395:TRP:NE1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:173:LEU:HD13	1:H:196:GLN:HE22	1.74	0.52
1:J:115:LYS:HG2	1:J:395:TRP:NE1	2.24	0.52
1:K:295:ILE:HG23	1:K:370:PHE:CE2	2.44	0.52
1:L:321:ILE:O	1:L:325:LEU:HD23	2.10	0.52
1:M:266:TYR:HD1	2:M:501:QRP:HAHA	1.74	0.52
1:M:320:GLN:NE2	1:M:392:SER:HB3	2.24	0.52
1:Q:171:PHE:CE1	1:Q:217:PRO:HB3	2.45	0.52
1:Q:320:GLN:HE22	1:Q:392:SER:HB3	1.75	0.52
2:Q:501:QRP:HB	3:Q:502:DST:C13	2.39	0.52
1:W:299:TRP:CD1	1:W:311:ILE:HG23	2.45	0.52
1:X:212:LYS:NZ	3:X:502:DST:P1	2.83	0.52
1:C:41:TYR:CZ	1:E:209:ILE:HD12	2.44	0.52
1:C:140:ASN:OD1	1:C:143:PRO:HG2	2.10	0.52
1:C:373:PRO:HG3	1:C:424:TRP:CZ3	2.45	0.52
1:A:173:LEU:HD12	1:A:173:LEU:N	2.25	0.52
1:E:122:ARG:HG2	1:E:202:ASP:OD1	2.10	0.52
1:E:161:THR:H	1:E:162:PRO:HD3	1.74	0.52
1:E:305:LEU:HD12	1:E:311:ILE:CD1	2.38	0.52
1:G:116:GLY:HA2	1:G:398:HIS:NE2	2.25	0.52
1:H:51:ARG:HB3	1:H:92:TYR:CG	2.44	0.52
1:H:167:LEU:O	1:H:171:PHE:HD2	1.91	0.52
1:I:99:THR:HG23	1:I:193:LEU:CD2	2.37	0.52
1:I:228:VAL:HG12	1:I:232:ILE:HD12	1.91	0.52
1:K:317:ARG:HB2	1:K:427:TYR:OH	2.10	0.52
1:M:209:ILE:HD12	1:P:41:TYR:CZ	2.44	0.52
1:N:372:LEU:O	1:N:424:TRP:HA	2.09	0.52
1:O:137:ASP:OD2	1:O:142:ILE:HG12	2.10	0.52
1:Q:100:ILE:O	2:Q:501:QRP:CD1	2.58	0.52
1:R:410:TYR:CD1	1:R:421:LEU:HD22	2.45	0.52
1:T:171:PHE:HE1	1:T:231:LEU:HD13	1.74	0.52
1:X:115:LYS:HE2	1:X:435:VAL:N	2.24	0.52
1:A:228:VAL:HG11	1:A:267:THR:CG2	2.39	0.52
1:G:115:LYS:HG2	1:G:395:TRP:HE1	1.75	0.52
1:G:120:LEU:HD21	1:G:205:PRO:HD3	1.92	0.52
1:O:147:LEU:HD23	1:O:199:PHE:CD2	2.44	0.52
1:P:415:ILE:HA	1:P:418:THR:CG2	2.40	0.52
1:S:419:THR:HG23	1:S:420:ARG:HG3	1.92	0.52
1:T:137:ASP:OD2	1:T:142:ILE:HG12	2.10	0.52
1:U:126:GLU:OE2	1:U:195:SER:HB2	2.09	0.52
1:U:360:HIS:ND1	1:U:361:PRO:HD2	2.25	0.52
1:W:206:ASP:OD1	1:W:207:GLY:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:290:VAL:HG23	1:X:294:LYS:HG2	1.91	0.52
1:X:321:ILE:O	1:X:325:LEU:HD23	2.10	0.52
1:X:374:VAL:CG1	1:X:382:VAL:HG11	2.40	0.52
1:V:79:PHE:CE2	1:W:42:HIS:HB2	2.45	0.52
1:V:321:ILE:HD11	1:V:389:PHE:CE2	2.45	0.52
1:E:390:TRP:CB	1:E:399:ALA:HB2	2.34	0.52
1:D:160:ASP:OD2	1:H:174:SER:HB2	2.10	0.52
1:D:161:THR:H	1:D:162:PRO:HD3	1.73	0.52
1:D:324:LEU:HB3	1:D:385:ALA:HB1	1.92	0.52
1:F:373:PRO:HG3	1:F:424:TRP:CZ3	2.45	0.52
1:I:274:VAL:HG22	1:I:275:GLU:N	2.25	0.52
1:I:321:ILE:CD1	1:I:437:MET:HE1	2.40	0.52
1:K:83:HIS:O	1:K:87:PRO:HG2	2.10	0.52
1:L:259:GLU:OE2	1:L:304:ARG:NH1	2.43	0.52
1:L:275:GLU:HG3	1:L:278:GLU:OE1	2.09	0.52
1:L:407:GLN:OE1	1:L:415:ILE:HG13	2.10	0.52
1:M:160:ASP:HB3	1:M:162:PRO:HD2	1.91	0.52
1:M:171:PHE:CE1	1:M:231:LEU:HD13	2.45	0.52
1:M:424:TRP:HB2	1:M:440:TYR:CD2	2.44	0.52
1:N:110:SER:O	1:N:121:LEU:HD12	2.10	0.52
1:O:127:PRO:HG3	1:O:147:LEU:HD23	1.92	0.52
1:Q:63:PHE:CE2	1:Q:109:PHE:HB2	2.45	0.52
1:U:171:PHE:HE1	1:U:231:LEU:HD13	1.75	0.52
1:W:369:LYS:HA	1:W:427:TYR:O	2.10	0.52
1:X:299:TRP:NE1	1:X:311:ILE:HG23	2.25	0.52
1:C:147:LEU:HD23	1:C:199:PHE:CD2	2.44	0.52
1:A:117:SER:O	1:A:118:HIS:HB3	2.10	0.52
1:V:318:LEU:HD12	1:V:427:TYR:CD2	2.45	0.52
1:E:360:HIS:ND1	1:E:361:PRO:HD2	2.25	0.52
1:D:418:THR:OG1	1:D:421:LEU:HG	2.10	0.52
1:F:154:LEU:HB3	1:F:156:LEU:CD1	2.40	0.52
1:F:292:TRP:CZ2	1:F:315:LEU:HD21	2.45	0.52
1:I:386:LEU:HD13	1:I:390:TRP:HE1	1.75	0.52
1:M:161:THR:H	1:M:162:PRO:HD3	1.75	0.52
1:N:390:TRP:HB2	1:N:399:ALA:CB	2.25	0.52
1:N:427:TYR:HD1	1:N:437:MET:HE2	1.75	0.52
1:O:290:VAL:HG23	1:O:294:LYS:CG	2.39	0.52
1:P:433:ARG:HG3	1:P:436:TYR:CZ	2.46	0.52
1:Q:208:ALA:HA	1:T:41:TYR:HH	1.75	0.52
1:Q:228:VAL:HG11	1:Q:267:THR:CG2	2.40	0.52
1:T:117:SER:O	1:T:118:HIS:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:SER:O	1:C:118:HIS:HB3	2.10	0.51
1:A:147:LEU:HD23	1:A:199:PHE:HD2	1.76	0.51
1:A:448:LEU:HD12	1:A:448:LEU:N	2.25	0.51
1:G:433:ARG:HG3	1:G:436:TYR:CZ	2.44	0.51
1:F:110:SER:O	1:F:121:LEU:HD12	2.10	0.51
1:F:387:ALA:HA	1:F:390:TRP:HD1	1.72	0.51
1:H:63:PHE:CE1	1:H:409:LEU:HD23	2.45	0.51
1:H:173:LEU:HD12	1:H:173:LEU:N	2.25	0.51
1:H:305:LEU:HD11	1:H:311:ILE:HG12	1.91	0.51
1:I:387:ALA:HA	1:I:390:TRP:HD1	1.75	0.51
1:I:420:ARG:HH12	1:I:448:LEU:HB2	1.75	0.51
1:L:70:GLY:HA3	1:L:73:GLN:HE22	1.73	0.51
1:L:85:LEU:HD22	1:L:125:PHE:CE1	2.44	0.51
1:L:321:ILE:CD1	1:L:437:MET:HE1	2.40	0.51
1:O:60:PHE:CE2	1:O:64:LEU:HD11	2.45	0.51
1:Q:282:LYS:HE3	1:Q:284:TYR:OH	2.10	0.51
1:R:85:LEU:HD22	1:R:125:PHE:CD1	2.46	0.51
1:S:418:THR:OG1	1:S:421:LEU:HG	2.09	0.51
1:W:360:HIS:ND1	1:W:361:PRO:HD2	2.25	0.51
1:X:115:LYS:HG2	1:X:395:TRP:NE1	2.25	0.51
1:A:115:LYS:HG2	1:A:395:TRP:CE2	2.45	0.51
1:G:70:GLY:HA3	1:G:73:GLN:HE22	1.75	0.51
1:B:193:LEU:N	1:B:193:LEU:HD12	2.26	0.51
1:D:127:PRO:HD2	1:D:144:ILE:HD13	1.91	0.51
1:F:266:TYR:HD1	2:F:501:QRP:HAHA	1.75	0.51
1:I:418:THR:OG1	1:I:421:LEU:HG	2.10	0.51
1:L:253:ILE:HD12	1:L:359:ILE:HD11	1.92	0.51
1:O:269:LEU:CD1	1:O:283:ILE:HG13	2.40	0.51
1:P:53:TRP:CH2	1:P:78:MET:CE	2.93	0.51
1:P:379:ASP:OD2	1:P:421:LEU:HB2	2.10	0.51
1:R:115:LYS:HE3	1:R:434:GLY:HA3	1.91	0.51
1:S:173:LEU:CD1	1:S:196:GLN:NE2	2.73	0.51
1:U:60:PHE:HE1	1:U:123:ILE:HD11	1.75	0.51
1:U:115:LYS:HG2	1:U:395:TRP:CE2	2.45	0.51
1:U:318:LEU:HD12	1:U:427:TYR:CD2	2.45	0.51
1:X:402:TYR:O	1:X:405:THR:N	2.43	0.51
1:G:288:THR:HG23	1:G:289:GLU:N	2.25	0.51
1:B:85:LEU:HB3	1:B:125:PHE:CE1	2.44	0.51
1:B:292:TRP:CZ2	1:B:319:LYS:HB2	2.45	0.51
1:I:292:TRP:HZ2	1:I:315:LEU:HD21	1.75	0.51
1:J:288:THR:HG23	1:J:289:GLU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:253:ILE:HD12	1:K:359:ILE:HD11	1.92	0.51
1:K:406:LEU:HD12	1:K:415:ILE:HD11	1.91	0.51
1:K:430:THR:HG22	1:K:432:LYS:H	1.76	0.51
1:L:382:VAL:O	1:L:386:LEU:HB2	2.10	0.51
1:M:85:LEU:HD22	1:M:125:PHE:CD1	2.45	0.51
1:M:115:LYS:HE2	1:M:435:VAL:H	1.75	0.51
1:P:117:SER:O	1:P:118:HIS:HB3	2.11	0.51
1:Q:426:SER:OG	1:Q:438:SER:HB2	2.09	0.51
1:S:167:LEU:HD12	1:S:167:LEU:N	2.26	0.51
1:T:448:LEU:HD12	1:T:448:LEU:N	2.26	0.51
1:A:63:PHE:CE2	1:A:109:PHE:HB2	2.46	0.51
1:A:115:LYS:HG2	1:A:395:TRP:CZ2	2.45	0.51
1:E:115:LYS:HE2	1:E:435:VAL:H	1.74	0.51
1:G:193:LEU:HD12	1:G:193:LEU:N	2.25	0.51
1:I:359:ILE:O	1:I:359:ILE:HG22	2.10	0.51
1:J:285:GLY:O	1:J:354:ILE:HG23	2.11	0.51
1:K:391:ASP:O	1:K:394:GLY:N	2.43	0.51
1:L:266:TYR:HD1	2:L:501:QRP:HAHA	1.75	0.51
1:N:448:LEU:HD12	1:N:448:LEU:N	2.25	0.51
1:O:229:GLY:HA3	1:O:263:TYR:CE2	2.46	0.51
1:O:261:THR:HG22	1:O:261:THR:O	2.10	0.51
1:Q:305:LEU:HD11	1:Q:311:ILE:HG12	1.91	0.51
1:S:171:PHE:CE1	1:S:231:LEU:HD13	2.44	0.51
1:T:305:LEU:HD23	1:T:305:LEU:H	1.75	0.51
1:U:252:LEU:CD2	1:U:301:LEU:HD23	2.40	0.51
1:X:117:SER:O	1:X:118:HIS:HB3	2.11	0.51
1:X:206:ASP:OD1	1:X:207:GLY:N	2.44	0.51
1:X:255:ASP:O	1:X:259:GLU:HG3	2.10	0.51
1:X:300:THR:O	1:X:305:LEU:HD23	2.09	0.51
1:A:239:ILE:HA	1:A:242:GLU:HB3	1.93	0.51
1:V:386:LEU:HD13	1:V:390:TRP:CE2	2.45	0.51
1:G:115:LYS:HE2	1:G:435:VAL:H	1.74	0.51
1:G:117:SER:O	1:G:118:HIS:HB3	2.10	0.51
1:G:212:LYS:NZ	3:G:502:DST:O4	2.43	0.51
1:B:175:LEU:HD11	1:F:275:GLU:CD	2.30	0.51
1:D:212:LYS:NZ	3:D:502:DST:P1	2.84	0.51
1:F:115:LYS:HA	1:F:395:TRP:CE2	2.45	0.51
1:H:305:LEU:HD12	1:H:311:ILE:HG12	1.91	0.51
1:H:410:TYR:CD1	1:H:421:LEU:HD22	2.46	0.51
1:J:102:ARG:HH11	1:J:375:HIS:CD2	2.29	0.51
1:J:127:PRO:HG3	1:J:147:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:TRP:CD2	1:K:89:LEU:HD13	2.46	0.51
1:K:261:THR:O	1:K:261:THR:HG22	2.10	0.51
1:K:374:VAL:HG11	1:K:382:VAL:HG11	1.91	0.51
1:L:117:SER:O	1:L:118:HIS:HB3	2.11	0.51
1:M:386:LEU:HD13	1:M:390:TRP:NE1	2.25	0.51
1:N:370:PHE:O	1:N:426:SER:HA	2.09	0.51
1:N:430:THR:HG22	1:N:432:LYS:H	1.74	0.51
1:P:379:ASP:CG	1:P:422:GLN:HG3	2.30	0.51
1:Q:305:LEU:HD23	1:Q:305:LEU:H	1.76	0.51
1:R:370:PHE:O	1:R:426:SER:HA	2.11	0.51
1:W:299:TRP:CH2	1:W:368:PRO:HG2	2.46	0.51
1:X:171:PHE:HE1	1:X:231:LEU:HD13	1.75	0.51
1:A:299:TRP:NE1	1:A:311:ILE:HG23	2.26	0.51
1:E:257:MET:HE3	1:E:263:TYR:N	2.26	0.51
1:G:46:THR:OG1	1:G:49:GLN:HG3	2.11	0.51
1:B:173:LEU:HD12	1:B:173:LEU:N	2.25	0.51
1:D:66:ALA:HB2	1:D:409:LEU:HD11	1.91	0.51
1:D:261:THR:HG22	1:D:261:THR:O	2.09	0.51
1:H:85:LEU:HD22	1:H:125:PHE:CE1	2.45	0.51
1:H:206:ASP:OD1	1:H:207:GLY:N	2.44	0.51
1:H:308:GLU:HB2	1:H:311:ILE:HD13	1.92	0.51
1:H:321:ILE:HG22	1:H:325:LEU:CD2	2.39	0.51
1:I:237:ARG:HA	1:I:240:ASP:OD2	2.10	0.51
1:I:311:ILE:H	1:I:311:ILE:HD12	1.76	0.51
1:J:127:PRO:HG3	1:J:147:LEU:CD2	2.40	0.51
1:J:308:GLU:CB	1:J:311:ILE:HD13	2.35	0.51
1:J:426:SER:OG	1:J:438:SER:HB2	2.11	0.51
1:J:427:TYR:HD1	1:J:437:MET:CE	2.23	0.51
1:N:140:ASN:OD1	1:N:143:PRO:HG2	2.11	0.51
1:N:167:LEU:HD23	1:N:269:LEU:HD23	1.92	0.51
1:P:173:LEU:HD12	1:P:173:LEU:N	2.26	0.51
1:R:127:PRO:HG3	1:R:147:LEU:CD2	2.41	0.51
1:S:200:GLY:N	1:S:212:LYS:O	2.40	0.51
1:T:160:ASP:HB3	1:T:162:PRO:HD2	1.92	0.51
1:U:110:SER:O	1:U:121:LEU:HD12	2.10	0.51
1:C:175:LEU:HD11	1:G:275:GLU:OE1	2.10	0.51
1:C:359:ILE:O	1:C:359:ILE:HG22	2.11	0.51
1:A:229:GLY:HA3	1:A:263:TYR:CE2	2.45	0.51
1:A:240:ASP:CG	1:A:247:THR:HG22	2.31	0.51
1:A:426:SER:O	1:A:437:MET:HA	2.10	0.51
1:V:85:LEU:HD22	1:V:125:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:PHE:HB3	1:G:121:LEU:HD13	1.92	0.51
1:G:299:TRP:NE1	1:G:311:ILE:HG23	2.25	0.51
1:B:252:LEU:CD2	1:B:301:LEU:HD23	2.41	0.51
1:I:42:HIS:HB2	1:L:79:PHE:HE2	1.76	0.51
1:K:60:PHE:HD1	1:K:109:PHE:CE1	2.27	0.51
1:M:60:PHE:CE1	1:M:123:ILE:HD11	2.45	0.51
1:M:303:GLY:O	1:M:306:ILE:HG13	2.10	0.51
1:N:240:ASP:CG	1:N:247:THR:HG22	2.31	0.51
1:O:81:PHE:HD1	1:O:85:LEU:HD12	1.76	0.51
1:P:320:GLN:HE22	1:P:392:SER:HB3	1.75	0.51
1:Q:52:TRP:CE3	1:Q:89:LEU:HD13	2.45	0.51
1:Q:410:TYR:CE1	1:Q:421:LEU:HD22	2.46	0.51
1:R:115:LYS:HE2	1:R:434:GLY:CA	2.36	0.51
1:S:115:LYS:HG2	1:S:395:TRP:CZ2	2.46	0.51
1:U:85:LEU:HB3	1:U:125:PHE:CE1	2.45	0.51
1:U:137:ASP:OD2	1:U:142:ILE:HG12	2.11	0.51
1:X:70:GLY:HA3	1:X:73:GLN:HE22	1.74	0.51
1:C:292:TRP:CZ2	1:C:319:LYS:HB2	2.44	0.51
1:A:386:LEU:HD13	1:A:390:TRP:CE2	2.46	0.51
1:V:266:TYR:CD1	2:V:501:QRP:HAHA	2.45	0.51
1:G:127:PRO:HG3	1:G:147:LEU:HD23	1.93	0.51
1:B:226:VAL:HG12	1:B:230:THR:OG1	2.10	0.51
1:D:41:TYR:HH	1:F:208:ALA:HA	1.74	0.51
1:D:285:GLY:HA3	1:D:355:TRP:CZ2	2.46	0.51
1:D:356:ASN:HB3	1:D:369:LYS:HB3	1.92	0.51
1:H:63:PHE:CE2	1:H:109:PHE:HB2	2.46	0.51
1:H:290:VAL:HG22	1:H:295:ILE:HG13	1.93	0.51
1:I:85:LEU:HB3	1:I:125:PHE:CE1	2.41	0.51
1:N:271:CYS:HB2	1:N:279:GLN:NE2	2.25	0.51
1:P:390:TRP:CZ3	1:P:395:TRP:CZ3	2.99	0.51
1:S:111:LEU:HD12	1:S:441:TYR:CE2	2.45	0.51
1:U:112:ASN:HD22	1:U:122:ARG:HH21	1.59	0.51
1:U:228:VAL:HG11	1:U:267:THR:HG23	1.92	0.51
1:U:420:ARG:HB2	1:U:447:TYR:CZ	2.43	0.51
1:W:231:LEU:HD12	1:W:232:ILE:N	2.26	0.51
1:X:266:TYR:HD1	2:X:501:QRP:HAHA	1.74	0.51
1:A:249:ALA:O	1:A:252:LEU:HB3	2.11	0.51
1:V:63:PHE:HE2	1:V:109:PHE:HB2	1.76	0.51
1:V:402:TYR:HB3	1:V:403:PRO:CD	2.36	0.51
1:G:237:ARG:O	1:G:240:ASP:HB2	2.11	0.51
1:G:373:PRO:HG3	1:G:424:TRP:CZ3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:TYR:CB	1:B:403:PRO:HD3	2.36	0.51
1:F:233:ALA:HA	1:F:250:PHE:CE2	2.45	0.51
1:I:115:LYS:HG2	1:I:395:TRP:NE1	2.26	0.51
1:J:173:LEU:HD12	1:J:173:LEU:N	2.26	0.51
1:M:83:HIS:O	1:M:87:PRO:HG2	2.11	0.51
1:M:108:GLU:HA	1:M:443:SER:CB	2.41	0.51
1:O:39:ALA:HB2	1:O:53:TRP:CZ2	2.46	0.51
1:Q:171:PHE:HE1	1:Q:231:LEU:HD13	1.76	0.51
1:S:102:ARG:NH1	1:S:375:HIS:CD2	2.79	0.51
1:S:126:GLU:OE2	1:S:195:SER:HB2	2.11	0.51
1:U:277:SER:HB3	1:U:278:GLU:OE1	2.11	0.51
1:U:288:THR:HG23	1:U:289:GLU:N	2.26	0.51
1:W:239:ILE:HA	1:W:242:GLU:HB3	1.93	0.51
1:W:430:THR:HG22	1:W:432:LYS:H	1.76	0.51
1:X:63:PHE:CE2	1:X:109:PHE:HB2	2.46	0.51
1:X:115:LYS:HG2	1:X:395:TRP:HE1	1.75	0.51
1:X:173:LEU:O	1:X:174:SER:OG	2.14	0.51
1:C:172:GLN:NE2	1:G:165:GLN:HG3	2.14	0.51
1:A:165:GLN:CG	1:E:172:GLN:HE22	2.12	0.51
1:A:237:ARG:O	1:A:240:ASP:HB2	2.11	0.51
1:V:175:LEU:HD11	1:X:275:GLU:CD	2.31	0.51
1:E:117:SER:O	1:E:118:HIS:HB3	2.10	0.51
1:I:102:ARG:HH11	1:I:375:HIS:CD2	2.29	0.51
1:K:387:ALA:HA	1:K:390:TRP:HD1	1.72	0.51
1:L:290:VAL:HG23	1:L:294:LYS:CG	2.41	0.51
1:M:174:SER:HB2	1:O:160:ASP:OD2	2.11	0.51
1:R:167:LEU:O	1:R:171:PHE:HD2	1.93	0.51
1:S:154:LEU:HB3	1:S:156:LEU:CD1	2.41	0.51
1:X:374:VAL:CG1	1:X:422:GLN:HG2	2.38	0.51
1:A:250:PHE:O	1:A:253:ILE:N	2.43	0.50
1:E:308:GLU:HB2	1:E:311:ILE:CD1	2.36	0.50
1:G:100:ILE:O	2:G:501:QRP:CD1	2.59	0.50
1:D:448:LEU:N	1:D:448:LEU:HD12	2.27	0.50
1:F:100:ILE:O	2:F:501:QRP:CD1	2.59	0.50
1:H:117:SER:O	1:H:118:HIS:HB3	2.12	0.50
1:J:266:TYR:HD1	2:J:501:QRP:HAHA	1.76	0.50
1:J:369:LYS:HA	1:J:427:TYR:O	2.11	0.50
1:K:66:ALA:HB2	1:K:409:LEU:HD11	1.93	0.50
1:K:115:LYS:HG2	1:K:395:TRP:CZ2	2.46	0.50
1:N:291:THR:O	1:N:295:ILE:HG13	2.12	0.50
1:N:360:HIS:ND1	1:N:361:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:127:PRO:HD2	1:P:144:ILE:HD13	1.91	0.50
1:Q:115:LYS:HG2	1:Q:395:TRP:HE1	1.75	0.50
1:Q:167:LEU:O	1:Q:171:PHE:HD2	1.93	0.50
1:Q:402:TYR:O	1:Q:405:THR:N	2.44	0.50
1:Q:420:ARG:HB2	1:Q:447:TYR:CZ	2.47	0.50
1:R:41:TYR:OH	1:S:208:ALA:HA	2.11	0.50
1:S:99:THR:HG23	1:S:193:LEU:CD2	2.39	0.50
1:S:102:ARG:HH11	1:S:375:HIS:CD2	2.29	0.50
1:U:160:ASP:HB3	1:U:162:PRO:HD2	1.93	0.50
1:W:171:PHE:CE1	1:W:231:LEU:HD13	2.45	0.50
1:W:370:PHE:O	1:W:426:SER:HA	2.11	0.50
1:E:47:ASN:C	1:E:47:ASN:HD22	2.12	0.50
1:E:275:GLU:HG3	1:E:278:GLU:OE1	2.11	0.50
1:B:116:GLY:CA	1:B:398:HIS:CE1	2.95	0.50
1:F:63:PHE:HE2	1:F:109:PHE:HB2	1.75	0.50
1:F:269:LEU:HD12	1:F:283:ILE:HG13	1.94	0.50
1:H:305:LEU:HD23	1:H:305:LEU:H	1.76	0.50
1:K:63:PHE:CE1	1:K:409:LEU:HD23	2.46	0.50
1:L:261:THR:HG22	1:L:261:THR:O	2.11	0.50
1:M:115:LYS:HG2	1:M:395:TRP:CE2	2.46	0.50
1:P:250:PHE:O	1:P:253:ILE:N	2.45	0.50
1:P:305:LEU:HD23	1:P:305:LEU:H	1.76	0.50
1:R:378:ASN:O	1:R:382:VAL:HG23	2.11	0.50
1:W:173:LEU:HD12	1:W:173:LEU:N	2.25	0.50
1:W:233:ALA:HA	1:W:250:PHE:CE2	2.45	0.50
1:C:85:LEU:HB3	1:C:125:PHE:CE1	2.43	0.50
1:A:175:LEU:HD11	1:E:275:GLU:CD	2.32	0.50
1:A:305:LEU:HD12	1:A:311:ILE:CD1	2.41	0.50
1:A:305:LEU:HD23	1:A:305:LEU:H	1.77	0.50
1:D:108:GLU:HA	1:D:443:SER:CB	2.41	0.50
1:D:115:LYS:HE2	1:D:435:VAL:H	1.75	0.50
1:D:410:TYR:CD1	1:D:421:LEU:HD22	2.46	0.50
1:F:315:LEU:O	1:F:315:LEU:HD23	2.11	0.50
1:F:402:TYR:O	1:F:405:THR:N	2.45	0.50
1:J:305:LEU:CD1	1:J:311:ILE:HG12	2.41	0.50
1:K:206:ASP:OD1	1:K:207:GLY:N	2.44	0.50
1:K:282:LYS:CB	1:K:284:TYR:HE1	2.24	0.50
1:L:295:ILE:HG23	1:L:370:PHE:HE2	1.76	0.50
1:M:110:SER:HB2	1:M:122:ARG:CB	2.19	0.50
1:M:239:ILE:O	1:M:243:ARG:N	2.31	0.50
1:N:308:GLU:HB2	1:N:311:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:229:GLY:HA3	1:Q:263:TYR:CD2	2.46	0.50
1:T:108:GLU:HA	1:T:443:SER:CB	2.42	0.50
1:U:46:THR:OG1	1:U:49:GLN:HG3	2.12	0.50
1:U:52:TRP:CE3	1:U:89:LEU:HD13	2.46	0.50
1:U:228:VAL:CG1	1:U:232:ILE:HD11	2.37	0.50
1:U:386:LEU:HD13	1:U:390:TRP:CE2	2.46	0.50
1:W:120:LEU:HD21	1:W:205:PRO:HD3	1.93	0.50
1:W:415:ILE:HA	1:W:418:THR:CG2	2.39	0.50
1:A:234:GLU:OE2	1:A:237:ARG:NH2	2.44	0.50
1:E:52:TRP:CE3	1:E:89:LEU:HD13	2.47	0.50
1:E:167:LEU:HD12	1:E:167:LEU:N	2.26	0.50
1:E:228:VAL:CG1	1:E:232:ILE:HD11	2.39	0.50
1:E:282:LYS:HE3	1:E:284:TYR:OH	2.11	0.50
1:B:115:LYS:HE2	1:B:435:VAL:N	2.23	0.50
1:B:229:GLY:HA3	1:B:263:TYR:CE2	2.47	0.50
1:B:317:ARG:HB2	1:B:427:TYR:OH	2.10	0.50
1:D:426:SER:O	1:D:437:MET:HA	2.11	0.50
1:F:53:TRP:CZ3	1:F:78:MET:CE	2.95	0.50
1:F:374:VAL:HG11	1:F:382:VAL:HG11	1.92	0.50
1:I:115:LYS:HE2	1:I:434:GLY:CA	2.38	0.50
1:I:269:LEU:CD1	1:I:283:ILE:HG13	2.42	0.50
1:K:51:ARG:HB3	1:K:92:TYR:CG	2.45	0.50
1:N:359:ILE:O	1:N:359:ILE:HG22	2.11	0.50
1:N:386:LEU:HD13	1:N:390:TRP:HE1	1.75	0.50
1:Q:66:ALA:HB2	1:Q:409:LEU:HD11	1.93	0.50
1:Q:239:ILE:O	1:Q:243:ARG:N	2.32	0.50
1:Q:428:SER:HB3	1:Q:436:TYR:CB	2.36	0.50
1:R:379:ASP:HB2	1:R:418:THR:HG23	1.92	0.50
1:R:415:ILE:CA	1:R:418:THR:HG22	2.39	0.50
1:X:448:LEU:HD12	1:X:448:LEU:N	2.26	0.50
1:A:382:VAL:O	1:A:386:LEU:HB2	2.11	0.50
1:E:240:ASP:CG	1:E:247:THR:HG22	2.32	0.50
1:E:418:THR:OG1	1:E:421:LEU:HG	2.10	0.50
1:G:232:ILE:O	1:G:236:VAL:HG23	2.11	0.50
1:G:284:TYR:N	1:G:284:TYR:HD1	2.09	0.50
1:B:256:TYR:CD2	1:B:301:LEU:HD12	2.45	0.50
1:I:63:PHE:CE2	1:I:109:PHE:CB	2.95	0.50
1:I:127:PRO:HG3	1:I:147:LEU:CD2	2.41	0.50
1:I:173:LEU:O	1:I:174:SER:OG	2.15	0.50
1:I:193:LEU:HD12	1:I:193:LEU:N	2.27	0.50
1:I:237:ARG:O	1:I:240:ASP:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:379:ASP:HB2	1:J:418:THR:CG2	2.34	0.50
1:J:386:LEU:HD13	1:J:390:TRP:CE2	2.46	0.50
2:M:501:QRP:HB	3:M:502:DST:C13	2.41	0.50
1:N:174:SER:HB2	1:P:160:ASP:OD2	2.12	0.50
1:O:115:LYS:HG2	1:O:395:TRP:CE2	2.47	0.50
1:P:107:ILE:HA	1:P:124:GLY:O	2.11	0.50
1:R:85:LEU:HB3	1:R:125:PHE:CE1	2.38	0.50
1:T:105:LEU:CD1	1:T:107:ILE:HG22	2.41	0.50
1:U:100:ILE:O	2:U:501:QRP:CD1	2.59	0.50
1:U:266:TYR:HD1	2:U:501:QRP:HAHA	1.76	0.50
1:W:321:ILE:O	1:W:325:LEU:HD23	2.12	0.50
1:X:53:TRP:CZ3	1:X:78:MET:CE	2.94	0.50
1:X:305:LEU:HD23	1:X:305:LEU:H	1.76	0.50
1:A:147:LEU:HD23	1:A:199:PHE:CD2	2.46	0.50
1:V:127:PRO:HG3	1:V:147:LEU:CD2	2.42	0.50
1:V:147:LEU:HD23	1:V:199:PHE:CD2	2.46	0.50
1:E:433:ARG:HG3	1:E:436:TYR:CZ	2.46	0.50
1:G:127:PRO:HD2	1:G:144:ILE:HD13	1.94	0.50
1:D:180:GLN:OE1	1:D:180:GLN:HA	2.12	0.50
1:I:46:THR:OG1	1:I:49:GLN:HG3	2.11	0.50
1:I:448:LEU:HD12	1:I:448:LEU:N	2.27	0.50
1:J:102:ARG:NH1	1:J:375:HIS:CD2	2.80	0.50
1:N:315:LEU:O	1:N:315:LEU:HD23	2.12	0.50
1:N:420:ARG:HB2	1:N:447:TYR:CZ	2.46	0.50
1:O:85:LEU:HD22	1:O:125:PHE:CE1	2.47	0.50
1:O:448:LEU:N	1:O:448:LEU:HD12	2.27	0.50
1:P:391:ASP:O	1:P:394:GLY:N	2.45	0.50
1:Q:60:PHE:HE1	1:Q:123:ILE:HD11	1.74	0.50
1:Q:112:ASN:ND2	1:Q:122:ARG:HH21	2.05	0.50
1:U:389:PHE:HE2	1:U:437:MET:HE1	1.75	0.50
1:W:282:LYS:HE3	1:W:284:TYR:OH	2.11	0.50
1:X:102:ARG:HH11	1:X:375:HIS:CD2	2.30	0.50
1:X:147:LEU:HD23	1:X:199:PHE:CD2	2.45	0.50
1:X:167:LEU:HD23	1:X:269:LEU:HD23	1.94	0.50
1:X:240:ASP:O	1:X:244:ASN:N	2.45	0.50
1:A:70:GLY:HA3	1:A:73:GLN:HE22	1.75	0.50
1:E:290:VAL:HG23	1:E:294:LYS:CG	2.42	0.50
1:D:229:GLY:HA3	1:D:263:TYR:CE2	2.46	0.50
1:H:115:LYS:CE	1:H:434:GLY:HA3	2.41	0.50
1:K:321:ILE:HG22	1:K:325:LEU:CD2	2.41	0.50
1:K:374:VAL:CG1	1:K:382:VAL:HG21	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:259:GLU:OE2	1:M:304:ARG:NH1	2.45	0.50
1:N:154:LEU:HB3	1:N:156:LEU:CD1	2.42	0.50
1:P:237:ARG:HA	1:P:240:ASP:OD2	2.11	0.50
1:P:292:TRP:CZ2	1:P:315:LEU:HD21	2.46	0.50
1:Q:53:TRP:CH2	1:Q:78:MET:CE	2.95	0.50
1:R:430:THR:HG22	1:R:432:LYS:H	1.76	0.50
1:S:100:ILE:O	2:S:501:QRP:CD1	2.59	0.50
1:S:281:LEU:C	1:S:281:LEU:HD12	2.32	0.50
1:T:402:TYR:O	1:T:405:THR:N	2.45	0.50
1:X:233:ALA:HA	1:X:250:PHE:CE2	2.46	0.50
1:C:305:LEU:CD1	1:C:311:ILE:HG12	2.41	0.50
1:A:85:LEU:HD22	1:A:125:PHE:CD1	2.47	0.50
1:A:160:ASP:HB3	1:A:162:PRO:HD2	1.94	0.50
1:G:212:LYS:NZ	3:G:502:DST:P1	2.84	0.50
1:D:386:LEU:HD13	1:D:390:TRP:CE2	2.47	0.50
1:H:290:VAL:HG11	1:H:353:ILE:HG12	1.94	0.50
1:J:172:GLN:CA	1:J:173:LEU:HD12	2.42	0.50
1:K:233:ALA:HA	1:K:250:PHE:CE2	2.46	0.50
1:K:270:SER:HB3	1:K:282:LYS:HB2	1.93	0.50
1:L:140:ASN:OD1	1:L:143:PRO:HG2	2.12	0.50
1:M:448:LEU:N	1:M:448:LEU:HD12	2.27	0.50
1:Q:299:TRP:NE1	1:Q:311:ILE:HG23	2.27	0.50
1:S:266:TYR:HD1	2:S:501:QRP:HAHA	1.75	0.50
1:T:173:LEU:HD12	1:T:173:LEU:N	2.27	0.50
1:T:176:SER:O	1:T:180:GLN:HB2	2.12	0.50
1:U:173:LEU:HD13	1:U:196:GLN:NE2	2.27	0.50
1:W:239:ILE:HD12	1:W:242:GLU:CG	2.41	0.50
1:X:228:VAL:CG1	1:X:232:ILE:HD11	2.36	0.50
1:X:371:TYR:OH	3:X:502:DST:O8	2.20	0.50
1:C:374:VAL:HG11	1:C:382:VAL:HG11	1.94	0.50
1:A:354:ILE:HB	1:A:371:TYR:HB2	1.94	0.50
1:G:305:LEU:HD23	1:G:305:LEU:H	1.77	0.50
1:H:299:TRP:NE1	1:H:311:ILE:HG23	2.27	0.50
1:H:320:GLN:HE22	1:H:392:SER:HB3	1.76	0.50
1:I:209:ILE:HD12	1:L:41:TYR:CZ	2.47	0.50
1:J:115:LYS:HE2	1:J:435:VAL:N	2.26	0.50
1:U:117:SER:O	1:U:118:HIS:HB3	2.12	0.50
1:C:209:ILE:HD12	1:E:41:TYR:CZ	2.46	0.49
1:C:369:LYS:HA	1:C:427:TYR:O	2.11	0.49
1:V:154:LEU:HB3	1:V:156:LEU:CD1	2.42	0.49
1:E:200:GLY:N	1:E:212:LYS:O	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:GLY:HA3	1:E:355:TRP:CZ2	2.47	0.49
1:G:282:LYS:HD2	1:G:356:ASN:HD21	1.77	0.49
1:B:284:TYR:N	1:B:284:TYR:HD1	2.10	0.49
1:F:117:SER:O	1:F:118:HIS:HB3	2.11	0.49
1:F:228:VAL:HG11	1:F:267:THR:HG23	1.94	0.49
1:H:239:ILE:HA	1:H:242:GLU:HB3	1.94	0.49
1:H:386:LEU:HD13	1:H:390:TRP:CE2	2.47	0.49
1:J:117:SER:O	1:J:118:HIS:HB3	2.11	0.49
1:K:281:LEU:C	1:K:281:LEU:HD12	2.33	0.49
1:K:321:ILE:O	1:K:325:LEU:HD23	2.11	0.49
1:M:290:VAL:HG23	1:M:294:LYS:CG	2.42	0.49
1:M:354:ILE:HG21	3:M:502:DST:C13	2.39	0.49
1:M:405:THR:O	1:M:409:LEU:HD13	2.12	0.49
1:N:292:TRP:CZ2	1:N:319:LYS:HB2	2.47	0.49
1:O:127:PRO:HG3	1:O:147:LEU:HD22	1.94	0.49
1:P:115:LYS:HG2	1:P:395:TRP:HE1	1.76	0.49
1:R:117:SER:O	1:R:118:HIS:HB3	2.12	0.49
1:R:321:ILE:HG22	1:R:325:LEU:CD2	2.39	0.49
1:S:288:THR:HG23	1:S:289:GLU:N	2.26	0.49
1:T:386:LEU:HD13	1:T:390:TRP:HE1	1.76	0.49
1:U:324:LEU:O	1:U:327:ILE:HG22	2.12	0.49
1:W:63:PHE:HE2	1:W:109:PHE:HB2	1.76	0.49
1:X:51:ARG:HB3	1:X:92:TYR:CG	2.47	0.49
1:X:237:ARG:HA	1:X:240:ASP:OD2	2.11	0.49
1:C:147:LEU:HD23	1:C:199:PHE:HD2	1.77	0.49
1:V:160:ASP:HB3	1:V:162:PRO:CD	2.42	0.49
1:V:305:LEU:CD1	1:V:311:ILE:HG12	2.42	0.49
1:V:374:VAL:CG1	1:V:382:VAL:HG21	2.38	0.49
1:E:36:GLN:OE1	1:E:58:SER:HA	2.13	0.49
1:E:321:ILE:HG22	1:E:325:LEU:CD2	2.41	0.49
1:G:105:LEU:CD1	1:G:107:ILE:HG22	2.42	0.49
1:F:73:GLN:OE1	1:F:73:GLN:N	2.45	0.49
1:F:85:LEU:HB3	1:F:125:PHE:CE1	2.47	0.49
1:H:288:THR:HG23	1:H:289:GLU:N	2.27	0.49
1:K:154:LEU:HB2	1:K:156:LEU:HD13	1.94	0.49
1:L:161:THR:H	1:L:162:PRO:HD3	1.75	0.49
1:L:200:GLY:N	1:L:212:LYS:O	2.38	0.49
1:L:308:GLU:HB2	1:L:311:ILE:CD1	2.37	0.49
1:N:211:VAL:HG12	1:N:273:PHE:CD2	2.47	0.49
1:N:389:PHE:HE2	1:N:437:MET:HE1	1.78	0.49
1:O:379:ASP:OD2	1:O:421:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:321:ILE:CG2	1:Q:325:LEU:HD23	2.42	0.49
1:R:324:LEU:O	1:R:327:ILE:HG22	2.12	0.49
1:T:382:VAL:O	1:T:386:LEU:HB2	2.13	0.49
1:U:206:ASP:OD1	1:U:207:GLY:N	2.45	0.49
1:X:426:SER:OG	1:X:438:SER:HB2	2.12	0.49
1:C:300:THR:O	1:C:305:LEU:HD23	2.11	0.49
1:C:354:ILE:HB	1:C:371:TYR:HB2	1.94	0.49
1:V:99:THR:HG23	1:V:193:LEU:CD2	2.28	0.49
1:V:206:ASP:OD1	1:V:207:GLY:N	2.45	0.49
1:V:300:THR:O	1:V:305:LEU:HD23	2.12	0.49
1:E:288:THR:HG23	1:E:289:GLU:N	2.26	0.49
1:E:448:LEU:HD12	1:E:448:LEU:N	2.27	0.49
1:G:211:VAL:HG12	1:G:273:PHE:CD2	2.47	0.49
1:B:239:ILE:HD12	1:B:242:GLU:CG	2.41	0.49
1:D:117:SER:O	1:D:118:HIS:HB3	2.11	0.49
1:D:221:ALA:CB	1:D:231:LEU:HD21	2.42	0.49
1:H:221:ALA:HB2	1:H:231:LEU:HD21	1.94	0.49
1:H:300:THR:O	1:H:305:LEU:HD23	2.13	0.49
1:I:117:SER:O	1:I:118:HIS:HB3	2.11	0.49
1:I:174:SER:OG	1:I:175:LEU:N	2.45	0.49
1:M:426:SER:O	1:M:437:MET:HG3	2.11	0.49
1:N:51:ARG:HB3	1:N:92:TYR:CG	2.47	0.49
1:N:112:ASN:ND2	1:N:122:ARG:HH21	2.05	0.49
1:N:115:LYS:HE2	1:N:434:GLY:CA	2.41	0.49
1:O:154:LEU:CB	1:O:156:LEU:HD13	2.42	0.49
1:P:351:SER:OG	1:P:373:PRO:HB3	2.13	0.49
1:Q:117:SER:O	1:Q:118:HIS:HB3	2.12	0.49
1:R:326:GLN:HG3	1:R:326:GLN:O	2.12	0.49
1:S:356:ASN:HB3	1:S:369:LYS:HB3	1.93	0.49
1:T:295:ILE:HG23	1:T:370:PHE:CE2	2.47	0.49
1:U:321:ILE:CD1	1:U:437:MET:HE2	2.43	0.49
1:W:147:LEU:HD23	1:W:199:PHE:HD2	1.77	0.49
1:C:63:PHE:CE1	1:C:409:LEU:HD23	2.47	0.49
1:C:81:PHE:CE2	1:C:86:ILE:HD11	2.48	0.49
1:E:369:LYS:HA	1:E:427:TYR:O	2.12	0.49
1:G:448:LEU:N	1:G:448:LEU:HD12	2.28	0.49
1:B:53:TRP:CZ3	1:B:78:MET:CE	2.95	0.49
1:B:127:PRO:HD2	1:B:144:ILE:HD13	1.94	0.49
1:D:140:ASN:OD1	1:D:143:PRO:HG2	2.12	0.49
1:F:305:LEU:CD1	1:F:311:ILE:HG12	2.42	0.49
1:H:295:ILE:HG23	1:H:370:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:66:ALA:HB2	1:J:409:LEU:HD11	1.93	0.49
1:J:109:PHE:CD2	1:J:443:SER:HB3	2.47	0.49
1:M:171:PHE:HE1	1:M:231:LEU:CD1	2.25	0.49
1:O:406:LEU:HD12	1:O:415:ILE:HD13	1.92	0.49
1:Q:162:PRO:HG2	1:S:174:SER:HB3	1.94	0.49
1:R:79:PHE:HE2	1:S:42:HIS:HB2	1.78	0.49
1:S:321:ILE:O	1:S:325:LEU:HD23	2.12	0.49
1:U:278:GLU:OE1	1:U:278:GLU:N	2.45	0.49
2:W:501:QRP:HB	3:W:502:DST:C13	2.42	0.49
1:C:120:LEU:HD21	1:C:205:PRO:HD3	1.94	0.49
1:G:240:ASP:CG	1:G:247:THR:HG22	2.33	0.49
1:B:79:PHE:CE2	1:H:42:HIS:HB2	2.47	0.49
1:B:227:PRO:O	1:B:230:THR:OG1	2.28	0.49
1:D:53:TRP:CZ3	1:D:78:MET:CE	2.96	0.49
1:D:255:ASP:O	1:D:259:GLU:HG3	2.13	0.49
1:D:305:LEU:CD1	1:D:311:ILE:HG12	2.43	0.49
1:D:433:ARG:HG3	1:D:436:TYR:CZ	2.48	0.49
1:F:52:TRP:CE2	1:F:89:LEU:HB3	2.47	0.49
1:F:212:LYS:NZ	3:F:502:DST:P1	2.86	0.49
1:F:295:ILE:HG23	1:F:370:PHE:CE2	2.46	0.49
1:I:305:LEU:HD12	1:I:311:ILE:HG12	1.94	0.49
1:J:119:ARG:N	1:J:119:ARG:HD2	2.27	0.49
1:K:324:LEU:HB3	1:K:385:ALA:HB1	1.93	0.49
1:L:234:GLU:OE2	1:L:237:ARG:NH2	2.44	0.49
1:M:321:ILE:HG22	1:M:325:LEU:CD2	2.42	0.49
1:M:402:TYR:O	1:M:405:THR:N	2.45	0.49
1:O:303:GLY:O	1:O:306:ILE:HG13	2.13	0.49
1:P:249:ALA:HB3	1:P:359:ILE:HG23	1.93	0.49
1:R:52:TRP:CE3	1:R:89:LEU:HD13	2.48	0.49
1:U:85:LEU:HD22	1:U:125:PHE:CD1	2.46	0.49
1:W:288:THR:HG23	1:W:289:GLU:N	2.26	0.49
1:C:269:LEU:CD1	1:C:283:ILE:HG13	2.43	0.49
1:A:83:HIS:NE2	1:G:83:HIS:NE2	2.45	0.49
1:E:66:ALA:HB2	1:E:409:LEU:HD11	1.95	0.49
1:F:173:LEU:HD13	1:F:196:GLN:NE2	2.26	0.49
1:H:285:GLY:O	1:H:354:ILE:HG23	2.13	0.49
1:I:268:PHE:CZ	1:I:284:TYR:CD2	3.01	0.49
1:L:239:ILE:HA	1:L:242:GLU:HB3	1.95	0.49
1:L:300:THR:O	1:L:305:LEU:HD23	2.13	0.49
1:M:99:THR:HG23	1:M:193:LEU:CD2	2.33	0.49
1:M:354:ILE:HB	1:M:371:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:373:PRO:HG3	1:N:424:TRP:HZ3	1.77	0.49
1:O:36:GLN:OE1	1:O:58:SER:HA	2.11	0.49
1:Q:119:ARG:HD2	1:Q:119:ARG:N	2.28	0.49
1:R:115:LYS:HE2	1:R:435:VAL:N	2.26	0.49
1:T:430:THR:HB	1:T:433:ARG:HB2	1.95	0.49
1:U:75:TYR:HE2	1:X:72:PRO:HA	1.78	0.49
1:W:359:ILE:O	1:W:359:ILE:HG22	2.12	0.49
1:W:448:LEU:N	1:W:448:LEU:HD12	2.28	0.49
1:V:209:ILE:HD12	1:W:41:TYR:CZ	2.48	0.49
1:V:391:ASP:O	1:V:394:GLY:N	2.45	0.49
1:G:127:PRO:HG3	1:G:147:LEU:CD2	2.43	0.49
1:H:154:LEU:HB3	1:H:156:LEU:HD13	1.95	0.49
1:H:406:LEU:HD12	1:H:415:ILE:HD11	1.93	0.49
1:I:75:TYR:CD2	1:L:75:TYR:HD2	2.16	0.49
1:J:209:ILE:HD12	1:K:41:TYR:CZ	2.48	0.49
1:M:390:TRP:CZ3	1:M:395:TRP:CZ3	3.00	0.49
1:O:173:LEU:CD1	1:O:196:GLN:NE2	2.76	0.49
1:P:369:LYS:O	1:P:370:PHE:HD1	1.95	0.49
1:T:282:LYS:CB	1:T:284:TYR:HE1	2.24	0.49
1:W:305:LEU:CD1	1:W:311:ILE:HG12	2.42	0.49
1:X:171:PHE:HE1	1:X:231:LEU:CD1	2.26	0.49
2:G:501:QRP:HB	3:G:502:DST:C13	2.42	0.49
1:B:47:ASN:HD22	1:D:95:LYS:NZ	2.11	0.49
1:D:275:GLU:CD	1:H:175:LEU:HD11	2.33	0.49
1:F:305:LEU:HD12	1:F:311:ILE:HD11	1.93	0.49
1:F:320:GLN:HB2	1:U:312:ILE:CG2	2.43	0.49
1:F:382:VAL:O	1:F:386:LEU:HB2	2.13	0.49
1:H:161:THR:H	1:H:162:PRO:HD3	1.76	0.49
1:J:268:PHE:CZ	1:J:284:TYR:CD2	3.01	0.49
1:J:275:GLU:HB2	1:L:175:LEU:HD21	1.95	0.49
1:K:115:LYS:HG2	1:K:395:TRP:CE2	2.48	0.49
1:K:410:TYR:OH	1:K:441:TYR:HB3	2.13	0.49
1:M:100:ILE:O	2:M:501:QRP:CD1	2.61	0.49
1:O:386:LEU:HD13	1:O:390:TRP:CE2	2.47	0.49
1:P:140:ASN:OD1	1:P:143:PRO:HG2	2.12	0.49
1:P:356:ASN:HB3	1:P:369:LYS:HB3	1.95	0.49
1:T:206:ASP:OD1	1:T:207:GLY:N	2.46	0.49
1:T:228:VAL:HG11	1:T:267:THR:HG23	1.95	0.49
1:X:426:SER:O	1:X:437:MET:HG3	2.12	0.49
1:X:433:ARG:HG3	1:X:436:TYR:OH	2.12	0.49
1:C:390:TRP:HB2	1:C:399:ALA:CB	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ARG:NH1	1:A:182:GLN:HB3	2.27	0.49
1:E:426:SER:O	1:E:437:MET:HA	2.12	0.49
1:G:48:ASP:CG	1:G:91:PRO:HA	2.33	0.49
1:G:53:TRP:CZ3	1:G:78:MET:CE	2.96	0.49
1:B:120:LEU:HD21	1:B:205:PRO:HD3	1.94	0.49
1:D:60:PHE:CE2	1:D:64:LEU:HD11	2.47	0.49
1:I:102:ARG:NH1	1:I:375:HIS:CD2	2.81	0.49
1:K:92:TYR:CD2	1:K:93:PRO:HD3	2.47	0.49
1:K:173:LEU:HD12	1:K:173:LEU:N	2.26	0.49
1:L:110:SER:HB2	1:L:122:ARG:CB	2.16	0.49
1:L:147:LEU:HD23	1:L:199:PHE:CD2	2.47	0.49
1:M:305:LEU:HD23	1:M:305:LEU:H	1.78	0.49
1:N:60:PHE:CE1	1:N:123:ILE:HD11	2.48	0.49
1:N:75:TYR:HD2	1:O:75:TYR:CD2	2.17	0.49
1:N:300:THR:O	1:N:305:LEU:HD23	2.13	0.49
1:O:382:VAL:O	1:O:386:LEU:HB2	2.13	0.49
1:P:386:LEU:HD13	1:P:390:TRP:HE1	1.76	0.49
1:Q:240:ASP:CG	1:Q:247:THR:HG22	2.32	0.49
1:R:48:ASP:CG	1:R:91:PRO:HA	2.32	0.49
2:T:501:QRP:HB	3:T:502:DST:C13	2.42	0.49
1:W:63:PHE:CE2	1:W:109:PHE:HB2	2.47	0.49
1:A:386:LEU:HD11	1:A:390:TRP:HZ2	1.78	0.49
1:E:60:PHE:CE1	1:E:123:ILE:HD11	2.48	0.49
1:E:147:LEU:HD23	1:E:199:PHE:HD2	1.78	0.49
1:B:321:ILE:HG22	1:B:325:LEU:CD2	2.42	0.49
1:B:371:TYR:OH	3:B:502:DST:O8	2.12	0.49
1:F:51:ARG:HB3	1:F:92:TYR:CG	2.48	0.49
1:J:70:GLY:HA3	1:J:73:GLN:OE1	2.12	0.49
1:K:266:TYR:HD1	2:K:501:QRP:HAHA	1.78	0.49
1:K:407:GLN:OE1	1:K:415:ILE:HG13	2.12	0.49
1:N:239:ILE:HA	1:N:242:GLU:HB3	1.95	0.49
1:N:275:GLU:CD	1:P:175:LEU:HD11	2.33	0.49
1:N:410:TYR:CD1	1:N:421:LEU:HD22	2.48	0.49
1:O:100:ILE:O	2:O:501:QRP:CD1	2.60	0.49
1:P:110:SER:O	1:P:121:LEU:HD12	2.12	0.49
1:Q:126:GLU:OE2	1:Q:195:SER:CB	2.61	0.49
1:U:386:LEU:HD13	1:U:390:TRP:HE1	1.77	0.49
1:X:140:ASN:OD1	1:X:143:PRO:HG2	2.13	0.49
1:C:266:TYR:CD1	2:C:501:QRP:HAHA	2.48	0.48
1:V:117:SER:O	1:V:118:HIS:HB3	2.13	0.48
1:V:161:THR:H	1:V:162:PRO:HD3	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:ARG:HH11	1:E:375:HIS:CD2	2.31	0.48
1:B:390:TRP:CZ3	1:B:395:TRP:CZ3	3.00	0.48
1:F:102:ARG:NH1	1:F:375:HIS:CD2	2.80	0.48
1:H:53:TRP:CZ3	1:H:78:MET:CE	2.96	0.48
1:I:52:TRP:CE2	1:I:89:LEU:HB3	2.48	0.48
1:I:370:PHE:O	1:I:426:SER:HA	2.13	0.48
1:I:428:SER:HB3	1:I:436:TYR:CB	2.32	0.48
1:K:115:LYS:HA	1:K:395:TRP:CE2	2.48	0.48
1:K:239:ILE:HA	1:K:242:GLU:HB3	1.95	0.48
1:K:255:ASP:O	1:K:259:GLU:HG3	2.12	0.48
1:L:237:ARG:HA	1:L:240:ASP:OD2	2.13	0.48
2:L:501:QRP:HB	3:L:502:DST:C13	2.43	0.48
1:O:231:LEU:HD12	1:O:232:ILE:N	2.28	0.48
1:O:266:TYR:HD1	2:O:501:QRP:HAHA	1.76	0.48
2:O:501:QRP:HB	3:O:502:DST:C13	2.43	0.48
1:Q:72:PRO:HA	1:T:75:TYR:HE2	1.78	0.48
1:Q:303:GLY:O	1:Q:306:ILE:HG13	2.13	0.48
1:U:115:LYS:HE2	1:U:434:GLY:CA	2.43	0.48
1:U:161:THR:H	1:U:162:PRO:HD3	1.75	0.48
1:W:386:LEU:HD13	1:W:390:TRP:CE2	2.48	0.48
1:X:239:ILE:HD12	1:X:242:GLU:CG	2.40	0.48
1:C:228:VAL:CG1	1:C:232:ILE:HD11	2.40	0.48
1:C:374:VAL:CG1	1:C:382:VAL:HG21	2.42	0.48
1:V:174:SER:HB2	1:X:160:ASP:OD2	2.13	0.48
1:E:292:TRP:HZ2	1:E:315:LEU:CD2	2.23	0.48
1:B:311:ILE:H	1:B:311:ILE:HD12	1.77	0.48
1:D:102:ARG:HH11	1:D:375:HIS:CD2	2.31	0.48
1:D:102:ARG:NH1	1:D:375:HIS:CD2	2.82	0.48
1:H:84:HIS:NE2	1:H:154:LEU:HD11	2.28	0.48
1:J:448:LEU:N	1:J:448:LEU:HD12	2.28	0.48
1:L:415:ILE:HA	1:L:418:THR:CG2	2.44	0.48
1:M:206:ASP:OD1	1:M:207:GLY:N	2.45	0.48
1:M:386:LEU:HD13	1:M:390:TRP:CE2	2.48	0.48
1:N:117:SER:O	1:N:118:HIS:HB3	2.13	0.48
1:N:147:LEU:HD23	1:N:199:PHE:CE2	2.49	0.48
1:P:240:ASP:CG	1:P:247:THR:HG22	2.34	0.48
1:P:426:SER:O	1:P:437:MET:HG3	2.14	0.48
1:R:127:PRO:HG3	1:R:147:LEU:HD23	1.95	0.48
1:S:105:LEU:CD1	1:S:107:ILE:HG22	2.43	0.48
1:S:369:LYS:HA	1:S:427:TYR:O	2.13	0.48
1:A:300:THR:O	1:A:305:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:O	1:A:318:LEU:HD23	2.13	0.48
1:V:175:LEU:HD11	1:X:275:GLU:OE1	2.13	0.48
1:E:81:PHE:CE2	1:E:86:ILE:HD11	2.48	0.48
1:G:290:VAL:HG22	1:G:295:ILE:HG13	1.95	0.48
1:G:370:PHE:O	1:G:426:SER:HA	2.13	0.48
1:B:448:LEU:N	1:B:448:LEU:HD12	2.27	0.48
1:D:420:ARG:HB2	1:D:447:TYR:CZ	2.48	0.48
1:H:126:GLU:OE2	1:H:195:SER:CB	2.61	0.48
1:J:212:LYS:NZ	3:J:502:DST:P1	2.85	0.48
1:L:320:GLN:HE22	1:L:392:SER:HB3	1.78	0.48
1:L:386:LEU:HD13	1:L:390:TRP:HE1	1.78	0.48
1:M:123:ILE:O	1:M:200:GLY:HA2	2.13	0.48
1:M:420:ARG:HB2	1:M:447:TYR:CZ	2.45	0.48
1:N:269:LEU:HD12	1:N:283:ILE:HG13	1.95	0.48
1:O:154:LEU:CB	1:O:156:LEU:CD1	2.91	0.48
1:O:250:PHE:O	1:O:253:ILE:N	2.46	0.48
1:P:300:THR:O	1:P:305:LEU:HD23	2.13	0.48
1:P:321:ILE:CD1	1:P:437:MET:HE1	2.43	0.48
1:R:175:LEU:HD11	1:T:275:GLU:OE1	2.12	0.48
1:R:212:LYS:NZ	3:R:502:DST:P1	2.86	0.48
1:R:402:TYR:O	1:R:405:THR:N	2.45	0.48
1:T:282:LYS:HB3	1:T:284:TYR:HE1	1.79	0.48
1:T:389:PHE:HE2	1:T:437:MET:HE3	1.77	0.48
1:W:237:ARG:HA	1:W:240:ASP:OD2	2.13	0.48
1:W:299:TRP:CD1	1:W:315:LEU:HB2	2.49	0.48
1:W:386:LEU:HD11	1:W:390:TRP:HZ2	1.76	0.48
1:X:427:TYR:HD1	1:X:437:MET:CE	2.27	0.48
1:X:433:ARG:HG3	1:X:436:TYR:CZ	2.49	0.48
1:V:119:ARG:N	1:V:119:ARG:HD2	2.29	0.48
1:V:228:VAL:CG1	1:V:232:ILE:HD11	2.40	0.48
1:G:112:ASN:ND2	1:G:122:ARG:HH21	2.12	0.48
1:G:303:GLY:O	1:G:306:ILE:HG13	2.13	0.48
1:B:63:PHE:CE2	1:B:109:PHE:HB2	2.48	0.48
1:B:231:LEU:HD12	1:B:232:ILE:N	2.28	0.48
1:B:232:ILE:O	1:B:236:VAL:HG23	2.13	0.48
1:B:402:TYR:O	1:B:405:THR:N	2.46	0.48
1:D:109:PHE:CD2	1:D:443:SER:HB3	2.47	0.48
1:D:171:PHE:HE1	1:D:231:LEU:CD1	2.26	0.48
1:D:303:GLY:O	1:D:306:ILE:HG13	2.14	0.48
1:F:300:THR:O	1:F:305:LEU:HD23	2.13	0.48
1:H:46:THR:OG1	1:H:49:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:386:LEU:CD1	1:I:390:TRP:HE1	2.27	0.48
1:J:389:PHE:CE2	1:J:393:LEU:HD11	2.48	0.48
1:K:100:ILE:O	2:K:501:QRP:CD1	2.61	0.48
1:K:269:LEU:CD1	1:K:283:ILE:HG13	2.44	0.48
1:L:378:ASN:O	1:L:382:VAL:HG23	2.12	0.48
1:M:47:ASN:HD22	1:N:95:LYS:NZ	2.11	0.48
1:M:102:ARG:NH1	1:M:375:HIS:CD2	2.81	0.48
1:N:259:GLU:OE2	1:N:304:ARG:NH1	2.46	0.48
1:N:382:VAL:O	1:N:386:LEU:HB2	2.13	0.48
1:P:100:ILE:HG13	1:P:101:SER:N	2.28	0.48
1:R:391:ASP:O	1:R:394:GLY:N	2.45	0.48
1:S:154:LEU:HB2	1:S:156:LEU:HD13	1.95	0.48
1:T:237:ARG:HA	1:T:240:ASP:OD2	2.13	0.48
1:U:250:PHE:O	1:U:253:ILE:N	2.47	0.48
1:W:117:SER:O	1:W:118:HIS:HB3	2.13	0.48
1:W:420:ARG:HB2	1:W:447:TYR:CZ	2.46	0.48
1:E:374:VAL:CG1	1:E:382:VAL:HG21	2.34	0.48
1:G:305:LEU:HD12	1:G:311:ILE:HG12	1.94	0.48
1:B:370:PHE:O	1:B:426:SER:HA	2.13	0.48
1:H:66:ALA:CB	1:H:409:LEU:HD11	2.43	0.48
1:H:420:ARG:HB2	1:H:447:TYR:CZ	2.45	0.48
1:H:430:THR:HG22	1:H:432:LYS:H	1.78	0.48
1:I:66:ALA:CB	1:I:409:LEU:HD11	2.41	0.48
1:I:299:TRP:NE1	1:I:311:ILE:HG23	2.26	0.48
1:J:63:PHE:HE2	1:J:109:PHE:HB2	1.78	0.48
1:J:167:LEU:HD12	1:J:167:LEU:N	2.29	0.48
1:M:428:SER:HB3	1:M:436:TYR:CB	2.39	0.48
1:N:228:VAL:CG1	1:N:232:ILE:HD11	2.38	0.48
1:O:171:PHE:HE1	1:O:231:LEU:CD1	2.27	0.48
1:Q:163:PHE:CD2	1:Q:279:GLN:NE2	2.82	0.48
1:R:75:TYR:CD2	1:S:75:TYR:HD2	2.22	0.48
1:R:255:ASP:HB3	1:R:304:ARG:NH1	2.29	0.48
1:T:53:TRP:CH2	1:T:78:MET:CE	2.97	0.48
1:T:268:PHE:CZ	1:T:284:TYR:CD2	3.01	0.48
1:W:386:LEU:HD11	1:W:390:TRP:CZ2	2.49	0.48
1:X:154:LEU:HB2	1:X:156:LEU:HD13	1.95	0.48
1:A:60:PHE:HE1	1:A:123:ILE:HD11	1.78	0.48
2:A:501:QRP:HB	3:A:502:DST:C13	2.44	0.48
1:V:275:GLU:HG3	1:V:278:GLU:OE1	2.14	0.48
1:V:324:LEU:O	1:V:327:ILE:HG22	2.14	0.48
1:V:390:TRP:CZ3	1:V:395:TRP:CZ3	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:GLY:O	1:E:354:ILE:HG23	2.14	0.48
1:G:239:ILE:HG13	1:G:239:ILE:O	2.13	0.48
1:D:172:GLN:HE22	1:H:165:GLN:CG	2.16	0.48
1:F:127:PRO:HD2	1:F:144:ILE:CD1	2.44	0.48
1:F:321:ILE:HG12	1:F:389:PHE:CD1	2.48	0.48
1:I:420:ARG:HB2	1:I:447:TYR:CZ	2.46	0.48
1:K:292:TRP:CZ2	1:K:315:LEU:HD21	2.47	0.48
1:K:354:ILE:HB	1:K:371:TYR:HB2	1.96	0.48
1:L:167:LEU:HD23	1:L:269:LEU:HD23	1.95	0.48
1:M:92:TYR:CB	1:M:93:PRO:HD3	2.44	0.48
1:S:160:ASP:HB3	1:S:162:PRO:HD2	1.95	0.48
1:S:321:ILE:HG22	1:S:325:LEU:HD23	1.95	0.48
1:X:120:LEU:HD21	1:X:205:PRO:HD3	1.96	0.48
1:C:89:LEU:HD22	1:C:106:PRO:HG2	1.95	0.48
1:V:269:LEU:CD1	1:V:283:ILE:HG13	2.43	0.48
1:G:174:SER:OG	1:G:175:LEU:N	2.47	0.48
1:B:237:ARG:O	1:B:240:ASP:HB2	2.14	0.48
1:I:79:PHE:CE2	1:L:42:HIS:HB2	2.48	0.48
1:I:300:THR:O	1:I:305:LEU:HD23	2.13	0.48
1:J:252:LEU:HD23	1:J:301:LEU:CD2	2.43	0.48
1:K:300:THR:O	1:K:305:LEU:HD23	2.14	0.48
1:L:285:GLY:O	1:L:354:ILE:HG23	2.14	0.48
1:O:424:TRP:HB2	1:O:440:TYR:CD2	2.49	0.48
1:P:36:GLN:OE1	1:P:58:SER:HA	2.13	0.48
1:P:52:TRP:CE3	1:P:89:LEU:HD13	2.48	0.48
1:Q:41:TYR:CZ	1:T:209:ILE:HD12	2.49	0.48
1:Q:266:TYR:HD1	2:Q:501:QRP:HAHA	1.78	0.48
1:Q:379:ASP:OD2	1:Q:421:LEU:HB2	2.14	0.48
1:Q:426:SER:O	1:Q:437:MET:HA	2.13	0.48
1:S:305:LEU:HD12	1:S:311:ILE:CD1	2.44	0.48
1:T:232:ILE:O	1:T:236:VAL:HG23	2.14	0.48
1:C:60:PHE:HE1	1:C:123:ILE:HD11	1.79	0.48
1:C:173:LEU:HD12	1:C:173:LEU:N	2.27	0.48
1:A:63:PHE:HE2	1:A:109:PHE:HB2	1.79	0.48
1:A:154:LEU:CB	1:A:156:LEU:HD13	2.43	0.48
1:A:209:ILE:C	1:A:210:LEU:HD12	2.34	0.48
1:A:420:ARG:HB2	1:A:447:TYR:CZ	2.49	0.48
1:E:70:GLY:HA3	1:E:73:GLN:HE22	1.78	0.48
1:G:102:ARG:HH11	1:G:375:HIS:CD2	2.32	0.48
1:G:180:GLN:HA	1:G:180:GLN:HE21	1.78	0.48
1:G:426:SER:O	1:G:437:MET:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:THR:OG1	1:B:421:LEU:HG	2.13	0.48
1:D:154:LEU:HB3	1:D:156:LEU:CD1	2.44	0.48
1:F:73:GLN:HG3	1:F:76:GLN:OE1	2.13	0.48
1:H:390:TRP:CZ3	1:H:395:TRP:CZ3	3.01	0.48
1:H:427:TYR:HD1	1:H:437:MET:HE2	1.78	0.48
1:K:390:TRP:CZ3	1:K:395:TRP:CZ3	3.02	0.48
1:L:389:PHE:HE2	1:L:437:MET:HE3	1.77	0.48
1:P:284:TYR:N	1:P:284:TYR:HD1	2.12	0.48
1:S:448:LEU:HD12	1:S:448:LEU:N	2.29	0.48
1:W:410:TYR:CD1	1:W:421:LEU:HD22	2.48	0.48
1:X:102:ARG:NH1	1:X:375:HIS:CD2	2.81	0.48
1:C:112:ASN:HD22	1:C:122:ARG:HH21	1.59	0.48
1:C:373:PRO:HG3	1:C:424:TRP:HZ3	1.79	0.48
1:E:147:LEU:HD23	1:E:199:PHE:CD2	2.49	0.48
1:G:108:GLU:HA	1:G:443:SER:OG	2.14	0.48
1:G:228:VAL:CG1	1:G:232:ILE:HD11	2.38	0.48
1:G:324:LEU:HB3	1:G:385:ALA:HB1	1.96	0.48
1:B:46:THR:OG1	1:B:49:GLN:HG3	2.14	0.48
1:B:167:LEU:HD23	1:B:269:LEU:HD23	1.96	0.48
1:D:126:GLU:OE2	1:D:195:SER:CB	2.62	0.48
1:D:160:ASP:HB3	1:D:162:PRO:HD2	1.96	0.48
1:D:430:THR:HG22	1:D:432:LYS:N	2.29	0.48
1:F:127:PRO:HG3	1:F:147:LEU:HD22	1.95	0.48
1:F:369:LYS:HA	1:F:427:TYR:O	2.13	0.48
1:H:112:ASN:ND2	1:H:122:ARG:HH21	2.11	0.48
1:I:163:PHE:O	1:I:167:LEU:HD13	2.14	0.48
1:I:171:PHE:HE1	1:I:231:LEU:HD13	1.78	0.48
1:I:275:GLU:CD	1:K:175:LEU:HD11	2.34	0.48
1:I:419:THR:HG23	1:I:420:ARG:HG3	1.94	0.48
1:I:433:ARG:HG3	1:I:436:TYR:CZ	2.48	0.48
1:J:115:LYS:HG2	1:J:395:TRP:HE1	1.79	0.48
1:J:311:ILE:H	1:J:311:ILE:HD12	1.77	0.48
1:L:284:TYR:N	1:L:284:TYR:HD1	2.12	0.48
1:M:117:SER:O	1:M:118:HIS:HB3	2.14	0.48
1:N:426:SER:O	1:N:437:MET:HG3	2.12	0.48
1:P:53:TRP:CZ3	1:P:78:MET:CE	2.97	0.48
1:P:112:ASN:ND2	1:P:122:ARG:HH21	2.09	0.48
1:Q:123:ILE:O	1:Q:200:GLY:HA2	2.14	0.48
1:Q:290:VAL:HG23	1:Q:294:LYS:CG	2.44	0.48
1:R:193:LEU:N	1:R:193:LEU:HD12	2.29	0.48
1:S:228:VAL:CG1	1:S:232:ILE:HD11	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:311:ILE:H	1:W:311:ILE:HD12	1.79	0.48
1:C:66:ALA:HB2	1:C:409:LEU:HD11	1.95	0.48
1:C:321:ILE:HD11	1:C:437:MET:HE1	1.95	0.48
1:A:321:ILE:HD11	1:A:437:MET:HE1	1.96	0.48
1:V:60:PHE:HD1	1:V:109:PHE:CE1	2.32	0.48
1:V:290:VAL:HG23	1:V:294:LYS:HB3	1.96	0.48
1:V:292:TRP:CZ2	1:V:319:LYS:HB2	2.48	0.48
1:V:433:ARG:HG3	1:V:436:TYR:OH	2.14	0.48
1:G:52:TRP:CE3	1:G:89:LEU:HD13	2.48	0.48
1:B:117:SER:O	1:B:118:HIS:HB3	2.13	0.48
1:D:240:ASP:CG	1:D:247:THR:HG22	2.34	0.48
1:D:374:VAL:HG11	1:D:382:VAL:HG11	1.95	0.48
1:F:354:ILE:HG21	3:F:502:DST:C13	2.40	0.48
1:F:386:LEU:HD13	1:F:390:TRP:CE2	2.49	0.48
1:I:318:LEU:HD12	1:I:427:TYR:HD2	1.79	0.48
1:J:147:LEU:HD23	1:J:199:PHE:HD2	1.79	0.48
1:J:410:TYR:CD1	1:J:421:LEU:HD22	2.49	0.48
1:K:115:LYS:HE2	1:K:434:GLY:CA	2.41	0.48
1:K:266:TYR:CD1	2:K:501:QRP:HAHA	2.48	0.48
1:K:305:LEU:CD1	1:K:311:ILE:HG12	2.43	0.48
1:L:127:PRO:HG3	1:L:147:LEU:CD2	2.43	0.48
1:M:229:GLY:HA3	1:M:263:TYR:CE2	2.49	0.48
1:O:63:PHE:CE2	1:O:109:PHE:HB2	2.48	0.48
1:O:115:LYS:HE2	1:O:435:VAL:N	2.28	0.48
1:O:172:GLN:CA	1:O:173:LEU:HD12	2.43	0.48
1:P:193:LEU:N	1:P:193:LEU:HD12	2.29	0.48
1:P:239:ILE:HA	1:P:242:GLU:HB3	1.94	0.48
1:Q:211:VAL:HG12	1:Q:273:PHE:CD2	2.48	0.48
1:Q:269:LEU:CD1	1:Q:283:ILE:HG13	2.44	0.48
1:R:275:GLU:OE1	1:T:175:LEU:HD11	2.13	0.48
1:T:305:LEU:HD11	1:T:311:ILE:HG12	1.95	0.48
1:T:430:THR:HG22	1:T:432:LYS:N	2.28	0.48
1:U:51:ARG:HB2	1:U:92:TYR:HB2	1.96	0.48
1:X:173:LEU:HD12	1:X:173:LEU:N	2.28	0.48
1:X:378:ASN:O	1:X:382:VAL:HG23	2.14	0.48
1:A:305:LEU:HD11	1:A:311:ILE:HG12	1.95	0.47
1:A:390:TRP:CZ3	1:A:395:TRP:CZ3	3.01	0.47
1:G:284:TYR:N	1:G:284:TYR:CD1	2.81	0.47
1:B:160:ASP:HB3	1:B:162:PRO:HD2	1.96	0.47
1:H:433:ARG:HD2	1:H:436:TYR:HE1	1.78	0.47
1:I:229:GLY:HA3	1:I:263:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:320:GLN:CB	1:I:320:GLN:NE2	2.76	0.47
1:K:282:LYS:HB3	1:K:284:TYR:HE1	1.78	0.47
1:N:256:TYR:CD2	1:N:301:LEU:HD12	2.49	0.47
1:N:369:LYS:O	1:N:370:PHE:HD1	1.97	0.47
1:O:320:GLN:HE22	1:O:392:SER:HB3	1.79	0.47
1:O:374:VAL:HG11	1:O:382:VAL:HG11	1.96	0.47
1:S:115:LYS:HE2	1:S:435:VAL:N	2.29	0.47
1:X:89:LEU:HD22	1:X:106:PRO:HG2	1.95	0.47
1:X:398:HIS:H	1:X:398:HIS:CD2	2.32	0.47
1:C:390:TRP:CZ3	1:C:395:TRP:CZ3	3.02	0.47
1:A:311:ILE:H	1:A:311:ILE:HD12	1.79	0.47
1:V:112:ASN:ND2	1:V:122:ARG:HH21	2.05	0.47
1:B:300:THR:HA	1:B:305:LEU:HD21	1.96	0.47
1:I:374:VAL:CG1	1:I:382:VAL:HG21	2.38	0.47
1:I:379:ASP:OD2	1:I:421:LEU:HB2	2.14	0.47
1:J:167:LEU:O	1:J:171:PHE:HD2	1.97	0.47
1:J:299:TRP:CZ2	1:J:368:PRO:HG2	2.50	0.47
1:K:237:ARG:HA	1:K:240:ASP:OD2	2.13	0.47
1:K:318:LEU:HD23	1:K:318:LEU:O	2.14	0.47
1:L:299:TRP:CD1	1:L:311:ILE:HG23	2.49	0.47
1:L:448:LEU:N	1:L:448:LEU:HD12	2.29	0.47
1:M:407:GLN:NE2	1:M:413:GLN:O	2.32	0.47
2:N:501:QRP:HB	3:N:502:DST:C13	2.44	0.47
1:O:379:ASP:OD2	1:O:421:LEU:N	2.45	0.47
1:R:60:PHE:CE1	1:R:123:ILE:HD11	2.50	0.47
1:S:320:GLN:CB	1:S:320:GLN:CD	2.76	0.47
1:T:172:GLN:CA	1:T:173:LEU:HD12	2.44	0.47
1:W:154:LEU:CB	1:W:156:LEU:CD1	2.91	0.47
1:X:250:PHE:O	1:X:253:ILE:N	2.47	0.47
1:V:321:ILE:CG1	1:V:389:PHE:CE1	2.98	0.47
1:I:233:ALA:HA	1:I:250:PHE:CE2	2.49	0.47
1:I:440:TYR:OH	3:I:502:DST:O7	2.16	0.47
1:J:292:TRP:HZ2	1:J:315:LEU:CD2	2.28	0.47
1:J:379:ASP:OD2	1:J:421:LEU:HB2	2.15	0.47
1:K:433:ARG:HG3	1:K:436:TYR:OH	2.13	0.47
1:L:212:LYS:NZ	3:L:502:DST:P1	2.88	0.47
1:L:268:PHE:CZ	1:L:284:TYR:CD2	3.02	0.47
1:M:240:ASP:CG	1:M:247:THR:HG22	2.34	0.47
1:M:300:THR:O	1:M:305:LEU:HD23	2.14	0.47
1:N:60:PHE:HD1	1:N:109:PHE:CE1	2.32	0.47
1:N:100:ILE:O	2:N:501:QRP:CD1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:175:LEU:HD11	1:P:275:GLU:OE1	2.14	0.47
1:P:115:LYS:HG2	1:P:395:TRP:CZ2	2.50	0.47
1:P:284:TYR:N	1:P:284:TYR:CD1	2.83	0.47
1:Q:371:TYR:OH	3:Q:502:DST:O7	2.17	0.47
1:R:102:ARG:HH11	1:R:375:HIS:CD2	2.32	0.47
1:S:53:TRP:CZ3	1:S:78:MET:CE	2.97	0.47
1:S:122:ARG:HG2	1:S:202:ASP:OD1	2.13	0.47
1:S:228:VAL:O	1:S:232:ILE:HG13	2.15	0.47
1:S:320:GLN:CG	1:S:320:GLN:HA	2.43	0.47
1:T:193:LEU:HD12	1:T:193:LEU:N	2.29	0.47
1:T:371:TYR:HA	1:T:425:ILE:O	2.14	0.47
1:U:311:ILE:H	1:U:311:ILE:HD12	1.80	0.47
1:U:354:ILE:HG21	3:U:502:DST:C13	2.41	0.47
1:C:83:HIS:O	1:C:87:PRO:HG2	2.14	0.47
1:C:278:GLU:N	1:C:278:GLU:OE1	2.47	0.47
1:A:324:LEU:HB3	1:A:385:ALA:HB1	1.95	0.47
1:E:109:PHE:CD2	1:E:443:SER:HB3	2.48	0.47
1:D:250:PHE:O	1:D:253:ILE:N	2.47	0.47
1:I:81:PHE:HD1	1:I:85:LEU:HD12	1.80	0.47
1:I:410:TYR:OH	1:I:441:TYR:HB3	2.15	0.47
1:J:147:LEU:HD23	1:J:199:PHE:CD2	2.49	0.47
1:K:63:PHE:HE2	1:K:109:PHE:HB2	1.79	0.47
1:K:102:ARG:NH1	1:K:375:HIS:CD2	2.82	0.47
1:L:108:GLU:HA	1:L:443:SER:CB	2.44	0.47
1:L:279:GLN:O	1:L:361:PRO:HD3	2.13	0.47
1:N:301:LEU:HD13	1:N:357:TYR:CE1	2.49	0.47
1:N:440:TYR:OH	3:N:502:DST:O7	2.18	0.47
1:O:321:ILE:O	1:O:325:LEU:HD23	2.15	0.47
1:O:359:ILE:O	1:O:359:ILE:HG22	2.14	0.47
1:O:402:TYR:O	1:O:405:THR:N	2.47	0.47
1:Q:115:LYS:HE2	1:Q:435:VAL:H	1.77	0.47
1:T:107:ILE:HA	1:T:124:GLY:O	2.13	0.47
1:T:321:ILE:CD1	1:T:437:MET:HE1	2.44	0.47
1:W:123:ILE:CD1	1:W:203:PHE:HE2	2.26	0.47
1:C:160:ASP:HB3	1:C:162:PRO:HD2	1.96	0.47
1:A:53:TRP:CH2	1:A:78:MET:CE	2.98	0.47
1:A:180:GLN:HE22	1:A:223:ALA:CA	2.27	0.47
1:A:386:LEU:CD1	1:A:390:TRP:HE1	2.27	0.47
1:V:160:ASP:HB3	1:V:162:PRO:HD2	1.95	0.47
1:B:63:PHE:HB3	1:B:121:LEU:HD13	1.96	0.47
1:D:83:HIS:O	1:D:87:PRO:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ASP:HB3	1:D:162:PRO:CD	2.44	0.47
1:H:120:LEU:HD21	1:H:205:PRO:HD3	1.94	0.47
1:H:212:LYS:NZ	3:H:502:DST:P1	2.87	0.47
1:H:284:TYR:N	1:H:284:TYR:HD1	2.13	0.47
1:H:311:ILE:HD12	1:H:311:ILE:H	1.80	0.47
1:H:379:ASP:OD2	1:H:421:LEU:HB2	2.14	0.47
1:J:126:GLU:OE2	1:J:195:SER:HB2	2.13	0.47
1:K:285:GLY:HA3	1:K:355:TRP:CE2	2.49	0.47
1:K:305:LEU:HD23	1:K:305:LEU:N	2.29	0.47
1:L:63:PHE:HE2	1:L:109:PHE:HB2	1.79	0.47
1:L:290:VAL:HG22	1:L:295:ILE:HG13	1.96	0.47
1:L:369:LYS:HA	1:L:427:TYR:O	2.15	0.47
1:N:99:THR:HG23	1:N:193:LEU:CD2	2.23	0.47
1:O:117:SER:O	1:O:118:HIS:HB3	2.14	0.47
1:P:301:LEU:HD13	1:P:357:TYR:CZ	2.49	0.47
1:Q:430:THR:HG22	1:Q:432:LYS:N	2.30	0.47
1:R:99:THR:HG23	1:R:193:LEU:CD2	2.30	0.47
1:R:173:LEU:O	1:R:174:SER:OG	2.18	0.47
1:T:354:ILE:HG21	3:T:502:DST:C13	2.43	0.47
1:T:391:ASP:O	1:T:394:GLY:N	2.47	0.47
1:T:415:ILE:HA	1:T:418:THR:CG2	2.45	0.47
1:T:426:SER:O	1:T:437:MET:HA	2.13	0.47
1:U:209:ILE:HD12	1:X:41:TYR:CZ	2.50	0.47
1:U:410:TYR:CD1	1:U:421:LEU:HD22	2.50	0.47
2:C:501:QRP:HB	3:C:502:DST:C13	2.44	0.47
1:G:63:PHE:CE2	1:G:109:PHE:CB	2.97	0.47
1:D:70:GLY:HA3	1:D:73:GLN:HE22	1.79	0.47
1:D:291:THR:O	1:D:295:ILE:HG13	2.14	0.47
1:D:375:HIS:H	1:D:423:SER:HA	1.79	0.47
1:F:240:ASP:CG	1:F:247:THR:HG22	2.35	0.47
1:H:234:GLU:OE2	1:H:237:ARG:NH2	2.47	0.47
1:I:386:LEU:HD13	1:I:390:TRP:CE2	2.49	0.47
1:J:46:THR:OG1	1:J:49:GLN:HG3	2.15	0.47
1:J:275:GLU:CD	1:L:175:LEU:HD11	2.35	0.47
1:K:371:TYR:HA	1:K:425:ILE:O	2.14	0.47
1:L:374:VAL:HG11	1:L:382:VAL:HG11	1.97	0.47
1:N:275:GLU:HG3	1:N:278:GLU:OE1	2.14	0.47
1:N:369:LYS:HA	1:N:427:TYR:O	2.14	0.47
1:P:53:TRP:CH2	1:P:78:MET:HE1	2.49	0.47
1:P:115:LYS:HE2	1:P:434:GLY:CA	2.40	0.47
1:P:171:PHE:HE1	1:P:231:LEU:CD1	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:232:ILE:O	1:Q:236:VAL:HG23	2.14	0.47
1:T:154:LEU:HB3	1:T:156:LEU:CD1	2.44	0.47
1:T:249:ALA:HB3	1:T:359:ILE:HG23	1.96	0.47
1:U:83:HIS:NE2	1:X:83:HIS:NE2	2.52	0.47
1:U:231:LEU:HD12	1:U:232:ILE:N	2.29	0.47
1:W:269:LEU:CD1	1:W:283:ILE:HG13	2.44	0.47
1:W:292:TRP:HZ2	1:W:315:LEU:HD21	1.79	0.47
1:X:324:LEU:HB3	1:X:385:ALA:HB1	1.97	0.47
1:C:127:PRO:HG3	1:C:147:LEU:CD2	2.45	0.47
1:C:253:ILE:HD12	1:C:359:ILE:HD11	1.97	0.47
1:A:115:LYS:HA	1:A:395:TRP:CE2	2.50	0.47
1:A:317:ARG:O	1:A:320:GLN:HB3	2.14	0.47
1:A:369:LYS:HA	1:A:427:TYR:O	2.15	0.47
1:V:373:PRO:HG3	1:V:424:TRP:CZ3	2.50	0.47
1:G:51:ARG:HB2	1:G:92:TYR:HB2	1.97	0.47
1:G:105:LEU:HD12	1:G:105:LEU:C	2.35	0.47
1:G:390:TRP:CZ3	1:G:395:TRP:CZ3	3.02	0.47
1:B:284:TYR:N	1:B:284:TYR:CD1	2.82	0.47
1:D:167:LEU:N	1:D:167:LEU:HD12	2.29	0.47
1:D:173:LEU:HD12	1:D:173:LEU:N	2.30	0.47
1:D:321:ILE:HD13	1:D:437:MET:HE1	1.96	0.47
1:F:299:TRP:CD1	1:F:311:ILE:HG23	2.50	0.47
1:H:369:LYS:HA	1:H:427:TYR:O	2.15	0.47
1:I:173:LEU:HD13	1:I:196:GLN:NE2	2.30	0.47
1:J:161:THR:H	1:J:162:PRO:HD3	1.77	0.47
1:J:221:ALA:HB2	1:J:231:LEU:HD21	1.97	0.47
1:J:321:ILE:O	1:J:325:LEU:HD23	2.15	0.47
1:K:95:LYS:NZ	1:L:47:ASN:ND2	2.62	0.47
1:K:373:PRO:HG3	1:K:424:TRP:HZ3	1.79	0.47
1:L:284:TYR:N	1:L:284:TYR:CD1	2.83	0.47
1:L:305:LEU:HD23	1:L:305:LEU:H	1.80	0.47
1:L:386:LEU:HD13	1:L:390:TRP:CE2	2.49	0.47
1:M:253:ILE:HD12	1:M:359:ILE:HD11	1.97	0.47
1:M:426:SER:O	1:M:437:MET:HA	2.14	0.47
1:N:45:PRO:HD2	1:N:49:GLN:OE1	2.15	0.47
1:N:303:GLY:O	1:N:306:ILE:HG13	2.14	0.47
1:O:60:PHE:HD1	1:O:109:PHE:CE1	2.33	0.47
1:O:420:ARG:HB2	1:O:447:TYR:CZ	2.47	0.47
1:P:370:PHE:O	1:P:426:SER:HA	2.15	0.47
1:Q:75:TYR:HE2	1:T:72:PRO:HA	1.80	0.47
1:Q:171:PHE:CE1	1:Q:231:LEU:HD13	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:176:SER:O	1:Q:180:GLN:HG2	2.14	0.47
1:Q:386:LEU:HD13	1:Q:390:TRP:CE2	2.49	0.47
1:R:266:TYR:CD1	2:R:501:QRP:HAHA	2.50	0.47
1:R:324:LEU:HB3	1:R:385:ALA:HB1	1.96	0.47
1:R:354:ILE:HG21	3:R:502:DST:C13	2.40	0.47
1:U:173:LEU:HD12	1:U:173:LEU:N	2.30	0.47
1:W:147:LEU:HD23	1:W:199:PHE:CD2	2.50	0.47
1:W:386:LEU:HD13	1:W:390:TRP:HE1	1.77	0.47
1:W:426:SER:O	1:W:437:MET:HG3	2.15	0.47
1:C:386:LEU:HD13	1:C:390:TRP:CE2	2.50	0.47
1:C:386:LEU:CD1	1:C:390:TRP:HE1	2.28	0.47
1:B:112:ASN:HD22	1:B:122:ARG:HH21	1.63	0.47
1:D:427:TYR:HD1	1:D:437:MET:HE2	1.80	0.47
1:F:72:PRO:HB2	1:F:73:GLN:OE1	2.15	0.47
1:F:406:LEU:HD12	1:F:415:ILE:HD11	1.93	0.47
1:H:448:LEU:HD12	1:H:448:LEU:N	2.30	0.47
1:I:83:HIS:NE2	1:L:83:HIS:NE2	2.50	0.47
1:I:173:LEU:HD12	1:I:173:LEU:N	2.29	0.47
1:I:206:ASP:O	1:I:208:ALA:N	2.46	0.47
1:J:257:MET:HE3	1:J:263:TYR:N	2.30	0.47
1:M:285:GLY:O	1:M:354:ILE:HG23	2.14	0.47
1:N:233:ALA:HA	1:N:250:PHE:CE2	2.50	0.47
1:N:374:VAL:CG1	1:N:382:VAL:HG21	2.42	0.47
1:Q:209:ILE:HD12	1:T:41:TYR:CZ	2.49	0.47
1:S:292:TRP:CZ2	1:S:319:LYS:HB2	2.50	0.47
1:T:81:PHE:HD1	1:T:85:LEU:HD12	1.80	0.47
1:U:126:GLU:OE2	1:U:195:SER:CB	2.62	0.47
1:W:317:ARG:HB2	1:W:427:TYR:OH	2.15	0.47
1:C:70:GLY:HA3	1:C:73:GLN:HE22	1.79	0.47
1:C:430:THR:HG22	1:C:432:LYS:H	1.80	0.47
1:A:60:PHE:CE2	1:A:64:LEU:HD11	2.50	0.47
1:V:115:LYS:HE2	1:V:435:VAL:N	2.30	0.47
1:V:211:VAL:HG12	1:V:273:PHE:CD2	2.50	0.47
1:V:227:PRO:O	1:V:230:THR:OG1	2.32	0.47
2:V:501:QRP:O	2:V:501:QRP:HE3	2.15	0.47
1:E:51:ARG:HB3	1:E:92:TYR:CG	2.50	0.47
1:E:83:HIS:O	1:E:87:PRO:HG2	2.15	0.47
1:E:228:VAL:O	1:E:232:ILE:HG13	2.14	0.47
1:B:102:ARG:NH1	1:B:375:HIS:CD2	2.83	0.47
1:B:275:GLU:OE1	1:F:175:LEU:HD11	2.15	0.47
1:B:418:THR:CG2	1:B:421:LEU:HD12	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:ASP:CG	1:H:247:THR:HG22	2.36	0.47
1:J:180:GLN:OE1	1:J:180:GLN:HA	2.15	0.47
1:J:206:ASP:OD1	1:J:207:GLY:N	2.47	0.47
1:K:127:PRO:CG	1:K:147:LEU:HD23	2.44	0.47
1:O:311:ILE:H	1:O:311:ILE:HD12	1.79	0.47
1:P:115:LYS:HE2	1:P:435:VAL:H	1.80	0.47
1:P:299:TRP:NE1	1:P:311:ILE:HG23	2.30	0.47
1:Q:356:ASN:HB3	1:Q:369:LYS:HB3	1.96	0.47
1:R:200:GLY:N	1:R:212:LYS:O	2.43	0.47
1:T:255:ASP:O	1:T:259:GLU:HG3	2.14	0.47
1:C:285:GLY:HA3	1:C:355:TRP:CE2	2.50	0.47
1:A:140:ASN:OD1	1:A:143:PRO:HG2	2.15	0.47
1:V:369:LYS:HA	1:V:427:TYR:O	2.15	0.47
1:V:410:TYR:CD1	1:V:421:LEU:HD22	2.50	0.47
1:E:370:PHE:O	1:E:426:SER:HA	2.15	0.47
1:E:412:ASP:OD1	1:E:413:GLN:N	2.48	0.47
1:G:102:ARG:NH1	1:G:375:HIS:CD2	2.83	0.47
1:B:426:SER:O	1:B:437:MET:HG3	2.15	0.47
1:D:278:GLU:OE1	1:D:278:GLU:N	2.47	0.47
1:D:386:LEU:HD11	1:D:390:TRP:HZ2	1.80	0.47
1:F:390:TRP:CZ3	1:F:395:TRP:CZ3	3.03	0.47
1:I:63:PHE:HB3	1:I:121:LEU:CD1	2.45	0.47
1:K:386:LEU:HD13	1:K:390:TRP:HE1	1.78	0.47
1:P:172:GLN:CA	1:P:173:LEU:HD12	2.45	0.47
1:P:373:PRO:HG3	1:P:424:TRP:CZ3	2.50	0.47
1:Q:305:LEU:HD12	1:Q:311:ILE:HD11	1.97	0.47
1:Q:305:LEU:HD12	1:Q:311:ILE:HG12	1.97	0.47
1:Q:318:LEU:HD12	1:Q:427:TYR:HD2	1.80	0.47
1:Q:321:ILE:HD13	1:Q:437:MET:HE1	1.96	0.47
1:R:266:TYR:HD1	2:R:501:QRP:HAHA	1.80	0.47
1:R:386:LEU:HD11	1:R:390:TRP:HZ2	1.80	0.47
1:U:212:LYS:HZ3	3:U:502:DST:P1	2.37	0.47
1:A:419:THR:HG23	1:A:420:ARG:HG3	1.97	0.46
1:E:231:LEU:HD12	1:E:232:ILE:N	2.30	0.46
1:G:274:VAL:HG22	1:G:275:GLU:N	2.30	0.46
1:G:278:GLU:OE1	1:G:278:GLU:N	2.48	0.46
1:D:100:ILE:O	2:D:501:QRP:CD1	2.63	0.46
1:D:172:GLN:CA	1:D:173:LEU:HD12	2.45	0.46
1:D:370:PHE:O	1:D:426:SER:HA	2.15	0.46
1:D:402:TYR:O	1:D:405:THR:N	2.48	0.46
1:F:115:LYS:HE2	1:F:435:VAL:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:430:THR:HG22	1:F:432:LYS:H	1.80	0.46
1:I:212:LYS:NZ	3:I:502:DST:P1	2.88	0.46
1:L:418:THR:OG1	1:L:421:LEU:HG	2.15	0.46
1:M:165:GLN:CG	1:O:172:GLN:HE22	2.13	0.46
1:N:212:LYS:NZ	3:N:502:DST:P1	2.88	0.46
1:P:100:ILE:O	2:P:501:QRP:CG	2.63	0.46
1:P:167:LEU:O	1:P:171:PHE:HD2	1.98	0.46
1:Q:53:TRP:CH2	1:Q:78:MET:HE1	2.50	0.46
1:Q:115:LYS:HG2	1:Q:395:TRP:CE2	2.50	0.46
1:R:140:ASN:OD1	1:R:143:PRO:HG2	2.15	0.46
1:R:167:LEU:HD23	1:R:269:LEU:HD23	1.96	0.46
1:S:268:PHE:CZ	1:S:284:TYR:CD2	3.03	0.46
1:T:63:PHE:CE2	1:T:109:PHE:CB	2.98	0.46
1:T:292:TRP:CZ2	1:T:315:LEU:HD21	2.50	0.46
1:U:212:LYS:NZ	3:U:502:DST:P1	2.88	0.46
1:U:305:LEU:HD11	1:U:311:ILE:HG12	1.97	0.46
1:W:160:ASP:HB3	1:W:162:PRO:HD2	1.97	0.46
1:W:320:GLN:NE2	1:W:392:SER:HB3	2.30	0.46
1:X:299:TRP:CZ2	1:X:368:PRO:HG2	2.50	0.46
1:C:448:LEU:HD12	1:C:448:LEU:H	1.78	0.46
1:A:100:ILE:O	2:A:501:QRP:CD1	2.63	0.46
1:A:303:GLY:O	1:A:306:ILE:HG13	2.15	0.46
1:V:173:LEU:HD12	1:V:173:LEU:N	2.28	0.46
1:E:45:PRO:HD2	1:E:49:GLN:OE1	2.15	0.46
1:E:240:ASP:OD2	1:E:247:THR:HG22	2.15	0.46
1:E:321:ILE:HD11	1:E:389:PHE:CE2	2.50	0.46
1:G:173:LEU:HD12	1:G:173:LEU:N	2.30	0.46
1:B:175:LEU:HD11	1:F:275:GLU:OE1	2.15	0.46
1:D:306:ILE:HD12	1:D:307:GLU:N	2.30	0.46
1:F:224:ALA:O	1:F:226:VAL:HG23	2.16	0.46
1:F:284:TYR:N	1:F:284:TYR:HD1	2.13	0.46
1:H:212:LYS:HB2	1:H:212:LYS:HE3	1.69	0.46
1:I:70:GLY:HA3	1:I:73:GLN:HE22	1.79	0.46
1:J:410:TYR:CE1	1:J:421:LEU:HD22	2.51	0.46
1:K:292:TRP:HZ2	1:K:315:LEU:HD21	1.81	0.46
1:L:160:ASP:HB3	1:L:162:PRO:HD3	1.97	0.46
1:M:85:LEU:HD22	1:M:125:PHE:CE1	2.50	0.46
1:M:212:LYS:NZ	3:M:502:DST:P1	2.88	0.46
1:N:226:VAL:HG12	1:N:230:THR:OG1	2.15	0.46
1:O:292:TRP:CZ2	1:O:319:LYS:HB2	2.50	0.46
1:O:295:ILE:HG23	1:O:370:PHE:HE2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:321:ILE:CG2	1:O:325:LEU:HD23	2.44	0.46
1:P:353:ILE:HD12	1:P:353:ILE:C	2.35	0.46
1:P:440:TYR:OH	3:P:502:DST:O8	2.34	0.46
1:R:126:GLU:OE2	1:R:195:SER:HB2	2.14	0.46
1:S:117:SER:O	1:S:118:HIS:HB3	2.15	0.46
1:S:290:VAL:HG22	1:S:295:ILE:HG13	1.97	0.46
1:S:295:ILE:HG23	1:S:370:PHE:HE2	1.79	0.46
1:T:281:LEU:C	1:T:281:LEU:HD12	2.35	0.46
1:U:53:TRP:CH2	1:U:78:MET:CE	2.99	0.46
1:X:389:PHE:CE2	1:X:437:MET:HE3	2.50	0.46
1:C:171:PHE:CE1	1:C:217:PRO:CB	2.97	0.46
1:V:63:PHE:CE1	1:V:409:LEU:HD23	2.50	0.46
1:V:354:ILE:HG21	3:V:502:DST:C13	2.43	0.46
1:V:402:TYR:O	1:V:405:THR:N	2.47	0.46
1:E:274:VAL:HG22	1:E:275:GLU:N	2.30	0.46
1:G:321:ILE:HG22	1:G:325:LEU:CD2	2.44	0.46
1:B:305:LEU:HD12	1:B:311:ILE:HG12	1.96	0.46
1:F:279:GLN:O	1:F:361:PRO:HD3	2.15	0.46
1:H:115:LYS:HG2	1:H:395:TRP:HE1	1.80	0.46
1:H:171:PHE:HE1	1:H:231:LEU:CD1	2.28	0.46
1:I:127:PRO:HG3	1:I:147:LEU:HD23	1.96	0.46
1:J:160:ASP:HB3	1:J:162:PRO:HD2	1.97	0.46
1:J:240:ASP:CG	1:J:247:THR:HG22	2.36	0.46
1:J:253:ILE:HD12	1:J:359:ILE:HD11	1.97	0.46
1:L:51:ARG:HB2	1:L:92:TYR:HB2	1.97	0.46
1:L:391:ASP:O	1:L:394:GLY:N	2.49	0.46
1:M:63:PHE:CE1	1:M:409:LEU:HD23	2.50	0.46
1:M:418:THR:OG1	1:M:421:LEU:HG	2.16	0.46
1:N:75:TYR:CD2	1:O:75:TYR:HD2	2.17	0.46
1:N:85:LEU:HD22	1:N:125:PHE:CD1	2.50	0.46
1:N:351:SER:OG	1:N:373:PRO:HB3	2.15	0.46
1:O:102:ARG:NH1	1:O:375:HIS:CD2	2.84	0.46
1:O:167:LEU:N	1:O:167:LEU:HD12	2.30	0.46
1:O:299:TRP:CH2	1:O:368:PRO:HG2	2.51	0.46
1:P:228:VAL:CG1	1:P:232:ILE:HD11	2.40	0.46
1:P:257:MET:HE1	1:P:355:TRP:CZ2	2.50	0.46
1:Q:228:VAL:CG1	1:Q:232:ILE:HD11	2.43	0.46
1:S:284:TYR:N	1:S:284:TYR:HD1	2.14	0.46
1:S:308:GLU:HB2	1:S:311:ILE:CD1	2.43	0.46
1:U:115:LYS:HE2	1:U:435:VAL:N	2.30	0.46
1:W:252:LEU:CD2	1:W:301:LEU:HD23	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:284:TYR:N	1:X:284:TYR:HD1	2.13	0.46
1:X:386:LEU:CD1	1:X:390:TRP:HE1	2.29	0.46
1:A:275:GLU:HG3	1:A:278:GLU:OE1	2.14	0.46
1:V:173:LEU:HB3	1:V:176:SER:HB2	1.97	0.46
1:V:321:ILE:HD13	1:V:437:MET:HE1	1.97	0.46
1:E:299:TRP:CD1	1:E:311:ILE:HG23	2.50	0.46
1:E:379:ASP:OD2	1:E:421:LEU:HB2	2.16	0.46
1:G:53:TRP:CH2	1:G:78:MET:CE	2.99	0.46
1:G:127:PRO:HB2	1:G:143:PRO:HB2	1.97	0.46
1:B:115:LYS:HG2	1:B:395:TRP:NE1	2.30	0.46
1:D:212:LYS:HZ3	3:D:502:DST:P1	2.37	0.46
1:H:52:TRP:CD2	1:H:89:LEU:HD13	2.50	0.46
1:H:102:ARG:NH1	1:H:375:HIS:CD2	2.84	0.46
1:I:110:SER:HB2	1:I:122:ARG:CB	2.16	0.46
1:I:111:LEU:O	1:I:438:SER:HA	2.14	0.46
1:I:430:THR:HG22	1:I:432:LYS:N	2.30	0.46
1:J:60:PHE:CE2	1:J:64:LEU:HD11	2.50	0.46
1:J:85:LEU:HB3	1:J:125:PHE:CE1	2.45	0.46
1:K:53:TRP:CZ3	1:K:78:MET:CE	2.98	0.46
1:K:299:TRP:CD1	1:K:311:ILE:HG23	2.50	0.46
1:K:356:ASN:HB3	1:K:369:LYS:HB3	1.96	0.46
1:N:326:GLN:O	1:N:326:GLN:HG3	2.16	0.46
1:N:386:LEU:HD13	1:N:390:TRP:CE2	2.50	0.46
1:O:373:PRO:HG3	1:O:424:TRP:CZ3	2.50	0.46
1:Q:300:THR:O	1:Q:305:LEU:HD23	2.15	0.46
1:W:300:THR:O	1:W:305:LEU:HD23	2.15	0.46
1:C:100:ILE:O	2:C:501:QRP:CG	2.64	0.46
1:C:324:LEU:HB3	1:C:385:ALA:HB1	1.97	0.46
1:E:154:LEU:HB2	1:E:156:LEU:HD13	1.96	0.46
1:D:81:PHE:CE2	1:D:86:ILE:HD11	2.51	0.46
1:D:249:ALA:HB3	1:D:359:ILE:HG23	1.98	0.46
1:I:81:PHE:CD1	1:I:85:LEU:HD12	2.51	0.46
1:I:369:LYS:HA	1:I:427:TYR:O	2.16	0.46
1:J:274:VAL:HG22	1:J:275:GLU:N	2.30	0.46
1:K:92:TYR:CB	1:K:93:PRO:HD3	2.45	0.46
1:L:100:ILE:HG13	1:L:101:SER:N	2.31	0.46
1:O:410:TYR:OH	1:O:441:TYR:HB3	2.16	0.46
1:S:270:SER:HB3	1:S:282:LYS:HB2	1.97	0.46
1:S:386:LEU:HD13	1:S:390:TRP:CE2	2.49	0.46
1:T:53:TRP:CZ3	1:T:78:MET:CE	2.99	0.46
1:T:303:GLY:O	1:T:306:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:171:PHE:CE1	1:U:231:LEU:HD13	2.50	0.46
1:X:52:TRP:CD2	1:X:89:LEU:HD13	2.51	0.46
1:X:137:ASP:OD2	1:X:142:ILE:HG12	2.15	0.46
1:A:102:ARG:NH1	1:A:375:HIS:CD2	2.83	0.46
1:A:306:ILE:HD12	1:A:307:GLU:HG3	1.98	0.46
1:V:109:PHE:CD2	1:V:443:SER:HB3	2.50	0.46
1:B:86:ILE:HB	1:B:87:PRO:HD3	1.98	0.46
1:F:55:GLU:OE2	1:F:446:THR:OG1	2.26	0.46
1:F:407:GLN:NE2	1:F:413:GLN:O	2.39	0.46
1:H:354:ILE:HG21	3:H:502:DST:H132	1.98	0.46
1:I:165:GLN:HG3	1:K:172:GLN:NE2	2.17	0.46
1:K:171:PHE:HE1	1:K:231:LEU:HD13	1.79	0.46
1:L:301:LEU:O	1:L:304:ARG:CG	2.63	0.46
1:M:53:TRP:CZ3	1:M:78:MET:CE	2.98	0.46
1:P:389:PHE:HE2	1:P:437:MET:HE3	1.79	0.46
1:Q:77:PHE:CD1	1:Q:203:PHE:CD1	3.04	0.46
1:Q:154:LEU:CB	1:Q:156:LEU:CD1	2.94	0.46
1:Q:224:ALA:O	1:Q:226:VAL:HG23	2.16	0.46
1:Q:275:GLU:CD	1:S:175:LEU:HD11	2.36	0.46
1:Q:320:GLN:NE2	1:Q:392:SER:HB3	2.30	0.46
1:Q:369:LYS:O	1:Q:370:PHE:HD1	1.99	0.46
1:R:390:TRP:HB2	1:R:399:ALA:CB	2.27	0.46
1:S:212:LYS:NZ	3:S:502:DST:P1	2.89	0.46
1:S:390:TRP:CZ3	1:S:395:TRP:CZ3	3.03	0.46
1:U:79:PHE:HE2	1:X:42:HIS:HB2	1.76	0.46
1:U:240:ASP:CG	1:U:247:THR:HG22	2.35	0.46
1:U:290:VAL:HG23	1:U:294:LYS:HG2	1.97	0.46
1:C:154:LEU:HB3	1:C:156:LEU:CD1	2.46	0.46
1:A:231:LEU:HD12	1:A:232:ILE:N	2.30	0.46
1:E:269:LEU:HD12	1:E:283:ILE:HG13	1.98	0.46
1:G:140:ASN:OD1	1:G:143:PRO:HG2	2.16	0.46
1:G:233:ALA:HA	1:G:250:PHE:CE2	2.50	0.46
1:D:107:ILE:HA	1:D:124:GLY:O	2.16	0.46
1:D:115:LYS:HG2	1:D:395:TRP:CE2	2.51	0.46
1:D:292:TRP:HZ2	1:D:315:LEU:CD2	2.25	0.46
1:I:45:PRO:HD2	1:I:49:GLN:OE1	2.15	0.46
1:J:233:ALA:HA	1:J:250:PHE:CE2	2.51	0.46
1:J:353:ILE:C	1:J:353:ILE:HD12	2.35	0.46
1:J:407:GLN:OE1	1:J:415:ILE:HG13	2.15	0.46
1:K:285:GLY:O	1:K:354:ILE:HG23	2.16	0.46
1:L:83:HIS:O	1:L:87:PRO:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:171:PHE:HE1	1:L:231:LEU:CD1	2.29	0.46
1:M:175:LEU:HD11	1:O:275:GLU:CD	2.36	0.46
1:N:142:ILE:HB	1:N:143:PRO:HD3	1.98	0.46
1:P:231:LEU:HD12	1:P:232:ILE:N	2.31	0.46
1:Q:53:TRP:CZ3	1:Q:78:MET:CE	2.99	0.46
1:Q:175:LEU:HD21	1:S:275:GLU:HB2	1.98	0.46
1:R:63:PHE:CE1	1:R:409:LEU:CD2	2.98	0.46
1:T:390:TRP:CZ3	1:T:395:TRP:CZ3	3.04	0.46
1:U:115:LYS:HG2	1:U:395:TRP:CZ2	2.50	0.46
1:U:193:LEU:N	1:U:193:LEU:HD12	2.30	0.46
2:U:501:QRP:HB	3:U:502:DST:C13	2.45	0.46
1:W:55:GLU:OE2	1:W:446:THR:HG23	2.16	0.46
1:W:301:LEU:O	1:W:304:ARG:CG	2.59	0.46
1:W:410:TYR:OH	1:W:441:TYR:HB3	2.16	0.46
1:X:92:TYR:O	1:X:94:GLN:N	2.48	0.46
1:C:275:GLU:HG3	1:C:278:GLU:OE1	2.15	0.46
1:A:320:GLN:HE22	1:A:392:SER:HB3	1.81	0.46
1:V:270:SER:HB3	1:V:282:LYS:HB2	1.97	0.46
1:V:351:SER:OG	1:V:373:PRO:HB3	2.15	0.46
1:I:305:LEU:HD11	1:I:311:ILE:HG12	1.98	0.46
1:K:94:GLN:OE1	1:K:106:PRO:HD3	2.16	0.46
1:K:212:LYS:NZ	3:K:502:DST:P1	2.89	0.46
1:K:318:LEU:HD12	1:K:427:TYR:CD2	2.50	0.46
1:L:55:GLU:OE2	1:L:446:THR:HG23	2.16	0.46
1:M:170:LYS:HZ3	1:M:238:THR:HG21	1.79	0.46
1:M:440:TYR:OH	3:M:502:DST:O8	2.25	0.46
1:O:94:GLN:HG3	1:O:94:GLN:O	2.15	0.46
1:O:274:VAL:HG22	1:O:275:GLU:N	2.31	0.46
1:P:240:ASP:O	1:P:244:ASN:N	2.49	0.46
1:Q:52:TRP:CE2	1:Q:89:LEU:HB3	2.51	0.46
1:Q:171:PHE:HE1	1:Q:231:LEU:CD1	2.29	0.46
1:R:119:ARG:HD2	1:R:119:ARG:N	2.31	0.46
1:S:305:LEU:HD12	1:S:311:ILE:HD11	1.98	0.46
1:U:108:GLU:HA	1:U:443:SER:OG	2.16	0.46
1:C:117:SER:O	1:C:118:HIS:CB	2.64	0.46
1:A:374:VAL:HG11	1:A:382:VAL:HG11	1.98	0.46
2:V:501:QRP:HB	3:V:502:DST:C13	2.46	0.46
1:E:284:TYR:N	1:E:284:TYR:HD1	2.14	0.46
1:B:321:ILE:HD13	1:B:437:MET:HE1	1.97	0.46
1:B:353:ILE:C	1:B:353:ILE:HD12	2.37	0.46
1:B:386:LEU:HD13	1:B:390:TRP:HE1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:VAL:HG23	1:D:294:LYS:CG	2.46	0.46
1:F:284:TYR:N	1:F:284:TYR:CD1	2.84	0.46
1:F:321:ILE:HD11	1:F:389:PHE:CE2	2.51	0.46
1:F:373:PRO:HG3	1:F:424:TRP:HZ3	1.80	0.46
1:H:284:TYR:N	1:H:284:TYR:CD1	2.84	0.46
1:H:321:ILE:O	1:H:325:LEU:HD23	2.16	0.46
1:H:353:ILE:HD12	1:H:353:ILE:C	2.35	0.46
1:K:78:MET:O	1:K:82:MET:HG3	2.16	0.46
1:K:167:LEU:HD23	1:K:269:LEU:HD23	1.98	0.46
1:M:173:LEU:HD13	1:M:196:GLN:HE22	1.81	0.46
1:M:321:ILE:O	1:M:325:LEU:HD23	2.16	0.46
1:N:175:LEU:HD11	1:P:275:GLU:CD	2.36	0.46
1:N:193:LEU:HD12	1:N:193:LEU:N	2.31	0.46
1:Q:55:GLU:OE2	1:Q:446:THR:HG23	2.16	0.46
1:R:240:ASP:CG	1:R:247:THR:HG22	2.36	0.46
1:S:115:LYS:HE3	1:S:434:GLY:HA3	1.97	0.46
1:T:389:PHE:CE2	1:T:393:LEU:HD11	2.51	0.46
1:U:320:GLN:NE2	1:U:392:SER:HB3	2.31	0.46
1:X:154:LEU:CB	1:X:156:LEU:CD1	2.94	0.46
1:X:292:TRP:CZ2	1:X:315:LEU:HD21	2.51	0.46
1:C:95:LYS:NZ	1:A:47:ASN:HD22	2.14	0.46
1:G:386:LEU:HD13	1:G:390:TRP:CE2	2.51	0.46
1:D:51:ARG:HB3	1:D:92:TYR:CG	2.51	0.46
1:D:321:ILE:HD11	1:D:389:PHE:CE2	2.51	0.46
1:D:407:GLN:NE2	1:D:413:GLN:O	2.41	0.46
1:F:291:THR:O	1:F:295:ILE:HG13	2.15	0.46
1:F:430:THR:HB	1:F:433:ARG:HB2	1.97	0.46
1:J:320:GLN:CB	1:J:320:GLN:CD	2.79	0.46
1:K:117:SER:O	1:K:118:HIS:CB	2.64	0.46
1:K:433:ARG:HG3	1:K:436:TYR:CZ	2.51	0.46
1:L:240:ASP:CG	1:L:247:THR:HG22	2.36	0.46
1:M:240:ASP:O	1:M:244:ASN:N	2.48	0.46
1:O:407:GLN:NE2	1:O:413:GLN:O	2.39	0.46
2:P:501:QRP:HB	3:P:502:DST:C13	2.46	0.46
1:Q:278:GLU:OE1	1:Q:278:GLU:N	2.49	0.46
1:R:269:LEU:HD12	1:R:282:LYS:O	2.16	0.46
1:S:170:LYS:NZ	1:S:238:THR:HG21	2.31	0.46
1:U:228:VAL:O	1:U:232:ILE:HG13	2.16	0.46
1:W:240:ASP:CG	1:W:247:THR:HG22	2.37	0.46
1:X:60:PHE:HD1	1:X:109:PHE:CE1	2.34	0.46
1:X:284:TYR:N	1:X:284:TYR:CD1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LEU:HD22	1:C:125:PHE:CD1	2.51	0.45
1:A:108:GLU:HA	1:A:443:SER:CB	2.46	0.45
1:A:317:ARG:HB2	1:A:427:TYR:OH	2.16	0.45
1:G:420:ARG:HB2	1:G:447:TYR:OH	2.16	0.45
1:D:83:HIS:NE2	1:F:83:HIS:NE2	2.48	0.45
1:F:285:GLY:O	1:F:354:ILE:HG23	2.16	0.45
1:F:390:TRP:O	1:F:394:GLY:N	2.49	0.45
1:H:374:VAL:HG11	1:H:422:GLN:HG3	1.98	0.45
1:I:239:ILE:HG13	1:I:239:ILE:O	2.16	0.45
1:I:255:ASP:O	1:I:259:GLU:HG3	2.16	0.45
1:I:303:GLY:O	1:I:306:ILE:HG13	2.15	0.45
1:I:320:GLN:CG	1:I:320:GLN:HA	2.43	0.45
1:O:390:TRP:CZ3	1:O:395:TRP:CZ3	3.03	0.45
1:O:419:THR:HG23	1:O:420:ARG:HG3	1.98	0.45
1:Q:233:ALA:HA	1:Q:250:PHE:CE2	2.51	0.45
1:Q:239:ILE:O	1:Q:239:ILE:HG13	2.16	0.45
1:R:108:GLU:HA	1:R:443:SER:CB	2.45	0.45
1:R:281:LEU:C	1:R:281:LEU:HD12	2.37	0.45
1:S:83:HIS:O	1:S:87:PRO:HG2	2.16	0.45
1:S:115:LYS:HG2	1:S:395:TRP:HE1	1.79	0.45
1:S:320:GLN:CB	1:S:320:GLN:NE2	2.79	0.45
1:W:126:GLU:OE2	1:W:195:SER:HB2	2.16	0.45
1:W:180:GLN:HE21	1:W:223:ALA:HA	1.82	0.45
1:X:173:LEU:HD13	1:X:196:GLN:HE22	1.80	0.45
1:X:379:ASP:OD2	1:X:421:LEU:HB2	2.16	0.45
1:V:249:ALA:HB3	1:V:359:ILE:HG23	1.98	0.45
1:G:115:LYS:HE2	1:G:434:GLY:CA	2.43	0.45
1:G:160:ASP:HB3	1:G:162:PRO:HD2	1.98	0.45
1:D:171:PHE:HE1	1:D:231:LEU:HD13	1.81	0.45
1:H:301:LEU:O	1:H:304:ARG:CG	2.64	0.45
1:H:427:TYR:HD1	1:H:437:MET:CE	2.30	0.45
1:I:365:PHE:HD2	1:I:366:PRO:O	1.99	0.45
1:M:119:ARG:N	1:M:119:ARG:HD2	2.32	0.45
1:O:53:TRP:CZ3	1:O:82:MET:HG2	2.51	0.45
1:R:115:LYS:HG2	1:R:395:TRP:CZ2	2.52	0.45
1:R:386:LEU:HD11	1:R:390:TRP:CZ2	2.50	0.45
1:R:387:ALA:HA	1:R:390:TRP:HD1	1.78	0.45
1:S:51:ARG:HB3	1:S:92:TYR:CG	2.52	0.45
1:S:110:SER:HB2	1:S:122:ARG:CB	2.13	0.45
1:T:164:PHE:CE2	1:T:168:LEU:HD11	2.51	0.45
1:U:237:ARG:O	1:U:240:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:239:ILE:HA	1:X:242:GLU:HB3	1.98	0.45
1:C:41:TYR:OH	1:E:208:ALA:HA	2.16	0.45
1:C:173:LEU:C	1:C:174:SER:HG	2.11	0.45
1:A:359:ILE:O	1:A:359:ILE:HG22	2.14	0.45
1:V:284:TYR:N	1:V:284:TYR:HD1	2.15	0.45
1:V:430:THR:HG22	1:V:432:LYS:N	2.31	0.45
1:E:154:LEU:CB	1:E:156:LEU:CD1	2.94	0.45
1:G:269:LEU:CD1	1:G:283:ILE:HG13	2.47	0.45
1:B:116:GLY:HA2	1:B:398:HIS:CE1	2.52	0.45
1:B:275:GLU:CD	1:F:175:LEU:HD11	2.37	0.45
1:B:324:LEU:O	1:B:327:ILE:HG22	2.16	0.45
1:D:77:PHE:CD1	1:D:203:PHE:HD1	2.35	0.45
1:D:301:LEU:HD13	1:D:357:TYR:CE1	2.51	0.45
1:H:85:LEU:HD22	1:H:125:PHE:CD1	2.52	0.45
1:H:249:ALA:O	1:H:252:LEU:HB3	2.17	0.45
1:I:115:LYS:HE2	1:I:435:VAL:H	1.82	0.45
1:J:402:TYR:HB3	1:J:403:PRO:CD	2.36	0.45
1:K:53:TRP:CH2	1:K:78:MET:CE	2.99	0.45
1:L:172:GLN:CA	1:L:173:LEU:HD12	2.47	0.45
1:L:305:LEU:HD12	1:L:311:ILE:HG12	1.97	0.45
1:N:402:TYR:O	1:N:405:THR:N	2.48	0.45
1:O:226:VAL:HG12	1:O:230:THR:OG1	2.16	0.45
1:P:228:VAL:O	1:P:232:ILE:HG13	2.16	0.45
1:P:274:VAL:HG22	1:P:275:GLU:N	2.32	0.45
1:R:147:LEU:HD23	1:R:199:PHE:HD2	1.81	0.45
1:R:175:LEU:HD11	1:T:275:GLU:CD	2.37	0.45
1:R:284:TYR:N	1:R:284:TYR:HD1	2.14	0.45
1:S:86:ILE:HB	1:S:87:PRO:HD3	1.98	0.45
1:S:274:VAL:HG22	1:S:275:GLU:N	2.31	0.45
1:U:63:PHE:CE2	1:U:109:PHE:CB	2.99	0.45
1:W:154:LEU:HB3	1:W:156:LEU:CD1	2.46	0.45
1:X:212:LYS:HZ2	3:X:502:DST:P1	2.39	0.45
1:X:430:THR:HG22	1:X:432:LYS:H	1.80	0.45
1:A:115:LYS:CE	1:A:434:GLY:HA3	2.45	0.45
1:A:315:LEU:HD23	1:A:315:LEU:C	2.35	0.45
1:E:278:GLU:OE1	1:E:278:GLU:N	2.49	0.45
1:E:284:TYR:N	1:E:284:TYR:CD1	2.85	0.45
1:E:374:VAL:HG11	1:E:422:GLN:CG	2.46	0.45
1:E:419:THR:HG23	1:E:420:ARG:HG3	1.98	0.45
1:G:428:SER:HB3	1:G:436:TYR:CB	2.36	0.45
1:D:174:SER:OG	1:D:175:LEU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:LEU:HB2	1:D:415:ILE:CG2	2.32	0.45
1:I:228:VAL:O	1:I:232:ILE:HG13	2.15	0.45
1:J:419:THR:HG23	1:J:420:ARG:HG3	1.97	0.45
1:L:102:ARG:NH1	1:L:375:HIS:CD2	2.85	0.45
1:M:115:LYS:HG2	1:M:395:TRP:CZ2	2.51	0.45
1:M:305:LEU:HD12	1:M:311:ILE:HG12	1.97	0.45
1:N:305:LEU:HD23	1:N:305:LEU:N	2.31	0.45
1:O:275:GLU:HG3	1:O:278:GLU:OE1	2.16	0.45
1:Q:48:ASP:CG	1:Q:91:PRO:HA	2.37	0.45
1:R:108:GLU:OE2	2:R:501:QRP:HD1	2.16	0.45
1:R:120:LEU:HD21	1:R:205:PRO:HD3	1.97	0.45
2:R:501:QRP:HE3	2:R:501:QRP:O	2.15	0.45
1:S:252:LEU:CD2	1:S:301:LEU:HD23	2.47	0.45
1:S:351:SER:OG	1:S:373:PRO:HB3	2.17	0.45
1:T:66:ALA:HB2	1:T:409:LEU:HD11	1.99	0.45
1:T:100:ILE:HG13	1:T:101:SER:N	2.32	0.45
1:T:163:PHE:CD2	1:T:279:GLN:NE2	2.84	0.45
1:U:300:THR:O	1:U:305:LEU:HD23	2.16	0.45
1:W:390:TRP:CZ3	1:W:395:TRP:CZ3	3.04	0.45
1:A:430:THR:HG22	1:A:432:LYS:N	2.31	0.45
1:V:239:ILE:HA	1:V:242:GLU:HB3	1.98	0.45
1:B:228:VAL:HG11	1:B:267:THR:HG23	1.98	0.45
1:B:270:SER:HB3	1:B:282:LYS:HB2	1.98	0.45
1:D:180:GLN:HE21	1:D:223:ALA:CB	2.27	0.45
1:F:374:VAL:CG1	1:F:382:VAL:HG21	2.45	0.45
1:H:53:TRP:CH2	1:H:78:MET:CE	2.99	0.45
1:I:140:ASN:OD1	1:I:143:PRO:HG2	2.16	0.45
1:I:147:LEU:HD23	1:I:199:PHE:HD2	1.82	0.45
1:I:354:ILE:HG21	3:I:502:DST:H132	1.97	0.45
1:I:402:TYR:O	1:I:405:THR:N	2.49	0.45
1:L:193:LEU:HD12	1:L:193:LEU:N	2.32	0.45
1:M:48:ASP:CG	1:M:91:PRO:HA	2.37	0.45
1:M:53:TRP:CH2	1:M:78:MET:CE	2.99	0.45
1:O:430:THR:HG22	1:O:432:LYS:N	2.32	0.45
1:P:170:LYS:NZ	1:P:238:THR:HG21	2.31	0.45
1:Q:160:ASP:CG	1:S:174:SER:HB2	2.36	0.45
1:Q:317:ARG:HB2	1:Q:427:TYR:OH	2.16	0.45
1:R:51:ARG:HB3	1:R:92:TYR:CG	2.51	0.45
2:R:501:QRP:HB	3:R:502:DST:C13	2.47	0.45
1:S:239:ILE:HA	1:S:242:GLU:HB3	1.98	0.45
1:T:379:ASP:CG	1:T:422:GLN:HG3	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:102:ARG:NH1	1:U:375:HIS:CD2	2.85	0.45
1:C:102:ARG:NH1	1:C:375:HIS:CD2	2.85	0.45
1:C:239:ILE:HA	1:C:242:GLU:HB3	1.99	0.45
1:A:391:ASP:O	1:A:394:GLY:N	2.50	0.45
1:A:426:SER:O	1:A:437:MET:HG3	2.16	0.45
1:V:48:ASP:CG	1:V:91:PRO:HA	2.37	0.45
1:E:154:LEU:CB	1:E:156:LEU:HD13	2.47	0.45
1:G:226:VAL:HG12	1:G:230:THR:OG1	2.16	0.45
1:G:391:ASP:O	1:G:394:GLY:N	2.50	0.45
1:B:427:TYR:HD1	1:B:437:MET:HE2	1.82	0.45
1:H:115:LYS:HG2	1:H:395:TRP:CZ2	2.51	0.45
1:H:160:ASP:HB3	1:H:162:PRO:HD3	1.98	0.45
1:J:108:GLU:HA	1:J:443:SER:CB	2.46	0.45
1:J:390:TRP:CZ3	1:J:395:TRP:CZ3	3.05	0.45
1:O:278:GLU:OE1	1:O:278:GLU:N	2.50	0.45
1:O:374:VAL:CG1	1:O:382:VAL:HG21	2.41	0.45
1:P:237:ARG:O	1:P:240:ASP:HB2	2.15	0.45
1:Q:249:ALA:HB3	1:Q:359:ILE:HG23	1.98	0.45
1:R:102:ARG:NH1	1:R:375:HIS:CD2	2.85	0.45
1:R:147:LEU:HD23	1:R:199:PHE:CD2	2.51	0.45
1:R:305:LEU:HD23	1:R:305:LEU:N	2.31	0.45
1:R:433:ARG:HG3	1:R:436:TYR:OH	2.17	0.45
1:S:85:LEU:HD22	1:S:125:PHE:CE1	2.52	0.45
1:S:112:ASN:ND2	1:S:122:ARG:HH21	2.08	0.45
1:S:282:LYS:HE3	1:S:284:TYR:OH	2.17	0.45
1:T:171:PHE:CE1	1:T:231:LEU:HD13	2.52	0.45
1:U:127:PRO:HG3	1:U:147:LEU:CD2	2.47	0.45
1:W:406:LEU:HD12	1:W:415:ILE:HD13	1.98	0.45
1:X:53:TRP:CZ3	1:X:78:MET:HE1	2.52	0.45
1:C:127:PRO:HD2	1:C:144:ILE:HD13	1.98	0.45
1:C:402:TYR:HB3	1:C:403:PRO:CD	2.41	0.45
1:A:266:TYR:HD1	2:A:501:QRP:HAHA	1.78	0.45
1:A:360:HIS:ND1	1:A:361:PRO:HD2	2.32	0.45
1:A:407:GLN:NE2	1:A:413:GLN:O	2.45	0.45
1:V:172:GLN:CA	1:V:173:LEU:HD12	2.47	0.45
1:V:426:SER:O	1:V:437:MET:HG3	2.15	0.45
1:E:193:LEU:N	1:E:193:LEU:HD12	2.32	0.45
1:E:412:ASP:OD1	1:E:413:GLN:HG2	2.17	0.45
1:G:252:LEU:CD2	1:G:301:LEU:HD23	2.47	0.45
1:G:424:TRP:HB2	1:G:440:TYR:CD2	2.52	0.45
1:B:51:ARG:HB3	1:B:92:TYR:CG	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LYS:HZ3	3:B:502:DST:P1	2.39	0.45
1:D:412:ASP:OD1	1:D:413:GLN:N	2.50	0.45
1:F:433:ARG:HD2	1:F:436:TYR:HE1	1.81	0.45
1:I:317:ARG:CZ	1:I:393:LEU:HD23	2.47	0.45
1:I:321:ILE:O	1:I:325:LEU:HD23	2.15	0.45
1:K:249:ALA:HB3	1:K:359:ILE:HG23	1.99	0.45
1:N:53:TRP:CZ3	1:N:78:MET:CE	3.00	0.45
1:N:102:ARG:NH1	1:N:375:HIS:CD2	2.85	0.45
1:N:317:ARG:HB2	1:N:427:TYR:OH	2.17	0.45
1:O:111:LEU:O	1:O:438:SER:HA	2.16	0.45
1:R:41:TYR:CZ	1:S:209:ILE:HD12	2.52	0.45
1:R:229:GLY:HA3	1:R:263:TYR:CD2	2.52	0.45
1:S:140:ASN:OD1	1:S:143:PRO:HG2	2.17	0.45
1:S:171:PHE:HE1	1:S:231:LEU:CD1	2.30	0.45
1:T:379:ASP:OD2	1:T:421:LEU:HB2	2.17	0.45
1:U:163:PHE:CD2	1:U:279:GLN:NE2	2.85	0.45
1:X:390:TRP:CZ3	1:X:395:TRP:CZ3	3.05	0.45
1:C:100:ILE:HB	2:C:501:QRP:CE2	2.47	0.45
1:C:219:LEU:HD22	1:C:219:LEU:N	2.31	0.45
1:A:257:MET:HE3	1:A:263:TYR:N	2.31	0.45
1:V:317:ARG:O	1:V:320:GLN:HB3	2.16	0.45
1:V:318:LEU:HB2	1:V:427:TYR:CE2	2.52	0.45
1:E:98:SER:OG	1:E:100:ILE:HG12	2.16	0.45
1:E:250:PHE:O	1:E:253:ILE:N	2.49	0.45
1:G:117:SER:O	1:G:118:HIS:CB	2.65	0.45
1:D:53:TRP:CH2	1:D:78:MET:HE2	2.52	0.45
1:D:252:LEU:CD2	1:D:301:LEU:HD23	2.47	0.45
1:J:299:TRP:CH2	1:J:368:PRO:HG2	2.51	0.45
1:K:284:TYR:N	1:K:284:TYR:HD1	2.15	0.45
1:L:163:PHE:CD2	1:L:279:GLN:NE2	2.85	0.45
1:L:237:ARG:O	1:L:240:ASP:HB2	2.17	0.45
1:O:115:LYS:HE3	1:O:434:GLY:HA3	1.98	0.45
1:R:353:ILE:C	1:R:353:ILE:HD12	2.37	0.45
1:T:240:ASP:CG	1:T:247:THR:HG22	2.38	0.45
1:T:269:LEU:CD1	1:T:283:ILE:HG13	2.47	0.45
1:T:353:ILE:C	1:T:353:ILE:HD12	2.37	0.45
1:U:71:LEU:HB3	1:U:72:PRO:HD3	1.99	0.45
1:U:317:ARG:O	1:U:320:GLN:HB3	2.17	0.45
1:W:70:GLY:HA3	1:W:73:GLN:OE1	2.16	0.45
1:W:123:ILE:HD12	1:W:203:PHE:CE2	2.52	0.45
1:W:237:ARG:O	1:W:240:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:311:ILE:HD12	1:X:311:ILE:H	1.81	0.45
1:X:317:ARG:HB2	1:X:427:TYR:OH	2.16	0.45
1:C:227:PRO:O	1:C:230:THR:OG1	2.34	0.45
1:C:284:TYR:N	1:C:284:TYR:HD1	2.14	0.45
1:A:321:ILE:CD1	1:A:437:MET:HE1	2.47	0.45
1:V:179:ARG:NH1	1:V:182:GLN:HB3	2.32	0.45
1:E:53:TRP:CZ3	1:E:82:MET:HG2	2.51	0.45
1:G:110:SER:O	1:G:121:LEU:HD12	2.16	0.45
1:G:242:GLU:O	1:G:243:ARG:CG	2.55	0.45
1:G:374:VAL:HG11	1:G:382:VAL:HG11	1.99	0.45
1:B:395:TRP:HB3	1:B:398:HIS:CB	2.46	0.45
1:D:116:GLY:CA	1:D:398:HIS:NE2	2.80	0.45
1:D:426:SER:O	1:D:437:MET:HG3	2.17	0.45
1:F:274:VAL:HG22	1:F:275:GLU:N	2.32	0.45
1:F:321:ILE:CD1	1:F:437:MET:HE1	2.46	0.45
1:H:117:SER:O	1:H:118:HIS:CB	2.65	0.45
1:H:321:ILE:HG12	1:H:389:PHE:CD1	2.52	0.45
1:J:154:LEU:HB3	1:J:156:LEU:CD1	2.46	0.45
1:J:252:LEU:CD2	1:J:301:LEU:HD23	2.47	0.45
1:J:271:CYS:CB	1:J:279:GLN:HE21	2.21	0.45
1:K:51:ARG:HB2	1:K:92:TYR:HB2	1.99	0.45
1:M:70:GLY:HA3	1:M:73:GLN:HE22	1.81	0.45
1:M:193:LEU:N	1:M:193:LEU:HD12	2.32	0.45
1:O:115:LYS:HG2	1:O:395:TRP:CZ2	2.51	0.45
1:O:239:ILE:HA	1:O:242:GLU:HB3	1.99	0.45
1:O:418:THR:OG1	1:O:421:LEU:HG	2.16	0.45
1:P:317:ARG:HB2	1:P:427:TYR:OH	2.16	0.45
1:R:305:LEU:CD1	1:R:311:ILE:HG12	2.47	0.45
1:U:390:TRP:CZ3	1:U:395:TRP:CZ3	3.04	0.45
1:W:212:LYS:HB2	1:W:212:LYS:HE3	1.73	0.45
1:C:237:ARG:HA	1:C:240:ASP:OD2	2.16	0.45
1:V:79:PHE:HZ	1:W:42:HIS:HD2	1.64	0.45
1:G:221:ALA:HB2	1:G:231:LEU:HD21	1.98	0.45
1:B:53:TRP:CZ3	1:B:78:MET:HE1	2.52	0.45
1:B:102:ARG:HH11	1:B:375:HIS:CD2	2.35	0.45
1:B:395:TRP:HB3	1:B:398:HIS:HB2	1.97	0.45
1:F:89:LEU:CD2	1:F:106:PRO:HG2	2.47	0.45
1:F:204:ASN:OD1	1:F:206:ASP:O	2.35	0.45
1:I:172:GLN:OE1	1:K:162:PRO:HA	2.17	0.45
1:I:179:ARG:NH1	1:I:182:GLN:HB3	2.32	0.45
1:K:284:TYR:N	1:K:284:TYR:CD1	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:305:LEU:HD12	1:M:311:ILE:CD1	2.48	0.45
1:N:428:SER:HB3	1:N:436:TYR:CB	2.41	0.45
1:O:426:SER:O	1:O:437:MET:HG3	2.17	0.45
1:Q:108:GLU:HA	1:Q:443:SER:CB	2.47	0.45
1:R:70:GLY:HA3	1:R:73:GLN:NE2	2.32	0.45
1:R:233:ALA:HA	1:R:250:PHE:CE2	2.52	0.45
1:S:285:GLY:O	1:S:354:ILE:HG23	2.16	0.45
1:S:420:ARG:HB2	1:S:447:TYR:CZ	2.51	0.45
1:T:51:ARG:HB3	1:T:92:TYR:CG	2.52	0.45
1:T:237:ARG:O	1:T:240:ASP:HB2	2.16	0.45
1:U:52:TRP:CE2	1:U:89:LEU:HB3	2.52	0.45
1:U:53:TRP:CZ3	1:U:78:MET:CE	2.99	0.45
1:C:115:LYS:HE2	1:C:435:VAL:N	2.32	0.44
1:C:305:LEU:HD12	1:C:311:ILE:HG12	1.97	0.44
1:A:424:TRP:HB2	1:A:440:TYR:HD2	1.81	0.44
1:A:427:TYR:HD1	1:A:437:MET:HE2	1.81	0.44
1:V:285:GLY:O	1:V:354:ILE:HG23	2.17	0.44
1:V:374:VAL:CG1	1:V:382:VAL:HG11	2.46	0.44
1:E:46:THR:OG1	1:E:49:GLN:HG3	2.17	0.44
1:E:212:LYS:HB2	1:E:212:LYS:HE3	1.70	0.44
1:G:231:LEU:HD12	1:G:232:ILE:N	2.32	0.44
1:G:295:ILE:HG23	1:G:370:PHE:HE2	1.81	0.44
1:B:100:ILE:HB	2:B:501:QRP:CE2	2.47	0.44
1:B:108:GLU:HA	1:B:443:SER:CB	2.47	0.44
1:B:321:ILE:HD11	1:B:437:MET:HE1	1.99	0.44
1:D:63:PHE:CE2	1:D:109:PHE:HB2	2.52	0.44
1:D:257:MET:HE3	1:D:263:TYR:N	2.32	0.44
1:F:255:ASP:HB3	1:F:304:ARG:NH1	2.32	0.44
1:H:110:SER:O	1:H:121:LEU:HD12	2.17	0.44
1:H:255:ASP:HB3	1:H:304:ARG:NH1	2.32	0.44
1:K:53:TRP:CH2	1:K:78:MET:HE2	2.52	0.44
1:K:108:GLU:HA	1:K:443:SER:CB	2.47	0.44
1:K:420:ARG:HH12	1:K:448:LEU:HB2	1.82	0.44
1:L:253:ILE:O	1:L:257:MET:HG2	2.17	0.44
1:L:320:GLN:NE2	1:L:392:SER:HB3	2.32	0.44
1:L:356:ASN:O	1:L:368:PRO:HA	2.17	0.44
1:M:126:GLU:OE2	1:M:195:SER:CB	2.65	0.44
1:M:299:TRP:CH2	1:M:368:PRO:HG2	2.52	0.44
1:N:102:ARG:HH11	1:N:375:HIS:CD2	2.35	0.44
1:N:284:TYR:N	1:N:284:TYR:HD1	2.16	0.44
1:P:233:ALA:HA	1:P:250:PHE:CE2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:300:THR:HA	1:P:305:LEU:HD21	1.99	0.44
2:Q:501:QRP:O	2:Q:501:QRP:HE3	2.17	0.44
1:R:63:PHE:CE2	1:R:109:PHE:CB	3.01	0.44
1:R:239:ILE:HA	1:R:242:GLU:HB3	1.99	0.44
1:R:252:LEU:CD2	1:R:301:LEU:HD23	2.48	0.44
1:R:360:HIS:ND1	1:R:361:PRO:HD2	2.32	0.44
1:S:232:ILE:O	1:S:236:VAL:HG23	2.17	0.44
1:T:351:SER:OG	1:T:373:PRO:HB3	2.17	0.44
1:T:420:ARG:HB2	1:T:447:TYR:OH	2.17	0.44
1:U:249:ALA:O	1:U:252:LEU:HB3	2.17	0.44
1:U:389:PHE:CE2	1:U:437:MET:HE1	2.51	0.44
1:W:212:LYS:NZ	3:W:502:DST:P1	2.90	0.44
1:X:148:LEU:HD21	1:X:165:GLN:OE1	2.17	0.44
1:C:63:PHE:CE2	1:C:109:PHE:HB2	2.52	0.44
1:C:174:SER:HB3	1:G:162:PRO:HG2	1.99	0.44
1:A:117:SER:O	1:A:118:HIS:CB	2.65	0.44
1:V:127:PRO:HG3	1:V:147:LEU:HD23	1.99	0.44
1:V:354:ILE:HB	1:V:371:TYR:HB2	1.99	0.44
1:E:100:ILE:O	2:E:501:QRP:CD1	2.64	0.44
1:E:108:GLU:HA	1:E:443:SER:CB	2.47	0.44
1:B:279:GLN:O	1:B:361:PRO:HD3	2.17	0.44
1:B:321:ILE:O	1:B:325:LEU:HD23	2.17	0.44
1:D:239:ILE:HA	1:D:242:GLU:HB3	1.99	0.44
1:H:356:ASN:HB3	1:H:369:LYS:HB3	1.99	0.44
1:H:405:THR:O	1:H:409:LEU:HD13	2.17	0.44
1:I:52:TRP:CE3	1:I:89:LEU:HD13	2.53	0.44
1:I:53:TRP:CH2	1:I:78:MET:CE	3.00	0.44
1:J:412:ASP:OD1	1:J:413:GLN:N	2.50	0.44
1:K:110:SER:O	1:K:121:LEU:HD12	2.17	0.44
1:K:379:ASP:OD2	1:K:421:LEU:HB2	2.16	0.44
1:L:53:TRP:CH2	1:L:78:MET:CE	3.00	0.44
1:L:110:SER:O	1:L:121:LEU:HD12	2.17	0.44
1:L:240:ASP:O	1:L:244:ASN:N	2.50	0.44
1:M:391:ASP:O	1:M:394:GLY:N	2.51	0.44
1:N:270:SER:HB3	1:N:282:LYS:HB2	1.98	0.44
1:O:354:ILE:HB	1:O:371:TYR:HB2	1.99	0.44
1:O:402:TYR:CB	1:O:403:PRO:HD3	2.40	0.44
1:Q:109:PHE:CD1	1:Q:123:ILE:HG12	2.52	0.44
1:R:299:TRP:CH2	1:R:368:PRO:HG2	2.52	0.44
1:S:163:PHE:CD2	1:S:279:GLN:NE2	2.85	0.44
1:S:284:TYR:N	1:S:284:TYR:CD1	2.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:311:ILE:H	1:T:311:ILE:HD12	1.81	0.44
1:W:53:TRP:CZ3	1:W:78:MET:CE	3.00	0.44
1:X:292:TRP:HZ2	1:X:315:LEU:HD21	1.82	0.44
1:C:284:TYR:N	1:C:284:TYR:CD1	2.85	0.44
1:A:174:SER:HB3	1:E:162:PRO:HG2	1.99	0.44
1:V:382:VAL:O	1:V:386:LEU:HB2	2.17	0.44
1:E:390:TRP:CZ3	1:E:395:TRP:CZ3	3.06	0.44
1:E:432:LYS:HZ2	1:E:433:ARG:HG2	1.82	0.44
1:B:84:HIS:NE2	1:B:154:LEU:HD11	2.32	0.44
1:B:212:LYS:NZ	3:B:502:DST:P1	2.90	0.44
1:D:410:TYR:OH	1:D:441:TYR:HB3	2.17	0.44
1:F:48:ASP:CG	1:F:91:PRO:HA	2.38	0.44
1:I:240:ASP:CG	1:I:247:THR:HG22	2.38	0.44
1:I:249:ALA:O	1:I:252:LEU:HB3	2.17	0.44
1:I:354:ILE:HB	1:I:371:TYR:HB2	1.99	0.44
1:J:252:LEU:HD23	1:J:301:LEU:HD21	1.99	0.44
1:J:415:ILE:HA	1:J:418:THR:CG2	2.46	0.44
2:J:501:QRP:HB	3:J:502:DST:C13	2.48	0.44
1:K:154:LEU:HB3	1:K:156:LEU:CD1	2.47	0.44
1:K:299:TRP:CH2	1:K:368:PRO:HG2	2.51	0.44
1:O:140:ASN:OD1	1:O:143:PRO:CG	2.63	0.44
1:O:257:MET:HE3	1:O:263:TYR:N	2.31	0.44
1:R:407:GLN:OE1	1:R:415:ILE:HG13	2.18	0.44
1:S:379:ASP:OD2	1:S:421:LEU:N	2.50	0.44
1:C:53:TRP:CZ3	1:C:78:MET:CE	3.00	0.44
1:A:42:HIS:HB2	1:G:79:PHE:HE2	1.80	0.44
1:A:212:LYS:NZ	3:A:502:DST:P1	2.91	0.44
1:A:321:ILE:O	1:A:325:LEU:HD23	2.17	0.44
1:V:154:LEU:CB	1:V:156:LEU:HD13	2.47	0.44
1:E:354:ILE:HB	1:E:371:TYR:HB2	2.00	0.44
1:D:275:GLU:CG	1:H:175:LEU:HD11	2.47	0.44
1:D:277:SER:HB3	1:D:278:GLU:OE1	2.17	0.44
1:H:115:LYS:HG2	1:H:395:TRP:CE2	2.52	0.44
1:J:212:LYS:HZ3	3:J:502:DST:P1	2.41	0.44
1:K:407:GLN:NE2	1:K:413:GLN:O	2.40	0.44
1:L:100:ILE:O	2:L:501:QRP:CG	2.66	0.44
1:M:63:PHE:CE2	1:M:109:PHE:CB	3.00	0.44
1:M:163:PHE:CE1	1:M:239:ILE:HG12	2.53	0.44
1:N:426:SER:OG	1:N:438:SER:HB2	2.18	0.44
1:O:100:ILE:HG13	1:O:101:SER:N	2.32	0.44
1:O:390:TRP:CH2	1:O:437:MET:SD	3.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:386:LEU:HD13	1:P:390:TRP:CE2	2.52	0.44
1:P:420:ARG:HB2	1:P:447:TYR:OH	2.18	0.44
1:P:426:SER:O	1:P:437:MET:HA	2.17	0.44
1:Q:102:ARG:NH1	1:Q:375:HIS:CD2	2.85	0.44
1:R:53:TRP:CH2	1:R:78:MET:CE	3.00	0.44
1:R:127:PRO:CG	1:R:147:LEU:HD23	2.47	0.44
1:R:315:LEU:HD23	1:R:315:LEU:C	2.38	0.44
1:S:299:TRP:NE1	1:S:311:ILE:HG23	2.32	0.44
1:U:63:PHE:CE1	1:U:409:LEU:CD2	2.99	0.44
1:X:356:ASN:OD1	1:X:357:TYR:N	2.51	0.44
1:C:317:ARG:HB2	1:C:427:TYR:OH	2.18	0.44
1:V:162:PRO:HA	1:X:172:GLN:OE1	2.17	0.44
1:D:173:LEU:CD1	1:D:196:GLN:NE2	2.80	0.44
1:D:206:ASP:OD1	1:D:207:GLY:N	2.50	0.44
1:H:163:PHE:CD2	1:H:279:GLN:NE2	2.86	0.44
1:H:232:ILE:O	1:H:236:VAL:HG23	2.17	0.44
1:I:285:GLY:HA3	1:I:355:TRP:CH2	2.53	0.44
1:K:410:TYR:CD1	1:K:421:LEU:HD22	2.51	0.44
2:K:501:QRP:HB	3:K:502:DST:C13	2.46	0.44
1:N:390:TRP:CZ3	1:N:395:TRP:CZ3	3.06	0.44
1:N:415:ILE:CA	1:N:418:THR:HG22	2.39	0.44
1:N:430:THR:HB	1:N:433:ARG:HB2	2.00	0.44
1:P:418:THR:OG1	1:P:421:LEU:HG	2.18	0.44
1:Q:390:TRP:CZ3	1:Q:395:TRP:CZ3	3.05	0.44
1:R:174:SER:OG	1:R:175:LEU:N	2.50	0.44
1:R:237:ARG:HA	1:R:240:ASP:OD2	2.17	0.44
1:S:257:MET:HE3	1:S:263:TYR:N	2.33	0.44
1:T:100:ILE:O	2:T:501:QRP:CG	2.66	0.44
1:U:249:ALA:HB3	1:U:359:ILE:HG23	1.99	0.44
1:W:317:ARG:O	1:W:320:GLN:HB3	2.17	0.44
1:W:354:ILE:HG21	3:W:502:DST:H132	1.99	0.44
1:X:63:PHE:CE1	1:X:409:LEU:CD2	3.01	0.44
1:X:115:LYS:HG2	1:X:395:TRP:CZ2	2.53	0.44
1:V:193:LEU:HD12	1:V:193:LEU:N	2.32	0.44
1:E:321:ILE:O	1:E:325:LEU:HD23	2.18	0.44
1:E:379:ASP:OD2	1:E:421:LEU:N	2.51	0.44
1:G:66:ALA:O	1:G:119:ARG:NH2	2.50	0.44
1:G:126:GLU:OE2	1:G:195:SER:HB2	2.17	0.44
1:B:171:PHE:HE1	1:B:231:LEU:HD13	1.83	0.44
1:F:170:LYS:NZ	1:F:238:THR:HG21	2.32	0.44
1:F:318:LEU:O	1:F:318:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:41:TYR:CZ	1:L:209:ILE:HD12	2.52	0.44
1:J:162:PRO:HG2	1:L:174:SER:HB3	2.00	0.44
1:M:127:PRO:HG3	1:M:147:LEU:HD22	1.99	0.44
1:M:228:VAL:CG1	1:M:232:ILE:HD11	2.43	0.44
1:M:292:TRP:CZ2	1:M:315:LEU:HD21	2.53	0.44
1:N:79:PHE:HE2	1:O:42:HIS:HB2	1.78	0.44
1:N:127:PRO:HG3	1:N:147:LEU:HD22	1.98	0.44
1:P:369:LYS:HA	1:P:427:TYR:O	2.17	0.44
1:R:66:ALA:HB2	1:R:409:LEU:HD11	2.00	0.44
1:R:271:CYS:HB2	1:R:279:GLN:NE2	2.25	0.44
1:R:284:TYR:N	1:R:284:TYR:CD1	2.85	0.44
1:S:154:LEU:CB	1:S:156:LEU:CD1	2.95	0.44
1:S:160:ASP:HB3	1:S:162:PRO:CD	2.48	0.44
1:S:275:GLU:HG3	1:S:278:GLU:OE1	2.17	0.44
1:T:231:LEU:O	1:T:235:ALA:N	2.46	0.44
1:U:237:ARG:HA	1:U:240:ASP:OD2	2.18	0.44
1:X:274:VAL:HG22	1:X:275:GLU:N	2.33	0.44
2:C:501:QRP:O	2:C:501:QRP:HE3	2.17	0.44
1:V:229:GLY:HA3	1:V:263:TYR:CE2	2.53	0.44
1:V:240:ASP:CG	1:V:247:THR:HG22	2.38	0.44
1:G:285:GLY:HA3	1:G:355:TRP:CE2	2.52	0.44
1:D:60:PHE:HD1	1:D:109:PHE:CE1	2.35	0.44
1:D:237:ARG:O	1:D:240:ASP:HB2	2.18	0.44
2:D:501:QRP:O	2:D:501:QRP:HE3	2.18	0.44
1:F:173:LEU:HD12	1:F:173:LEU:N	2.31	0.44
1:F:320:GLN:NE2	1:F:392:SER:CB	2.79	0.44
1:F:321:ILE:CG1	1:F:389:PHE:CE1	3.00	0.44
1:I:63:PHE:CD2	1:I:109:PHE:HB3	2.52	0.44
1:I:292:TRP:CZ2	1:I:319:LYS:HB2	2.52	0.44
1:J:354:ILE:HB	1:J:371:TYR:HB2	1.99	0.44
1:N:48:ASP:CG	1:N:91:PRO:HA	2.38	0.44
1:N:379:ASP:OD2	1:N:421:LEU:HB2	2.18	0.44
2:N:501:QRP:O	2:N:501:QRP:HE3	2.18	0.44
1:O:269:LEU:HD12	1:O:283:ILE:HG13	2.00	0.44
1:S:85:LEU:HB3	1:S:125:PHE:CE1	2.48	0.44
1:T:253:ILE:HD12	1:T:359:ILE:HD11	2.00	0.44
1:T:374:VAL:CG1	1:T:382:VAL:HG21	2.48	0.44
1:U:371:TYR:HA	1:U:425:ILE:O	2.17	0.44
1:W:389:PHE:CE2	1:W:437:MET:HE3	2.50	0.44
1:X:126:GLU:OE2	1:X:195:SER:HB2	2.17	0.44
1:X:170:LYS:HZ3	1:X:238:THR:HG21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:173:LEU:HD13	1:X:196:GLN:NE2	2.33	0.44
1:C:305:LEU:HD23	1:C:305:LEU:N	2.33	0.44
1:A:147:LEU:HD12	1:A:147:LEU:O	2.18	0.44
1:V:51:ARG:HD3	1:V:92:TYR:HD2	1.79	0.44
1:E:268:PHE:CZ	1:E:284:TYR:CD2	3.05	0.44
1:G:100:ILE:O	2:G:501:QRP:HA	2.17	0.44
1:B:353:ILE:HG13	1:B:353:ILE:O	2.18	0.44
1:B:420:ARG:HB2	1:B:447:TYR:OH	2.18	0.44
1:F:102:ARG:HH11	1:F:375:HIS:CD2	2.36	0.44
1:F:117:SER:O	1:F:118:HIS:CB	2.66	0.44
1:H:53:TRP:CH2	1:H:78:MET:HE2	2.53	0.44
1:J:386:LEU:HD11	1:J:390:TRP:HZ2	1.83	0.44
1:K:369:LYS:HA	1:K:427:TYR:O	2.18	0.44
1:L:142:ILE:HB	1:L:143:PRO:HD3	1.98	0.44
1:M:221:ALA:HB2	1:M:231:LEU:HD21	2.00	0.44
1:M:229:GLY:HA3	1:M:263:TYR:CD2	2.52	0.44
1:M:269:LEU:HD12	1:M:282:LYS:O	2.18	0.44
1:M:291:THR:O	1:M:295:ILE:HG13	2.18	0.44
1:M:324:LEU:O	1:M:327:ILE:HG22	2.18	0.44
1:N:173:LEU:HD12	1:N:173:LEU:N	2.31	0.44
1:O:83:HIS:O	1:O:87:PRO:HG2	2.17	0.44
1:O:285:GLY:HA3	1:O:355:TRP:CE2	2.53	0.44
1:P:51:ARG:HB3	1:P:92:TYR:CG	2.52	0.44
1:P:275:GLU:HG3	1:P:278:GLU:OE1	2.17	0.44
1:Q:60:PHE:CE2	1:Q:64:LEU:HD11	2.52	0.44
1:Q:109:PHE:HD1	1:Q:123:ILE:HG12	1.83	0.44
1:Q:115:LYS:HE2	1:Q:434:GLY:CA	2.41	0.44
1:Q:176:SER:O	1:Q:180:GLN:CG	2.66	0.44
1:R:303:GLY:O	1:R:306:ILE:HG13	2.17	0.44
1:S:389:PHE:HE2	1:S:437:MET:HE1	1.80	0.44
1:T:250:PHE:O	1:T:253:ILE:N	2.51	0.44
1:T:257:MET:HE3	1:T:263:TYR:N	2.33	0.44
1:U:242:GLU:O	1:U:243:ARG:CG	2.56	0.44
1:W:86:ILE:HB	1:W:87:PRO:HD3	1.98	0.44
1:X:282:LYS:CB	1:X:284:TYR:HE1	2.30	0.44
1:X:324:LEU:O	1:X:327:ILE:HG22	2.18	0.44
1:C:232:ILE:O	1:C:236:VAL:HG23	2.18	0.44
1:V:66:ALA:HB2	1:V:409:LEU:HD11	2.00	0.44
1:V:100:ILE:O	2:V:501:QRP:CD1	2.66	0.44
1:E:81:PHE:HD1	1:E:85:LEU:HD12	1.82	0.44
1:E:281:LEU:C	1:E:281:LEU:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:PHE:CD2	1:G:109:PHE:HB3	2.53	0.44
1:B:41:TYR:CZ	1:H:209:ILE:CD1	3.00	0.44
1:F:126:GLU:OE2	1:F:195:SER:HB2	2.18	0.44
1:J:79:PHE:HE2	1:K:42:HIS:HB2	1.83	0.44
1:J:239:ILE:CD1	1:J:242:GLU:HG2	2.47	0.44
1:L:100:ILE:HB	2:L:501:QRP:CE2	2.48	0.44
1:L:278:GLU:OE1	1:L:278:GLU:N	2.50	0.44
1:M:47:ASN:ND2	1:N:95:LYS:NZ	2.65	0.44
1:M:53:TRP:CZ3	1:M:78:MET:HE1	2.53	0.44
1:M:128:VAL:HG12	1:M:129:SER:N	2.33	0.44
1:N:419:THR:HG23	1:N:420:ARG:HG3	2.00	0.44
1:P:321:ILE:HD11	1:P:437:MET:HE1	1.99	0.44
1:Q:92:TYR:CB	1:Q:93:PRO:HD3	2.48	0.44
1:Q:239:ILE:CD1	1:Q:242:GLU:CG	2.95	0.44
1:R:212:LYS:HZ2	3:R:502:DST:P1	2.41	0.44
1:R:426:SER:OG	1:R:438:SER:HB2	2.18	0.44
1:T:117:SER:O	1:T:118:HIS:CB	2.66	0.44
1:T:233:ALA:HB2	1:T:254:ASN:ND2	2.33	0.44
1:U:112:ASN:ND2	1:U:122:ARG:HH21	2.16	0.44
1:X:92:TYR:CB	1:X:93:PRO:HD3	2.46	0.44
1:C:110:SER:O	1:C:121:LEU:HD12	2.18	0.43
1:C:173:LEU:HD13	1:C:196:GLN:NE2	2.30	0.43
1:A:284:TYR:N	1:A:284:TYR:HD1	2.16	0.43
1:A:415:ILE:HA	1:A:418:THR:CG2	2.48	0.43
1:V:112:ASN:HB2	1:V:122:ARG:HE	1.82	0.43
1:E:63:PHE:CE2	1:E:109:PHE:CB	2.99	0.43
1:G:279:GLN:O	1:G:361:PRO:HD3	2.18	0.43
1:G:321:ILE:HD11	1:G:389:PHE:CE2	2.52	0.43
1:B:410:TYR:CD1	1:B:421:LEU:HD22	2.53	0.43
1:F:229:GLY:HA3	1:F:263:TYR:CE2	2.53	0.43
1:F:371:TYR:HA	1:F:425:ILE:O	2.18	0.43
1:H:274:VAL:HG22	1:H:275:GLU:N	2.32	0.43
1:I:53:TRP:CH2	1:I:78:MET:HE1	2.53	0.43
1:J:382:VAL:O	1:J:386:LEU:HB2	2.18	0.43
1:K:147:LEU:HD23	1:K:199:PHE:CD2	2.53	0.43
1:K:193:LEU:HD12	1:K:193:LEU:N	2.33	0.43
1:L:117:SER:O	1:L:118:HIS:CB	2.66	0.43
1:M:53:TRP:CH2	1:M:78:MET:HE1	2.53	0.43
1:M:109:PHE:CD1	1:M:123:ILE:HG12	2.53	0.43
1:N:118:HIS:HD2	1:N:119:ARG:O	2.01	0.43
1:N:317:ARG:CZ	1:N:393:LEU:HD23	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:85:LEU:HD22	1:O:125:PHE:CD1	2.53	0.43
1:P:92:TYR:O	1:P:94:GLN:N	2.50	0.43
1:P:402:TYR:HB3	1:P:403:PRO:CD	2.39	0.43
1:P:412:ASP:OD1	1:P:413:GLN:N	2.51	0.43
1:R:226:VAL:HG12	1:R:230:THR:OG1	2.18	0.43
1:S:60:PHE:CE2	1:S:64:LEU:HD11	2.53	0.43
1:S:204:ASN:CB	1:S:205:PRO:HD2	2.48	0.43
1:T:173:LEU:HD13	1:T:196:GLN:NE2	2.33	0.43
1:T:321:ILE:HD11	1:T:437:MET:HE1	1.99	0.43
1:U:77:PHE:CD1	1:U:203:PHE:CD1	3.06	0.43
1:U:233:ALA:HA	1:U:250:PHE:CE2	2.53	0.43
1:W:36:GLN:OE1	1:W:58:SER:HA	2.18	0.43
1:W:171:PHE:HE1	1:W:231:LEU:CD1	2.28	0.43
1:W:250:PHE:O	1:W:253:ILE:N	2.51	0.43
1:W:373:PRO:HG3	1:W:424:TRP:HZ3	1.82	0.43
1:X:275:GLU:HG3	1:X:278:GLU:OE1	2.17	0.43
1:A:41:TYR:CZ	1:G:209:ILE:HD12	2.53	0.43
1:A:321:ILE:HD11	1:A:389:PHE:CZ	2.53	0.43
1:V:128:VAL:HG12	1:V:129:SER:N	2.33	0.43
1:E:39:ALA:HB2	1:E:53:TRP:CZ2	2.54	0.43
1:E:212:LYS:NZ	3:E:502:DST:P1	2.91	0.43
1:G:100:ILE:O	2:G:501:QRP:CG	2.66	0.43
1:G:167:LEU:N	1:G:167:LEU:HD12	2.33	0.43
1:G:257:MET:HE3	1:G:263:TYR:N	2.32	0.43
1:B:115:LYS:HE3	1:B:434:GLY:HA3	2.00	0.43
1:B:171:PHE:CE1	1:B:231:LEU:HD13	2.53	0.43
1:F:79:PHE:HA	1:F:82:MET:HE2	2.01	0.43
2:F:501:QRP:HB	3:F:502:DST:C13	2.47	0.43
1:H:386:LEU:HD11	1:H:390:TRP:HZ2	1.83	0.43
1:I:239:ILE:O	1:I:242:GLU:HB3	2.18	0.43
1:L:102:ARG:HH11	1:L:375:HIS:CD2	2.37	0.43
1:M:212:LYS:HZ3	3:M:502:DST:P1	2.41	0.43
1:M:228:VAL:HG11	1:M:267:THR:HG23	2.00	0.43
1:N:172:GLN:CA	1:N:173:LEU:HD12	2.48	0.43
1:N:430:THR:HG22	1:N:432:LYS:N	2.32	0.43
1:O:115:LYS:HA	1:O:395:TRP:CE2	2.53	0.43
1:P:115:LYS:HA	1:P:395:TRP:CE2	2.53	0.43
1:Q:85:LEU:HD22	1:Q:125:PHE:CD1	2.53	0.43
1:Q:154:LEU:CB	1:Q:156:LEU:HD13	2.48	0.43
1:R:154:LEU:HB3	1:R:156:LEU:CD1	2.48	0.43
1:R:420:ARG:HB2	1:R:447:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:292:TRP:CZ2	1:S:315:LEU:HD21	2.52	0.43
1:S:374:VAL:HG11	1:S:382:VAL:HG11	2.00	0.43
1:T:115:LYS:HG2	1:T:395:TRP:NE1	2.32	0.43
1:T:174:SER:OG	1:T:175:LEU:N	2.51	0.43
1:T:305:LEU:HD12	1:T:311:ILE:CD1	2.48	0.43
1:W:51:ARG:HB3	1:W:92:TYR:CG	2.53	0.43
1:W:60:PHE:CE2	1:W:64:LEU:HD11	2.53	0.43
1:W:154:LEU:HB2	1:W:156:LEU:CD1	2.48	0.43
1:X:92:TYR:CD2	1:X:93:PRO:HD3	2.53	0.43
1:X:374:VAL:CG1	1:X:382:VAL:HG21	2.48	0.43
1:C:51:ARG:HB2	1:C:92:TYR:HB2	2.00	0.43
1:A:51:ARG:HB2	1:A:92:TYR:HB2	1.99	0.43
1:A:53:TRP:CH2	1:A:78:MET:HE1	2.53	0.43
1:A:305:LEU:HD12	1:A:311:ILE:HG12	1.98	0.43
1:V:102:ARG:NH1	1:V:375:HIS:CD2	2.87	0.43
1:D:110:SER:O	1:D:121:LEU:HD12	2.18	0.43
1:D:174:SER:HB2	1:H:160:ASP:CG	2.38	0.43
1:H:200:GLY:N	1:H:212:LYS:O	2.43	0.43
1:H:318:LEU:HD23	1:H:318:LEU:C	2.38	0.43
1:H:354:ILE:HB	1:H:371:TYR:HB2	2.01	0.43
1:I:112:ASN:ND2	1:I:122:ARG:HH21	2.12	0.43
1:I:306:ILE:HG13	1:I:306:ILE:H	1.67	0.43
1:J:53:TRP:CZ3	1:J:78:MET:CE	3.01	0.43
1:J:100:ILE:O	2:J:501:QRP:HA	2.18	0.43
1:K:252:LEU:CD2	1:K:301:LEU:HD23	2.48	0.43
1:K:274:VAL:HG22	1:K:275:GLU:N	2.34	0.43
1:L:257:MET:HE1	1:L:355:TRP:CZ2	2.54	0.43
1:M:212:LYS:HB2	1:M:212:LYS:HE3	1.79	0.43
1:M:305:LEU:HD11	1:M:311:ILE:HG12	1.99	0.43
1:N:253:ILE:CD1	1:N:359:ILE:HD11	2.42	0.43
1:O:108:GLU:HA	1:O:443:SER:CB	2.48	0.43
1:O:305:LEU:CD1	1:O:311:ILE:HG12	2.47	0.43
1:O:308:GLU:HB2	1:O:311:ILE:CD1	2.43	0.43
1:Q:71:LEU:HB3	1:Q:72:PRO:HD3	1.99	0.43
1:R:386:LEU:CD1	1:R:390:TRP:HE1	2.31	0.43
1:R:426:SER:O	1:R:437:MET:HG3	2.17	0.43
1:S:427:TYR:HD1	1:S:437:MET:HE2	1.83	0.43
1:T:269:LEU:HD12	1:T:282:LYS:O	2.17	0.43
1:T:285:GLY:HA3	1:T:355:TRP:CE2	2.53	0.43
1:T:324:LEU:HB3	1:T:385:ALA:HB1	2.00	0.43
1:U:321:ILE:HG13	1:U:389:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:92:TYR:CB	1:W:93:PRO:HD3	2.46	0.43
1:W:115:LYS:HE2	1:W:435:VAL:N	2.33	0.43
1:W:386:LEU:CD1	1:W:390:TRP:HE1	2.31	0.43
1:X:39:ALA:HB2	1:X:53:TRP:CZ2	2.54	0.43
1:X:115:LYS:HA	1:X:395:TRP:CE2	2.54	0.43
1:C:252:LEU:CD2	1:C:301:LEU:HD23	2.48	0.43
1:C:402:TYR:CB	1:C:403:PRO:HD3	2.41	0.43
1:C:406:LEU:CD1	1:C:415:ILE:HD11	2.49	0.43
1:A:240:ASP:O	1:A:244:ASN:N	2.52	0.43
1:V:387:ALA:HA	1:V:390:TRP:HD1	1.82	0.43
1:E:224:ALA:O	1:E:226:VAL:HG23	2.18	0.43
1:E:410:TYR:OH	1:E:441:TYR:HB3	2.18	0.43
1:E:415:ILE:HA	1:E:418:THR:CG2	2.47	0.43
1:G:63:PHE:CE1	1:G:409:LEU:CD2	3.01	0.43
1:D:77:PHE:CD1	1:D:203:PHE:CD1	3.06	0.43
1:D:374:VAL:HG11	1:D:422:GLN:CG	2.48	0.43
1:D:386:LEU:CD1	1:D:390:TRP:CZ2	3.01	0.43
1:H:402:TYR:HB3	1:H:403:PRO:CD	2.37	0.43
1:H:406:LEU:HD12	1:H:415:ILE:HD13	2.00	0.43
1:J:386:LEU:HD13	1:J:390:TRP:HE1	1.79	0.43
1:J:418:THR:OG1	1:J:421:LEU:HG	2.18	0.43
1:L:111:LEU:O	1:L:438:SER:HA	2.18	0.43
1:M:154:LEU:HB3	1:M:156:LEU:CD1	2.49	0.43
1:M:174:SER:HB3	1:O:162:PRO:HG2	2.00	0.43
1:N:290:VAL:HG23	1:N:294:LYS:HB3	2.01	0.43
1:N:433:ARG:HG3	1:N:436:TYR:OH	2.18	0.43
1:O:299:TRP:NE1	1:O:311:ILE:HG23	2.33	0.43
1:R:317:ARG:HB2	1:R:427:TYR:OH	2.18	0.43
1:U:123:ILE:HD12	1:U:203:PHE:CE2	2.53	0.43
1:W:228:VAL:CG1	1:W:232:ILE:HD11	2.46	0.43
1:W:295:ILE:HG23	1:W:370:PHE:HE2	1.83	0.43
1:X:100:ILE:O	2:X:501:QRP:HA	2.18	0.43
1:A:284:TYR:N	1:A:284:TYR:CD1	2.86	0.43
1:V:274:VAL:HG22	1:V:275:GLU:N	2.33	0.43
1:V:305:LEU:HD23	1:V:305:LEU:N	2.33	0.43
1:E:291:THR:O	1:E:295:ILE:HG13	2.18	0.43
1:G:228:VAL:O	1:G:232:ILE:HG13	2.19	0.43
1:D:275:GLU:CD	1:D:277:SER:H	2.21	0.43
1:H:415:ILE:HA	1:H:418:THR:CG2	2.49	0.43
1:I:390:TRP:CZ3	1:I:395:TRP:CZ3	3.06	0.43
1:J:86:ILE:HB	1:J:87:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:100:ILE:O	2:J:501:QRP:CD1	2.66	0.43
1:J:224:ALA:O	1:J:226:VAL:HG23	2.18	0.43
1:J:365:PHE:HD2	1:J:366:PRO:O	2.01	0.43
1:K:369:LYS:O	1:K:370:PHE:HD1	2.01	0.43
1:L:229:GLY:HA3	1:L:263:TYR:CD2	2.53	0.43
1:L:321:ILE:HG22	1:L:325:LEU:CD2	2.47	0.43
1:L:386:LEU:HD11	1:L:390:TRP:HZ2	1.83	0.43
1:M:282:LYS:HE3	1:M:284:TYR:OH	2.18	0.43
1:Q:86:ILE:HB	1:Q:87:PRO:HD3	2.01	0.43
1:Q:108:GLU:HA	1:Q:443:SER:OG	2.19	0.43
1:Q:154:LEU:HB2	1:Q:156:LEU:HD13	1.99	0.43
1:Q:324:LEU:HB3	1:Q:385:ALA:HB1	2.00	0.43
1:Q:354:ILE:HG21	3:Q:502:DST:C13	2.43	0.43
1:S:249:ALA:HB3	1:S:359:ILE:HG23	2.00	0.43
1:T:53:TRP:CH2	1:T:78:MET:HE2	2.53	0.43
1:U:356:ASN:HB3	1:U:369:LYS:HB3	2.00	0.43
1:X:53:TRP:HZ3	1:X:78:MET:CE	2.31	0.43
1:C:212:LYS:HE3	1:C:212:LYS:HB2	1.78	0.43
1:V:250:PHE:O	1:V:253:ILE:N	2.50	0.43
1:V:390:TRP:HB2	1:V:399:ALA:CB	2.29	0.43
1:E:105:LEU:CD1	1:E:107:ILE:HG22	2.49	0.43
1:G:315:LEU:HD23	1:G:315:LEU:C	2.38	0.43
1:B:84:HIS:CE1	1:B:154:LEU:HD11	2.54	0.43
1:F:163:PHE:CD2	1:F:279:GLN:NE2	2.87	0.43
1:H:108:GLU:HA	1:H:443:SER:CB	2.48	0.43
1:I:51:ARG:HB2	1:I:92:TYR:HB2	2.01	0.43
1:J:281:LEU:C	1:J:281:LEU:HD12	2.39	0.43
1:L:386:LEU:CD1	1:L:390:TRP:HE1	2.31	0.43
1:L:390:TRP:CZ3	1:L:395:TRP:CZ3	3.05	0.43
1:M:51:ARG:HB3	1:M:92:TYR:CG	2.54	0.43
1:M:402:TYR:O	1:M:405:THR:HB	2.19	0.43
1:N:63:PHE:CE2	1:N:109:PHE:CB	3.02	0.43
1:O:120:LEU:CD2	1:O:205:PRO:HD3	2.49	0.43
1:O:233:ALA:HA	1:O:250:PHE:CE2	2.54	0.43
1:O:391:ASP:O	1:O:394:GLY:N	2.51	0.43
1:P:324:LEU:O	1:P:327:ILE:HG22	2.18	0.43
1:Q:390:TRP:HB2	1:Q:399:ALA:CB	2.35	0.43
1:R:179:ARG:NH1	1:R:182:GLN:HB3	2.34	0.43
1:S:390:TRP:CH2	1:S:437:MET:SD	3.12	0.43
1:T:386:LEU:HD11	1:T:390:TRP:HZ2	1.83	0.43
1:W:281:LEU:C	1:W:281:LEU:HD12	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:117:SER:O	1:X:118:HIS:CB	2.67	0.43
1:C:275:GLU:CD	1:C:277:SER:H	2.20	0.43
1:C:418:THR:OG1	1:C:421:LEU:HG	2.18	0.43
1:C:426:SER:OG	1:C:438:SER:HB2	2.18	0.43
1:A:174:SER:OG	1:A:175:LEU:N	2.52	0.43
1:V:171:PHE:HE1	1:V:231:LEU:HD13	1.84	0.43
1:V:284:TYR:N	1:V:284:TYR:CD1	2.86	0.43
1:E:229:GLY:HA3	1:E:263:TYR:CD2	2.53	0.43
1:G:92:TYR:CB	1:G:93:PRO:HD3	2.48	0.43
1:B:428:SER:HB3	1:B:436:TYR:CB	2.45	0.43
1:D:281:LEU:C	1:D:281:LEU:HD12	2.38	0.43
1:F:299:TRP:CD1	1:F:315:LEU:HB2	2.54	0.43
1:F:321:ILE:O	1:F:325:LEU:HD23	2.19	0.43
1:H:306:ILE:H	1:H:306:ILE:HG13	1.67	0.43
1:H:386:LEU:CD1	1:H:390:TRP:HE1	2.27	0.43
1:I:167:LEU:O	1:I:171:PHE:CD2	2.68	0.43
1:I:224:ALA:O	1:I:226:VAL:HG23	2.19	0.43
1:I:275:GLU:OE1	1:K:175:LEU:CD1	2.67	0.43
1:J:48:ASP:CG	1:J:91:PRO:HA	2.39	0.43
1:J:83:HIS:O	1:J:87:PRO:HG2	2.19	0.43
1:K:147:LEU:HD23	1:K:199:PHE:HD2	1.84	0.43
1:K:426:SER:O	1:K:437:MET:HA	2.18	0.43
1:L:360:HIS:ND1	1:L:361:PRO:HD2	2.33	0.43
1:N:115:LYS:HA	1:N:395:TRP:CE2	2.53	0.43
1:O:53:TRP:HZ3	1:O:82:MET:HG2	1.84	0.43
1:O:163:PHE:CD2	1:O:279:GLN:NE2	2.87	0.43
1:P:257:MET:HE3	1:P:263:TYR:N	2.34	0.43
1:P:386:LEU:CD1	1:P:390:TRP:HE1	2.32	0.43
2:P:501:QRP:O	2:P:501:QRP:HE3	2.19	0.43
1:R:60:PHE:HD1	1:R:109:PHE:CE1	2.37	0.43
1:R:141:ARG:NH1	1:R:145:THR:HG21	2.33	0.43
1:S:305:LEU:HD23	1:S:305:LEU:N	2.32	0.43
1:T:102:ARG:HH11	1:T:375:HIS:CD2	2.37	0.43
1:T:284:TYR:N	1:T:284:TYR:CD1	2.87	0.43
1:X:221:ALA:HB2	1:X:231:LEU:HD21	2.01	0.43
1:C:115:LYS:HE2	1:C:434:GLY:CA	2.42	0.43
1:C:240:ASP:CG	1:C:247:THR:HG22	2.39	0.43
1:C:242:GLU:O	1:C:243:ARG:CG	2.56	0.43
1:A:290:VAL:HG23	1:A:294:LYS:CG	2.49	0.43
1:E:107:ILE:HA	1:E:124:GLY:O	2.19	0.43
1:E:128:VAL:HG12	1:E:129:SER:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:LEU:CD2	1:E:301:LEU:HD23	2.48	0.43
1:E:321:ILE:CD1	1:E:437:MET:HE2	2.49	0.43
1:E:386:LEU:CD1	1:E:390:TRP:CZ2	3.02	0.43
1:F:379:ASP:OD2	1:F:421:LEU:HB2	2.17	0.43
1:F:420:ARG:HB2	1:F:447:TYR:OH	2.19	0.43
1:H:428:SER:HB3	1:H:436:TYR:CB	2.36	0.43
1:I:373:PRO:HG3	1:I:424:TRP:CZ3	2.54	0.43
1:J:277:SER:HB3	1:J:278:GLU:OE1	2.18	0.43
1:L:204:ASN:OD1	1:L:206:ASP:O	2.37	0.43
1:M:250:PHE:O	1:M:253:ILE:N	2.49	0.43
1:N:53:TRP:CH2	1:N:78:MET:CE	3.02	0.43
1:O:92:TYR:CB	1:O:93:PRO:HD3	2.46	0.43
1:O:115:LYS:HE2	1:O:434:GLY:CA	2.43	0.43
1:O:305:LEU:HD23	1:O:305:LEU:N	2.32	0.43
1:P:359:ILE:HG22	1:P:359:ILE:O	2.18	0.43
1:Q:100:ILE:O	2:Q:501:QRP:HA	2.19	0.43
1:R:228:VAL:O	1:R:232:ILE:HG13	2.19	0.43
1:R:292:TRP:HZ2	1:R:315:LEU:CD2	2.31	0.43
1:R:386:LEU:HD13	1:R:390:TRP:CE2	2.54	0.43
1:S:233:ALA:HA	1:S:250:PHE:CE2	2.54	0.43
1:U:321:ILE:O	1:U:325:LEU:HD23	2.17	0.43
1:C:102:ARG:HH11	1:C:375:HIS:CD2	2.36	0.43
1:C:292:TRP:HZ2	1:C:315:LEU:CD2	2.30	0.43
1:C:390:TRP:O	1:C:394:GLY:N	2.52	0.43
1:V:46:THR:OG1	1:V:49:GLN:HG3	2.19	0.43
1:V:110:SER:O	1:V:121:LEU:HD12	2.19	0.43
1:V:175:LEU:CD1	1:X:275:GLU:OE1	2.67	0.43
1:V:212:LYS:NZ	3:V:502:DST:O5	2.52	0.43
1:E:221:ALA:HB2	1:E:231:LEU:HD21	2.00	0.43
1:G:321:ILE:CD1	1:G:437:MET:HE1	2.48	0.43
1:B:115:LYS:HG2	1:B:395:TRP:CZ2	2.54	0.43
1:D:306:ILE:HG13	1:D:306:ILE:H	1.68	0.43
1:H:140:ASN:OD1	1:H:143:PRO:HG2	2.18	0.43
1:H:171:PHE:CE1	1:H:231:LEU:HD13	2.54	0.43
1:J:320:GLN:CG	1:J:320:GLN:HA	2.43	0.43
1:K:105:LEU:HD12	1:K:105:LEU:C	2.39	0.43
1:K:229:GLY:HA2	1:K:232:ILE:HB	2.00	0.43
1:K:291:THR:O	1:K:295:ILE:HG13	2.18	0.43
2:L:501:QRP:O	2:L:501:QRP:HE3	2.19	0.43
1:M:233:ALA:HA	1:M:250:PHE:CE2	2.54	0.43
1:M:239:ILE:CA	1:M:242:GLU:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:60:PHE:HE1	1:N:123:ILE:HD11	1.83	0.43
1:O:77:PHE:CD1	1:O:203:PHE:CD1	3.07	0.43
1:O:85:LEU:HB3	1:O:125:PHE:CE1	2.49	0.43
1:Q:373:PRO:HG3	1:Q:424:TRP:CZ3	2.53	0.43
1:R:257:MET:HE1	1:R:355:TRP:HZ2	1.83	0.43
1:R:318:LEU:HD12	1:R:427:TYR:CD2	2.54	0.43
1:T:99:THR:HG23	1:T:193:LEU:CD2	2.33	0.43
1:T:321:ILE:HD11	1:T:389:PHE:CE2	2.53	0.43
1:U:324:LEU:HB3	1:U:385:ALA:HB1	2.01	0.43
1:W:374:VAL:HG11	1:W:382:VAL:HG11	2.01	0.43
1:X:321:ILE:HD11	1:X:437:MET:HE1	2.00	0.43
1:V:212:LYS:NZ	3:V:502:DST:P1	2.91	0.43
1:V:315:LEU:HD23	1:V:315:LEU:C	2.39	0.43
1:B:92:TYR:CB	1:B:93:PRO:HD3	2.49	0.43
1:B:386:LEU:CD1	1:B:390:TRP:HE1	2.32	0.43
1:D:326:GLN:HG3	1:D:326:GLN:O	2.19	0.43
1:H:242:GLU:O	1:H:243:ARG:CG	2.57	0.43
1:H:257:MET:HE3	1:H:263:TYR:N	2.34	0.43
1:I:117:SER:O	1:I:118:HIS:CB	2.67	0.43
1:J:140:ASN:OD1	1:J:143:PRO:HG2	2.17	0.43
1:K:173:LEU:HD13	1:K:196:GLN:NE2	2.34	0.43
1:K:315:LEU:O	1:K:315:LEU:HD23	2.18	0.43
1:O:81:PHE:CD1	1:O:85:LEU:HD12	2.53	0.43
1:O:142:ILE:N	1:O:143:PRO:CD	2.82	0.43
1:O:292:TRP:CZ3	1:O:318:LEU:HD22	2.54	0.43
1:O:389:PHE:CE2	1:O:437:MET:HE1	2.48	0.43
1:P:53:TRP:CH2	1:P:78:MET:HE2	2.54	0.43
1:P:108:GLU:HA	1:P:443:SER:OG	2.18	0.43
1:Q:206:ASP:O	1:Q:208:ALA:N	2.50	0.43
1:R:107:ILE:HA	1:R:124:GLY:O	2.19	0.43
1:R:112:ASN:ND2	1:R:122:ARG:HH21	2.16	0.43
1:R:180:GLN:OE1	1:R:180:GLN:HA	2.18	0.43
1:R:351:SER:OG	1:R:373:PRO:HB3	2.19	0.43
1:S:111:LEU:O	1:S:438:SER:HA	2.18	0.43
1:T:63:PHE:CD2	1:T:109:PHE:HB3	2.53	0.43
1:W:60:PHE:CE1	1:W:123:ILE:HD11	2.54	0.43
1:W:389:PHE:CE2	1:W:393:LEU:HD11	2.54	0.43
1:X:112:ASN:ND2	1:X:122:ARG:HH21	2.14	0.43
1:X:141:ARG:O	1:X:141:ARG:HG2	2.19	0.43
1:A:46:THR:OG1	1:A:49:GLN:HG3	2.19	0.42
1:V:154:LEU:HB2	1:V:156:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:228:VAL:HG11	1:V:267:THR:HG23	2.01	0.42
1:V:275:GLU:CD	1:V:277:SER:H	2.22	0.42
1:E:53:TRP:HZ3	1:E:82:MET:HG2	1.84	0.42
1:B:117:SER:O	1:B:118:HIS:CB	2.67	0.42
1:B:242:GLU:O	1:B:243:ARG:CG	2.57	0.42
1:B:269:LEU:CD1	1:B:283:ILE:HG13	2.49	0.42
1:D:300:THR:HA	1:D:305:LEU:HD21	2.00	0.42
1:D:391:ASP:O	1:D:394:GLY:N	2.52	0.42
1:F:77:PHE:CD1	1:F:203:PHE:CD1	3.07	0.42
1:I:60:PHE:HD1	1:I:109:PHE:CE1	2.36	0.42
1:J:420:ARG:HB2	1:J:447:TYR:OH	2.19	0.42
1:K:36:GLN:OE1	1:K:58:SER:HA	2.18	0.42
1:L:108:GLU:HA	1:L:443:SER:OG	2.19	0.42
1:L:171:PHE:HE1	1:L:231:LEU:HD13	1.84	0.42
1:L:179:ARG:NH1	1:L:182:GLN:HB3	2.34	0.42
1:L:212:LYS:HZ3	3:L:502:DST:P1	2.42	0.42
1:M:52:TRP:CE2	1:M:89:LEU:HB3	2.54	0.42
1:M:252:LEU:CD2	1:M:301:LEU:HD23	2.49	0.42
1:M:386:LEU:CD1	1:M:390:TRP:CZ2	3.02	0.42
1:N:154:LEU:CB	1:N:156:LEU:CD1	2.97	0.42
1:N:315:LEU:HD23	1:N:315:LEU:C	2.40	0.42
1:O:102:ARG:HH11	1:O:375:HIS:CD2	2.37	0.42
1:O:227:PRO:O	1:O:230:THR:OG1	2.28	0.42
1:O:281:LEU:C	1:O:281:LEU:HD12	2.39	0.42
1:O:321:ILE:HG22	1:O:325:LEU:CD2	2.49	0.42
1:P:282:LYS:CB	1:P:284:TYR:HE1	2.31	0.42
1:P:440:TYR:OH	3:P:502:DST:O7	2.34	0.42
1:Q:100:ILE:HB	2:Q:501:QRP:CE2	2.49	0.42
1:Q:237:ARG:O	1:Q:240:ASP:HB2	2.19	0.42
1:R:212:LYS:HE3	1:R:212:LYS:HB2	1.80	0.42
1:R:372:LEU:O	1:R:424:TRP:HA	2.18	0.42
1:W:52:TRP:CE2	1:W:89:LEU:HB3	2.54	0.42
1:W:100:ILE:O	2:W:501:QRP:CD1	2.67	0.42
1:W:167:LEU:N	1:W:167:LEU:HD12	2.34	0.42
1:X:154:LEU:HB3	1:X:156:LEU:CD1	2.49	0.42
1:X:282:LYS:HB2	1:X:284:TYR:HE1	1.83	0.42
1:C:71:LEU:HB3	1:C:72:PRO:HD3	2.00	0.42
1:A:418:THR:OG1	1:A:421:LEU:HG	2.18	0.42
1:V:420:ARG:HH12	1:V:448:LEU:HB2	1.85	0.42
1:E:102:ARG:NH1	1:E:375:HIS:CD2	2.87	0.42
1:E:402:TYR:O	1:E:405:THR:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:292:TRP:CZ2	1:G:319:LYS:HB2	2.54	0.42
1:L:66:ALA:CB	1:L:409:LEU:HD11	2.48	0.42
1:L:291:THR:O	1:L:295:ILE:HG13	2.19	0.42
1:L:321:ILE:HD11	1:L:389:PHE:CE2	2.54	0.42
1:L:359:ILE:O	1:L:359:ILE:HG22	2.19	0.42
1:L:419:THR:HG23	1:L:420:ARG:HG3	2.01	0.42
1:M:353:ILE:HG13	1:M:353:ILE:O	2.18	0.42
1:N:255:ASP:HB3	1:N:304:ARG:NH1	2.33	0.42
1:N:353:ILE:C	1:N:353:ILE:HD12	2.39	0.42
1:P:115:LYS:HG2	1:P:395:TRP:CE2	2.54	0.42
1:P:270:SER:HB3	1:P:282:LYS:HB2	2.01	0.42
1:R:283:ILE:N	1:R:283:ILE:HD12	2.34	0.42
1:R:299:TRP:CZ2	1:R:368:PRO:HG2	2.55	0.42
1:S:100:ILE:O	2:S:501:QRP:CG	2.67	0.42
1:S:430:THR:HG22	1:S:432:LYS:N	2.35	0.42
2:S:501:QRP:HB	3:S:502:DST:C13	2.50	0.42
1:T:299:TRP:NE1	1:T:311:ILE:HG23	2.34	0.42
1:T:435:VAL:HG11	1:T:437:MET:HE3	2.00	0.42
1:U:75:TYR:CD2	1:X:75:TYR:HD2	2.17	0.42
1:U:107:ILE:HA	1:U:124:GLY:O	2.19	0.42
1:U:305:LEU:HD23	1:U:305:LEU:H	1.84	0.42
1:W:255:ASP:O	1:W:259:GLU:HG3	2.19	0.42
1:X:63:PHE:HB3	1:X:121:LEU:HD13	2.00	0.42
1:X:108:GLU:HA	1:X:443:SER:OG	2.19	0.42
1:X:387:ALA:HA	1:X:390:TRP:HD1	1.81	0.42
1:A:92:TYR:CB	1:A:93:PRO:HD3	2.47	0.42
1:E:117:SER:O	1:E:118:HIS:CB	2.67	0.42
1:E:300:THR:O	1:E:305:LEU:HD23	2.19	0.42
1:E:320:GLN:HE22	1:E:392:SER:HB3	1.84	0.42
1:G:402:TYR:O	1:G:405:THR:N	2.52	0.42
1:B:252:LEU:HD23	1:B:301:LEU:CD2	2.49	0.42
1:B:386:LEU:HD13	1:B:390:TRP:CE2	2.54	0.42
1:D:115:LYS:HG2	1:D:395:TRP:CZ2	2.54	0.42
1:D:255:ASP:HB3	1:D:304:ARG:NH1	2.34	0.42
1:F:278:GLU:OE1	1:F:278:GLU:N	2.51	0.42
1:F:369:LYS:O	1:F:370:PHE:HD1	2.02	0.42
1:H:63:PHE:HE2	1:H:109:PHE:HB2	1.84	0.42
1:H:253:ILE:CD1	1:H:359:ILE:HD11	2.48	0.42
1:H:324:LEU:O	1:H:327:ILE:HG22	2.19	0.42
1:H:424:TRP:HB2	1:H:440:TYR:CD2	2.54	0.42
1:L:92:TYR:CB	1:L:93:PRO:HD3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:167:LEU:O	1:L:171:PHE:HD2	2.02	0.42
1:M:318:LEU:HD23	1:M:318:LEU:C	2.40	0.42
1:N:240:ASP:O	1:N:244:ASN:N	2.51	0.42
1:P:117:SER:O	1:P:118:HIS:CB	2.67	0.42
1:P:163:PHE:CD2	1:P:279:GLN:NE2	2.87	0.42
1:P:356:ASN:OD1	1:P:357:TYR:N	2.52	0.42
1:Q:105:LEU:HD13	1:Q:107:ILE:HG22	1.99	0.42
1:Q:115:LYS:HG2	1:Q:395:TRP:CZ2	2.53	0.42
1:R:321:ILE:HD11	1:R:437:MET:HE1	2.01	0.42
1:R:374:VAL:CG1	1:R:382:VAL:HG21	2.44	0.42
1:S:300:THR:O	1:S:305:LEU:HD23	2.19	0.42
1:T:100:ILE:O	2:T:501:QRP:HA	2.19	0.42
1:T:321:ILE:O	1:T:325:LEU:HD23	2.19	0.42
1:W:128:VAL:HG12	1:W:129:SER:N	2.34	0.42
1:X:63:PHE:HE2	1:X:109:PHE:HB2	1.82	0.42
1:X:100:ILE:HG13	1:X:101:SER:N	2.34	0.42
1:X:126:GLU:O	1:X:128:VAL:HG23	2.19	0.42
1:C:369:LYS:NZ	3:C:502:DST:O4	2.47	0.42
1:A:160:ASP:HB3	1:A:162:PRO:CD	2.50	0.42
1:V:275:GLU:OE1	1:X:175:LEU:CD1	2.68	0.42
1:E:300:THR:HA	1:E:305:LEU:HD21	2.01	0.42
1:E:315:LEU:HD23	1:E:315:LEU:C	2.39	0.42
1:G:419:THR:HG23	1:G:420:ARG:HG3	2.00	0.42
1:D:171:PHE:CE1	1:D:231:LEU:HD13	2.54	0.42
1:D:193:LEU:HD12	1:D:193:LEU:N	2.35	0.42
1:D:221:ALA:CA	1:D:231:LEU:HD21	2.50	0.42
1:F:239:ILE:O	1:F:239:ILE:HG13	2.20	0.42
1:H:108:GLU:OE2	2:H:501:QRP:HD1	2.19	0.42
1:J:63:PHE:CE1	1:J:409:LEU:HD23	2.54	0.42
1:J:85:LEU:O	1:J:89:LEU:HG	2.20	0.42
1:K:81:PHE:CE2	1:K:86:ILE:HD11	2.55	0.42
1:K:237:ARG:O	1:K:240:ASP:HB2	2.19	0.42
1:L:406:LEU:HD12	1:L:415:ILE:HD11	2.01	0.42
1:M:102:ARG:HH11	1:M:375:HIS:CD2	2.37	0.42
1:Q:237:ARG:HA	1:Q:240:ASP:OD2	2.19	0.42
1:S:229:GLY:HA3	1:S:263:TYR:CE2	2.55	0.42
1:T:284:TYR:N	1:T:284:TYR:HD1	2.18	0.42
1:T:300:THR:O	1:T:305:LEU:HD23	2.19	0.42
1:T:386:LEU:CD1	1:T:390:TRP:HE1	2.32	0.42
1:T:418:THR:OG1	1:T:421:LEU:HG	2.19	0.42
2:X:501:QRP:O	2:X:501:QRP:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:351:SER:CB	1:V:375:HIS:NE2	2.83	0.42
1:E:211:VAL:HG12	1:E:273:PHE:CD2	2.54	0.42
1:E:299:TRP:CZ2	1:E:368:PRO:HG2	2.55	0.42
1:E:386:LEU:HD11	1:E:390:TRP:HZ2	1.84	0.42
1:G:52:TRP:CE2	1:G:89:LEU:HB3	2.55	0.42
1:G:321:ILE:O	1:G:325:LEU:HD23	2.19	0.42
1:G:410:TYR:CD1	1:G:421:LEU:HD22	2.54	0.42
1:G:418:THR:CG2	1:G:421:LEU:HD12	2.33	0.42
1:B:379:ASP:OD2	1:B:421:LEU:N	2.52	0.42
1:D:237:ARG:HA	1:D:240:ASP:OD2	2.19	0.42
1:D:353:ILE:O	1:D:353:ILE:HG13	2.20	0.42
1:F:154:LEU:HB2	1:F:156:LEU:HD13	2.01	0.42
1:F:252:LEU:CD2	1:F:301:LEU:HD23	2.50	0.42
1:I:226:VAL:HG12	1:I:230:THR:OG1	2.19	0.42
1:J:353:ILE:O	1:J:353:ILE:HG13	2.19	0.42
1:L:315:LEU:HD23	1:L:315:LEU:C	2.39	0.42
1:O:60:PHE:CE1	1:O:123:ILE:HD11	2.55	0.42
1:Q:100:ILE:O	2:Q:501:QRP:CG	2.67	0.42
1:Q:315:LEU:O	1:Q:315:LEU:HD23	2.19	0.42
1:Q:317:ARG:O	1:Q:320:GLN:HB3	2.20	0.42
1:Q:402:TYR:HB3	1:Q:403:PRO:CD	2.35	0.42
1:Q:418:THR:OG1	1:Q:421:LEU:HG	2.20	0.42
1:R:321:ILE:HG12	1:R:389:PHE:CD1	2.54	0.42
1:R:390:TRP:CZ3	1:R:395:TRP:CZ3	3.07	0.42
1:S:227:PRO:O	1:S:230:THR:OG1	2.29	0.42
1:S:353:ILE:C	1:S:353:ILE:HD12	2.40	0.42
2:S:501:QRP:O	2:S:501:QRP:HE3	2.20	0.42
1:U:52:TRP:CD2	1:U:89:LEU:HD13	2.54	0.42
1:U:86:ILE:HB	1:U:87:PRO:HD3	2.02	0.42
1:U:407:GLN:NE2	1:U:413:GLN:O	2.40	0.42
1:U:430:THR:HG22	1:U:432:LYS:H	1.85	0.42
1:W:306:ILE:H	1:W:306:ILE:HG13	1.71	0.42
1:X:369:LYS:NZ	3:X:502:DST:O4	2.52	0.42
1:C:239:ILE:O	1:C:239:ILE:HG13	2.20	0.42
1:A:228:VAL:O	1:A:232:ILE:HG13	2.20	0.42
1:B:305:LEU:HD23	1:B:305:LEU:H	1.84	0.42
1:D:122:ARG:HG2	1:D:202:ASP:OD1	2.19	0.42
1:D:300:THR:O	1:D:305:LEU:HD23	2.20	0.42
1:D:318:LEU:C	1:D:318:LEU:HD23	2.40	0.42
1:J:237:ARG:O	1:J:240:ASP:HB2	2.20	0.42
1:J:374:VAL:HG11	1:J:422:GLN:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:ARG:NH1	1:K:145:THR:HG21	2.34	0.42
1:M:271:CYS:CB	1:M:279:GLN:HE21	2.20	0.42
1:M:386:LEU:HD11	1:M:390:TRP:HZ2	1.84	0.42
1:P:92:TYR:CB	1:P:93:PRO:HD3	2.48	0.42
1:P:282:LYS:HB2	1:P:284:TYR:HE1	1.84	0.42
1:T:306:ILE:HG13	1:T:306:ILE:H	1.64	0.42
1:T:379:ASP:HB3	1:T:422:GLN:HE21	1.84	0.42
1:U:174:SER:OG	1:U:175:LEU:N	2.53	0.42
1:U:292:TRP:CZ2	1:U:315:LEU:HD21	2.54	0.42
1:W:127:PRO:HG3	1:W:147:LEU:HD22	2.01	0.42
1:X:386:LEU:HD13	1:X:390:TRP:CE2	2.55	0.42
1:C:274:VAL:HG22	1:C:275:GLU:N	2.34	0.42
1:C:321:ILE:O	1:C:325:LEU:HD23	2.19	0.42
1:V:118:HIS:HD2	1:V:119:ARG:O	2.02	0.42
1:G:239:ILE:HA	1:G:242:GLU:HB3	2.02	0.42
1:B:275:GLU:OE1	1:F:175:LEU:CD1	2.68	0.42
1:B:300:THR:C	1:B:305:LEU:CD2	2.88	0.42
1:B:420:ARG:HH12	1:B:448:LEU:HB2	1.84	0.42
1:D:53:TRP:CH2	1:D:78:MET:CE	3.02	0.42
1:F:239:ILE:HA	1:F:242:GLU:HB3	2.02	0.42
1:H:108:GLU:OE2	2:H:501:QRP:CD1	2.67	0.42
1:I:324:LEU:O	1:I:327:ILE:HG22	2.20	0.42
1:J:111:LEU:O	1:J:438:SER:HA	2.20	0.42
1:J:154:LEU:HB2	1:J:156:LEU:HD13	2.01	0.42
1:J:175:LEU:HD11	1:L:275:GLU:CD	2.40	0.42
1:K:242:GLU:O	1:K:243:ARG:CG	2.57	0.42
1:L:100:ILE:O	2:L:501:QRP:HA	2.20	0.42
1:M:115:LYS:HE2	1:M:435:VAL:N	2.35	0.42
1:M:154:LEU:HB2	1:M:156:LEU:HD13	2.00	0.42
1:N:229:GLY:HA3	1:N:263:TYR:CE2	2.55	0.42
1:N:374:VAL:CG1	1:N:382:VAL:HG11	2.48	0.42
1:Q:301:LEU:O	1:Q:304:ARG:CG	2.67	0.42
2:Q:501:QRP:CB	3:Q:502:DST:C14	2.98	0.42
1:R:420:ARG:HH12	1:R:448:LEU:HB2	1.84	0.42
1:T:102:ARG:NH1	1:T:375:HIS:CD2	2.88	0.42
1:T:231:LEU:HD12	1:T:232:ILE:N	2.35	0.42
1:X:66:ALA:O	1:X:119:ARG:NH2	2.53	0.42
1:X:212:LYS:HB2	1:X:212:LYS:HE3	1.78	0.42
1:X:371:TYR:HA	1:X:425:ILE:O	2.20	0.42
1:A:172:GLN:CA	1:A:173:LEU:HD12	2.50	0.42
1:A:386:LEU:CD1	1:A:390:TRP:CZ2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LEU:CD1	1:A:390:TRP:NE1	2.82	0.42
1:V:257:MET:HE3	1:V:263:TYR:N	2.34	0.42
1:E:127:PRO:HD2	1:E:144:ILE:HD13	2.02	0.42
1:E:239:ILE:HA	1:E:242:GLU:HB3	2.02	0.42
1:E:295:ILE:HG23	1:E:370:PHE:HE2	1.85	0.42
1:G:154:LEU:CB	1:G:156:LEU:CD1	2.98	0.42
1:B:282:LYS:HB2	1:B:284:TYR:HE1	1.84	0.42
1:D:92:TYR:CB	1:D:93:PRO:HD3	2.49	0.42
1:D:224:ALA:O	1:D:226:VAL:HG23	2.19	0.42
1:H:219:LEU:HD22	1:H:219:LEU:N	2.34	0.42
1:H:271:CYS:CB	1:H:279:GLN:HE21	2.22	0.42
1:H:380:LEU:HB2	1:H:415:ILE:CG2	2.35	0.42
1:J:154:LEU:CB	1:J:156:LEU:CD1	2.98	0.42
1:J:160:ASP:CG	1:L:174:SER:HB2	2.39	0.42
1:J:412:ASP:OD1	1:J:413:GLN:HG2	2.20	0.42
1:K:390:TRP:CH2	1:K:437:MET:SD	3.13	0.42
1:K:448:LEU:HD12	1:K:448:LEU:H	1.83	0.42
1:L:89:LEU:HD22	1:L:106:PRO:HG2	2.01	0.42
1:L:318:LEU:HD12	1:L:427:TYR:CD2	2.55	0.42
1:M:239:ILE:O	1:M:242:GLU:HB3	2.19	0.42
1:N:252:LEU:CD2	1:N:301:LEU:HD23	2.49	0.42
1:R:359:ILE:HG22	1:R:359:ILE:O	2.20	0.42
1:U:212:LYS:HB2	1:U:212:LYS:HE3	1.69	0.42
1:W:193:LEU:HD12	1:W:193:LEU:N	2.34	0.42
1:W:386:LEU:CD1	1:W:390:TRP:CZ2	3.03	0.42
1:W:402:TYR:CB	1:W:403:PRO:HD3	2.42	0.42
1:W:419:THR:HG23	1:W:420:ARG:HG3	2.02	0.42
1:X:252:LEU:CD2	1:X:301:LEU:HD23	2.49	0.42
1:X:290:VAL:HG23	1:X:294:LYS:HB3	2.00	0.42
1:X:353:ILE:HD12	1:X:353:ILE:C	2.40	0.42
1:X:386:LEU:CD1	1:X:390:TRP:NE1	2.81	0.42
1:X:420:ARG:HB2	1:X:447:TYR:OH	2.19	0.42
1:C:317:ARG:CZ	1:C:393:LEU:HD23	2.50	0.42
1:A:433:ARG:HD2	1:A:436:TYR:HE1	1.84	0.42
1:G:379:ASP:OD2	1:G:421:LEU:N	2.51	0.42
1:B:115:LYS:HE2	1:B:434:GLY:CA	2.46	0.42
1:D:305:LEU:HD12	1:D:311:ILE:HD11	2.01	0.42
1:F:359:ILE:O	1:F:359:ILE:HG22	2.19	0.42
1:H:172:GLN:CA	1:H:173:LEU:HD12	2.50	0.42
1:H:374:VAL:HG11	1:H:382:VAL:HG11	2.00	0.42
1:H:433:ARG:HD2	1:H:436:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:154:LEU:CB	1:I:156:LEU:CD1	2.98	0.42
1:I:239:ILE:HA	1:I:242:GLU:HB3	2.02	0.42
1:J:300:THR:O	1:J:305:LEU:HD23	2.20	0.42
1:K:303:GLY:O	1:K:306:ILE:HG13	2.20	0.42
1:K:433:ARG:HD2	1:K:436:TYR:HE1	1.85	0.42
1:L:53:TRP:HH2	1:L:78:MET:HE2	1.84	0.42
1:M:173:LEU:HD13	1:M:196:GLN:NE2	2.35	0.42
1:M:268:PHE:CZ	1:M:284:TYR:CD2	3.08	0.42
1:M:269:LEU:CD1	1:M:283:ILE:HG13	2.50	0.42
1:N:284:TYR:N	1:N:284:TYR:CD1	2.87	0.42
1:O:86:ILE:HB	1:O:87:PRO:HD3	2.00	0.42
1:O:212:LYS:HB2	1:O:212:LYS:HE3	1.83	0.42
1:O:284:TYR:N	1:O:284:TYR:HD1	2.18	0.42
1:Q:51:ARG:HB2	1:Q:92:TYR:HB2	2.02	0.42
1:Q:63:PHE:CE1	1:Q:409:LEU:CD2	3.02	0.42
1:R:227:PRO:O	1:R:230:THR:OG1	2.27	0.42
1:R:321:ILE:CG2	1:R:325:LEU:HD23	2.45	0.42
1:S:127:PRO:CG	1:S:147:LEU:HD23	2.49	0.42
1:S:321:ILE:CD1	1:S:437:MET:HE1	2.50	0.42
1:U:102:ARG:HH11	1:U:375:HIS:CD2	2.37	0.42
1:U:240:ASP:O	1:U:244:ASN:N	2.52	0.42
1:U:275:GLU:CD	1:W:175:LEU:HD11	2.40	0.42
1:U:275:GLU:HG3	1:U:278:GLU:OE1	2.20	0.42
1:U:386:LEU:CD1	1:U:390:TRP:HE1	2.32	0.42
1:W:433:ARG:HD2	1:W:436:TYR:HE1	1.85	0.42
1:X:320:GLN:HE22	1:X:392:SER:HB3	1.85	0.42
1:X:354:ILE:HB	1:X:371:TYR:HB2	2.02	0.42
1:X:415:ILE:CA	1:X:418:THR:HG22	2.41	0.42
1:C:51:ARG:CB	1:C:92:TYR:CG	3.03	0.42
1:A:386:LEU:HD11	1:A:390:TRP:CZ2	2.54	0.42
1:E:365:PHE:HD2	1:E:366:PRO:O	2.02	0.42
2:G:501:QRP:HB	3:G:502:DST:H131	2.01	0.42
1:B:212:LYS:HB2	1:B:212:LYS:HE3	1.81	0.42
1:D:354:ILE:HB	1:D:371:TYR:HB2	2.02	0.42
1:D:365:PHE:HD2	1:D:366:PRO:O	2.02	0.42
1:I:100:ILE:O	2:I:501:QRP:CG	2.68	0.42
1:I:285:GLY:HA3	1:I:355:TRP:CE2	2.53	0.42
1:J:77:PHE:CD1	1:J:203:PHE:CD1	3.08	0.42
1:J:141:ARG:NH2	1:J:172:GLN:NE2	2.67	0.42
1:J:237:ARG:HA	1:J:240:ASP:OD2	2.20	0.42
1:K:215:VAL:O	1:K:268:PHE:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:279:GLN:O	1:K:361:PRO:HD3	2.18	0.42
1:K:311:ILE:H	1:K:311:ILE:HD12	1.85	0.42
1:K:326:GLN:HG3	1:K:326:GLN:O	2.19	0.42
1:K:389:PHE:CE2	1:K:437:MET:HE3	2.48	0.42
1:M:52:TRP:CD2	1:M:89:LEU:HD13	2.55	0.42
1:M:211:VAL:HG12	1:M:273:PHE:CD2	2.55	0.42
1:M:356:ASN:HB3	1:M:369:LYS:HB3	2.01	0.42
2:M:501:QRP:O	2:M:501:QRP:HE3	2.20	0.42
1:N:63:PHE:CD2	1:N:109:PHE:HB3	2.54	0.42
1:N:128:VAL:HG12	1:N:129:SER:N	2.34	0.42
1:P:141:ARG:NH2	1:P:172:GLN:NE2	2.67	0.42
1:P:321:ILE:O	1:P:325:LEU:HD23	2.20	0.42
1:R:240:ASP:O	1:R:244:ASN:N	2.52	0.42
1:S:141:ARG:NH2	1:S:172:GLN:NE2	2.68	0.42
1:S:257:MET:HE1	1:S:355:TRP:CZ2	2.54	0.42
1:T:52:TRP:CE3	1:T:89:LEU:HD13	2.54	0.42
1:T:203:PHE:HD1	1:T:209:ILE:HG13	1.85	0.42
1:T:301:LEU:O	1:T:304:ARG:CG	2.66	0.42
1:U:117:SER:O	1:U:118:HIS:CB	2.68	0.42
1:U:140:ASN:OD1	1:U:143:PRO:HG2	2.19	0.42
1:W:45:PRO:HD2	1:W:49:GLN:OE1	2.19	0.42
1:W:204:ASN:OD1	1:W:206:ASP:O	2.38	0.42
1:X:105:LEU:HB2	1:X:106:PRO:HD2	2.01	0.42
1:C:266:TYR:HD1	2:C:501:QRP:HAHA	1.84	0.41
1:A:295:ILE:HG23	1:A:370:PHE:CE2	2.50	0.41
1:E:301:LEU:HD13	1:E:357:TYR:CE1	2.54	0.41
1:E:353:ILE:C	1:E:353:ILE:HD12	2.40	0.41
1:E:371:TYR:HA	1:E:425:ILE:O	2.20	0.41
1:B:292:TRP:HZ2	1:B:315:LEU:HD21	1.85	0.41
1:D:117:SER:O	1:D:118:HIS:CB	2.67	0.41
1:D:317:ARG:HB2	1:D:427:TYR:OH	2.19	0.41
1:F:154:LEU:CB	1:F:156:LEU:CD1	2.98	0.41
1:H:249:ALA:HB3	1:H:359:ILE:HG23	2.02	0.41
1:H:290:VAL:O	1:H:290:VAL:HG13	2.20	0.41
1:H:315:LEU:HD23	1:H:315:LEU:C	2.40	0.41
2:H:501:QRP:CG	3:H:502:DST:H142	2.50	0.41
1:I:326:GLN:O	1:I:326:GLN:HG3	2.21	0.41
1:J:269:LEU:HD12	1:J:283:ILE:HG13	2.01	0.41
1:K:360:HIS:ND1	1:K:361:PRO:HD2	2.35	0.41
1:K:402:TYR:CB	1:K:403:PRO:HD3	2.42	0.41
1:K:440:TYR:OH	3:K:502:DST:O8	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:110:SER:O	1:M:121:LEU:HD12	2.20	0.41
1:M:117:SER:O	1:M:118:HIS:CB	2.68	0.41
1:M:127:PRO:HG3	1:M:147:LEU:CD2	2.50	0.41
1:M:231:LEU:HD12	1:M:232:ILE:N	2.34	0.41
1:M:317:ARG:O	1:M:320:GLN:HB3	2.20	0.41
1:N:52:TRP:CE2	1:N:89:LEU:HB3	2.55	0.41
1:N:175:LEU:CD1	1:P:275:GLU:OE1	2.68	0.41
1:O:99:THR:HG23	1:O:193:LEU:CD2	2.40	0.41
1:O:295:ILE:HG23	1:O:370:PHE:CE2	2.54	0.41
1:P:108:GLU:HA	1:P:443:SER:CB	2.50	0.41
1:P:305:LEU:HD12	1:P:311:ILE:HG12	2.00	0.41
1:Q:240:ASP:O	1:Q:244:ASN:N	2.52	0.41
1:Q:351:SER:OG	1:Q:373:PRO:HB3	2.19	0.41
1:R:282:LYS:CB	1:R:284:TYR:HE1	2.33	0.41
1:S:172:GLN:HA	1:S:173:LEU:HD12	2.02	0.41
1:U:53:TRP:CH2	1:U:78:MET:HE2	2.55	0.41
1:U:170:LYS:HZ3	1:U:238:THR:HG21	1.83	0.41
1:U:206:ASP:O	1:U:208:ALA:N	2.51	0.41
1:W:172:GLN:CA	1:W:173:LEU:HD12	2.49	0.41
1:C:45:PRO:HD2	1:C:49:GLN:OE1	2.20	0.41
1:C:229:GLY:HA2	1:C:232:ILE:HB	2.02	0.41
1:C:415:ILE:CA	1:C:418:THR:HG22	2.44	0.41
1:A:100:ILE:HG13	1:A:101:SER:N	2.36	0.41
1:A:233:ALA:HA	1:A:250:PHE:CE2	2.56	0.41
1:A:269:LEU:CD1	1:A:283:ILE:HG13	2.50	0.41
1:V:239:ILE:O	1:V:239:ILE:HG13	2.20	0.41
1:E:92:TYR:CB	1:E:93:PRO:HD3	2.48	0.41
1:E:299:TRP:CH2	1:E:368:PRO:HG2	2.55	0.41
1:G:253:ILE:HD12	1:G:359:ILE:HD11	2.01	0.41
1:B:206:ASP:O	1:B:208:ALA:N	2.52	0.41
1:B:296:ALA:HA	1:B:315:LEU:HD11	2.01	0.41
1:D:128:VAL:HG12	1:D:129:SER:N	2.35	0.41
1:F:354:ILE:HB	1:F:371:TYR:HB2	2.03	0.41
1:F:419:THR:HG23	1:F:420:ARG:HG3	2.01	0.41
1:K:102:ARG:HH11	1:K:375:HIS:CD2	2.39	0.41
1:K:402:TYR:HB3	1:K:403:PRO:CD	2.43	0.41
1:L:274:VAL:HG22	1:L:275:GLU:N	2.35	0.41
1:L:353:ILE:O	1:L:353:ILE:HG13	2.20	0.41
1:M:237:ARG:O	1:M:240:ASP:HB2	2.20	0.41
1:N:66:ALA:HB2	1:N:409:LEU:HD11	2.02	0.41
1:Q:36:GLN:OE1	1:Q:58:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:117:SER:O	1:Q:118:HIS:CB	2.68	0.41
1:Q:268:PHE:CZ	1:Q:284:TYR:CD2	3.08	0.41
1:Q:321:ILE:HD11	1:Q:437:MET:HE1	2.01	0.41
1:R:44:PHE:HD2	1:R:50:GLU:OE1	2.03	0.41
1:R:115:LYS:HG2	1:R:395:TRP:CE2	2.55	0.41
1:R:374:VAL:CG1	1:R:422:GLN:HG2	2.45	0.41
1:S:240:ASP:CG	1:S:247:THR:HG22	2.41	0.41
1:S:402:TYR:CB	1:S:403:PRO:HD3	2.43	0.41
1:U:154:LEU:HB3	1:U:156:LEU:CD1	2.50	0.41
1:U:154:LEU:HB2	1:U:156:LEU:HD13	2.01	0.41
1:U:410:TYR:CE1	1:U:421:LEU:HD22	2.55	0.41
1:W:66:ALA:CB	1:W:409:LEU:HD11	2.50	0.41
1:W:242:GLU:O	1:W:243:ARG:CG	2.59	0.41
1:C:320:GLN:HE22	1:C:392:SER:CB	2.33	0.41
1:C:321:ILE:HG12	1:C:389:PHE:CD1	2.55	0.41
1:C:386:LEU:HD13	1:C:390:TRP:HE1	1.85	0.41
1:A:120:LEU:HD21	1:A:205:PRO:HD3	2.02	0.41
1:A:290:VAL:HG23	1:A:294:LYS:HG2	2.02	0.41
1:A:373:PRO:HG3	1:A:424:TRP:CZ3	2.55	0.41
1:V:51:ARG:CB	1:V:92:TYR:CG	3.04	0.41
1:V:282:LYS:HB2	1:V:284:TYR:HE1	1.85	0.41
1:B:53:TRP:HZ3	1:B:78:MET:CE	2.32	0.41
1:D:274:VAL:HG22	1:D:275:GLU:N	2.35	0.41
1:D:321:ILE:CG2	1:D:325:LEU:HD23	2.50	0.41
1:F:126:GLU:OE2	1:F:195:SER:CB	2.68	0.41
1:H:303:GLY:O	1:H:306:ILE:HG13	2.20	0.41
1:I:108:GLU:HA	1:I:443:SER:OG	2.20	0.41
1:J:160:ASP:HB3	1:J:162:PRO:CD	2.50	0.41
1:J:239:ILE:HD12	1:J:242:GLU:CG	2.47	0.41
1:J:321:ILE:HG22	1:J:325:LEU:CD2	2.50	0.41
1:J:402:TYR:O	1:J:405:THR:HB	2.20	0.41
1:K:433:ARG:NE	1:K:436:TYR:OH	2.53	0.41
1:L:430:THR:HG22	1:L:432:LYS:N	2.35	0.41
1:M:163:PHE:CD2	1:M:279:GLN:NE2	2.88	0.41
1:M:290:VAL:HG23	1:M:294:LYS:HG2	2.02	0.41
1:N:114:GLN:OE1	1:N:436:TYR:HD1	2.03	0.41
1:N:301:LEU:HD13	1:N:357:TYR:CZ	2.55	0.41
1:N:321:ILE:HG12	1:N:389:PHE:CD1	2.54	0.41
1:O:204:ASN:C	1:O:204:ASN:OD1	2.58	0.41
1:O:239:ILE:O	1:O:242:GLU:HB3	2.19	0.41
1:Q:164:PHE:CE2	1:Q:168:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:354:ILE:HB	1:R:371:TYR:HB2	2.01	0.41
1:S:94:GLN:O	1:S:94:GLN:HG3	2.19	0.41
1:T:115:LYS:HE2	1:T:435:VAL:H	1.84	0.41
1:T:211:VAL:HG12	1:T:273:PHE:CE2	2.55	0.41
1:T:321:ILE:HG22	1:T:325:LEU:CD2	2.48	0.41
1:W:123:ILE:CD1	1:W:203:PHE:CE2	3.04	0.41
1:W:379:ASP:OD2	1:W:421:LEU:HB2	2.20	0.41
1:A:63:PHE:CE1	1:A:409:LEU:CD2	3.03	0.41
1:A:200:GLY:N	1:A:212:LYS:O	2.47	0.41
1:V:115:LYS:HE3	1:V:434:GLY:HA3	2.00	0.41
1:V:174:SER:HB2	1:X:160:ASP:CG	2.41	0.41
1:V:292:TRP:HZ2	1:V:315:LEU:CD2	2.28	0.41
1:V:351:SER:HB3	1:V:375:HIS:NE2	2.35	0.41
1:E:63:PHE:CD2	1:E:109:PHE:HB3	2.56	0.41
1:E:115:LYS:HG2	1:E:395:TRP:CE2	2.56	0.41
1:E:204:ASN:OD1	1:E:206:ASP:O	2.39	0.41
1:G:299:TRP:CZ2	1:G:368:PRO:HG2	2.55	0.41
1:B:63:PHE:CE1	1:B:409:LEU:CD2	3.03	0.41
1:D:379:ASP:OD2	1:D:421:LEU:HB2	2.21	0.41
1:F:410:TYR:CD1	1:F:421:LEU:HD22	2.56	0.41
1:H:51:ARG:HB2	1:H:92:TYR:HB2	2.03	0.41
1:H:115:LYS:HE2	1:H:435:VAL:H	1.86	0.41
1:H:160:ASP:HB3	1:H:162:PRO:HD2	2.01	0.41
1:H:320:GLN:NE2	1:H:392:SER:HB3	2.36	0.41
1:I:51:ARG:CB	1:I:92:TYR:CG	3.03	0.41
1:I:172:GLN:CA	1:I:173:LEU:HD12	2.50	0.41
1:I:270:SER:HB3	1:I:282:LYS:HB2	2.02	0.41
1:I:284:TYR:N	1:I:284:TYR:HD1	2.18	0.41
1:K:92:TYR:HD2	1:K:93:PRO:HD3	1.84	0.41
2:K:501:QRP:HB	3:K:502:DST:H131	2.02	0.41
1:N:92:TYR:O	1:N:94:GLN:N	2.53	0.41
1:O:249:ALA:O	1:O:252:LEU:HB3	2.20	0.41
1:O:301:LEU:O	1:O:304:ARG:CG	2.64	0.41
1:P:257:MET:CE	1:P:355:TRP:CZ2	3.04	0.41
1:R:275:GLU:CD	1:T:175:LEU:HD11	2.40	0.41
1:S:123:ILE:HD12	1:S:203:PHE:CE2	2.56	0.41
1:S:127:PRO:HG3	1:S:147:LEU:HD22	1.99	0.41
1:S:242:GLU:O	1:S:243:ARG:CG	2.59	0.41
1:U:92:TYR:CB	1:U:93:PRO:HD3	2.48	0.41
1:U:119:ARG:N	1:U:119:ARG:HD2	2.35	0.41
1:U:123:ILE:HD12	1:U:203:PHE:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:109:PHE:CD2	1:W:443:SER:HB3	2.55	0.41
1:X:55:GLU:OE2	1:X:446:THR:HG23	2.20	0.41
1:X:359:ILE:HG22	1:X:359:ILE:O	2.19	0.41
1:C:38:LEU:HD22	1:E:79:PHE:CD1	2.56	0.41
1:V:53:TRP:CH2	1:V:78:MET:CE	3.03	0.41
1:V:53:TRP:CZ3	1:V:78:MET:CE	3.04	0.41
1:V:290:VAL:HG23	1:V:294:LYS:CB	2.49	0.41
1:V:351:SER:HG	1:V:373:PRO:HB3	1.84	0.41
1:V:402:TYR:CB	1:V:403:PRO:HD3	2.36	0.41
1:E:119:ARG:N	1:E:119:ARG:HD2	2.36	0.41
1:G:228:VAL:HG11	1:G:267:THR:HG23	2.02	0.41
1:B:147:LEU:HD23	1:B:199:PHE:CD2	2.55	0.41
1:D:351:SER:OG	1:D:373:PRO:HB3	2.20	0.41
1:F:53:TRP:HZ3	1:F:78:MET:CE	2.33	0.41
1:F:108:GLU:HA	1:F:443:SER:CB	2.51	0.41
1:F:127:PRO:HB2	1:F:143:PRO:HB2	2.01	0.41
1:F:305:LEU:HD23	1:F:305:LEU:N	2.35	0.41
1:F:390:TRP:HB2	1:F:399:ALA:CB	2.29	0.41
1:H:268:PHE:CZ	1:H:284:TYR:CD2	3.07	0.41
1:I:430:THR:HB	1:I:433:ARG:HB2	2.03	0.41
1:K:100:ILE:O	2:K:501:QRP:CG	2.69	0.41
1:K:128:VAL:HG12	1:K:129:SER:N	2.35	0.41
1:L:233:ALA:HB2	1:L:254:ASN:ND2	2.35	0.41
1:L:295:ILE:HG23	1:L:370:PHE:CE2	2.55	0.41
1:M:112:ASN:ND2	1:M:122:ARG:HH21	2.17	0.41
1:M:278:GLU:N	1:M:278:GLU:OE1	2.54	0.41
1:M:321:ILE:CG2	1:M:325:LEU:HD23	2.47	0.41
1:N:109:PHE:CD2	1:N:443:SER:HB3	2.55	0.41
1:N:237:ARG:HA	1:N:240:ASP:OD2	2.21	0.41
1:O:290:VAL:HG23	1:O:294:LYS:HB3	2.02	0.41
1:O:426:SER:OG	1:O:438:SER:HB2	2.21	0.41
1:Q:110:SER:HB2	1:Q:122:ARG:CB	2.25	0.41
1:R:175:LEU:CD1	1:T:275:GLU:OE1	2.68	0.41
1:R:209:ILE:HD12	1:S:41:TYR:CZ	2.55	0.41
1:R:300:THR:O	1:R:305:LEU:HD23	2.20	0.41
1:S:81:PHE:HD1	1:S:85:LEU:HD12	1.86	0.41
1:S:147:LEU:HD23	1:S:199:PHE:HD2	1.85	0.41
1:T:239:ILE:HA	1:T:242:GLU:HB3	2.02	0.41
1:X:386:LEU:HD13	1:X:390:TRP:HE1	1.86	0.41
1:C:48:ASP:CG	1:C:91:PRO:HA	2.41	0.41
1:C:179:ARG:NH1	1:C:182:GLN:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:VAL:HG11	1:A:422:GLN:HG3	2.03	0.41
1:E:81:PHE:CD1	1:E:85:LEU:HD12	2.56	0.41
1:E:239:ILE:O	1:E:239:ILE:HG13	2.20	0.41
1:E:267:THR:O	1:E:267:THR:HG23	2.20	0.41
1:D:282:LYS:HE3	1:D:284:TYR:OH	2.21	0.41
1:D:390:TRP:CZ3	1:D:395:TRP:CZ3	3.09	0.41
1:F:140:ASN:OD1	1:F:143:PRO:HD2	2.21	0.41
1:F:226:VAL:HG12	1:F:230:THR:OG1	2.21	0.41
1:H:100:ILE:HG13	1:H:101:SER:N	2.36	0.41
1:J:117:SER:O	1:J:118:HIS:CB	2.68	0.41
1:J:204:ASN:OD1	1:J:206:ASP:O	2.38	0.41
1:K:255:ASP:HB3	1:K:304:ARG:NH1	2.35	0.41
1:M:292:TRP:HZ2	1:M:315:LEU:HD21	1.85	0.41
1:N:375:HIS:H	1:N:423:SER:HA	1.84	0.41
1:O:100:ILE:O	2:O:501:QRP:CG	2.69	0.41
1:O:300:THR:O	1:O:305:LEU:HD23	2.20	0.41
1:O:369:LYS:NZ	3:O:502:DST:O4	2.45	0.41
2:O:501:QRP:HE3	2:O:501:QRP:O	2.21	0.41
1:P:292:TRP:HZ2	1:P:315:LEU:HD21	1.86	0.41
1:Q:51:ARG:HB3	1:Q:92:TYR:CG	2.55	0.41
1:Q:53:TRP:HH2	1:Q:78:MET:CE	2.34	0.41
1:Q:318:LEU:HD23	1:Q:318:LEU:C	2.41	0.41
1:R:92:TYR:CB	1:R:93:PRO:HD3	2.48	0.41
1:R:105:LEU:HB2	1:R:106:PRO:HD2	2.02	0.41
1:R:274:VAL:HG22	1:R:275:GLU:N	2.35	0.41
1:R:386:LEU:CD1	1:R:390:TRP:NE1	2.82	0.41
1:S:174:SER:OG	1:S:175:LEU:N	2.54	0.41
1:S:257:MET:HE1	1:S:355:TRP:HZ2	1.84	0.41
1:S:292:TRP:CZ3	1:S:318:LEU:HD22	2.56	0.41
1:S:373:PRO:HG3	1:S:424:TRP:CZ3	2.56	0.41
1:T:386:LEU:HD11	1:T:390:TRP:CZ2	2.56	0.41
1:U:239:ILE:CD1	1:U:242:GLU:CG	2.96	0.41
1:C:237:ARG:O	1:C:240:ASP:HB2	2.21	0.41
1:A:426:SER:OG	1:A:438:SER:HB2	2.21	0.41
1:V:107:ILE:HA	1:V:124:GLY:O	2.21	0.41
1:V:324:LEU:HB3	1:V:385:ALA:HB1	2.02	0.41
1:E:374:VAL:HG11	1:E:382:VAL:HG11	2.02	0.41
1:G:86:ILE:HB	1:G:87:PRO:HD3	2.03	0.41
1:G:100:ILE:HB	2:G:501:QRP:CE2	2.50	0.41
1:G:239:ILE:CD1	1:G:242:GLU:CG	2.95	0.41
1:B:100:ILE:O	2:B:501:QRP:CG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:GLN:HE21	1:D:223:ALA:CA	2.33	0.41
1:H:179:ARG:NH1	1:H:182:GLN:HB3	2.36	0.41
1:H:214:TYR:CD2	2:H:501:QRP:HH2	2.55	0.41
1:I:284:TYR:N	1:I:284:TYR:CD1	2.88	0.41
1:K:154:LEU:CB	1:K:156:LEU:CD1	2.99	0.41
1:K:301:LEU:HD13	1:K:357:TYR:CE1	2.56	0.41
1:L:52:TRP:NE1	1:L:92:TYR:HA	2.34	0.41
1:L:128:VAL:HG12	1:L:129:SER:N	2.35	0.41
1:M:317:ARG:HB2	1:M:427:TYR:OH	2.20	0.41
1:O:128:VAL:HG12	1:O:129:SER:N	2.35	0.41
1:Q:53:TRP:CZ3	1:Q:78:MET:HE1	2.55	0.41
1:Q:239:ILE:CA	1:Q:242:GLU:HB3	2.50	0.41
1:R:275:GLU:OE1	1:T:175:LEU:CD1	2.69	0.41
1:R:275:GLU:HG3	1:R:278:GLU:OE1	2.20	0.41
1:S:108:GLU:HA	1:S:443:SER:CB	2.50	0.41
1:S:315:LEU:HD23	1:S:315:LEU:C	2.40	0.41
1:T:92:TYR:CB	1:T:93:PRO:HD3	2.50	0.41
1:T:242:GLU:O	1:T:243:ARG:CG	2.59	0.41
1:U:123:ILE:CD1	1:U:203:PHE:HE2	2.34	0.41
1:U:321:ILE:CG2	1:U:325:LEU:HD23	2.51	0.41
1:W:117:SER:O	1:W:118:HIS:CB	2.68	0.41
1:W:353:ILE:HG13	1:W:353:ILE:O	2.20	0.41
1:A:115:LYS:HE2	1:A:435:VAL:H	1.86	0.41
1:V:52:TRP:CE2	1:V:89:LEU:HB3	2.55	0.41
2:B:501:QRP:HB	3:B:502:DST:C12	2.50	0.41
1:J:386:LEU:CD1	1:J:390:TRP:HE1	2.34	0.41
1:K:154:LEU:CB	1:K:156:LEU:HD13	2.51	0.41
1:M:239:ILE:CD1	1:M:242:GLU:CG	2.95	0.41
1:M:389:PHE:HE2	1:M:437:MET:HE1	1.86	0.41
1:N:92:TYR:CB	1:N:93:PRO:HD3	2.49	0.41
1:N:239:ILE:O	1:N:239:ILE:HG13	2.21	0.41
1:N:299:TRP:CD1	1:N:315:LEU:HB2	2.56	0.41
1:O:53:TRP:CZ3	1:O:78:MET:CE	3.03	0.41
1:O:306:ILE:HG13	1:O:306:ILE:H	1.65	0.41
1:S:295:ILE:HG23	1:S:370:PHE:CE2	2.55	0.41
1:T:66:ALA:O	1:T:119:ARG:NH2	2.54	0.41
1:T:211:VAL:O	1:T:273:PHE:HD2	2.04	0.41
1:U:299:TRP:NE1	1:U:311:ILE:HG23	2.35	0.41
1:X:321:ILE:CG2	1:X:325:LEU:CD2	2.99	0.41
1:X:424:TRP:HB2	1:X:440:TYR:HB2	2.03	0.41
2:X:501:QRP:CG	3:X:502:DST:H142	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ASN:OD1	1:C:143:PRO:HD2	2.21	0.41
1:C:173:LEU:HB3	1:C:176:SER:HB2	2.02	0.41
1:C:269:LEU:HD12	1:C:282:LYS:O	2.20	0.41
1:C:317:ARG:O	1:C:320:GLN:HB3	2.21	0.41
1:A:255:ASP:O	1:A:259:GLU:HG3	2.21	0.41
1:A:257:MET:HE1	1:A:355:TRP:CZ2	2.56	0.41
1:A:290:VAL:O	1:A:290:VAL:HG13	2.21	0.41
1:V:95:LYS:NZ	1:U:47:ASN:ND2	2.68	0.41
1:V:420:ARG:HB2	1:V:447:TYR:CZ	2.50	0.41
1:V:430:THR:HB	1:V:433:ARG:HB2	2.03	0.41
1:E:226:VAL:HG12	1:E:230:THR:OG1	2.21	0.41
1:E:353:ILE:O	1:E:353:ILE:HG13	2.21	0.41
1:E:386:LEU:HD13	1:E:390:TRP:CZ2	2.56	0.41
1:G:115:LYS:HE2	1:G:435:VAL:N	2.36	0.41
1:G:301:LEU:O	1:G:304:ARG:CG	2.65	0.41
1:G:326:GLN:O	1:G:326:GLN:HG3	2.21	0.41
1:B:162:PRO:HG2	1:F:174:SER:HB3	2.02	0.41
1:B:172:GLN:CA	1:B:173:LEU:HD12	2.51	0.41
1:B:255:ASP:HB3	1:B:304:ARG:NH1	2.36	0.41
1:B:282:LYS:CB	1:B:284:TYR:HE1	2.33	0.41
1:B:372:LEU:HA	1:B:373:PRO:HD3	1.96	0.41
1:D:299:TRP:CZ2	1:D:368:PRO:HG2	2.56	0.41
1:D:369:LYS:O	1:D:370:PHE:HD1	2.04	0.41
1:D:395:TRP:HB3	1:D:398:HIS:CD2	2.53	0.41
1:F:92:TYR:O	1:F:94:GLN:N	2.54	0.41
1:F:100:ILE:O	2:F:501:QRP:CG	2.69	0.41
1:F:257:MET:HE3	1:F:263:TYR:N	2.36	0.41
1:H:174:SER:OG	1:H:175:LEU:N	2.54	0.41
1:H:426:SER:O	1:H:437:MET:HA	2.21	0.41
1:I:84:HIS:NE2	1:I:154:LEU:HD11	2.35	0.41
1:I:212:LYS:HE3	1:I:212:LYS:HB2	1.81	0.41
1:J:51:ARG:HB2	1:J:92:TYR:HB2	2.03	0.41
1:J:92:TYR:CB	1:J:93:PRO:HD3	2.51	0.41
1:K:89:LEU:HD22	1:K:106:PRO:HG2	2.03	0.41
1:K:232:ILE:O	1:K:236:VAL:HG23	2.21	0.41
1:K:240:ASP:O	1:K:244:ASN:N	2.54	0.41
1:K:254:ASN:HD22	1:K:254:ASN:C	2.24	0.41
1:L:154:LEU:CB	1:L:156:LEU:HD13	2.51	0.41
1:M:389:PHE:CE2	1:M:393:LEU:HD11	2.56	0.41
1:O:237:ARG:HA	1:O:240:ASP:OD2	2.20	0.41
1:P:123:ILE:HD12	1:P:203:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:154:LEU:HB2	1:P:156:LEU:HD13	2.03	0.41
1:P:160:ASP:HB3	1:P:162:PRO:CD	2.49	0.41
1:P:373:PRO:HG3	1:P:424:TRP:HZ3	1.86	0.41
1:P:427:TYR:HD1	1:P:437:MET:CE	2.34	0.41
1:Q:77:PHE:CD1	1:Q:203:PHE:HD1	2.39	0.41
1:Q:83:HIS:O	1:Q:87:PRO:HG2	2.21	0.41
1:Q:172:GLN:HE22	1:S:165:GLN:CG	2.22	0.41
1:Q:209:ILE:C	1:Q:210:LEU:HD12	2.41	0.41
1:Q:281:LEU:HD11	1:Q:359:ILE:HD12	2.01	0.41
1:Q:285:GLY:O	1:Q:354:ILE:HG23	2.20	0.41
1:Q:448:LEU:HD12	1:Q:448:LEU:H	1.85	0.41
1:R:278:GLU:OE1	1:R:278:GLU:N	2.54	0.41
1:R:299:TRP:CD1	1:R:311:ILE:HG23	2.56	0.41
1:R:321:ILE:O	1:R:325:LEU:HD23	2.20	0.41
1:S:231:LEU:HD12	1:S:232:ILE:N	2.36	0.41
1:S:237:ARG:HA	1:S:240:ASP:OD2	2.20	0.41
1:S:269:LEU:HD12	1:S:283:ILE:HG13	2.02	0.41
1:S:412:ASP:OD1	1:S:413:GLN:N	2.54	0.41
1:T:271:CYS:CB	1:T:279:GLN:HE21	2.18	0.41
1:U:175:LEU:HD11	1:W:275:GLU:CD	2.41	0.41
1:U:232:ILE:O	1:U:236:VAL:HG23	2.21	0.41
1:U:386:LEU:HD11	1:U:390:TRP:HZ2	1.86	0.41
1:U:419:THR:HG23	1:U:420:ARG:HG3	2.02	0.41
1:U:428:SER:HB3	1:U:436:TYR:CB	2.48	0.41
1:U:440:TYR:OH	3:U:502:DST:O8	2.18	0.41
1:W:212:LYS:HZ2	3:W:502:DST:P1	2.44	0.41
1:W:296:ALA:HA	1:W:315:LEU:HD11	2.03	0.41
1:W:412:ASP:OD1	1:W:413:GLN:N	2.54	0.41
1:X:86:ILE:N	1:X:87:PRO:CD	2.84	0.41
1:X:257:MET:HE3	1:X:263:TYR:N	2.36	0.41
1:C:208:ALA:HA	1:E:41:TYR:HH	1.83	0.41
1:V:102:ARG:HH11	1:V:375:HIS:CD2	2.39	0.41
1:V:237:ARG:HA	1:V:240:ASP:OD2	2.21	0.41
1:E:160:ASP:HB3	1:E:162:PRO:CD	2.51	0.41
1:E:215:VAL:O	1:E:268:PHE:HB2	2.20	0.41
1:G:154:LEU:HB3	1:G:156:LEU:CD1	2.51	0.41
1:G:255:ASP:O	1:G:259:GLU:HG3	2.20	0.41
1:B:229:GLY:HA3	1:B:263:TYR:CD2	2.56	0.41
1:B:305:LEU:HD12	1:B:311:ILE:CD1	2.51	0.41
1:F:154:LEU:CB	1:F:156:LEU:HD13	2.51	0.41
1:F:239:ILE:O	1:F:242:GLU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:294:LYS:O	1:F:298:MET:HG3	2.21	0.41
1:H:92:TYR:CB	1:H:93:PRO:HD3	2.47	0.41
1:H:321:ILE:HD11	1:H:437:MET:HE1	2.02	0.41
1:H:420:ARG:HH12	1:H:448:LEU:HB2	1.85	0.41
1:I:171:PHE:CE1	1:I:231:LEU:HD13	2.55	0.41
1:J:212:LYS:HB2	1:J:212:LYS:HE3	1.80	0.41
1:M:105:LEU:HD13	1:M:107:ILE:HG22	2.03	0.41
1:O:63:PHE:HE2	1:O:109:PHE:HB2	1.86	0.41
1:P:53:TRP:HH2	1:P:78:MET:HE2	1.85	0.41
1:P:154:LEU:HB3	1:P:156:LEU:CD1	2.51	0.41
1:P:255:ASP:O	1:P:259:GLU:HG3	2.21	0.41
1:P:301:LEU:O	1:P:304:ARG:CG	2.68	0.41
1:Q:391:ASP:O	1:Q:394:GLY:N	2.54	0.41
1:U:418:THR:OG1	1:U:421:LEU:HG	2.20	0.41
1:W:224:ALA:O	1:W:226:VAL:HG23	2.20	0.41
1:X:321:ILE:HG12	1:X:389:PHE:CD1	2.56	0.41
1:C:206:ASP:O	1:C:208:ALA:N	2.50	0.40
1:A:112:ASN:ND2	1:A:122:ARG:HH21	2.13	0.40
1:A:160:ASP:CG	1:E:174:SER:HB2	2.42	0.40
1:V:51:ARG:HB2	1:V:92:TYR:HB2	2.03	0.40
1:V:257:MET:HE1	1:V:355:TRP:CZ2	2.56	0.40
1:G:123:ILE:HD12	1:G:203:PHE:CE2	2.56	0.40
1:B:100:ILE:HG13	1:B:101:SER:N	2.36	0.40
1:B:239:ILE:HA	1:B:242:GLU:HB3	2.03	0.40
1:B:402:TYR:HB3	1:B:403:PRO:CD	2.38	0.40
1:H:180:GLN:O	1:H:181:LEU:C	2.57	0.40
1:H:269:LEU:HD12	1:H:283:ILE:HG13	1.99	0.40
1:H:305:LEU:HD12	1:H:311:ILE:CG1	2.50	0.40
1:H:378:ASN:O	1:H:382:VAL:HG23	2.21	0.40
1:H:410:TYR:OH	1:H:441:TYR:HB3	2.21	0.40
1:J:305:LEU:HD23	1:J:305:LEU:N	2.35	0.40
1:J:430:THR:HG22	1:J:432:LYS:N	2.34	0.40
1:K:112:ASN:ND2	1:K:122:ARG:HH21	2.10	0.40
1:L:173:LEU:HB3	1:L:176:SER:HB2	2.03	0.40
1:L:389:PHE:CE2	1:L:393:LEU:HD11	2.56	0.40
1:M:200:GLY:N	1:M:212:LYS:O	2.46	0.40
1:M:274:VAL:HG22	1:M:275:GLU:N	2.36	0.40
1:P:66:ALA:CB	1:P:409:LEU:HD11	2.52	0.40
1:P:371:TYR:HA	1:P:425:ILE:O	2.21	0.40
1:Q:239:ILE:O	1:Q:242:GLU:HB3	2.21	0.40
1:R:117:SER:O	1:R:118:HIS:CB	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:249:ALA:HB3	1:R:359:ILE:HG23	2.03	0.40
1:T:212:LYS:NZ	3:T:502:DST:P1	2.94	0.40
1:T:239:ILE:HG13	1:T:239:ILE:O	2.21	0.40
1:T:420:ARG:HH12	1:T:448:LEU:HB2	1.86	0.40
1:U:170:LYS:HZ1	1:U:238:THR:HG21	1.83	0.40
1:U:318:LEU:C	1:U:318:LEU:HD23	2.41	0.40
1:W:89:LEU:HD22	1:W:106:PRO:HG2	2.03	0.40
1:W:354:ILE:HB	1:W:371:TYR:HB2	2.03	0.40
1:X:257:MET:HG3	1:X:263:TYR:CE1	2.56	0.40
1:C:53:TRP:CH2	1:C:78:MET:HE2	2.56	0.40
1:A:119:ARG:HD2	1:A:119:ARG:N	2.37	0.40
1:A:154:LEU:HB2	1:A:156:LEU:HD13	2.03	0.40
1:A:274:VAL:HG22	1:A:275:GLU:N	2.35	0.40
1:V:86:ILE:HB	1:V:87:PRO:HD3	2.02	0.40
1:V:115:LYS:HE2	1:V:434:GLY:CA	2.46	0.40
1:V:123:ILE:CD1	1:V:203:PHE:HE2	2.35	0.40
1:V:303:GLY:O	1:V:306:ILE:HG13	2.20	0.40
1:V:326:GLN:O	1:V:326:GLN:HG3	2.22	0.40
1:E:410:TYR:CD1	1:E:421:LEU:HD22	2.55	0.40
1:G:369:LYS:O	1:G:370:PHE:HD1	2.03	0.40
1:B:171:PHE:CE1	1:B:217:PRO:CB	3.00	0.40
1:D:100:ILE:O	2:D:501:QRP:CG	2.69	0.40
1:D:175:LEU:CD1	1:H:275:GLU:OE1	2.70	0.40
1:D:212:LYS:HD2	1:D:214:TYR:OH	2.21	0.40
1:D:320:GLN:HE22	1:D:392:SER:HB3	1.86	0.40
1:F:379:ASP:OD2	1:F:421:LEU:N	2.53	0.40
1:H:60:PHE:HD1	1:H:109:PHE:CE1	2.39	0.40
1:H:154:LEU:HB2	1:H:156:LEU:HD13	2.04	0.40
1:J:63:PHE:CE2	1:J:109:PHE:CB	3.04	0.40
1:J:371:TYR:HA	1:J:425:ILE:O	2.21	0.40
1:L:420:ARG:HB2	1:L:447:TYR:OH	2.21	0.40
1:M:306:ILE:HG13	1:M:306:ILE:H	1.60	0.40
1:N:100:ILE:HB	2:N:501:QRP:CE2	2.50	0.40
1:N:386:LEU:CD1	1:N:390:TRP:HE1	2.34	0.40
1:O:240:ASP:CG	1:O:247:THR:HG22	2.42	0.40
1:P:126:GLU:OE2	1:P:195:SER:CB	2.70	0.40
1:Q:53:TRP:HH2	1:Q:78:MET:HE2	1.86	0.40
1:Q:174:SER:OG	1:Q:175:LEU:N	2.55	0.40
1:Q:212:LYS:NZ	3:Q:502:DST:O6	2.54	0.40
1:Q:250:PHE:O	1:Q:253:ILE:N	2.51	0.40
1:R:321:ILE:CG1	1:R:389:PHE:CE1	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:418:THR:CG2	1:R:421:LEU:HD12	2.46	0.40
1:R:430:THR:HG22	1:R:432:LYS:N	2.36	0.40
1:T:171:PHE:CE1	1:T:217:PRO:CB	2.99	0.40
1:T:433:ARG:HD2	1:T:436:TYR:HE1	1.85	0.40
1:U:100:ILE:O	2:U:501:QRP:CG	2.68	0.40
1:U:239:ILE:O	1:U:239:ILE:HG13	2.22	0.40
1:U:301:LEU:O	1:U:304:ARG:CG	2.64	0.40
1:W:102:ARG:NH1	1:W:375:HIS:CD2	2.90	0.40
1:W:266:TYR:HD1	2:W:501:QRP:HAHA	1.86	0.40
1:W:398:HIS:H	1:W:398:HIS:CD2	2.39	0.40
1:X:154:LEU:HB2	1:X:156:LEU:CD1	2.51	0.40
1:X:254:ASN:HD22	1:X:254:ASN:C	2.23	0.40
1:C:60:PHE:HD1	1:C:109:PHE:CE1	2.38	0.40
1:C:108:GLU:HA	1:C:443:SER:CB	2.51	0.40
1:C:300:THR:C	1:C:305:LEU:HD21	2.41	0.40
1:V:111:LEU:O	1:V:438:SER:HA	2.21	0.40
1:V:291:THR:O	1:V:295:ILE:HG13	2.21	0.40
1:E:174:SER:OG	1:E:175:LEU:N	2.54	0.40
1:E:390:TRP:HB2	1:E:399:ALA:CB	2.38	0.40
1:G:63:PHE:HB3	1:G:121:LEU:CD1	2.52	0.40
1:G:229:GLY:HA3	1:G:263:TYR:CD2	2.56	0.40
1:G:410:TYR:OH	1:G:441:TYR:HB3	2.21	0.40
1:F:203:PHE:CD1	1:F:209:ILE:HG13	2.56	0.40
1:F:219:LEU:HD22	1:F:219:LEU:N	2.36	0.40
1:F:228:VAL:HG11	1:F:267:THR:CG2	2.50	0.40
1:I:66:ALA:O	1:I:119:ARG:NH2	2.55	0.40
1:I:204:ASN:OD1	1:I:206:ASP:O	2.39	0.40
1:I:321:ILE:HG22	1:I:325:LEU:CD2	2.51	0.40
1:J:105:LEU:CD1	1:J:107:ILE:HG22	2.51	0.40
1:K:60:PHE:CE2	1:K:64:LEU:HD11	2.56	0.40
1:K:249:ALA:O	1:K:252:LEU:HB3	2.22	0.40
1:K:300:THR:HA	1:K:305:LEU:HD21	2.04	0.40
1:K:369:LYS:HE2	1:K:428:SER:HB2	2.02	0.40
1:L:233:ALA:HA	1:L:250:PHE:CE2	2.56	0.40
1:L:321:ILE:HD13	1:L:437:MET:HE1	2.01	0.40
1:N:275:GLU:OE1	1:P:175:LEU:CD1	2.69	0.40
1:N:282:LYS:HB2	1:N:284:TYR:HE1	1.86	0.40
1:N:402:TYR:CB	1:N:403:PRO:HD3	2.35	0.40
1:O:282:LYS:CB	1:O:284:TYR:HE1	2.35	0.40
1:O:284:TYR:N	1:O:284:TYR:CD1	2.89	0.40
1:O:410:TYR:CD1	1:O:421:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:102:ARG:HH11	1:P:375:HIS:CD2	2.40	0.40
1:S:154:LEU:CB	1:S:156:LEU:HD13	2.50	0.40
1:S:212:LYS:HZ3	3:S:502:DST:P1	2.45	0.40
1:S:257:MET:HG3	1:S:263:TYR:CE1	2.55	0.40
1:S:380:LEU:CB	1:S:415:ILE:HG22	2.40	0.40
1:T:70:GLY:HA3	1:T:73:GLN:NE2	2.35	0.40
1:U:174:SER:HB3	1:W:162:PRO:HG2	2.03	0.40
1:W:94:GLN:O	1:W:94:GLN:HG3	2.20	0.40
1:W:229:GLY:HA3	1:W:263:TYR:CD2	2.56	0.40
1:X:66:ALA:CB	1:X:409:LEU:HD11	2.51	0.40
2:X:501:QRP:HB	3:X:502:DST:C13	2.51	0.40
1:A:231:LEU:O	1:A:235:ALA:N	2.49	0.40
1:A:412:ASP:OD1	1:A:413:GLN:N	2.55	0.40
1:V:147:LEU:HD12	1:V:147:LEU:O	2.22	0.40
1:E:89:LEU:HD22	1:E:106:PRO:HG2	2.03	0.40
1:E:164:PHE:CE2	1:E:168:LEU:HD11	2.56	0.40
1:B:253:ILE:HD11	1:B:366:PRO:CG	2.51	0.40
1:D:275:GLU:HG2	1:H:175:LEU:HD11	2.03	0.40
1:F:160:ASP:HB3	1:F:162:PRO:CD	2.50	0.40
1:I:147:LEU:HD23	1:I:199:PHE:CD2	2.56	0.40
1:J:229:GLY:HA3	1:J:263:TYR:CD2	2.56	0.40
1:J:321:ILE:CG2	1:J:325:LEU:HD23	2.51	0.40
1:M:92:TYR:CD2	1:M:93:PRO:HD3	2.56	0.40
1:M:373:PRO:HG3	1:M:424:TRP:CZ3	2.56	0.40
1:N:115:LYS:HG2	1:N:395:TRP:CE2	2.56	0.40
1:N:115:LYS:HE3	1:N:434:GLY:HA3	1.99	0.40
1:N:117:SER:O	1:N:118:HIS:CB	2.69	0.40
1:O:51:ARG:HB3	1:O:92:TYR:CG	2.57	0.40
1:P:315:LEU:HD23	1:P:315:LEU:C	2.41	0.40
1:U:221:ALA:HB2	1:U:231:LEU:HD21	2.04	0.40
1:W:111:LEU:O	1:W:438:SER:HA	2.21	0.40
1:W:324:LEU:HB3	1:W:385:ALA:HB1	2.03	0.40
1:W:324:LEU:CD1	1:W:389:PHE:HB2	2.52	0.40
1:X:60:PHE:CE2	1:X:64:LEU:HD11	2.57	0.40
1:X:174:SER:OG	1:X:175:LEU:N	2.54	0.40
1:X:204:ASN:CB	1:X:205:PRO:HD2	2.50	0.40
1:X:321:ILE:HD13	1:X:437:MET:HE1	2.04	0.40
1:C:279:GLN:O	1:C:361:PRO:HD3	2.21	0.40
1:A:433:ARG:NE	1:A:436:TYR:OH	2.54	0.40
1:A:448:LEU:HD12	1:A:448:LEU:H	1.86	0.40
1:E:234:GLU:OE2	1:E:237:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:321:ILE:CG2	1:G:325:LEU:HD23	2.49	0.40
1:B:174:SER:OG	1:B:175:LEU:N	2.54	0.40
1:B:211:VAL:HG12	1:B:273:PHE:CD2	2.56	0.40
1:D:120:LEU:CD2	1:D:205:PRO:HD3	2.48	0.40
1:D:269:LEU:HD12	1:D:282:LYS:O	2.21	0.40
1:F:299:TRP:CD1	1:F:315:LEU:HD12	2.57	0.40
1:F:386:LEU:HD13	1:F:390:TRP:HE1	1.86	0.40
1:I:53:TRP:CZ3	1:I:78:MET:CE	3.04	0.40
1:I:63:PHE:CE1	1:I:409:LEU:CD2	3.03	0.40
1:I:249:ALA:O	1:I:253:ILE:HG13	2.21	0.40
1:I:288:THR:CG2	1:I:289:GLU:H	2.33	0.40
1:J:228:VAL:CG1	1:J:232:ILE:HD11	2.47	0.40
1:J:284:TYR:N	1:J:284:TYR:CD1	2.90	0.40
1:J:311:ILE:HD12	1:J:311:ILE:N	2.36	0.40
1:K:252:LEU:HD23	1:K:301:LEU:CD2	2.52	0.40
1:K:386:LEU:HD13	1:K:390:TRP:CE2	2.55	0.40
1:M:371:TYR:HA	1:M:425:ILE:O	2.22	0.40
1:M:390:TRP:O	1:M:394:GLY:N	2.55	0.40
1:M:410:TYR:CD1	1:M:421:LEU:HD22	2.56	0.40
1:N:114:GLN:OE1	1:N:436:TYR:CD1	2.74	0.40
1:N:320:GLN:HE22	1:N:392:SER:CB	2.32	0.40
1:N:420:ARG:HH12	1:N:448:LEU:HB2	1.87	0.40
1:O:232:ILE:O	1:O:236:VAL:HG23	2.21	0.40
1:P:126:GLU:OE2	1:P:195:SER:HB2	2.22	0.40
1:P:226:VAL:HG12	1:P:230:THR:OG1	2.22	0.40
1:P:324:LEU:HB3	1:P:385:ALA:HB1	2.03	0.40
1:Q:288:THR:CG2	1:Q:289:GLU:H	2.31	0.40
1:Q:290:VAL:HG22	1:Q:295:ILE:HG13	2.04	0.40
1:R:108:GLU:OE2	2:R:501:QRP:CD1	2.70	0.40
1:R:257:MET:HE1	1:R:355:TRP:CZ2	2.57	0.40
1:R:419:THR:HG23	1:R:420:ARG:HG3	2.04	0.40
1:S:278:GLU:OE1	1:S:278:GLU:N	2.55	0.40
1:U:204:ASN:OD1	1:U:206:ASP:O	2.40	0.40
1:W:418:THR:OG1	1:W:421:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/472 (81%)	356 (93%)	22 (6%)	3 (1%)	19	57
1	B	381/472 (81%)	358 (94%)	20 (5%)	3 (1%)	19	57
1	C	381/472 (81%)	357 (94%)	21 (6%)	3 (1%)	19	57
1	D	381/472 (81%)	359 (94%)	19 (5%)	3 (1%)	19	57
1	E	381/472 (81%)	358 (94%)	20 (5%)	3 (1%)	19	57
1	F	381/472 (81%)	357 (94%)	21 (6%)	3 (1%)	19	57
1	G	381/472 (81%)	357 (94%)	21 (6%)	3 (1%)	19	57
1	H	381/472 (81%)	360 (94%)	18 (5%)	3 (1%)	19	57
1	I	381/472 (81%)	359 (94%)	19 (5%)	3 (1%)	19	57
1	J	381/472 (81%)	357 (94%)	21 (6%)	3 (1%)	19	57
1	K	381/472 (81%)	357 (94%)	21 (6%)	3 (1%)	19	57
1	L	381/472 (81%)	358 (94%)	19 (5%)	4 (1%)	15	53
1	M	381/472 (81%)	359 (94%)	19 (5%)	3 (1%)	19	57
1	N	381/472 (81%)	359 (94%)	19 (5%)	3 (1%)	19	57
1	O	381/472 (81%)	358 (94%)	20 (5%)	3 (1%)	19	57
1	P	381/472 (81%)	359 (94%)	19 (5%)	3 (1%)	19	57
1	Q	381/472 (81%)	361 (95%)	17 (4%)	3 (1%)	19	57
1	R	381/472 (81%)	359 (94%)	19 (5%)	3 (1%)	19	57
1	S	381/472 (81%)	359 (94%)	19 (5%)	3 (1%)	19	57
1	T	381/472 (81%)	359 (94%)	18 (5%)	4 (1%)	15	53
1	U	381/472 (81%)	360 (94%)	18 (5%)	3 (1%)	19	57
1	V	381/472 (81%)	359 (94%)	19 (5%)	3 (1%)	19	57
1	W	381/472 (81%)	359 (94%)	19 (5%)	3 (1%)	19	57
1	X	381/472 (81%)	359 (94%)	18 (5%)	4 (1%)	15	53
All	All	9144/11328 (81%)	8603 (94%)	466 (5%)	75 (1%)	19	57

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	118	HIS
1	C	275	GLU
1	A	118	HIS
1	A	275	GLU
1	V	118	HIS
1	V	275	GLU
1	E	118	HIS
1	E	275	GLU
1	G	118	HIS
1	G	275	GLU
1	B	118	HIS
1	B	275	GLU
1	D	118	HIS
1	D	275	GLU
1	F	118	HIS
1	F	275	GLU
1	H	118	HIS
1	H	275	GLU
1	I	118	HIS
1	I	275	GLU
1	J	118	HIS
1	J	275	GLU
1	K	118	HIS
1	K	275	GLU
1	L	118	HIS
1	L	275	GLU
1	M	118	HIS
1	M	275	GLU
1	N	118	HIS
1	N	275	GLU
1	O	118	HIS
1	O	275	GLU
1	P	118	HIS
1	P	275	GLU
1	Q	118	HIS
1	Q	275	GLU
1	R	118	HIS
1	R	275	GLU
1	S	118	HIS
1	S	275	GLU
1	T	118	HIS
1	T	275	GLU

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Mol	Chain	Res	Type
1	U	118	HIS
1	U	275	GLU
1	W	118	HIS
1	W	275	GLU
1	X	118	HIS
1	X	275	GLU
1	C	34	PRO
1	A	34	PRO
1	V	34	PRO
1	E	34	PRO
1	G	34	PRO
1	B	34	PRO
1	D	34	PRO
1	F	34	PRO
1	H	34	PRO
1	I	34	PRO
1	J	34	PRO
1	K	34	PRO
1	L	34	PRO
1	M	34	PRO
1	N	34	PRO
1	P	34	PRO
1	Q	34	PRO
1	R	34	PRO
1	T	34	PRO
1	U	34	PRO
1	W	34	PRO
1	X	34	PRO
1	O	34	PRO
1	S	34	PRO
1	L	174	SER
1	X	93	PRO
1	T	93	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/408 (83%)	335 (99%)	4 (1%)	71	90
1	B	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	C	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	D	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	E	339/408 (83%)	335 (99%)	4 (1%)	71	90
1	F	339/408 (83%)	334 (98%)	5 (2%)	65	87
1	G	339/408 (83%)	334 (98%)	5 (2%)	65	87
1	H	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	I	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	J	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	K	339/408 (83%)	335 (99%)	4 (1%)	71	90
1	L	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	M	339/408 (83%)	335 (99%)	4 (1%)	71	90
1	N	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	O	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	P	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	Q	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	R	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	S	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	T	339/408 (83%)	334 (98%)	5 (2%)	65	87
1	U	339/408 (83%)	335 (99%)	4 (1%)	71	90
1	V	339/408 (83%)	336 (99%)	3 (1%)	78	92
1	W	339/408 (83%)	335 (99%)	4 (1%)	71	90
1	X	339/408 (83%)	335 (99%)	4 (1%)	71	90
All	All	8136/9792 (83%)	8051 (99%)	85 (1%)	76	91

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	119	ARG
1	C	284	TYR
1	C	353	ILE
1	A	119	ARG
1	A	254	ASN
1	A	284	TYR

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Mol	Chain	Res	Type
1	A	353	ILE
1	V	119	ARG
1	V	284	TYR
1	V	353	ILE
1	E	47	ASN
1	E	119	ARG
1	E	284	TYR
1	E	353	ILE
1	G	119	ARG
1	G	180	GLN
1	G	254	ASN
1	G	284	TYR
1	G	353	ILE
1	B	119	ARG
1	B	284	TYR
1	B	353	ILE
1	D	119	ARG
1	D	284	TYR
1	D	353	ILE
1	F	119	ARG
1	F	180	GLN
1	F	254	ASN
1	F	284	TYR
1	F	353	ILE
1	H	119	ARG
1	H	284	TYR
1	H	353	ILE
1	I	119	ARG
1	I	284	TYR
1	I	353	ILE
1	J	119	ARG
1	J	284	TYR
1	J	353	ILE
1	K	119	ARG
1	K	254	ASN
1	K	284	TYR
1	K	353	ILE
1	L	119	ARG
1	L	284	TYR
1	L	353	ILE
1	M	119	ARG
1	M	284	TYR

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Mol	Chain	Res	Type
1	M	353	ILE
1	M	422	GLN
1	N	119	ARG
1	N	284	TYR
1	N	353	ILE
1	O	119	ARG
1	O	284	TYR
1	O	353	ILE
1	P	119	ARG
1	P	284	TYR
1	P	422	GLN
1	Q	119	ARG
1	Q	284	TYR
1	Q	353	ILE
1	R	119	ARG
1	R	284	TYR
1	R	353	ILE
1	S	119	ARG
1	S	180	GLN
1	S	284	TYR
1	T	119	ARG
1	T	180	GLN
1	T	284	TYR
1	T	353	ILE
1	T	422	GLN
1	U	119	ARG
1	U	254	ASN
1	U	284	TYR
1	U	353	ILE
1	W	119	ARG
1	W	254	ASN
1	W	284	TYR
1	W	353	ILE
1	X	119	ARG
1	X	254	ASN
1	X	284	TYR
1	X	353	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	73	GLN

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Mol	Chain	Res	Type
1	C	172	GLN
1	C	196	GLN
1	C	279	GLN
1	A	73	GLN
1	A	172	GLN
1	A	180	GLN
1	A	196	GLN
1	A	279	GLN
1	V	73	GLN
1	V	172	GLN
1	V	196	GLN
1	V	279	GLN
1	E	47	ASN
1	E	73	GLN
1	E	172	GLN
1	E	196	GLN
1	E	279	GLN
1	G	47	ASN
1	G	73	GLN
1	G	172	GLN
1	G	180	GLN
1	G	279	GLN
1	B	47	ASN
1	B	73	GLN
1	B	172	GLN
1	B	196	GLN
1	B	279	GLN
1	B	398	HIS
1	D	73	GLN
1	D	172	GLN
1	D	180	GLN
1	D	196	GLN
1	D	279	GLN
1	F	172	GLN
1	F	180	GLN
1	F	196	GLN
1	F	279	GLN
1	F	320	GLN
1	F	422	GLN
1	H	73	GLN
1	H	172	GLN
1	H	196	GLN

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Mol	Chain	Res	Type
1	H	279	GLN
1	I	73	GLN
1	I	172	GLN
1	I	196	GLN
1	I	254	ASN
1	I	279	GLN
1	J	172	GLN
1	J	196	GLN
1	J	279	GLN
1	K	73	GLN
1	K	172	GLN
1	K	196	GLN
1	K	279	GLN
1	L	47	ASN
1	L	73	GLN
1	L	172	GLN
1	L	196	GLN
1	M	73	GLN
1	M	172	GLN
1	M	180	GLN
1	M	196	GLN
1	M	279	GLN
1	N	172	GLN
1	N	279	GLN
1	O	114	GLN
1	O	172	GLN
1	O	196	GLN
1	O	279	GLN
1	O	422	GLN
1	P	73	GLN
1	P	172	GLN
1	P	196	GLN
1	P	279	GLN
1	P	320	GLN
1	P	422	GLN
1	Q	73	GLN
1	Q	172	GLN
1	Q	279	GLN
1	Q	422	GLN
1	R	73	GLN
1	R	172	GLN
1	R	279	GLN

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Mol	Chain	Res	Type
1	S	73	GLN
1	S	172	GLN
1	S	180	GLN
1	S	196	GLN
1	S	279	GLN
1	T	73	GLN
1	T	172	GLN
1	T	180	GLN
1	T	196	GLN
1	T	279	GLN
1	T	422	GLN
1	U	47	ASN
1	U	73	GLN
1	U	172	GLN
1	U	196	GLN
1	U	279	GLN
1	W	42	HIS
1	W	172	GLN
1	W	196	GLN
1	W	279	GLN
1	X	73	GLN
1	X	172	GLN
1	X	196	GLN
1	X	279	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

48 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	QRP	F	501	-	23,24,24	3.15	7 (30%)	31,35,35	1.48	3 (9%)
2	QRP	U	501	-	23,24,24	3.02	7 (30%)	31,35,35	1.33	3 (9%)
2	QRP	W	501	-	23,24,24	3.05	8 (34%)	31,35,35	1.39	3 (9%)
3	DST	N	502	-	9,13,13	1.69	3 (33%)	11,19,19	1.37	2 (18%)
3	DST	I	502	-	9,13,13	1.54	2 (22%)	11,19,19	1.51	3 (27%)
3	DST	V	502	-	9,13,13	1.45	2 (22%)	11,19,19	1.34	1 (9%)
3	DST	U	502	-	9,13,13	1.59	3 (33%)	11,19,19	1.42	2 (18%)
2	QRP	E	501	-	23,24,24	3.13	9 (39%)	31,35,35	1.45	4 (12%)
3	DST	J	502	-	9,13,13	1.63	3 (33%)	11,19,19	1.49	2 (18%)
3	DST	P	502	-	9,13,13	1.91	3 (33%)	11,19,19	1.28	1 (9%)
3	DST	X	502	-	9,13,13	1.59	2 (22%)	11,19,19	1.25	2 (18%)
3	DST	A	502	-	9,13,13	1.70	4 (44%)	11,19,19	1.47	3 (27%)
2	QRP	M	501	-	23,24,24	2.96	7 (30%)	31,35,35	1.20	2 (6%)
3	DST	R	502	-	9,13,13	1.55	2 (22%)	11,19,19	1.24	1 (9%)
2	QRP	O	501	-	23,24,24	3.00	7 (30%)	31,35,35	1.37	3 (9%)
2	QRP	I	501	-	23,24,24	3.06	8 (34%)	31,35,35	1.46	4 (12%)
2	QRP	G	501	-	23,24,24	3.08	8 (34%)	31,35,35	1.42	3 (9%)
2	QRP	P	501	-	23,24,24	3.04	8 (34%)	31,35,35	1.31	2 (6%)
2	QRP	L	501	-	23,24,24	3.10	8 (34%)	31,35,35	1.42	4 (12%)
2	QRP	D	501	-	23,24,24	3.15	8 (34%)	31,35,35	1.47	2 (6%)
3	DST	D	502	-	9,13,13	1.40	1 (11%)	11,19,19	1.54	4 (36%)
3	DST	T	502	-	9,13,13	1.87	4 (44%)	11,19,19	1.16	1 (9%)
3	DST	G	502	-	9,13,13	1.44	1 (11%)	11,19,19	1.47	2 (18%)
2	QRP	S	501	-	23,24,24	3.05	8 (34%)	31,35,35	1.42	3 (9%)
2	QRP	Q	501	-	23,24,24	3.01	7 (30%)	31,35,35	1.30	3 (9%)
3	DST	B	502	-	9,13,13	1.59	3 (33%)	11,19,19	1.59	3 (27%)
3	DST	M	502	-	9,13,13	1.58	4 (44%)	11,19,19	1.35	2 (18%)
3	DST	K	502	-	9,13,13	1.62	3 (33%)	11,19,19	1.30	1 (9%)
2	QRP	A	501	-	23,24,24	2.92	6 (26%)	31,35,35	1.27	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DST	W	502	-	9,13,13	1.66	4 (44%)	11,19,19	1.50	2 (18%)
2	QRP	R	501	-	23,24,24	3.07	8 (34%)	31,35,35	1.65	4 (12%)
2	QRP	T	501	-	23,24,24	3.14	7 (30%)	31,35,35	1.38	4 (12%)
3	DST	F	502	-	9,13,13	1.45	1 (11%)	11,19,19	1.52	2 (18%)
3	DST	C	502	-	9,13,13	1.74	3 (33%)	11,19,19	1.46	1 (9%)
2	QRP	B	501	-	23,24,24	3.17	7 (30%)	31,35,35	1.41	5 (16%)
3	DST	E	502	-	9,13,13	1.42	1 (11%)	11,19,19	1.39	2 (18%)
3	DST	L	502	-	9,13,13	1.55	2 (22%)	11,19,19	1.66	2 (18%)
2	QRP	N	501	-	23,24,24	3.11	9 (39%)	31,35,35	1.39	3 (9%)
2	QRP	V	501	-	23,24,24	3.13	10 (43%)	31,35,35	1.40	2 (6%)
2	QRP	H	501	-	23,24,24	3.05	8 (34%)	31,35,35	1.40	4 (12%)
3	DST	O	502	-	9,13,13	1.61	1 (11%)	11,19,19	1.40	2 (18%)
2	QRP	C	501	-	23,24,24	3.03	8 (34%)	31,35,35	1.44	3 (9%)
2	QRP	X	501	-	23,24,24	3.02	7 (30%)	31,35,35	1.41	5 (16%)
3	DST	Q	502	-	9,13,13	1.47	2 (22%)	11,19,19	1.48	2 (18%)
2	QRP	J	501	-	23,24,24	3.11	7 (30%)	31,35,35	1.39	3 (9%)
2	QRP	K	501	-	23,24,24	3.03	7 (30%)	31,35,35	1.40	3 (9%)
3	DST	S	502	-	9,13,13	1.82	3 (33%)	11,19,19	1.34	3 (27%)
3	DST	H	502	-	9,13,13	1.58	2 (22%)	11,19,19	1.52	3 (27%)

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
2	QRP	F	501	-	-	2/3/30/30	0/4/4/4
2	QRP	U	501	-	-	2/3/30/30	0/4/4/4
2	QRP	W	501	-	-	2/3/30/30	0/4/4/4
3	DST	N	502	-	-	3/7/13/13	-
3	DST	I	502	-	-	1/7/13/13	-
3	DST	V	502	-	-	2/7/13/13	-
3	DST	U	502	-	-	2/7/13/13	-
2	QRP	E	501	-	-	2/3/30/30	0/4/4/4
3	DST	J	502	-	-	2/7/13/13	-
3	DST	P	502	-	-	2/7/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DST	X	502	-	-	2/7/13/13	-
3	DST	A	502	-	-	1/7/13/13	-
2	QRP	M	501	-	-	2/3/30/30	0/4/4/4
3	DST	R	502	-	-	2/7/13/13	-
2	QRP	O	501	-	-	2/3/30/30	0/4/4/4
2	QRP	I	501	-	-	2/3/30/30	0/4/4/4
2	QRP	G	501	-	-	2/3/30/30	0/4/4/4
2	QRP	P	501	-	-	2/3/30/30	0/4/4/4
2	QRP	L	501	-	-	2/3/30/30	0/4/4/4
2	QRP	D	501	-	-	2/3/30/30	0/4/4/4
3	DST	D	502	-	-	1/7/13/13	-
3	DST	T	502	-	-	2/7/13/13	-
3	DST	G	502	-	-	1/7/13/13	-
2	QRP	S	501	-	-	2/3/30/30	0/4/4/4
2	QRP	Q	501	-	-	2/3/30/30	0/4/4/4
3	DST	B	502	-	-	1/7/13/13	-
3	DST	M	502	-	-	1/7/13/13	-
3	DST	K	502	-	-	1/7/13/13	-
2	QRP	A	501	-	-	2/3/30/30	0/4/4/4
3	DST	W	502	-	-	2/7/13/13	-
2	QRP	R	501	-	-	2/3/30/30	0/4/4/4
2	QRP	T	501	-	-	2/3/30/30	0/4/4/4
3	DST	F	502	-	-	1/7/13/13	-
3	DST	C	502	-	-	2/7/13/13	-
2	QRP	B	501	-	-	2/3/30/30	0/4/4/4
3	DST	E	502	-	-	2/7/13/13	-
3	DST	L	502	-	-	1/7/13/13	-
2	QRP	N	501	-	-	2/3/30/30	0/4/4/4
2	QRP	V	501	-	-	2/3/30/30	0/4/4/4
2	QRP	H	501	-	-	2/3/30/30	0/4/4/4
3	DST	O	502	-	-	1/7/13/13	-
2	QRP	C	501	-	-	2/3/30/30	0/4/4/4
2	QRP	X	501	-	-	2/3/30/30	0/4/4/4
3	DST	Q	502	-	-	2/7/13/13	-
2	QRP	J	501	-	-	2/3/30/30	0/4/4/4
2	QRP	K	501	-	-	2/3/30/30	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DST	S	502	-	-	2/7/13/13	-
3	DST	H	502	-	-	2/7/13/13	-

All (243) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	QRP	CAN-N	10.07	1.49	1.33
2	D	501	QRP	CAN-N	9.97	1.49	1.33
2	T	501	QRP	CAN-N	9.83	1.48	1.33
2	F	501	QRP	CAN-N	9.82	1.48	1.33
2	E	501	QRP	CAN-N	9.73	1.48	1.33
2	J	501	QRP	CAN-N	9.69	1.48	1.33
2	L	501	QRP	CAN-N	9.67	1.48	1.33
2	G	501	QRP	CAN-N	9.60	1.48	1.33
2	S	501	QRP	CAN-N	9.53	1.48	1.33
2	W	501	QRP	CAN-N	9.45	1.48	1.33
2	I	501	QRP	CAN-N	9.40	1.48	1.33
2	V	501	QRP	CAN-N	9.38	1.48	1.33
2	R	501	QRP	CAN-N	9.35	1.48	1.33
2	N	501	QRP	CAN-N	9.31	1.48	1.33
2	C	501	QRP	CAN-N	9.29	1.48	1.33
2	U	501	QRP	CAN-N	9.24	1.47	1.33
2	Q	501	QRP	CAN-N	9.23	1.47	1.33
2	K	501	QRP	CAN-N	9.21	1.47	1.33
2	H	501	QRP	CAN-N	9.16	1.47	1.33
2	P	501	QRP	CAN-N	9.16	1.47	1.33
2	O	501	QRP	CAN-N	9.14	1.47	1.33
2	M	501	QRP	CAN-N	8.97	1.47	1.33
2	A	501	QRP	CAN-N	8.72	1.47	1.33
2	X	501	QRP	CAN-N	8.57	1.46	1.33
2	X	501	QRP	CD1-NE1	-7.07	1.22	1.36
2	R	501	QRP	CD1-NE1	-6.92	1.22	1.36
2	V	501	QRP	CD1-NE1	-6.91	1.22	1.36
2	H	501	QRP	CD1-NE1	-6.83	1.22	1.36
2	P	501	QRP	CD1-NE1	-6.80	1.22	1.36
2	A	501	QRP	CD1-NE1	-6.79	1.22	1.36
2	N	501	QRP	CD1-NE1	-6.76	1.22	1.36
2	I	501	QRP	CD1-NE1	-6.72	1.22	1.36
2	D	501	QRP	CD1-NE1	-6.71	1.22	1.36
2	K	501	QRP	CD1-NE1	-6.70	1.22	1.36
2	U	501	QRP	CD1-NE1	-6.69	1.23	1.36
2	E	501	QRP	CD1-NE1	-6.66	1.23	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	501	QRP	CD1-NE1	-6.63	1.23	1.36
2	T	501	QRP	CD1-NE1	-6.62	1.23	1.36
2	B	501	QRP	CD1-NE1	-6.62	1.23	1.36
2	Q	501	QRP	CD1-NE1	-6.62	1.23	1.36
2	F	501	QRP	CD1-NE1	-6.62	1.23	1.36
2	W	501	QRP	CD1-NE1	-6.61	1.23	1.36
2	C	501	QRP	CD1-NE1	-6.60	1.23	1.36
2	L	501	QRP	CD1-NE1	-6.57	1.23	1.36
2	O	501	QRP	CD1-NE1	-6.55	1.23	1.36
2	J	501	QRP	CD1-NE1	-6.51	1.23	1.36
2	S	501	QRP	CD1-NE1	-6.49	1.23	1.36
2	G	501	QRP	CD1-NE1	-6.49	1.23	1.36
2	F	501	QRP	C-NAU	5.53	1.46	1.34
2	G	501	QRP	C-NAU	5.34	1.45	1.34
2	B	501	QRP	C-NAU	5.26	1.45	1.34
2	E	501	QRP	C-NAU	5.24	1.45	1.34
2	S	501	QRP	C-NAU	5.21	1.45	1.34
2	L	501	QRP	C-NAU	5.19	1.45	1.34
2	T	501	QRP	C-NAU	5.18	1.45	1.34
2	J	501	QRP	C-NAU	5.17	1.45	1.34
2	D	501	QRP	C-NAU	5.09	1.45	1.34
2	N	501	QRP	C-NAU	5.06	1.45	1.34
2	V	501	QRP	C-NAU	4.98	1.45	1.34
2	W	501	QRP	C-NAU	4.97	1.45	1.34
2	Q	501	QRP	C-NAU	4.96	1.45	1.34
2	X	501	QRP	C-NAU	4.91	1.45	1.34
2	H	501	QRP	C-NAU	4.87	1.44	1.34
2	U	501	QRP	C-NAU	4.86	1.44	1.34
2	I	501	QRP	C-NAU	4.86	1.44	1.34
2	K	501	QRP	C-NAU	4.85	1.44	1.34
2	O	501	QRP	C-NAU	4.84	1.44	1.34
2	P	501	QRP	C-NAU	4.83	1.44	1.34
2	C	501	QRP	C-NAU	4.81	1.44	1.34
2	M	501	QRP	C-NAU	4.80	1.44	1.34
2	V	501	QRP	CE2-NE1	-4.64	1.24	1.38
2	R	501	QRP	C-NAU	4.60	1.44	1.34
2	N	501	QRP	CE2-NE1	-4.47	1.24	1.38
2	X	501	QRP	CE2-NE1	-4.46	1.24	1.38
2	A	501	QRP	C-NAU	4.44	1.44	1.34
2	E	501	QRP	CE2-NE1	-4.35	1.25	1.38
2	D	501	QRP	CE2-NE1	-4.34	1.25	1.38
2	P	501	QRP	CE2-NE1	-4.29	1.25	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	QRP	CE2-NE1	-4.26	1.25	1.38
2	J	501	QRP	CE2-NE1	-4.26	1.25	1.38
2	I	501	QRP	CE2-NE1	-4.25	1.25	1.38
2	R	501	QRP	CE2-NE1	-4.25	1.25	1.38
2	W	501	QRP	CE2-NE1	-4.23	1.25	1.38
2	U	501	QRP	CE2-NE1	-4.20	1.25	1.38
2	K	501	QRP	CE2-NE1	-4.18	1.25	1.38
2	T	501	QRP	CE2-NE1	-4.17	1.25	1.38
2	A	501	QRP	CE2-NE1	-4.16	1.25	1.38
2	B	501	QRP	CE2-NE1	-4.16	1.25	1.38
2	G	501	QRP	CE2-NE1	-4.15	1.25	1.38
2	F	501	QRP	CE2-NE1	-4.14	1.25	1.38
2	C	501	QRP	CE2-NE1	-4.12	1.25	1.38
2	M	501	QRP	CE2-NE1	-4.09	1.26	1.38
2	O	501	QRP	CE2-NE1	-4.07	1.26	1.38
2	Q	501	QRP	CE2-NE1	-4.04	1.26	1.38
2	L	501	QRP	CE2-NE1	-3.98	1.26	1.38
2	S	501	QRP	CE2-NE1	-3.97	1.26	1.38
3	S	502	DST	P3-O8	-3.15	1.48	1.56
3	T	502	DST	P3-O8	-2.99	1.49	1.56
3	O	502	DST	P3-O8	-2.95	1.49	1.56
3	P	502	DST	C14-C12	2.91	1.58	1.50
3	P	502	DST	P3-O8	-2.88	1.49	1.56
3	C	502	DST	P3-O8	-2.80	1.49	1.56
3	J	502	DST	C14-C12	2.78	1.57	1.50
2	X	501	QRP	OAA-CAN	-2.76	1.17	1.23
3	N	502	DST	C14-C12	2.75	1.57	1.50
2	V	501	QRP	CZ2-CE2	-2.67	1.37	1.41
3	F	502	DST	C14-C12	2.63	1.57	1.50
3	X	502	DST	C14-C12	2.58	1.57	1.50
2	N	501	QRP	CZ2-CE2	-2.56	1.37	1.41
3	I	502	DST	P3-O8	-2.56	1.50	1.56
2	C	501	QRP	CZ2-CE2	-2.55	1.37	1.41
3	H	502	DST	P3-O8	-2.55	1.50	1.56
3	U	502	DST	C14-C12	2.52	1.57	1.50
3	T	502	DST	C14-C12	2.52	1.57	1.50
2	P	501	QRP	CZ2-CE2	-2.50	1.37	1.41
3	E	502	DST	P3-O8	-2.47	1.50	1.56
3	L	502	DST	C14-C12	2.45	1.57	1.50
3	W	502	DST	C14-C12	2.45	1.57	1.50
3	R	502	DST	P3-O8	-2.45	1.50	1.56
2	X	501	QRP	CZ2-CE2	-2.44	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	501	QRP	OAA-CAN	-2.44	1.18	1.23
2	A	501	QRP	OAA-CAN	-2.43	1.18	1.23
2	O	501	QRP	OAA-CAN	-2.41	1.18	1.23
3	P	502	DST	C13-C12	2.41	1.56	1.50
3	N	502	DST	C13-C12	2.41	1.56	1.50
3	D	502	DST	P3-O8	-2.40	1.50	1.56
3	N	502	DST	P3-O8	-2.39	1.50	1.56
2	U	501	QRP	CZ2-CE2	-2.39	1.37	1.41
2	I	501	QRP	OAA-CAN	-2.38	1.18	1.23
2	R	501	QRP	OAA-CAN	-2.38	1.18	1.23
3	K	502	DST	C14-C12	2.37	1.56	1.50
3	J	502	DST	C13-C12	2.37	1.56	1.50
2	D	501	QRP	CZ2-CE2	-2.36	1.37	1.41
3	B	502	DST	C14-C12	2.36	1.56	1.50
2	F	501	QRP	CZ2-CE2	-2.35	1.37	1.41
3	C	502	DST	C14-C12	2.35	1.56	1.50
3	A	502	DST	P3-O8	-2.35	1.50	1.56
2	H	501	QRP	OAA-CAN	-2.34	1.18	1.23
3	L	502	DST	C13-C12	2.33	1.56	1.50
3	A	502	DST	C14-C12	2.33	1.56	1.50
2	T	501	QRP	CZ2-CE2	-2.33	1.37	1.41
3	R	502	DST	C14-C12	2.33	1.56	1.50
3	U	502	DST	C13-C12	2.33	1.56	1.50
3	Q	502	DST	C14-C12	2.32	1.56	1.50
2	I	501	QRP	CZ2-CE2	-2.30	1.37	1.41
2	E	501	QRP	CZ2-CE2	-2.29	1.37	1.41
2	W	501	QRP	OAA-CAN	-2.28	1.18	1.23
2	S	501	QRP	OAA-CAN	-2.28	1.18	1.23
2	G	501	QRP	CZ2-CE2	-2.28	1.37	1.41
2	K	501	QRP	CZ2-CE2	-2.28	1.37	1.41
3	K	502	DST	P1-O4	-2.27	1.46	1.54
3	M	502	DST	C14-C12	2.26	1.56	1.50
2	J	501	QRP	CZ2-CE2	-2.26	1.37	1.41
3	W	502	DST	P3-O8	-2.26	1.51	1.56
2	R	501	QRP	CZ2-CE2	-2.25	1.38	1.41
2	M	501	QRP	CZ2-CE2	-2.24	1.38	1.41
2	Q	501	QRP	CZ2-CE2	-2.23	1.38	1.41
2	R	501	QRP	CAH-CAJ	2.23	1.59	1.51
2	J	501	QRP	OAA-CAN	-2.23	1.19	1.23
2	B	501	QRP	CZ2-CE2	-2.22	1.38	1.41
2	T	501	QRP	CAH-CAJ	2.22	1.59	1.51
2	O	501	QRP	CAH-CAJ	2.21	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	501	QRP	CAH-CAJ	2.20	1.59	1.51
3	S	502	DST	C14-C12	2.20	1.56	1.50
2	H	501	QRP	CZ2-CE2	-2.20	1.38	1.41
2	H	501	QRP	CAH-CAJ	2.20	1.59	1.51
2	F	501	QRP	CAH-CAJ	2.20	1.59	1.51
2	U	501	QRP	OAA-CAN	-2.20	1.19	1.23
2	V	501	QRP	CZ3-CE3	2.20	1.41	1.36
2	P	501	QRP	OAA-CAN	-2.19	1.19	1.23
3	V	502	DST	C14-C12	2.19	1.56	1.50
2	E	501	QRP	OAA-CAN	-2.19	1.19	1.23
3	S	502	DST	P1-O4	-2.18	1.46	1.54
2	J	501	QRP	CAH-CAJ	2.18	1.59	1.51
2	V	501	QRP	OAA-CAN	-2.17	1.19	1.23
2	G	501	QRP	CAH-CAJ	2.17	1.59	1.51
3	B	502	DST	C10-S9	-2.17	1.81	1.84
2	Q	501	QRP	OAA-CAN	-2.17	1.19	1.23
2	O	501	QRP	CZ2-CE2	-2.17	1.38	1.41
2	K	501	QRP	OAA-CAN	-2.16	1.19	1.23
2	M	501	QRP	OAA-CAN	-2.16	1.19	1.23
2	N	501	QRP	O-C	-2.16	1.18	1.22
3	V	502	DST	P3-O8	-2.16	1.51	1.56
2	G	501	QRP	OAA-CAN	-2.16	1.19	1.23
2	E	501	QRP	CZ3-CE3	2.16	1.41	1.36
2	E	501	QRP	CE3-CD2	-2.15	1.37	1.42
2	D	501	QRP	CAH-CAJ	2.15	1.59	1.51
2	I	501	QRP	CAH-CAJ	2.15	1.59	1.51
2	C	501	QRP	OAA-CAN	-2.15	1.19	1.23
3	C	502	DST	C13-C12	2.14	1.56	1.50
2	L	501	QRP	CAH-CAJ	2.14	1.59	1.51
3	K	502	DST	C13-C12	2.14	1.56	1.50
2	L	501	QRP	CZ3-CE3	2.13	1.41	1.36
3	J	502	DST	P3-O8	-2.13	1.51	1.56
3	M	502	DST	P3-O8	-2.12	1.51	1.56
2	A	501	QRP	CZ2-CE2	-2.12	1.38	1.41
3	H	502	DST	C14-C12	2.11	1.56	1.50
3	W	502	DST	P1-O4	-2.11	1.46	1.54
3	G	502	DST	C14-C12	2.11	1.56	1.50
3	T	502	DST	C13-C12	2.11	1.56	1.50
2	V	501	QRP	CE3-CD2	-2.10	1.37	1.42
2	W	501	QRP	CAH-CAJ	2.10	1.59	1.51
2	N	501	QRP	CAH-CAJ	2.10	1.59	1.51
2	P	501	QRP	CAH-CAJ	2.10	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	501	QRP	CZ3-CE3	2.10	1.41	1.36
2	B	501	QRP	CAH-CAJ	2.10	1.59	1.51
2	T	501	QRP	OAA-CAN	-2.10	1.19	1.23
2	E	501	QRP	CAH-CAJ	2.09	1.59	1.51
2	W	501	QRP	CZ2-CE2	-2.09	1.38	1.41
3	W	502	DST	C13-C12	2.09	1.56	1.50
2	L	501	QRP	OAA-CAN	-2.09	1.19	1.23
3	X	502	DST	C13-C12	2.09	1.56	1.50
3	A	502	DST	C10-S9	-2.09	1.81	1.84
2	K	501	QRP	CAH-CAJ	2.08	1.59	1.51
2	F	501	QRP	OAA-CAN	-2.08	1.19	1.23
2	C	501	QRP	CAH-CAJ	2.08	1.59	1.51
3	A	502	DST	C13-C12	2.06	1.55	1.50
2	Q	501	QRP	CAH-CAJ	2.06	1.58	1.51
3	I	502	DST	C14-C12	2.06	1.55	1.50
2	U	501	QRP	CAH-CAJ	2.06	1.58	1.51
2	D	501	QRP	CZ3-CE3	2.06	1.41	1.36
2	X	501	QRP	CAH-CAJ	2.06	1.58	1.51
2	R	501	QRP	CZ3-CE3	2.05	1.41	1.36
2	G	501	QRP	CZ3-CE3	2.05	1.41	1.36
2	W	501	QRP	CZ3-CE3	2.04	1.41	1.36
3	B	502	DST	P3-O8	-2.04	1.51	1.56
2	N	501	QRP	CZ3-CE3	2.04	1.41	1.36
2	P	501	QRP	CE3-CD2	-2.04	1.38	1.42
2	L	501	QRP	CZ2-CE2	-2.03	1.38	1.41
2	I	501	QRP	CZ3-CE3	2.03	1.41	1.36
2	S	501	QRP	CZ2-CE2	-2.03	1.38	1.41
3	Q	502	DST	C13-C12	2.03	1.55	1.50
3	T	502	DST	P1-O4	-2.02	1.47	1.54
2	V	501	QRP	CAH-CAJ	2.02	1.58	1.51
2	D	501	QRP	OAA-CAN	-2.02	1.19	1.23
3	M	502	DST	P1-O4	-2.01	1.47	1.54
2	V	501	QRP	CAI-CAT	-2.01	1.49	1.53
3	M	502	DST	C13-C12	2.01	1.55	1.50
2	C	501	QRP	O-C	-2.01	1.18	1.22
2	M	501	QRP	CAH-CAJ	2.00	1.58	1.51
3	U	502	DST	P1-O4	-2.00	1.47	1.54
2	H	501	QRP	CZ3-CE3	2.00	1.41	1.36
2	B	501	QRP	OAA-CAN	-2.00	1.19	1.23

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	501	QRP	CAI-CAT-NAU	5.66	111.43	103.03
2	D	501	QRP	CAI-CAT-NAU	4.97	110.42	103.03
2	F	501	QRP	CAI-CAT-NAU	4.94	110.37	103.03
2	N	501	QRP	CAI-CAT-NAU	4.79	110.15	103.03
2	C	501	QRP	CAI-CAT-NAU	4.78	110.13	103.03
2	V	501	QRP	CAI-CAT-NAU	4.73	110.05	103.03
2	O	501	QRP	CAI-CAT-NAU	4.57	109.81	103.03
2	G	501	QRP	CAI-CAT-NAU	4.51	109.72	103.03
2	S	501	QRP	CAI-CAT-NAU	4.43	109.61	103.03
2	U	501	QRP	CAI-CAT-NAU	4.30	109.42	103.03
2	J	501	QRP	CAI-CAT-NAU	4.23	109.31	103.03
2	I	501	QRP	CAI-CAT-NAU	4.21	109.28	103.03
2	L	501	QRP	CAI-CAT-NAU	4.19	109.25	103.03
2	K	501	QRP	CAI-CAT-NAU	4.19	109.25	103.03
2	H	501	QRP	CAI-CAT-NAU	4.17	109.22	103.03
2	T	501	QRP	CAI-CAT-NAU	4.16	109.20	103.03
2	B	501	QRP	CAI-CAT-NAU	4.05	109.05	103.03
2	X	501	QRP	CAI-CAT-NAU	4.04	109.02	103.03
2	E	501	QRP	CAI-CAT-NAU	3.93	108.86	103.03
2	W	501	QRP	CAI-CAT-NAU	3.86	108.76	103.03
2	P	501	QRP	CAI-CAT-NAU	3.82	108.70	103.03
2	Q	501	QRP	CAI-CAT-NAU	3.61	108.39	103.03
3	F	502	DST	C14-C12-C13	3.55	122.44	114.60
2	B	501	QRP	O-C-NAU	-3.42	118.09	123.03
3	Q	502	DST	C14-C12-C13	3.36	122.02	114.60
2	A	501	QRP	CAI-CAT-NAU	3.33	107.97	103.03
2	L	501	QRP	O-C-NAU	-3.31	118.25	123.03
2	M	501	QRP	CAI-CAT-NAU	3.29	107.91	103.03
3	W	502	DST	C14-C12-C13	3.24	121.75	114.60
3	L	502	DST	C14-C12-C13	3.21	121.69	114.60
3	C	502	DST	C14-C12-C13	3.20	121.66	114.60
2	I	501	QRP	O-C-NAU	-3.13	118.51	123.03
2	T	501	QRP	O-C-NAU	-3.08	118.58	123.03
3	N	502	DST	C14-C12-C13	3.06	121.37	114.60
2	K	501	QRP	O-C-NAU	-3.03	118.66	123.03
2	R	501	QRP	CG-CB-CA	3.02	119.36	113.45
3	V	502	DST	C14-C12-C13	3.01	121.25	114.60
3	B	502	DST	C14-C12-C13	2.98	121.19	114.60
2	A	501	QRP	O-C-NAU	-2.97	118.73	123.03
2	H	501	QRP	O-C-NAU	-2.95	118.77	123.03
2	P	501	QRP	O-C-NAU	-2.95	118.78	123.03
3	U	502	DST	C14-C12-C13	2.91	121.04	114.60
3	I	502	DST	O6-P1-O4	2.87	118.60	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	502	DST	O6-P1-O4	2.85	118.55	107.64
3	A	502	DST	C14-C12-C13	2.84	120.88	114.60
3	J	502	DST	C14-C12-C13	2.81	120.82	114.60
3	G	502	DST	C14-C12-C13	2.79	120.77	114.60
2	J	501	QRP	O-C-NAU	-2.78	119.01	123.03
3	M	502	DST	C14-C12-C13	2.77	120.72	114.60
3	I	502	DST	C14-C12-C13	2.75	120.69	114.60
3	P	502	DST	C14-C12-C13	2.72	120.61	114.60
2	W	501	QRP	O-C-NAU	-2.71	119.12	123.03
3	B	502	DST	O6-P1-O4	2.69	117.92	107.64
2	R	501	QRP	O-C-NAU	-2.69	119.15	123.03
3	O	502	DST	C14-C12-C13	2.67	120.50	114.60
3	H	502	DST	O6-P1-O4	2.67	117.83	107.64
2	X	501	QRP	CAN-CAT-NAU	-2.65	105.69	112.33
3	K	502	DST	C14-C12-C13	2.65	120.45	114.60
3	G	502	DST	O6-P1-O4	2.61	117.62	107.64
2	Q	501	QRP	O-C-NAU	-2.61	119.26	123.03
2	G	501	QRP	CAN-CAT-NAU	-2.59	105.84	112.33
2	I	501	QRP	CAN-CAT-NAU	-2.56	105.91	112.33
3	S	502	DST	C14-C12-C13	2.54	120.22	114.60
2	C	501	QRP	CAN-CAT-NAU	-2.50	106.08	112.33
2	E	501	QRP	O-C-NAU	-2.49	119.43	123.03
3	H	502	DST	C13-C12-C11	-2.49	115.45	122.65
2	D	501	QRP	CAN-CAT-NAU	-2.48	106.12	112.33
2	F	501	QRP	CAN-CAT-NAU	-2.47	106.14	112.33
3	A	502	DST	O6-P1-O4	2.46	117.03	107.64
3	H	502	DST	C14-C12-C13	2.44	120.00	114.60
2	S	501	QRP	CAN-CAT-NAU	-2.40	106.31	112.33
2	E	501	QRP	CZ3-CH2-CZ2	-2.39	117.09	120.44
2	U	501	QRP	CAN-CAT-NAU	-2.38	106.37	112.33
2	O	501	QRP	CAN-CAT-NAU	-2.38	106.38	112.33
2	S	501	QRP	O-C-NAU	-2.36	119.62	123.03
2	E	501	QRP	CAN-CAT-NAU	-2.36	106.43	112.33
2	X	501	QRP	CG-CB-CA	2.35	118.04	113.45
2	F	501	QRP	O-C-NAU	-2.34	119.64	123.03
2	W	501	QRP	CAN-CAT-NAU	-2.34	106.48	112.33
2	K	501	QRP	CAN-CAT-NAU	-2.33	106.49	112.33
3	R	502	DST	C14-C12-C13	2.33	119.74	114.60
2	J	501	QRP	CAN-CAT-NAU	-2.32	106.54	112.33
3	O	502	DST	C13-C12-C11	-2.31	115.97	122.65
2	N	501	QRP	CAN-CAT-NAU	-2.31	106.56	112.33
2	O	501	QRP	O-C-NAU	-2.30	119.70	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	502	DST	O6-P1-O2	2.29	112.31	104.64
3	X	502	DST	C14-C12-C13	2.28	119.64	114.60
3	F	502	DST	C13-C12-C11	-2.27	116.08	122.65
3	W	502	DST	C13-C12-C11	-2.25	116.14	122.65
2	C	501	QRP	O-C-NAU	-2.25	119.78	123.03
2	N	501	QRP	O-C-NAU	-2.24	119.79	123.03
2	G	501	QRP	O-C-NAU	-2.24	119.80	123.03
3	T	502	DST	C14-C12-C13	2.21	119.48	114.60
2	H	501	QRP	CG-CB-CA	2.21	117.77	113.45
2	T	501	QRP	CAN-CAT-NAU	-2.20	106.82	112.33
2	M	501	QRP	CAN-CAT-NAU	-2.19	106.85	112.33
3	D	502	DST	C14-C12-C13	2.17	119.39	114.60
2	Q	501	QRP	CAN-CAT-NAU	-2.17	106.91	112.33
2	X	501	QRP	O-C-NAU	-2.16	119.91	123.03
2	B	501	QRP	CAN-CAT-NAU	-2.16	106.93	112.33
3	D	502	DST	O4-P1-O2	2.14	111.80	104.64
3	S	502	DST	O6-P1-O5	2.13	119.03	110.68
2	B	501	QRP	CG-CB-CA	-2.13	109.28	113.45
3	E	502	DST	C14-C12-C13	2.13	119.30	114.60
2	V	501	QRP	CAN-CAT-NAU	-2.12	107.01	112.33
3	B	502	DST	C13-C12-C11	-2.12	116.52	122.65
3	S	502	DST	C13-C12-C11	-2.12	116.52	122.65
2	R	501	QRP	CAN-CAT-NAU	-2.11	107.06	112.33
3	N	502	DST	C13-C12-C11	-2.10	116.57	122.65
2	T	501	QRP	C-CA-N	-2.10	108.69	112.60
2	L	501	QRP	CG-CB-CA	-2.10	109.34	113.45
3	Q	502	DST	C13-C12-C11	-2.08	116.62	122.65
2	L	501	QRP	CAN-CAT-NAU	-2.08	107.12	112.33
3	A	502	DST	C13-C12-C11	-2.08	116.64	122.65
3	E	502	DST	O6-P1-O5	2.08	118.82	110.68
3	D	502	DST	C13-C12-C11	-2.08	116.65	122.65
2	X	501	QRP	C-CA-N	-2.08	108.73	112.60
3	M	502	DST	O6-P1-O5	2.07	118.79	110.68
2	I	501	QRP	C-CA-N	-2.06	108.75	112.60
3	U	502	DST	O6-P1-O5	2.06	118.76	110.68
3	D	502	DST	O6-P1-O5	2.05	118.70	110.68
2	B	501	QRP	C-CA-N	-2.05	108.78	112.60
3	X	502	DST	C13-C12-C11	-2.04	116.75	122.65
2	H	501	QRP	CAN-CAT-NAU	-2.03	107.24	112.33
2	U	501	QRP	O-C-NAU	-2.02	120.11	123.03
3	I	502	DST	C13-C12-C11	-2.02	116.82	122.65

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	QRP	C-CA-CB-CG
2	C	501	QRP	N-CA-CB-CG
2	A	501	QRP	C-CA-CB-CG
2	A	501	QRP	N-CA-CB-CG
2	V	501	QRP	C-CA-CB-CG
2	V	501	QRP	N-CA-CB-CG
2	E	501	QRP	C-CA-CB-CG
2	E	501	QRP	N-CA-CB-CG
2	G	501	QRP	C-CA-CB-CG
2	G	501	QRP	N-CA-CB-CG
2	B	501	QRP	C-CA-CB-CG
2	B	501	QRP	N-CA-CB-CG
2	D	501	QRP	C-CA-CB-CG
2	D	501	QRP	N-CA-CB-CG
2	F	501	QRP	C-CA-CB-CG
2	F	501	QRP	N-CA-CB-CG
2	H	501	QRP	C-CA-CB-CG
2	H	501	QRP	N-CA-CB-CG
2	I	501	QRP	C-CA-CB-CG
2	I	501	QRP	N-CA-CB-CG
2	J	501	QRP	C-CA-CB-CG
2	J	501	QRP	N-CA-CB-CG
2	K	501	QRP	C-CA-CB-CG
2	K	501	QRP	N-CA-CB-CG
2	L	501	QRP	C-CA-CB-CG
2	L	501	QRP	N-CA-CB-CG
2	M	501	QRP	C-CA-CB-CG
2	M	501	QRP	N-CA-CB-CG
2	N	501	QRP	C-CA-CB-CG
2	N	501	QRP	N-CA-CB-CG
2	O	501	QRP	C-CA-CB-CG
2	O	501	QRP	N-CA-CB-CG
2	P	501	QRP	C-CA-CB-CG
2	P	501	QRP	N-CA-CB-CG
2	Q	501	QRP	C-CA-CB-CG
2	Q	501	QRP	N-CA-CB-CG
2	R	501	QRP	C-CA-CB-CG
2	R	501	QRP	N-CA-CB-CG
2	S	501	QRP	C-CA-CB-CG
2	S	501	QRP	N-CA-CB-CG
2	T	501	QRP	C-CA-CB-CG
2	T	501	QRP	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	U	501	QRP	C-CA-CB-CG
2	U	501	QRP	N-CA-CB-CG
2	W	501	QRP	C-CA-CB-CG
2	W	501	QRP	N-CA-CB-CG
2	X	501	QRP	C-CA-CB-CG
2	X	501	QRP	N-CA-CB-CG
3	C	502	DST	P3-O2-P1-O4
3	V	502	DST	P3-O2-P1-O4
3	V	502	DST	P3-O2-P1-O6
3	B	502	DST	P3-O2-P1-O6
3	J	502	DST	P3-O2-P1-O4
3	L	502	DST	P3-O2-P1-O6
3	N	502	DST	P3-O2-P1-O4
3	O	502	DST	P3-O2-P1-O4
3	P	502	DST	P3-O2-P1-O4
3	P	502	DST	P3-O2-P1-O6
3	Q	502	DST	P3-O2-P1-O4
3	R	502	DST	P3-O2-P1-O4
3	R	502	DST	P3-O2-P1-O6
3	S	502	DST	P3-O2-P1-O4
3	T	502	DST	P3-O2-P1-O6
3	U	502	DST	P3-O2-P1-O4
3	W	502	DST	P3-O2-P1-O4
3	X	502	DST	P3-O2-P1-O6
3	D	502	DST	P3-O2-P1-O5
3	F	502	DST	P3-O2-P1-O5
3	K	502	DST	P3-O2-P1-O5
3	H	502	DST	P3-O2-P1-O5
3	M	502	DST	P3-O2-P1-O5
3	T	502	DST	P3-O2-P1-O4
3	X	502	DST	P3-O2-P1-O4
3	E	502	DST	P3-O2-P1-O5
3	J	502	DST	P3-O2-P1-O5
3	N	502	DST	P3-O2-P1-O5
3	Q	502	DST	P3-O2-P1-O5
3	S	502	DST	P3-O2-P1-O5
3	W	502	DST	P3-O2-P1-O5
3	A	502	DST	P3-O2-P1-O6
3	E	502	DST	P3-O2-P1-O4
3	G	502	DST	P3-O2-P1-O6
3	H	502	DST	P3-O2-P1-O6
3	I	502	DST	P3-O2-P1-O6

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Mol	Chain	Res	Type	Atoms
3	N	502	DST	P3-O2-P1-O6
3	C	502	DST	P3-O2-P1-O5
3	U	502	DST	P3-O2-P1-O5

There are no ring outliers.

48 monomers are involved in 254 short contacts:

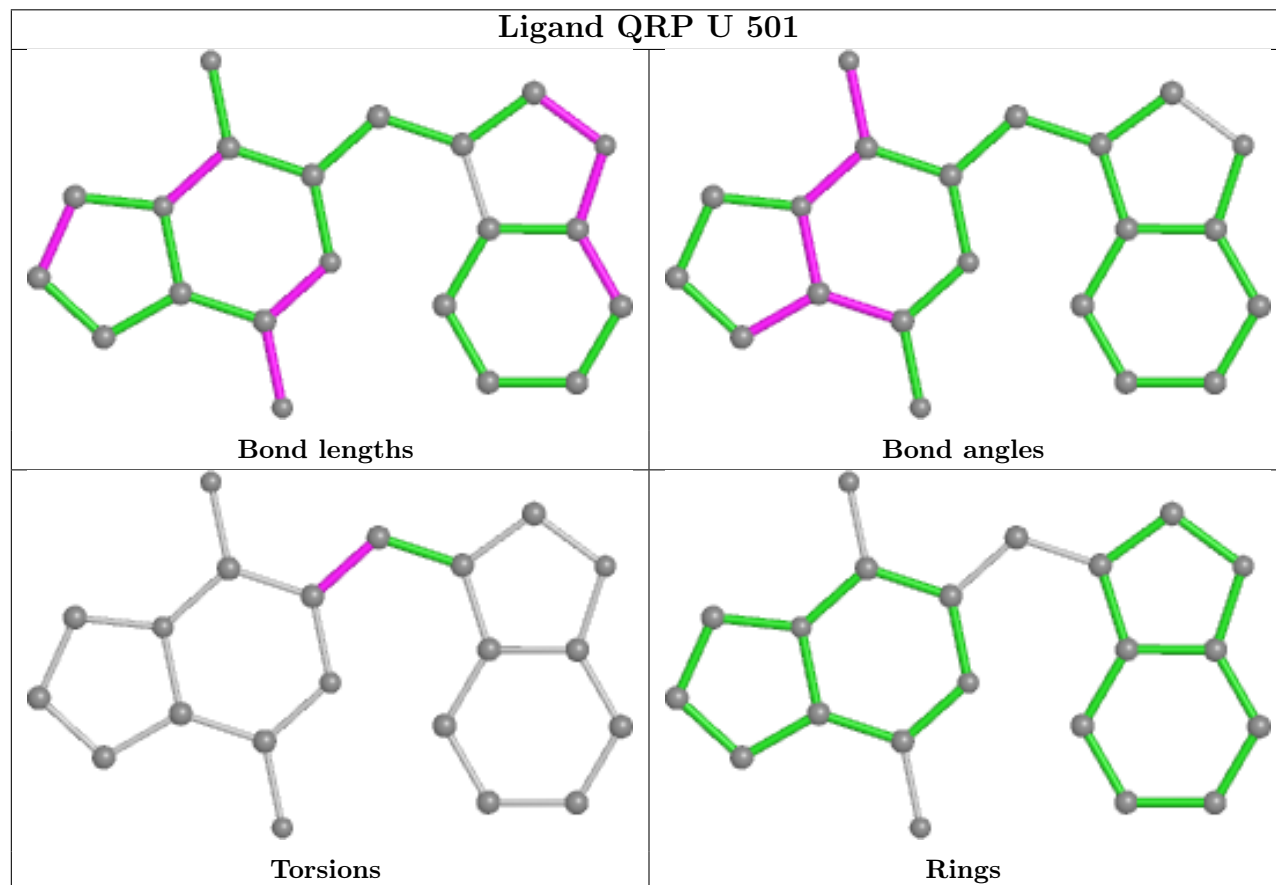
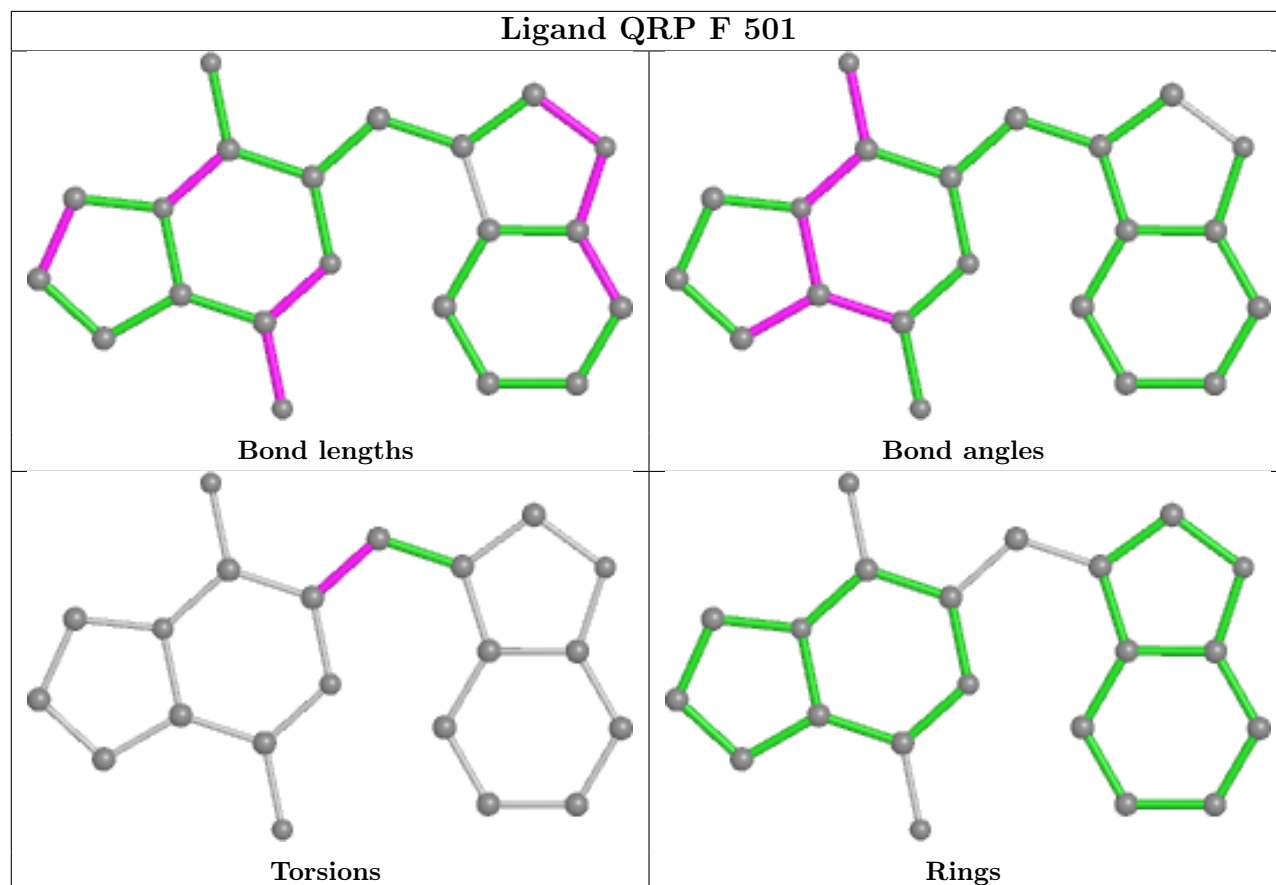
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	QRP	5	0
2	U	501	QRP	5	0
2	W	501	QRP	4	0
3	N	502	DST	6	0
3	I	502	DST	5	0
3	V	502	DST	6	0
3	U	502	DST	8	0
2	E	501	QRP	3	0
3	J	502	DST	5	0
3	P	502	DST	5	0
3	X	502	DST	9	0
3	A	502	DST	5	0
2	M	501	QRP	5	0
3	R	502	DST	9	0
2	O	501	QRP	6	0
2	I	501	QRP	5	0
2	G	501	QRP	8	0
2	P	501	QRP	5	0
2	L	501	QRP	8	0
2	D	501	QRP	5	0
3	D	502	DST	5	0
3	T	502	DST	6	0
3	G	502	DST	5	0
2	S	501	QRP	6	0
2	Q	501	QRP	9	0
3	B	502	DST	7	0
3	M	502	DST	9	0
3	K	502	DST	7	0
2	A	501	QRP	4	0
3	W	502	DST	5	0
2	R	501	QRP	7	0
2	T	501	QRP	6	0
3	F	502	DST	6	0
3	C	502	DST	4	0

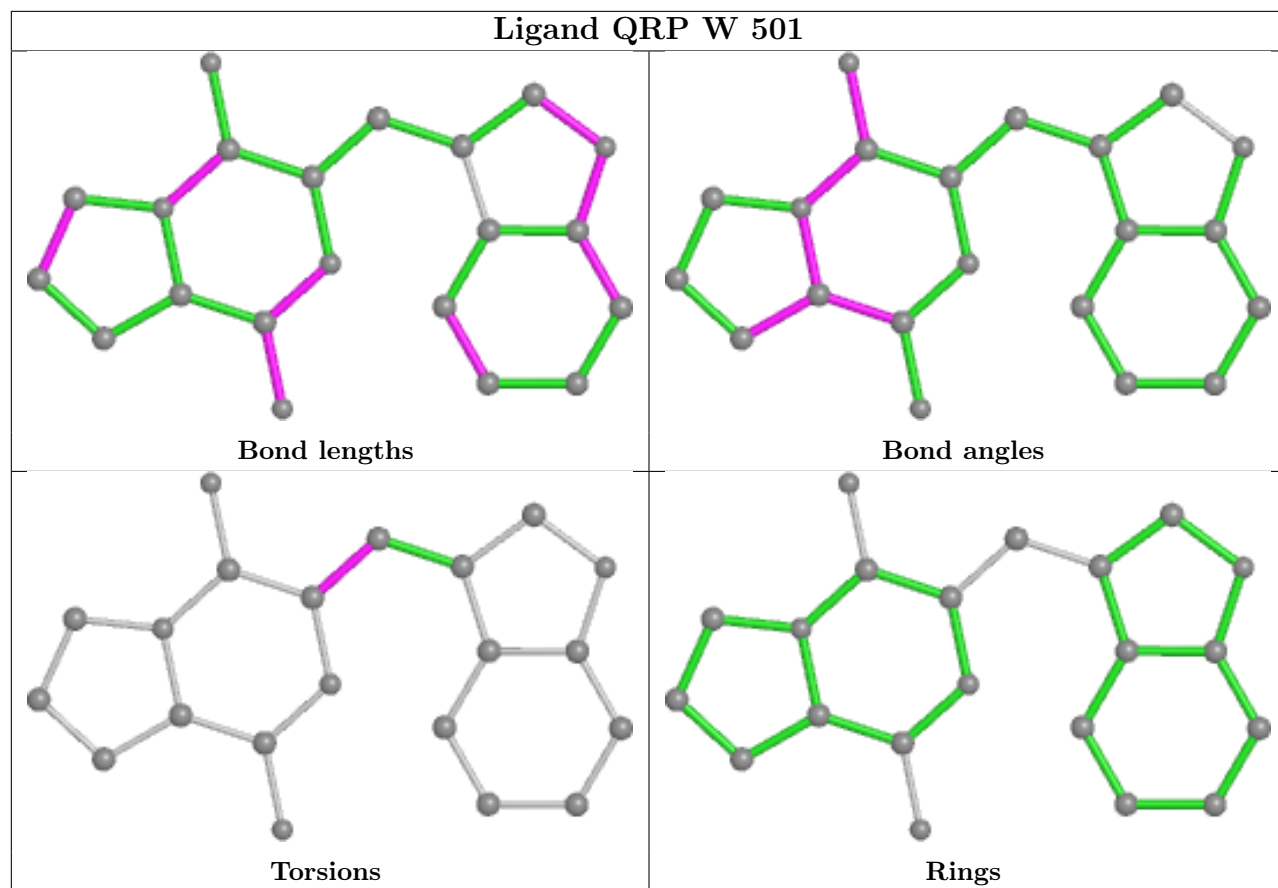
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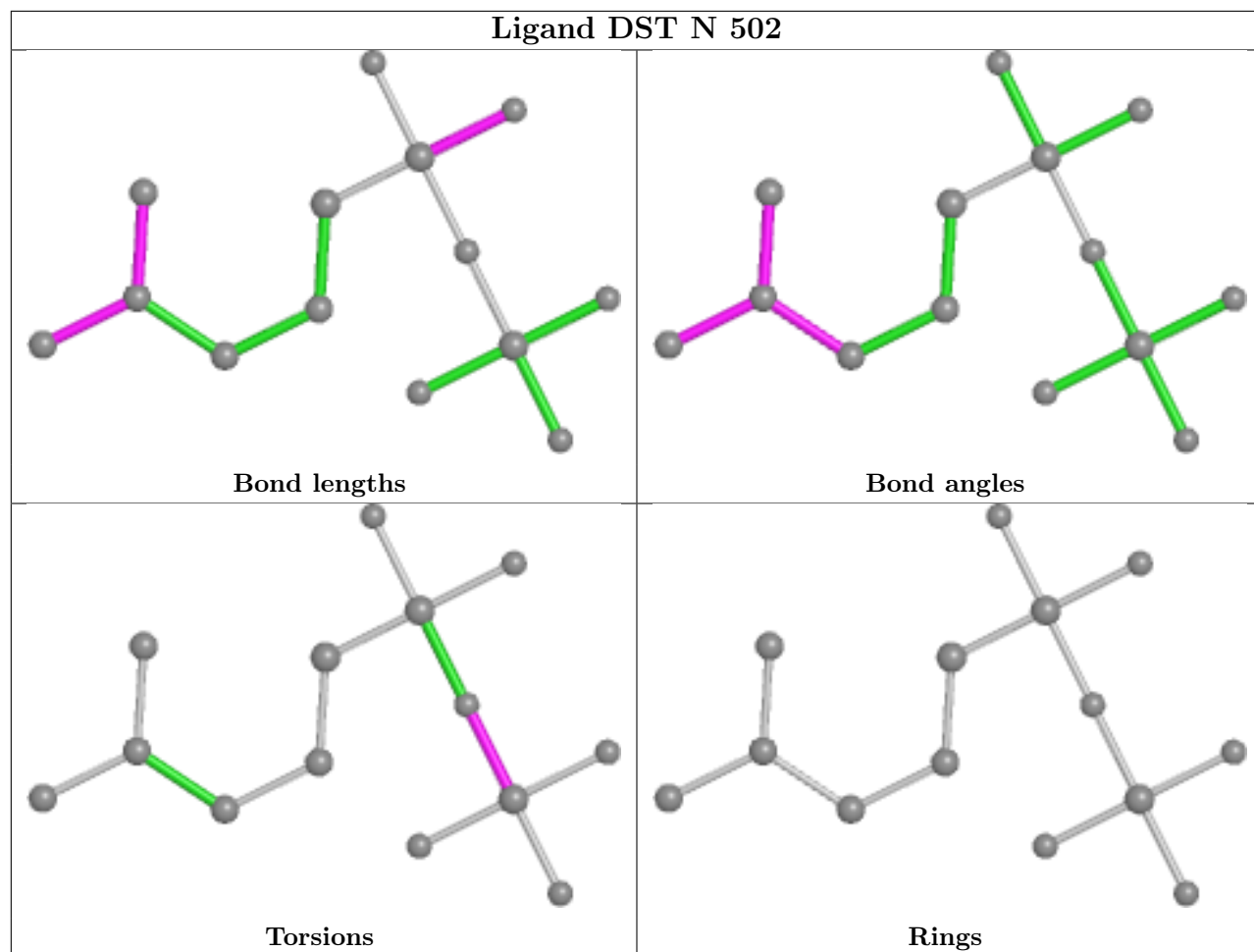
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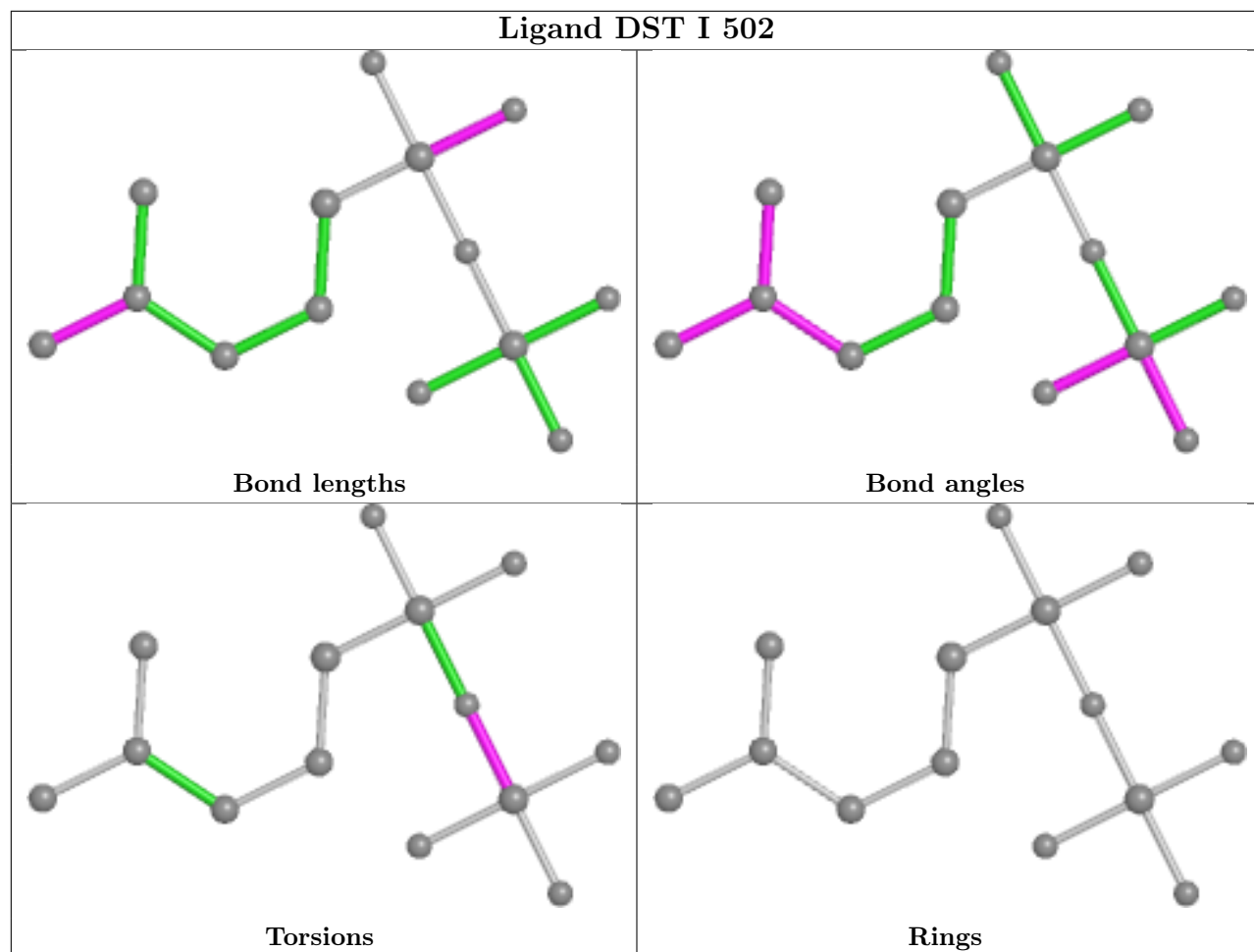
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	QRP	7	0
3	E	502	DST	3	0
3	L	502	DST	5	0
2	N	501	QRP	6	0
2	V	501	QRP	5	0
2	H	501	QRP	7	0
3	O	502	DST	6	0
2	C	501	QRP	7	0
2	X	501	QRP	7	0
3	Q	502	DST	7	0
2	J	501	QRP	5	0
2	K	501	QRP	6	0
3	S	502	DST	5	0
3	H	502	DST	5	0

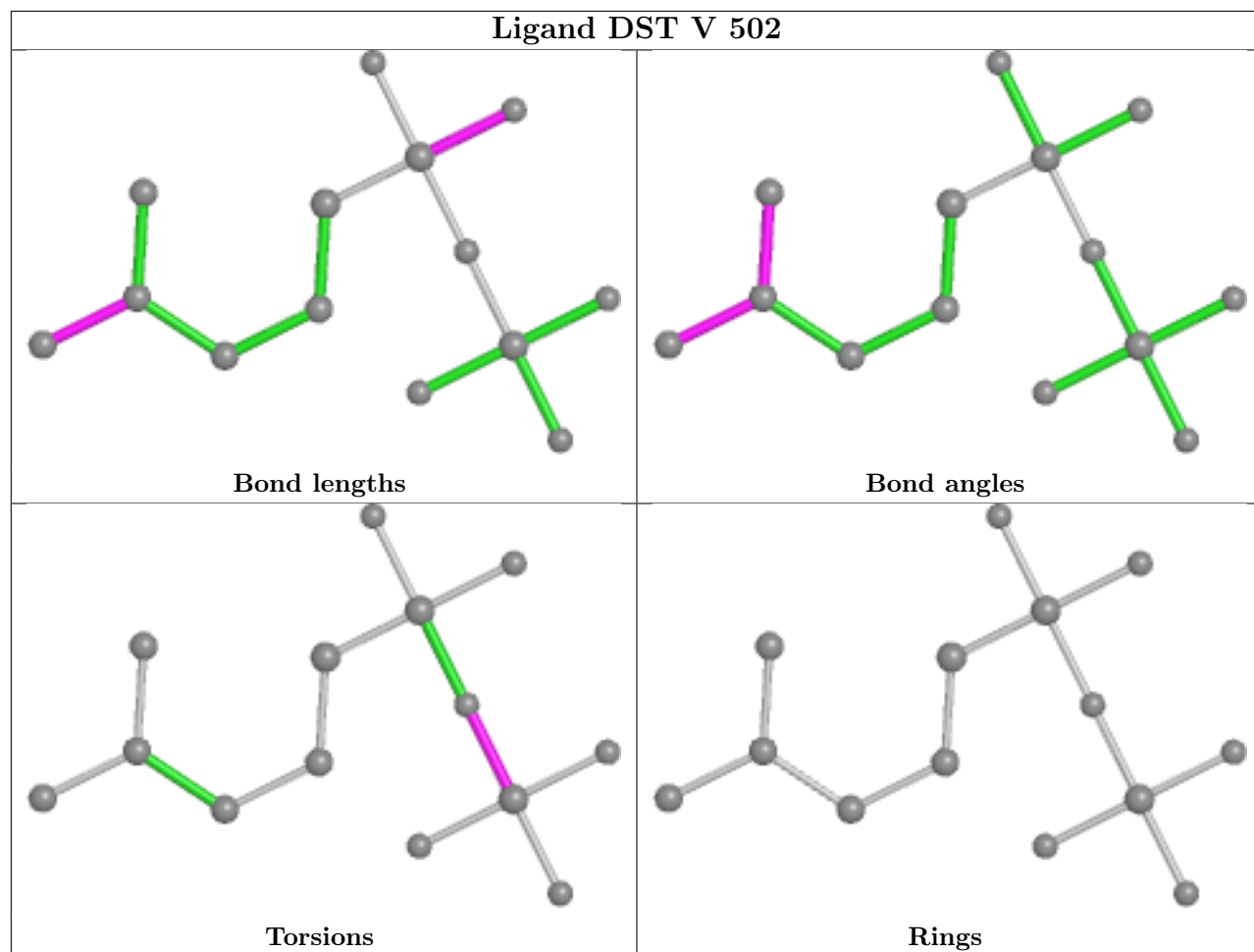
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

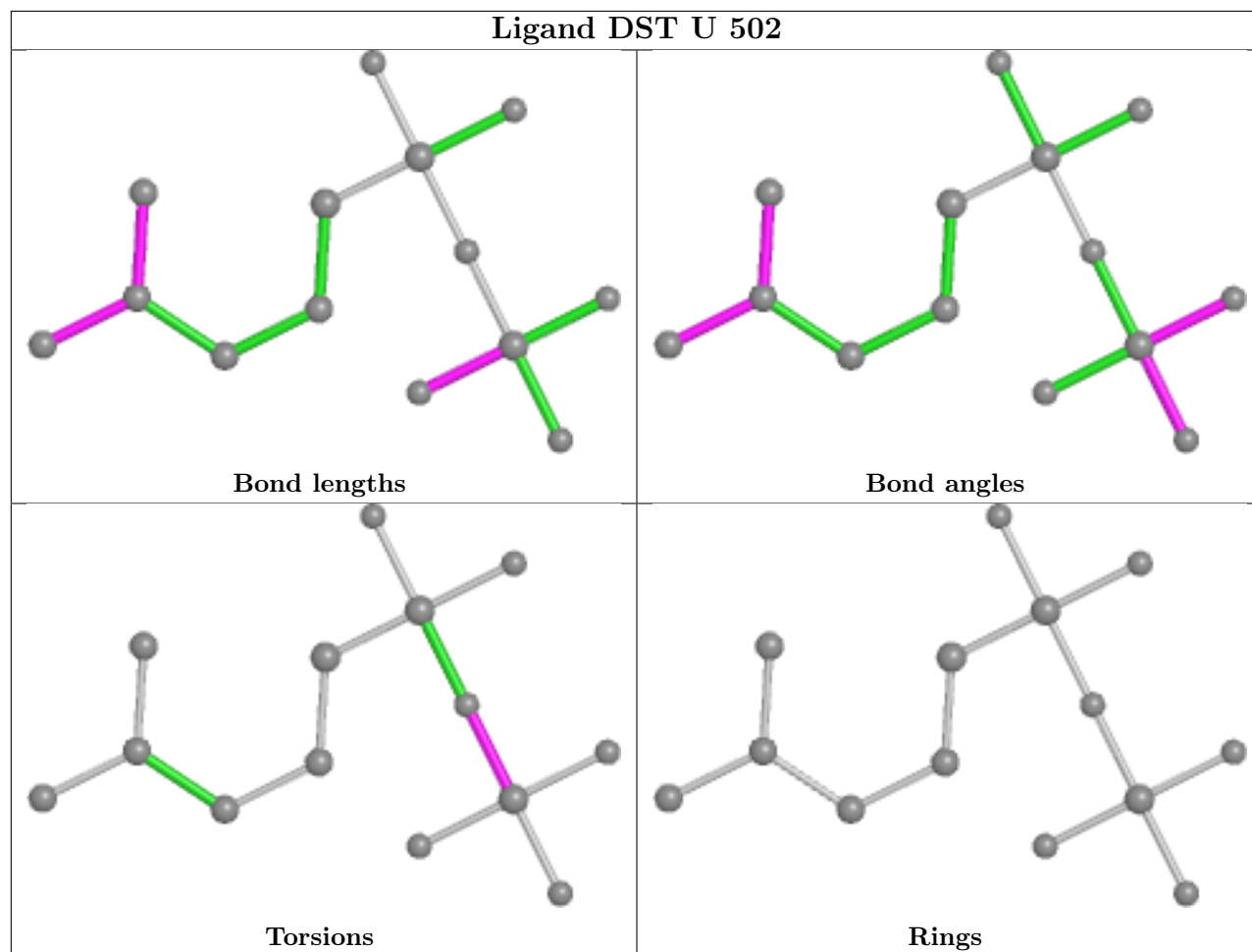


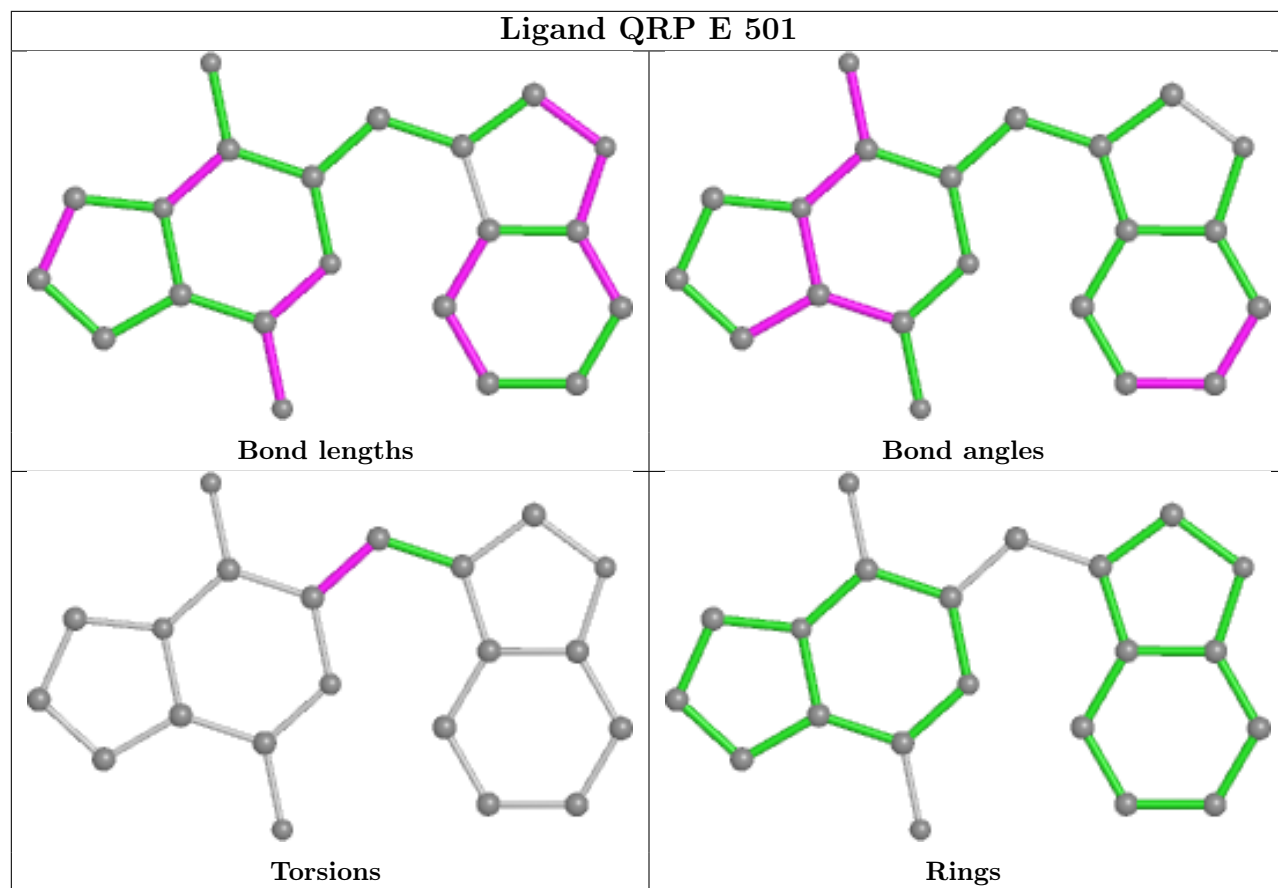


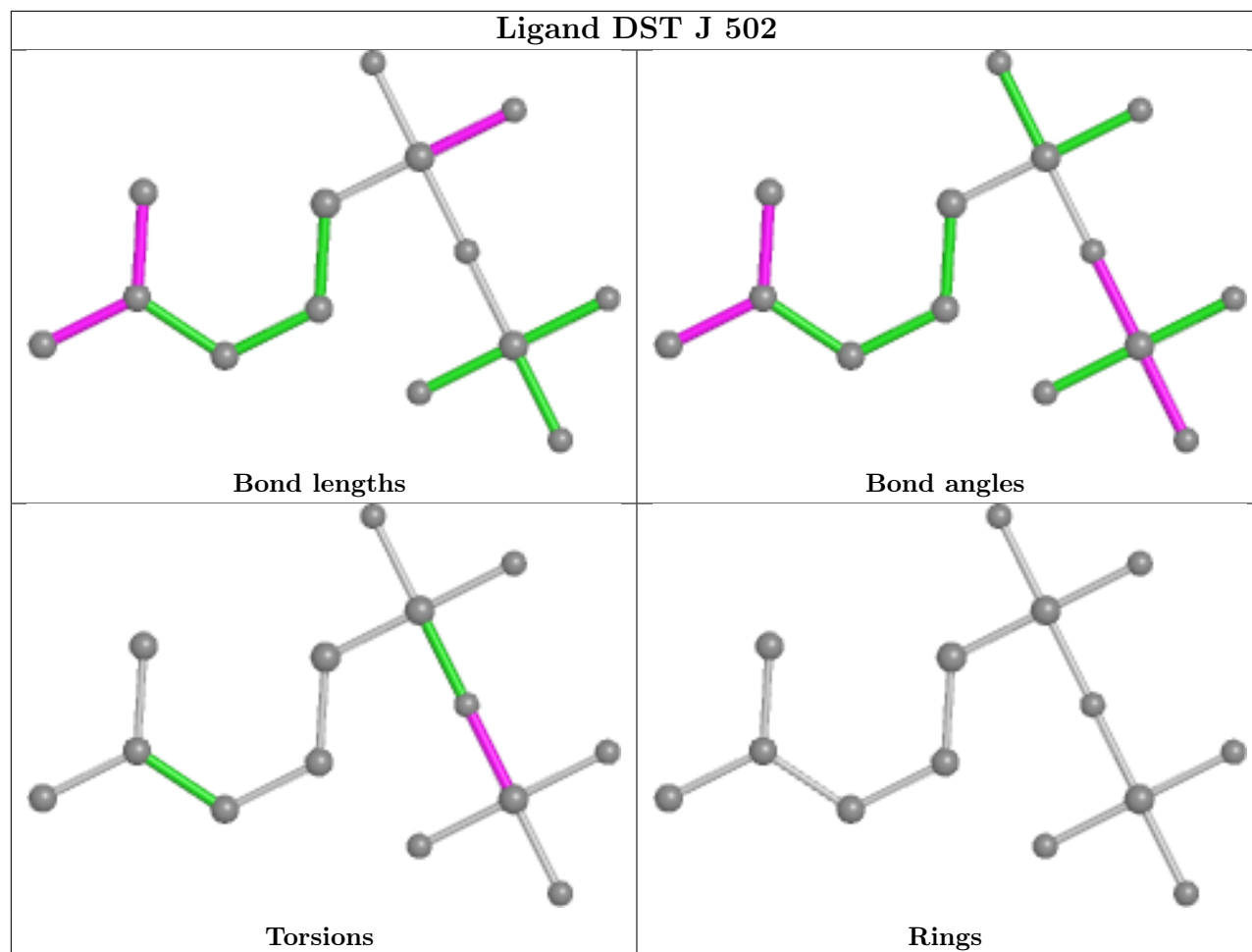


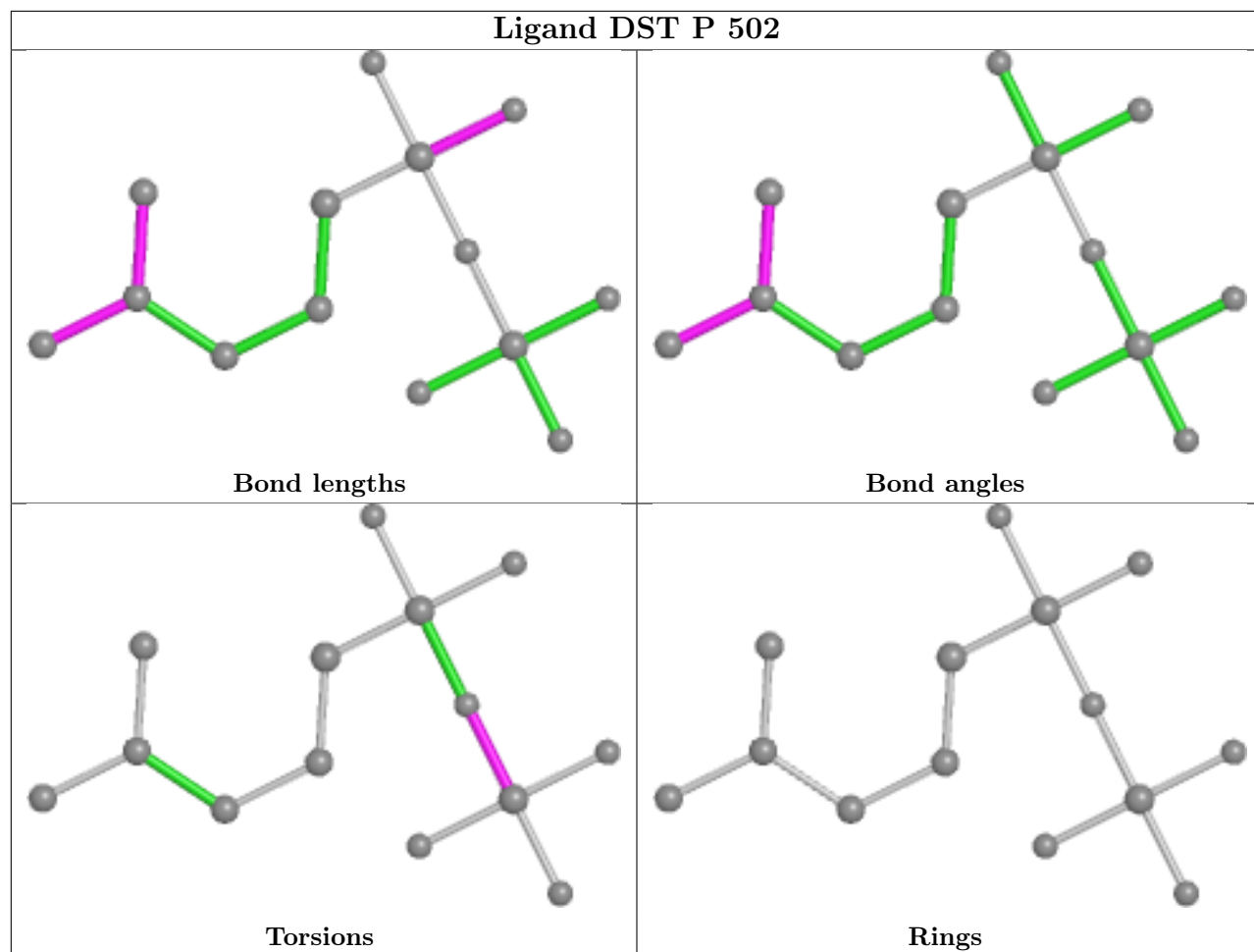


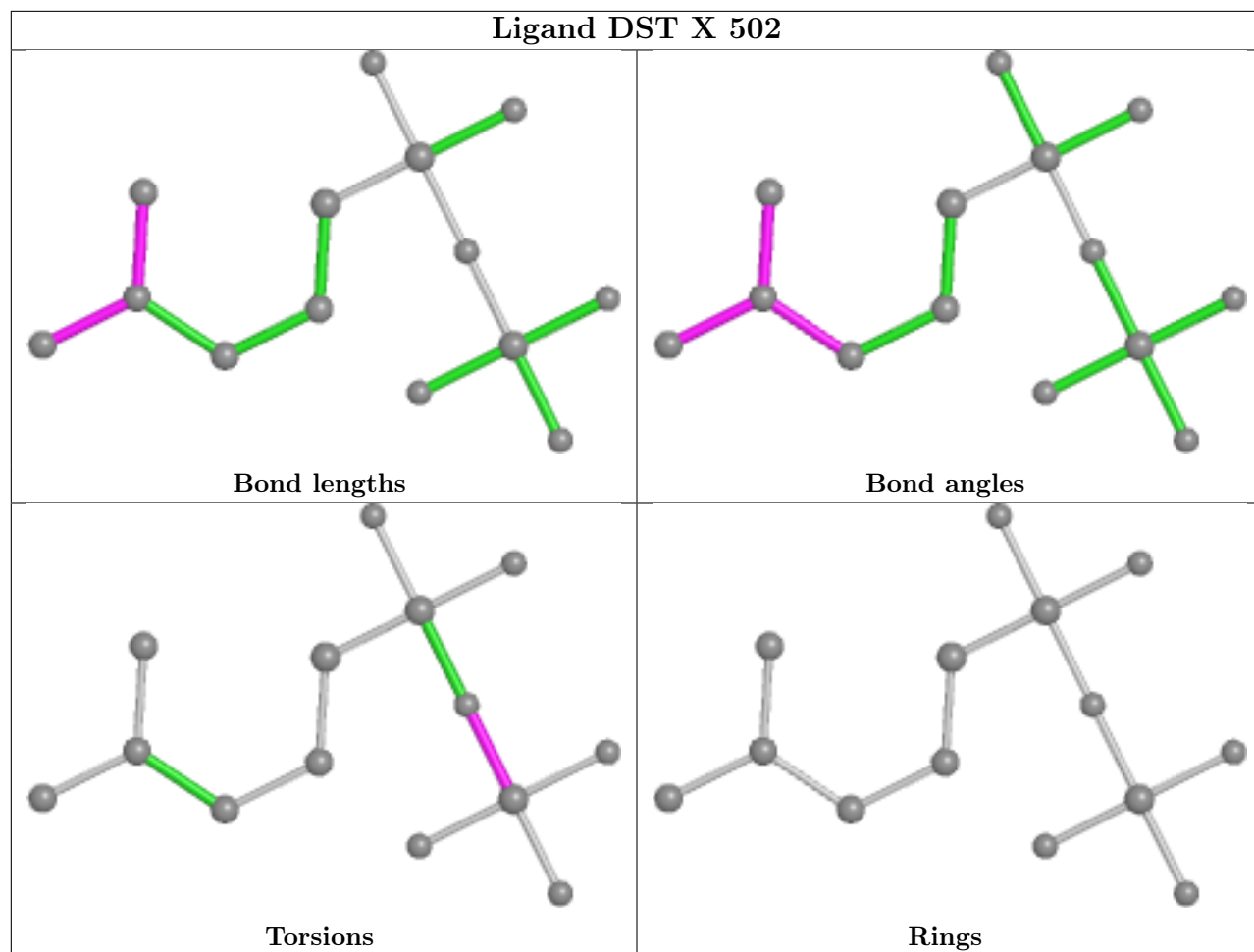


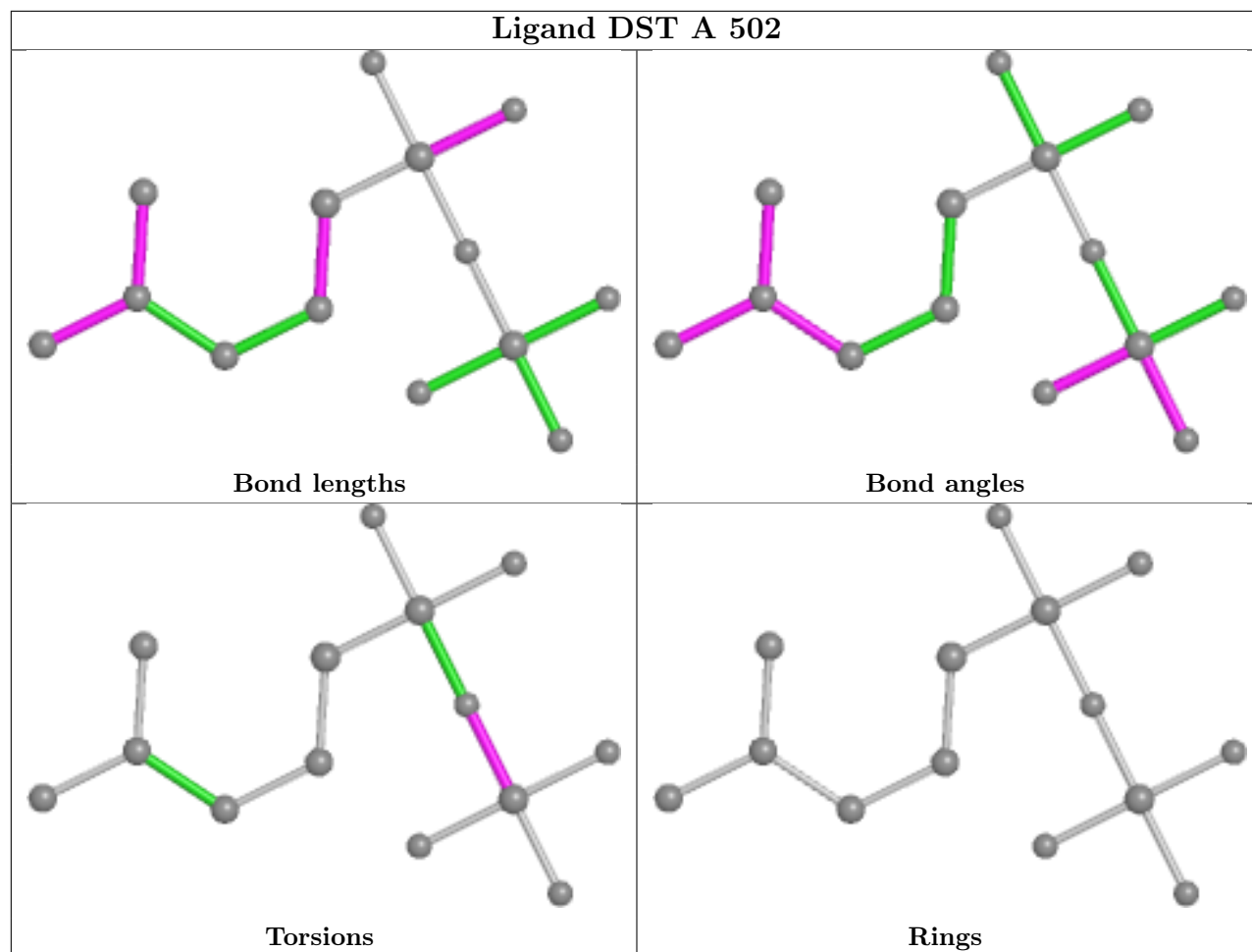


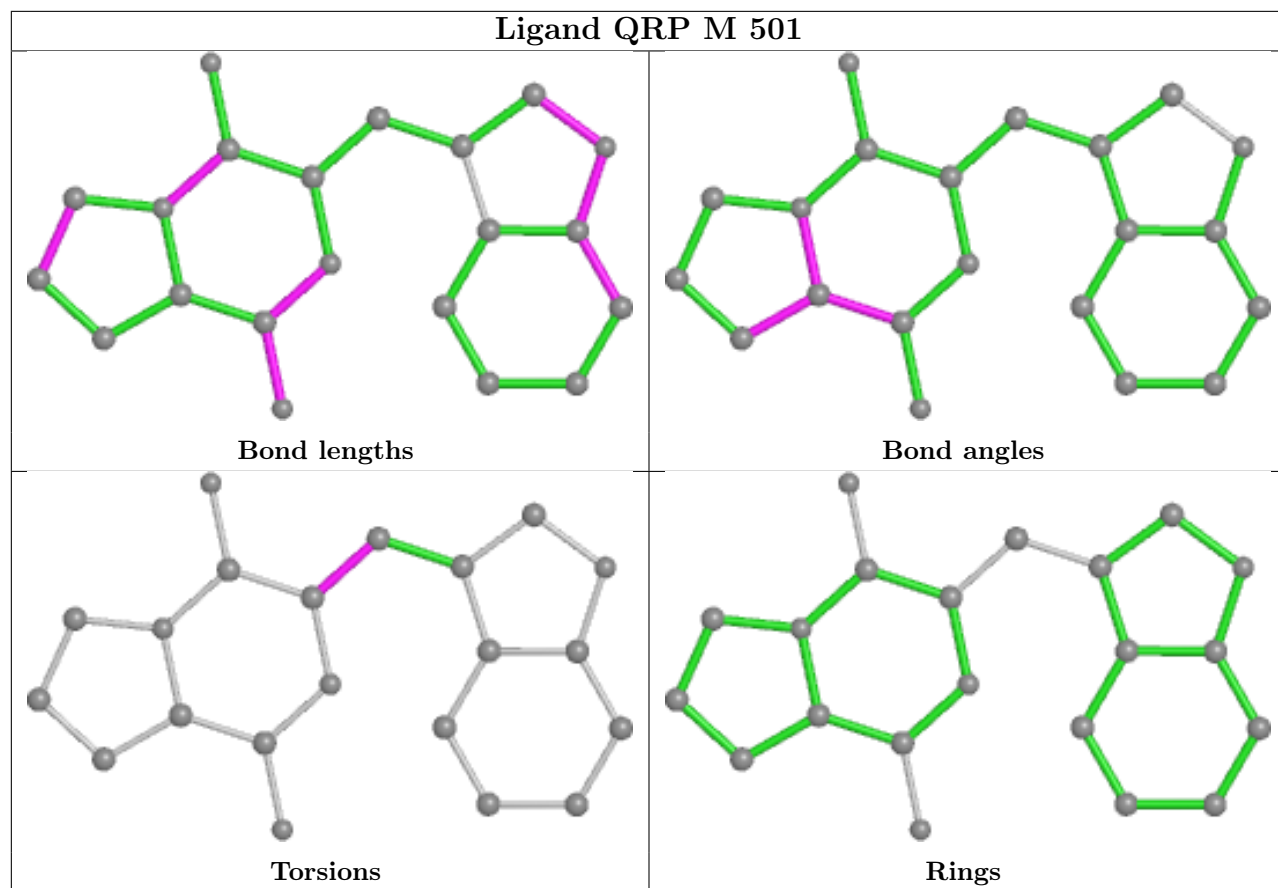


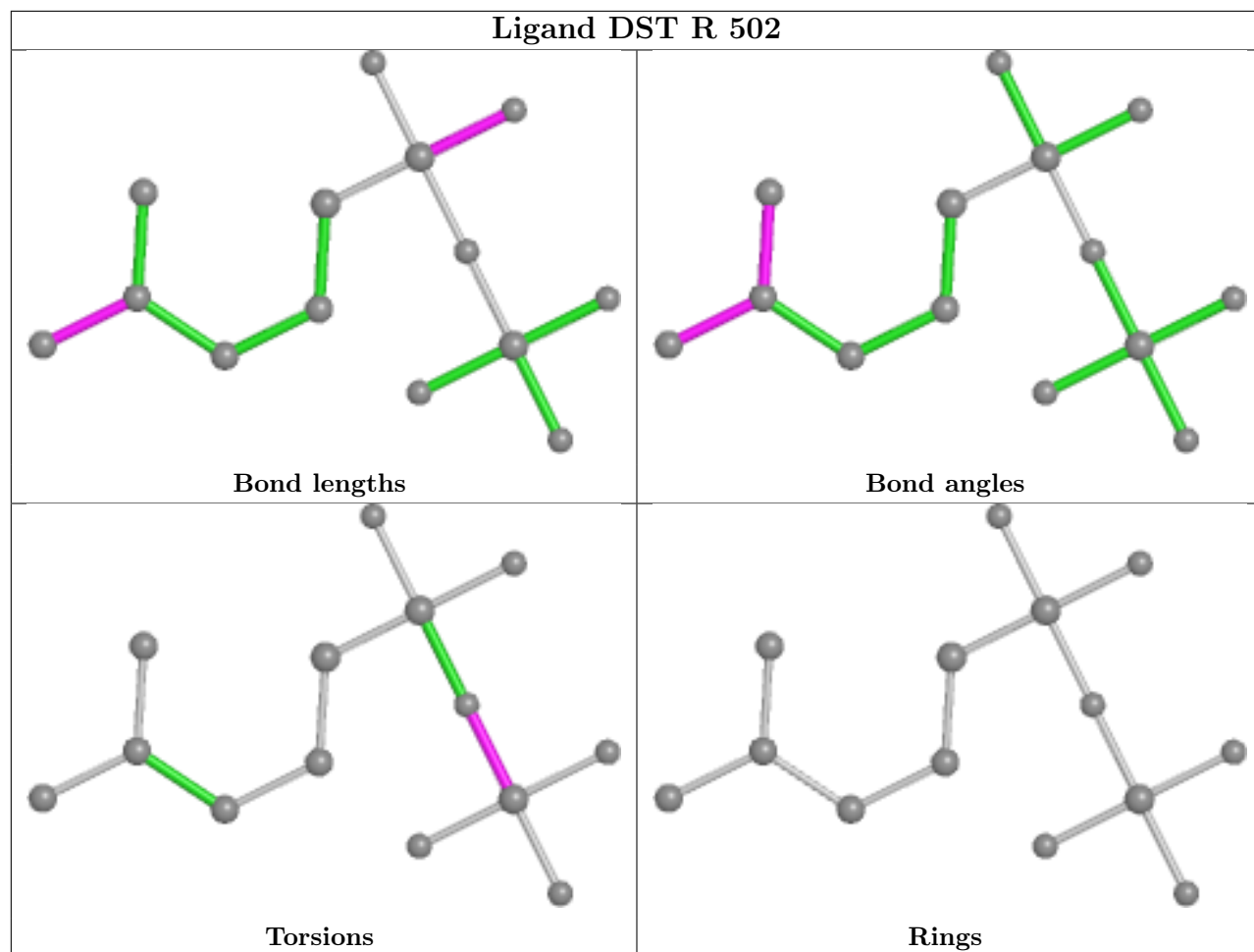


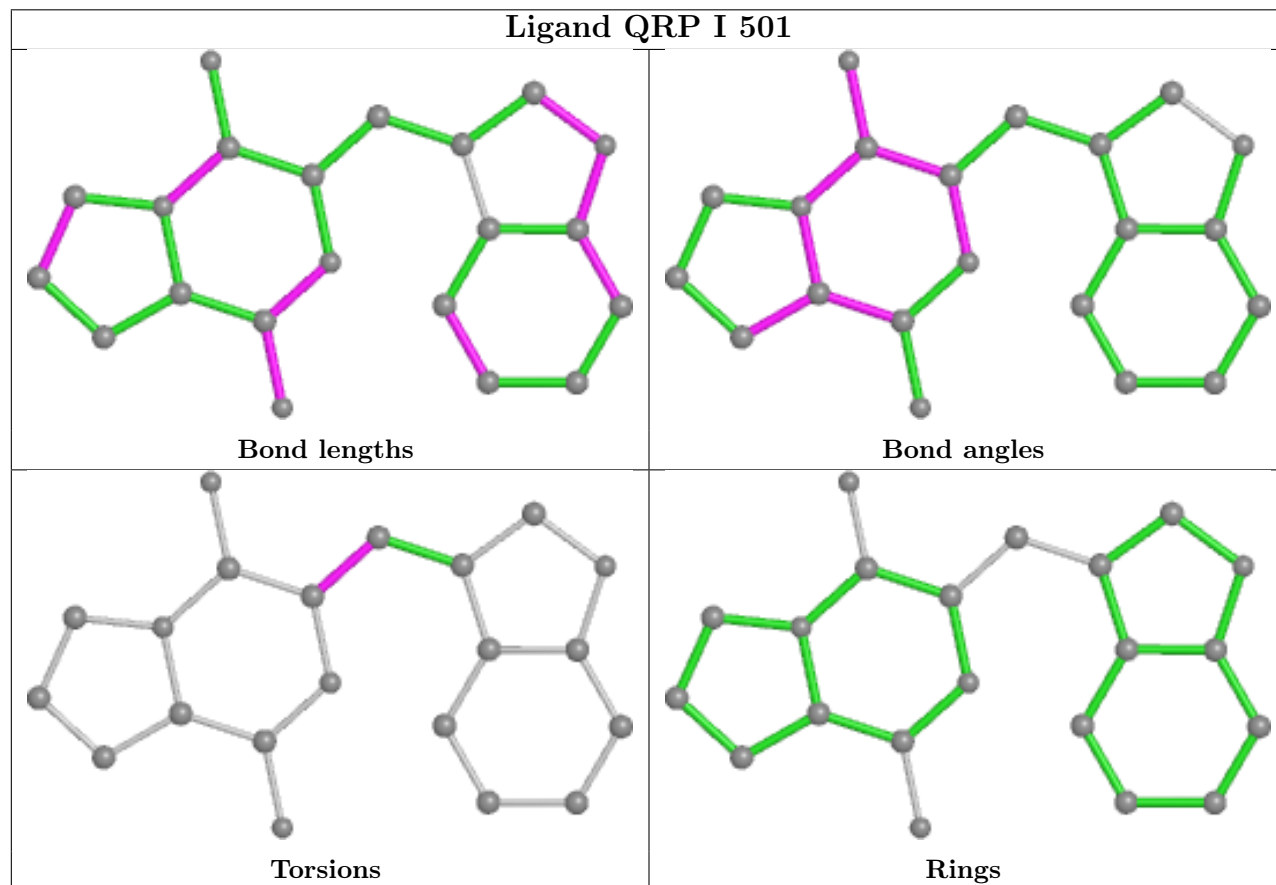
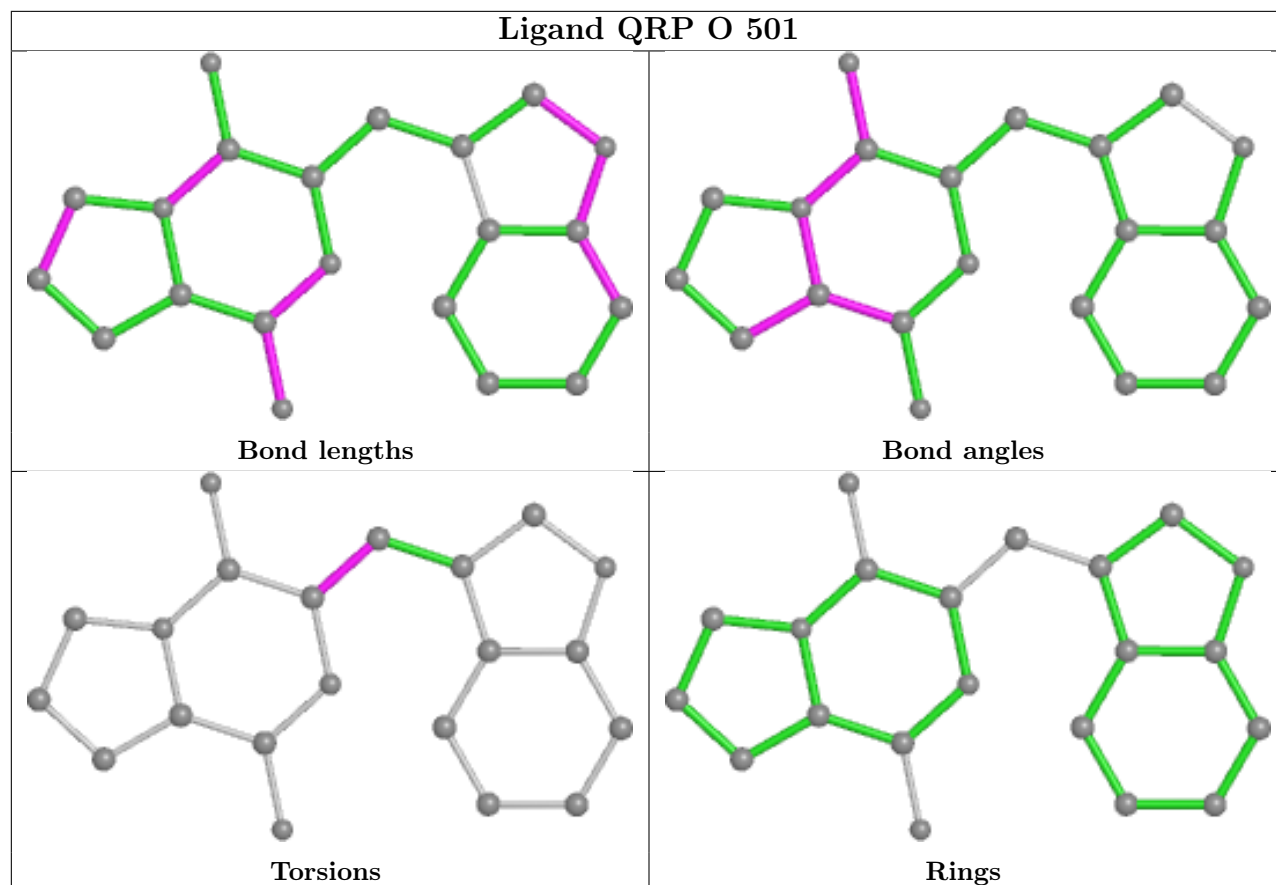


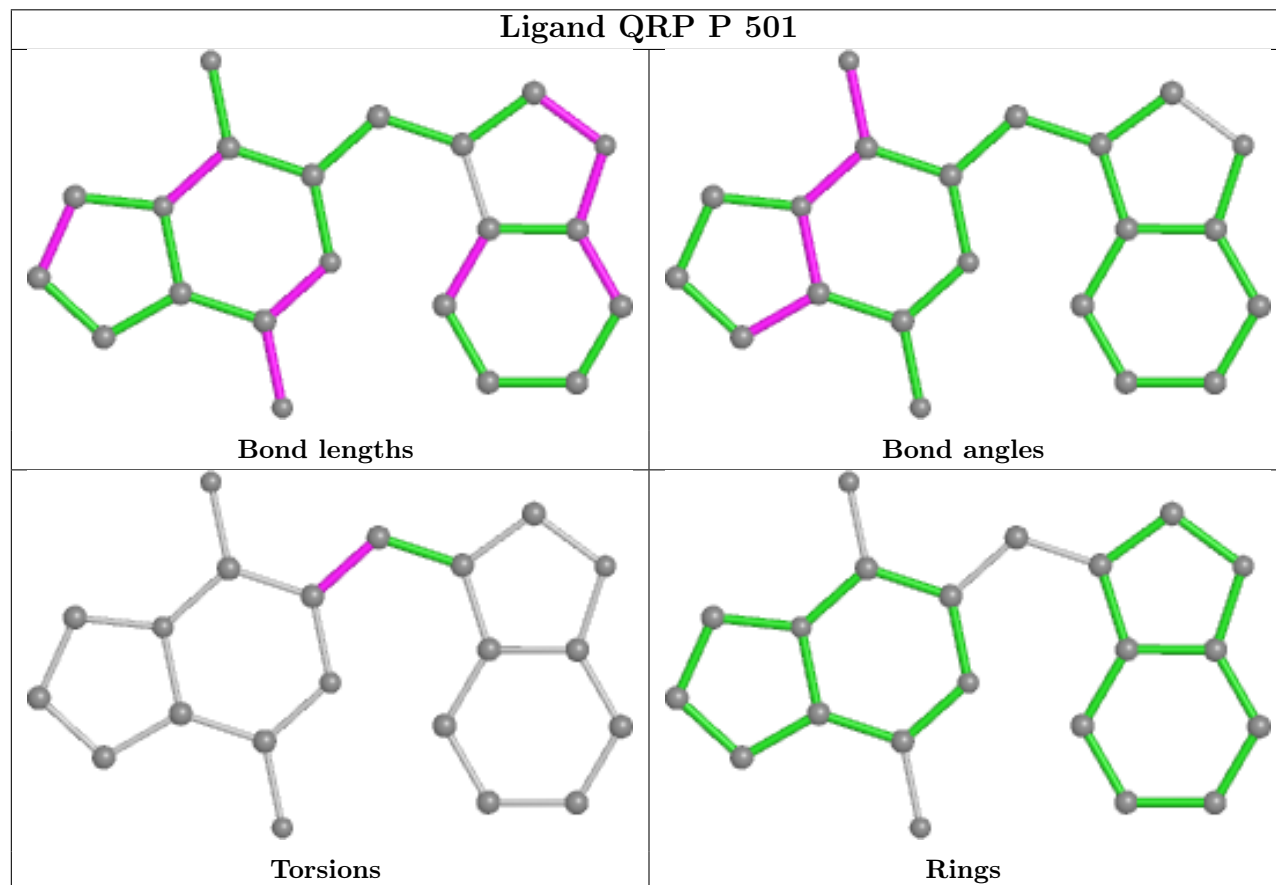
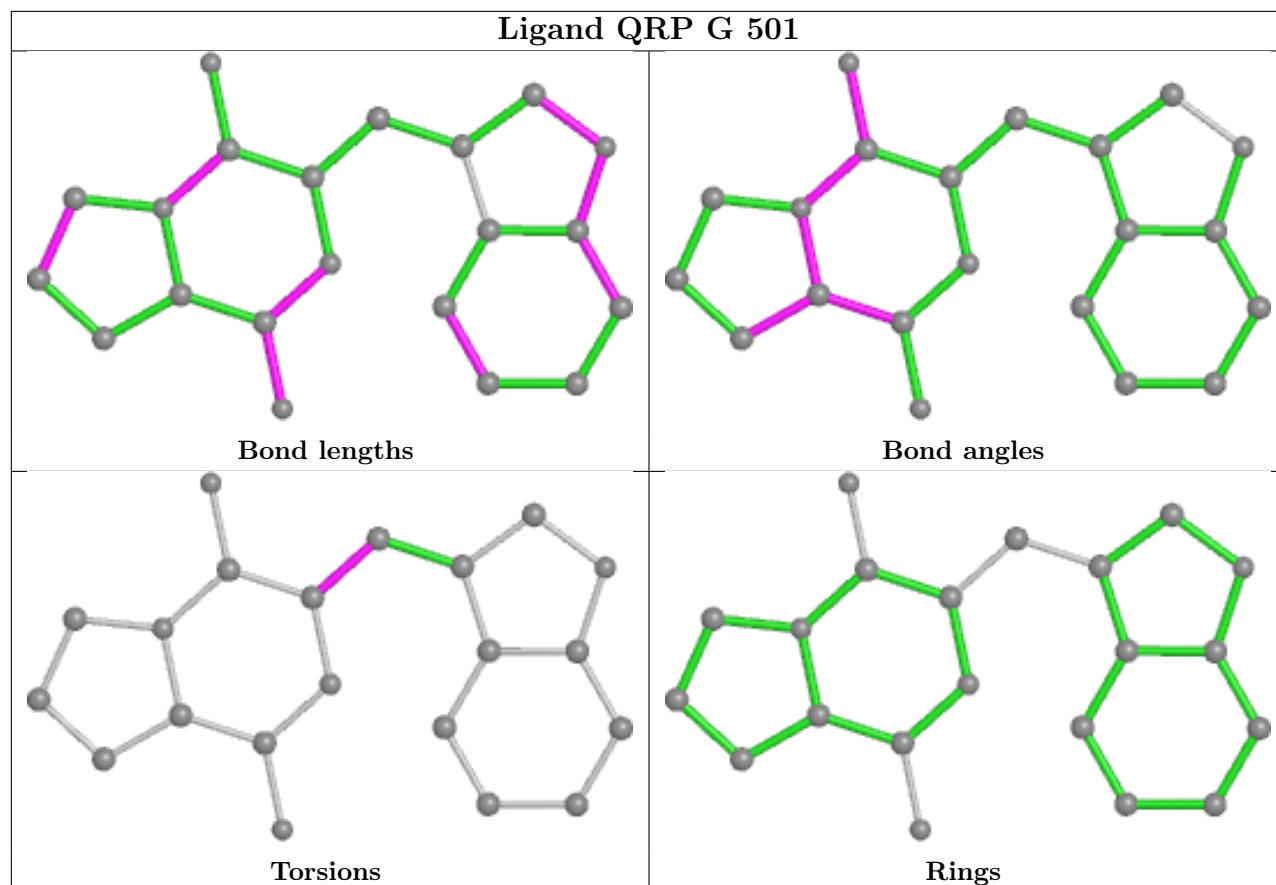


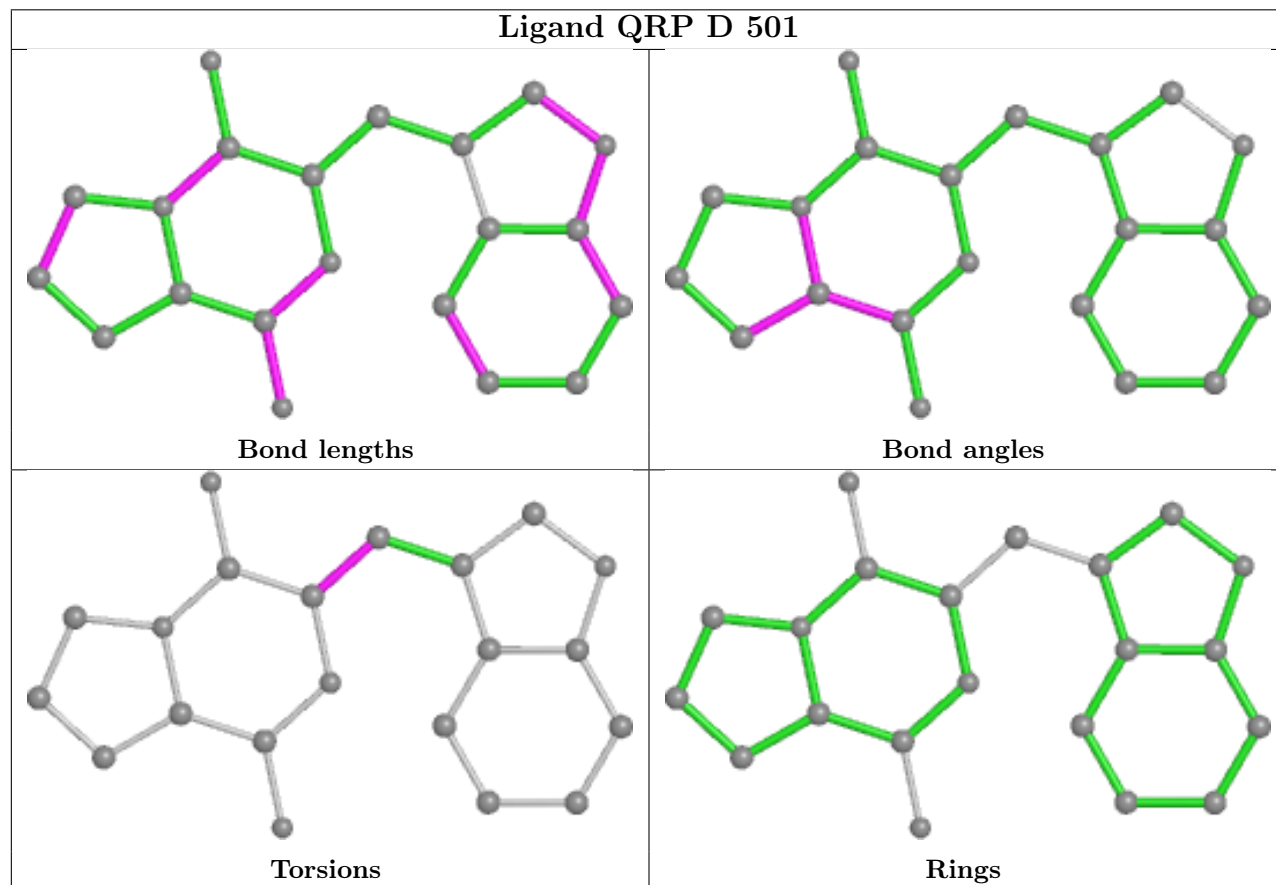
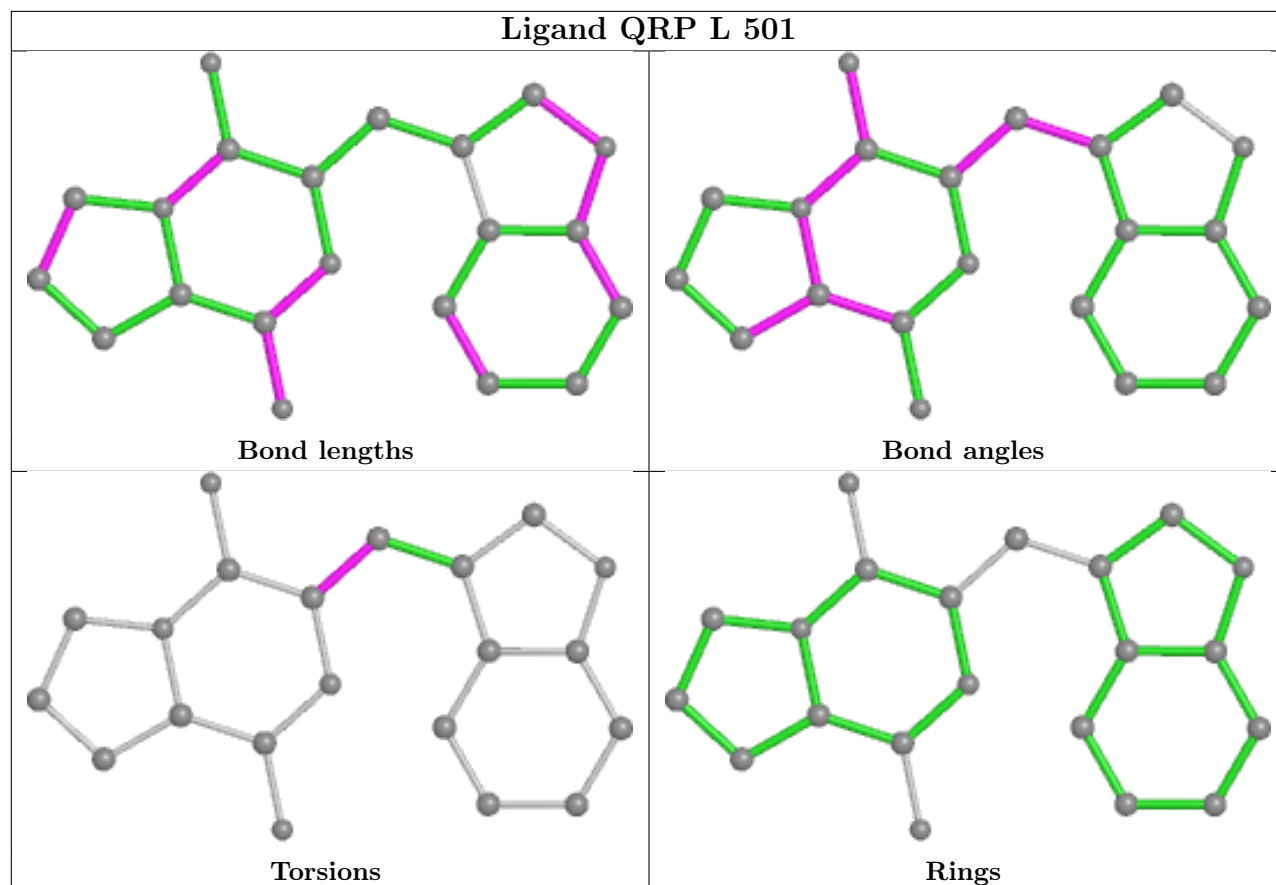


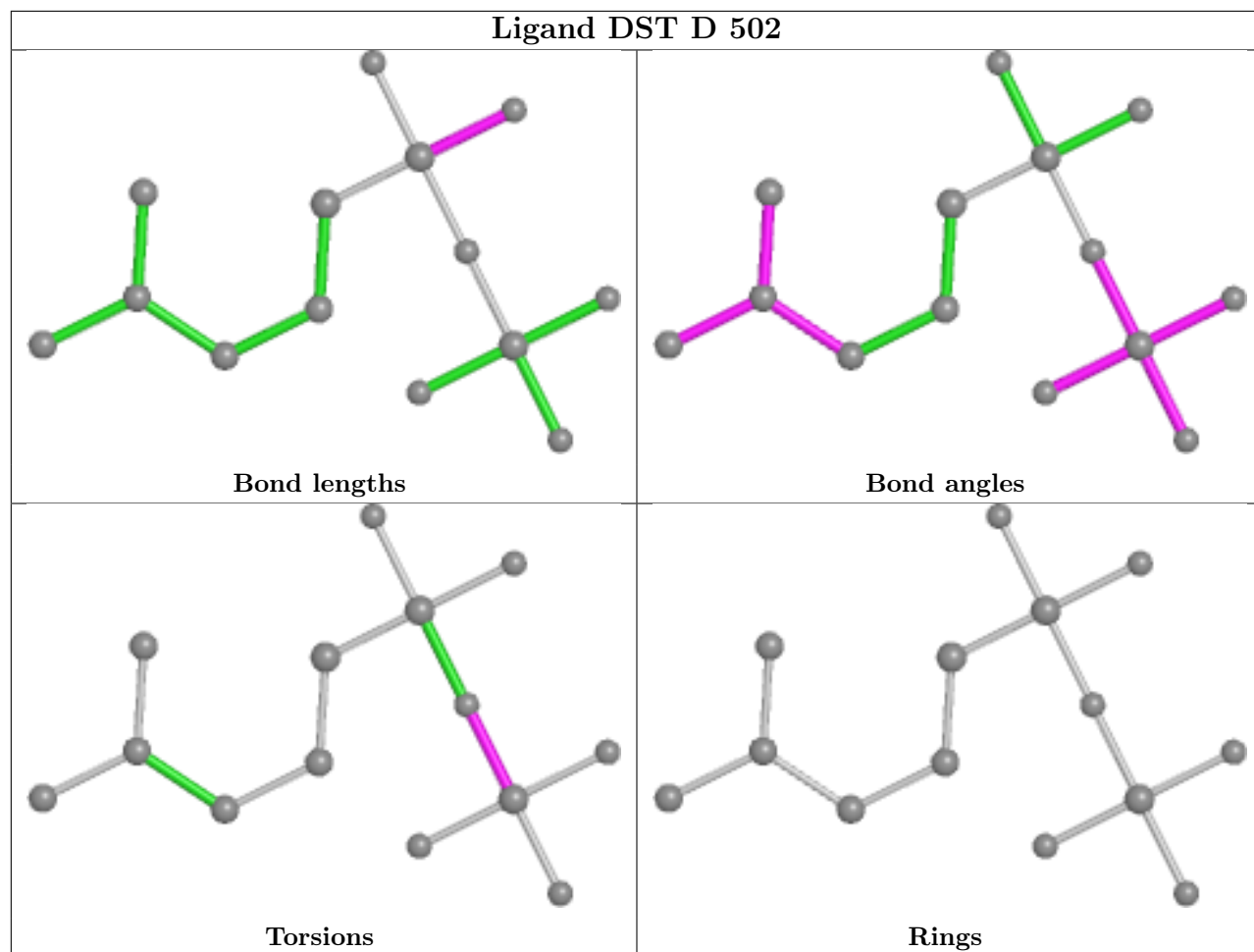


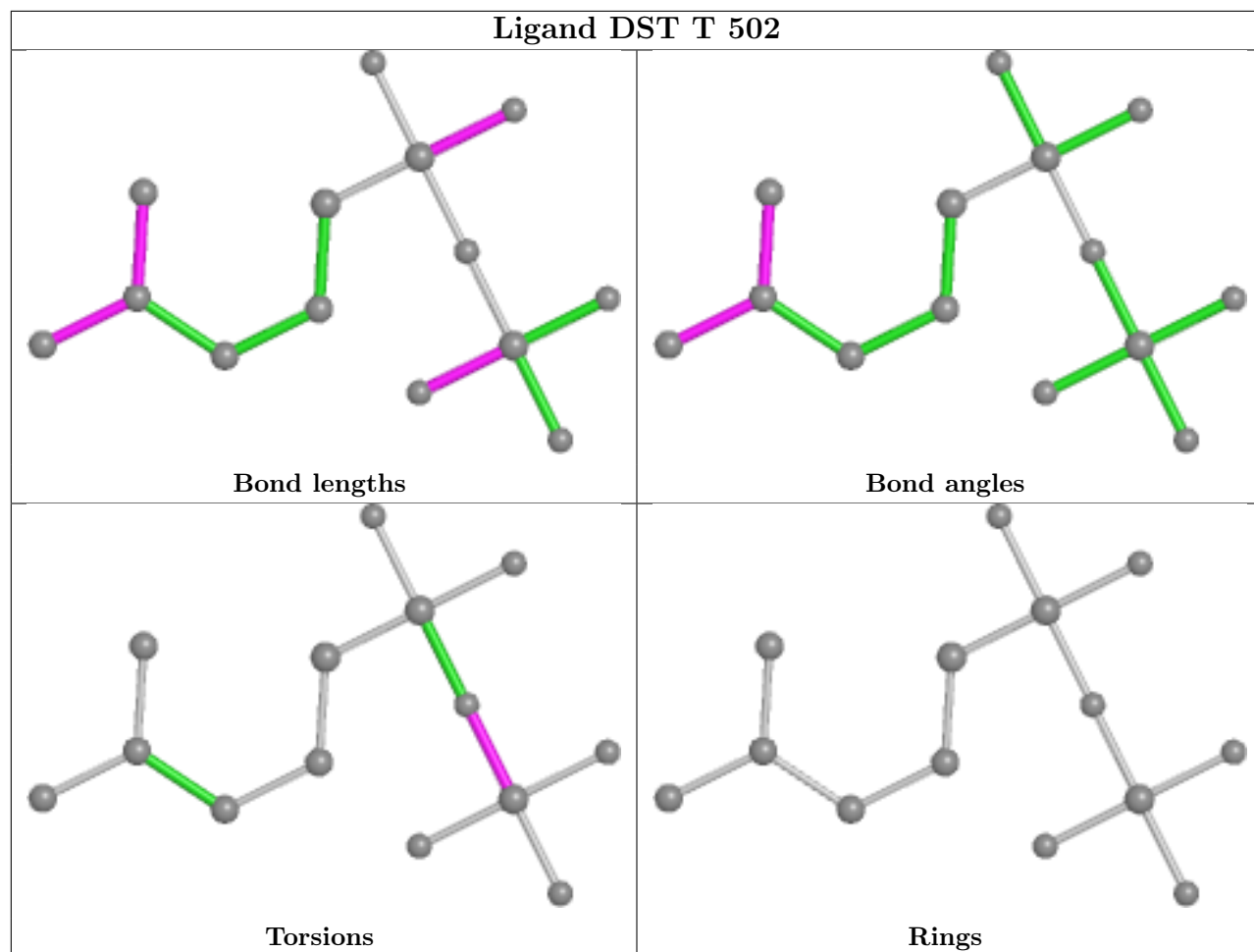


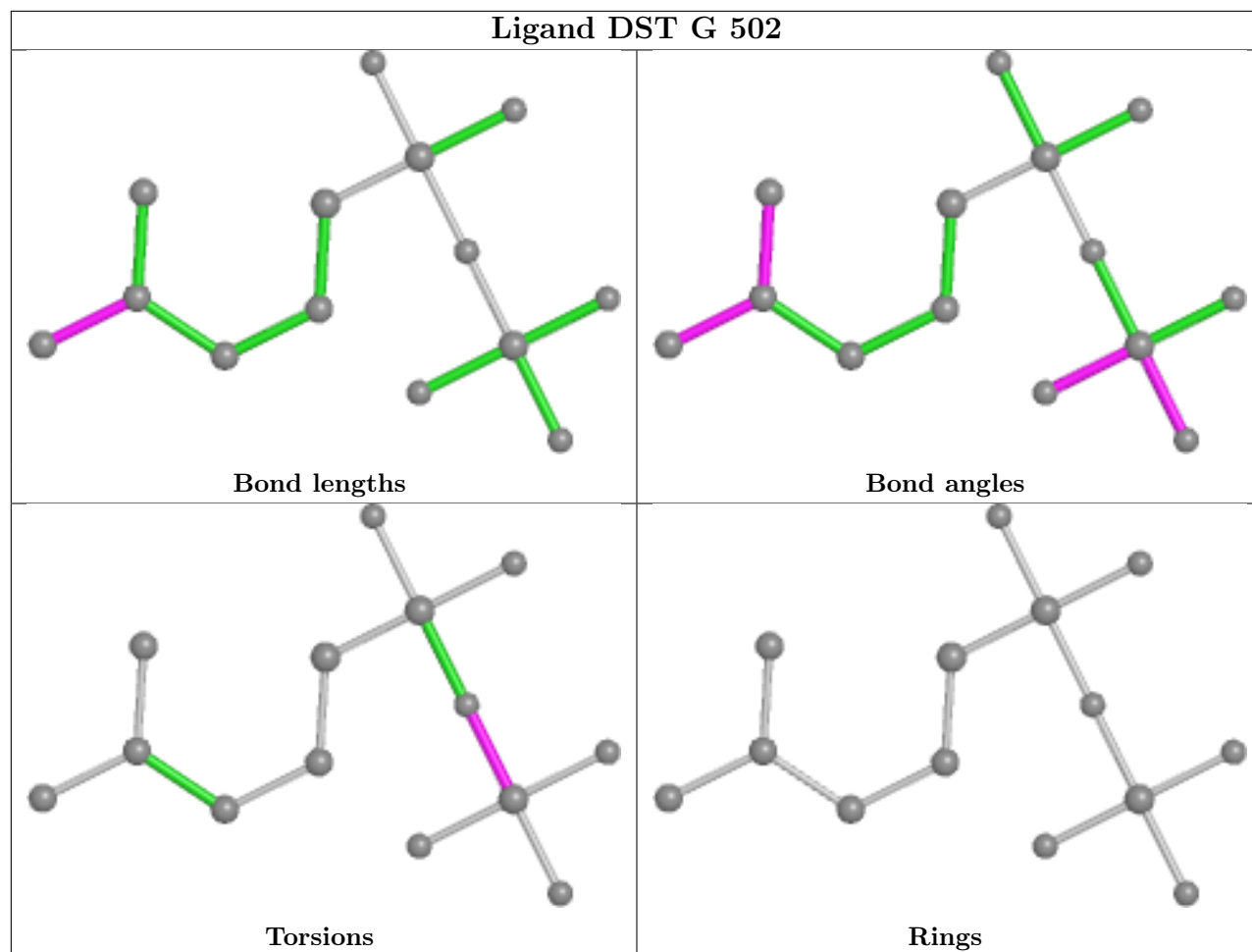


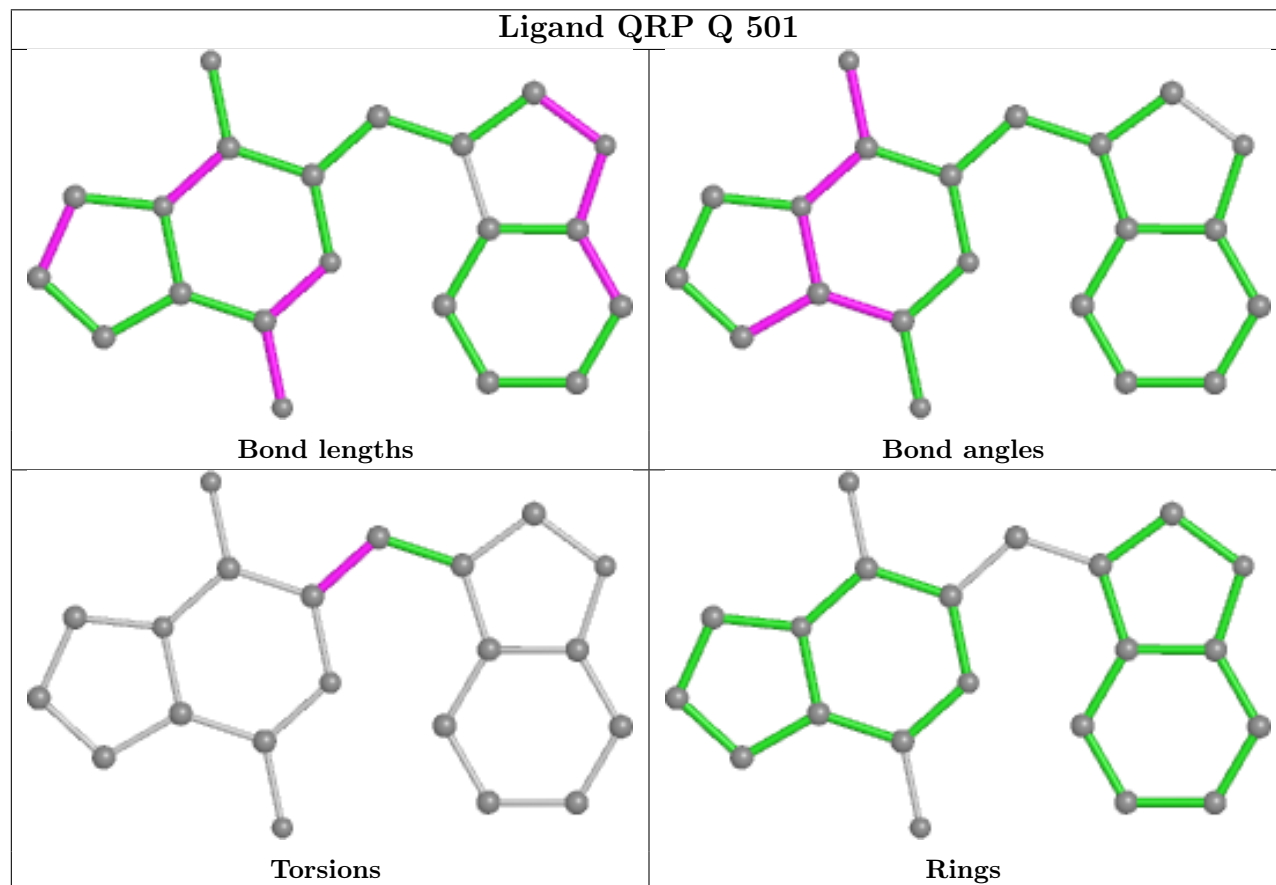
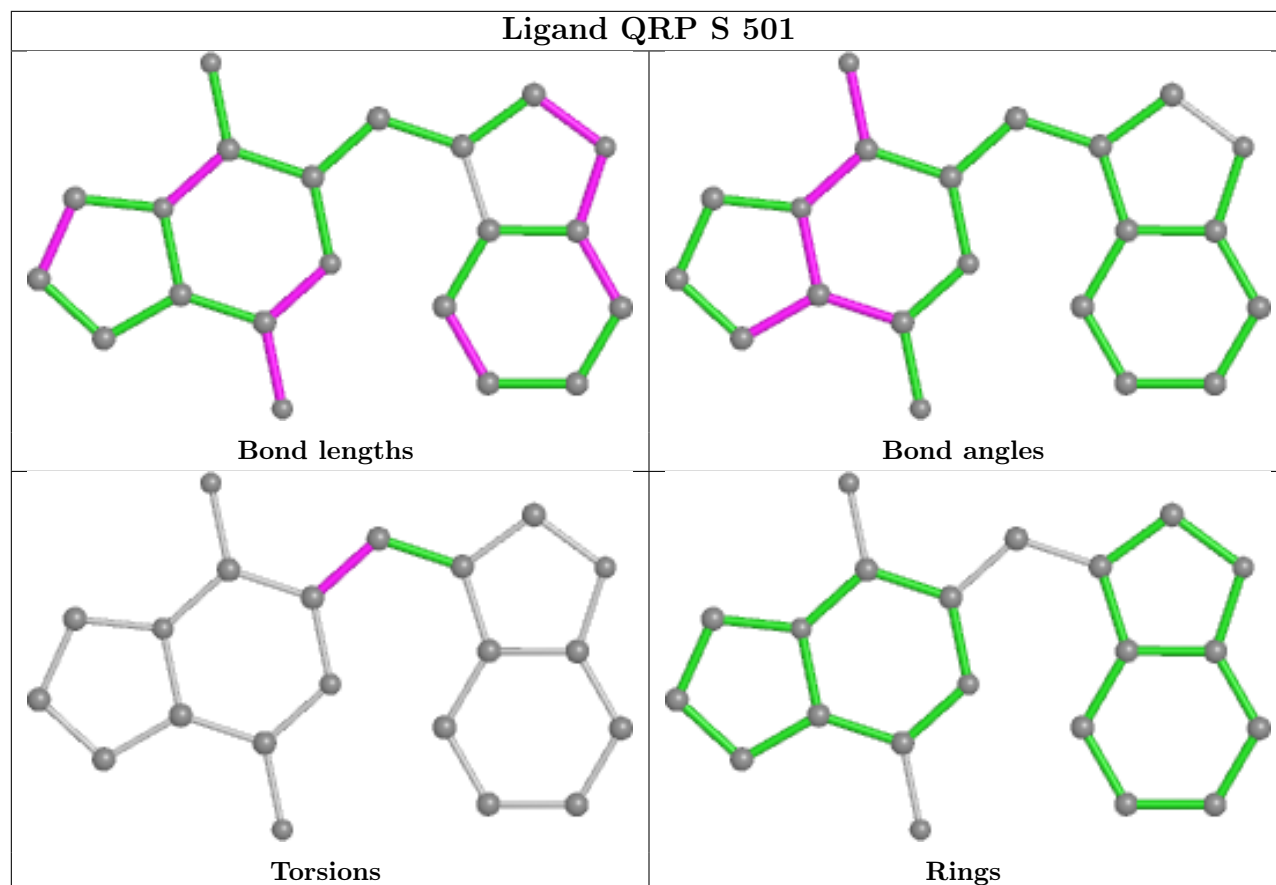


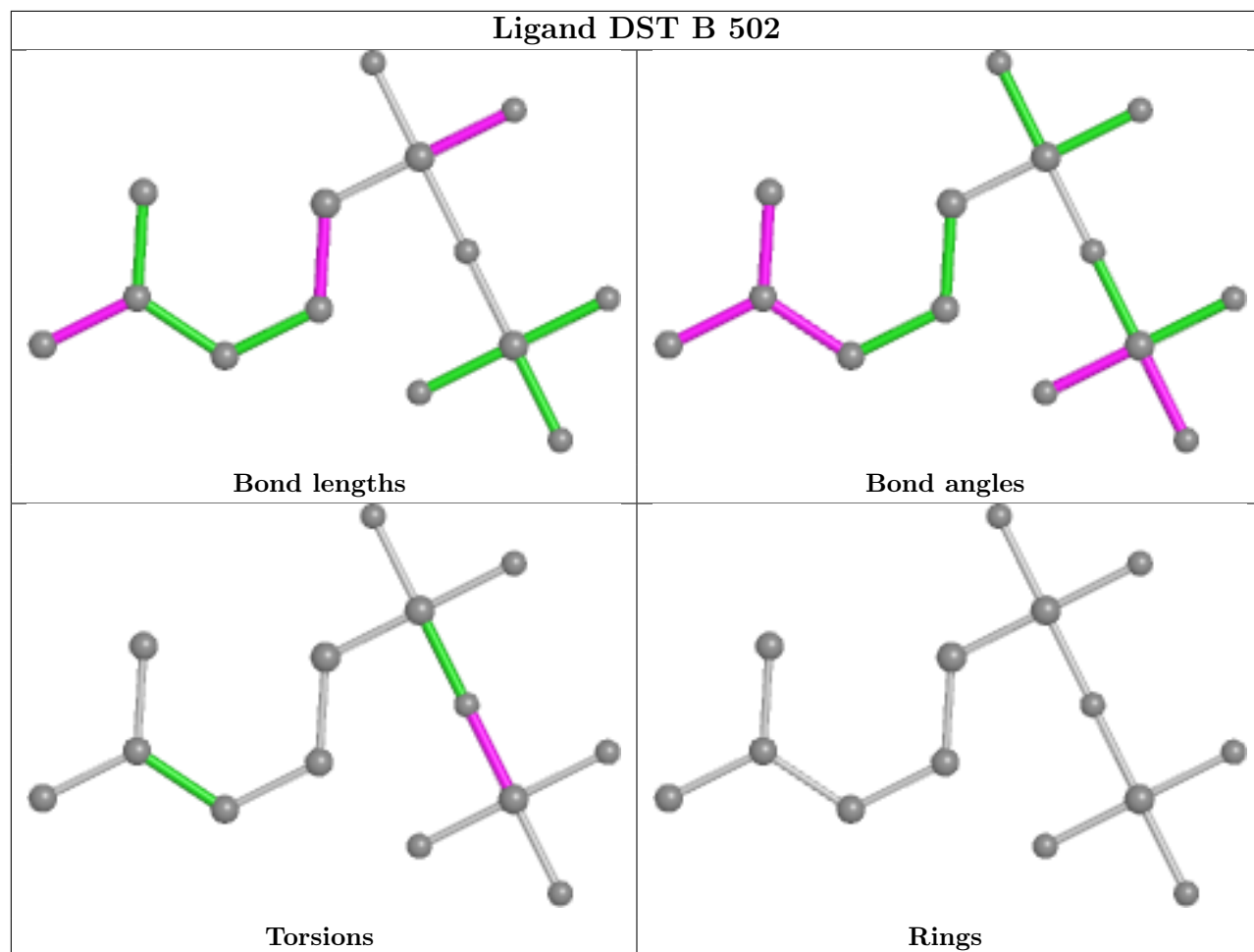


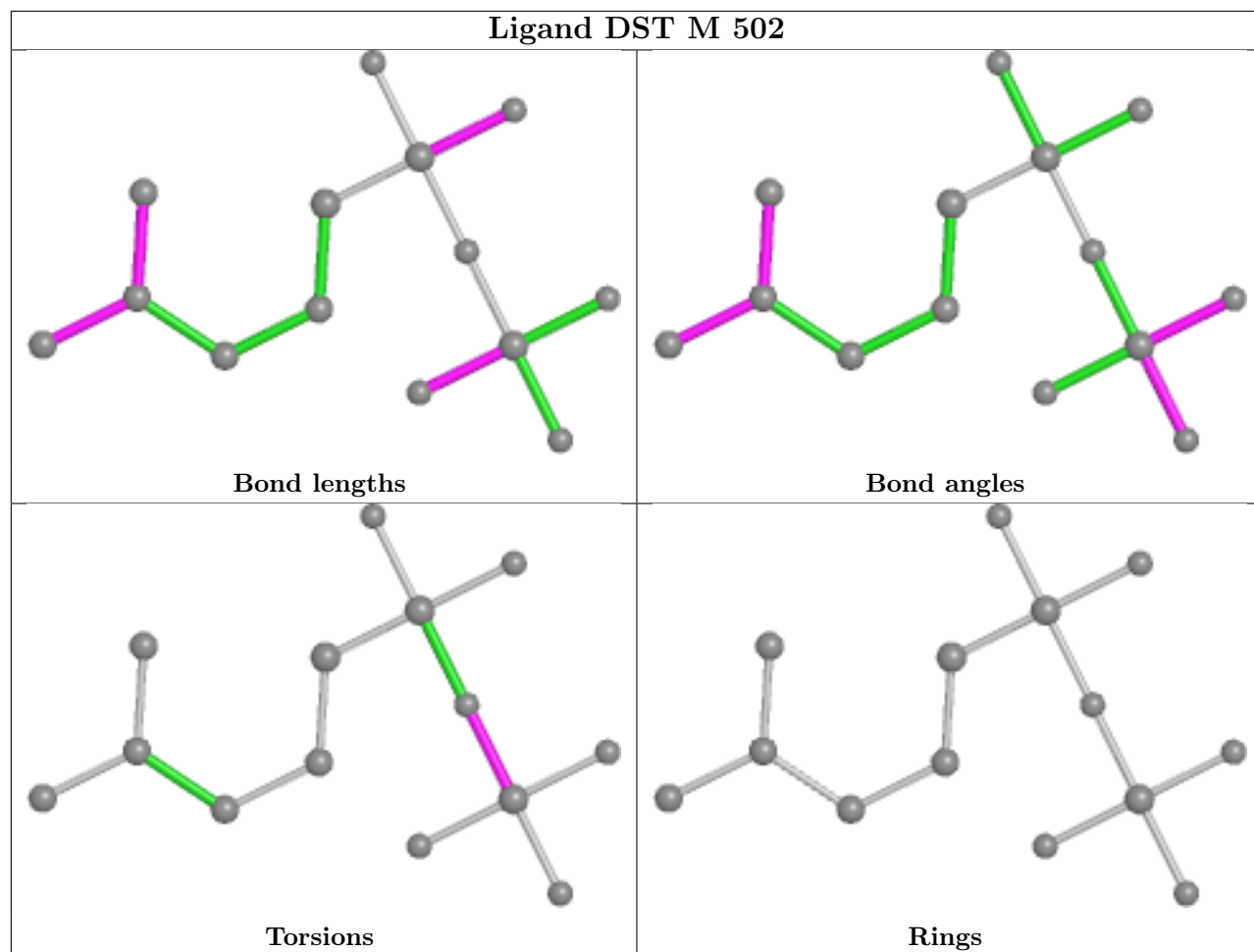


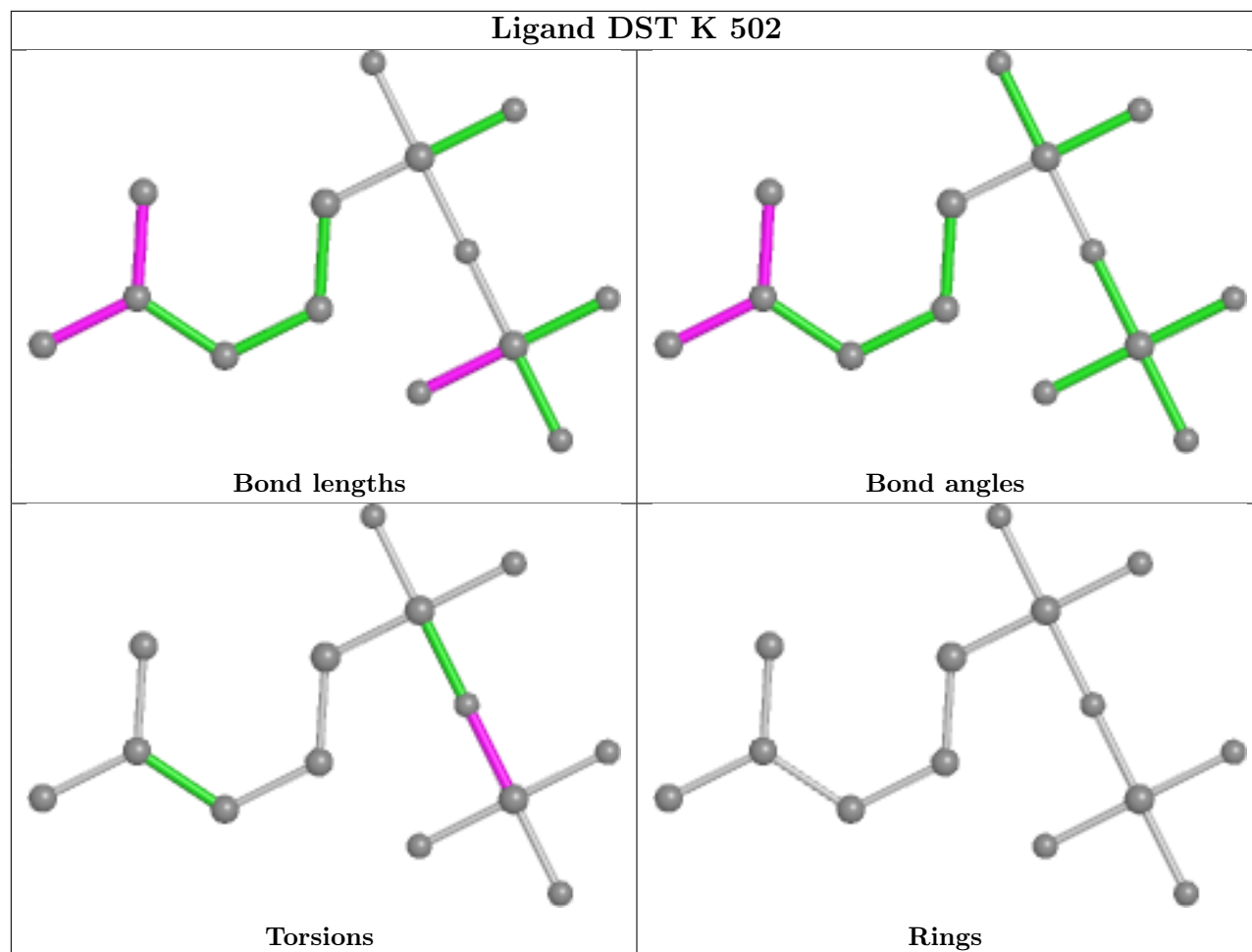


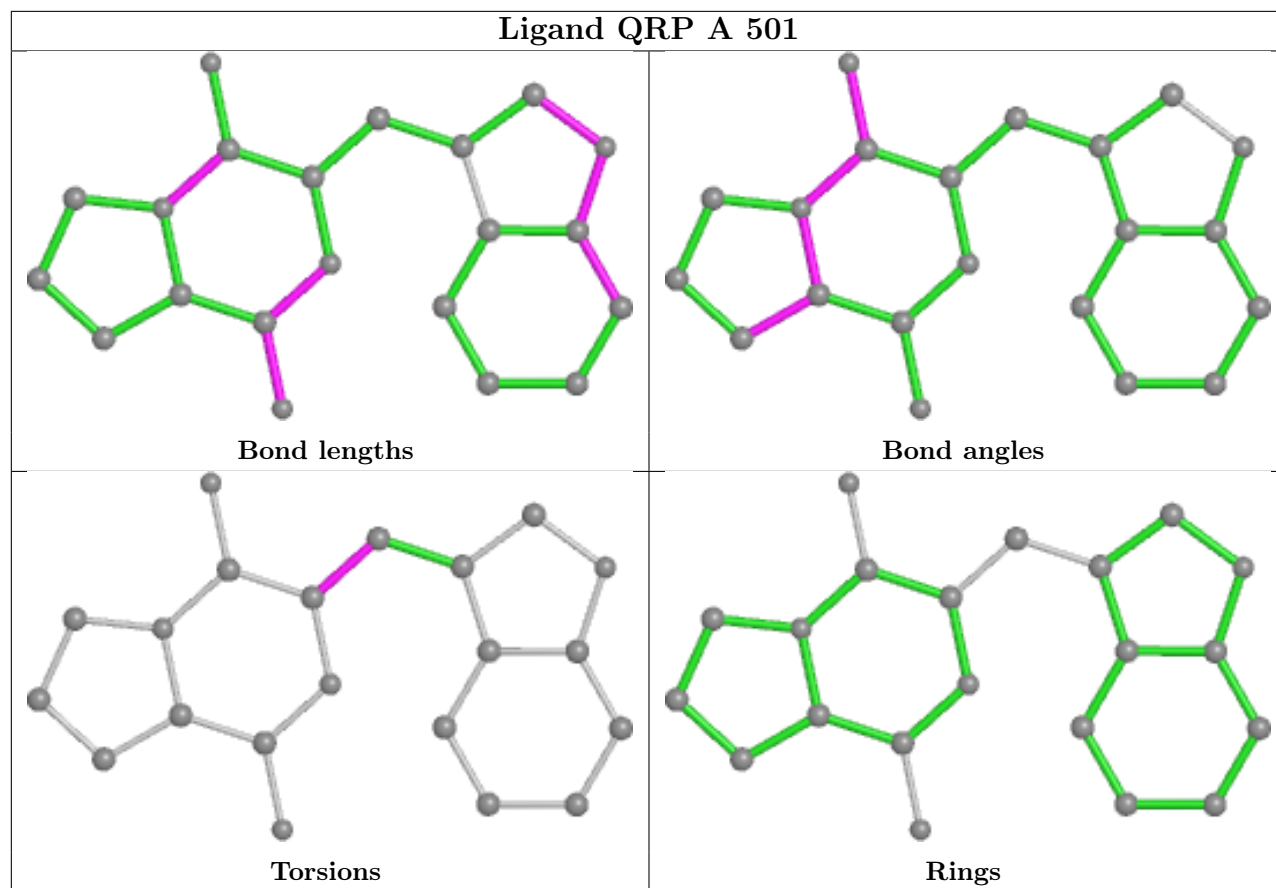


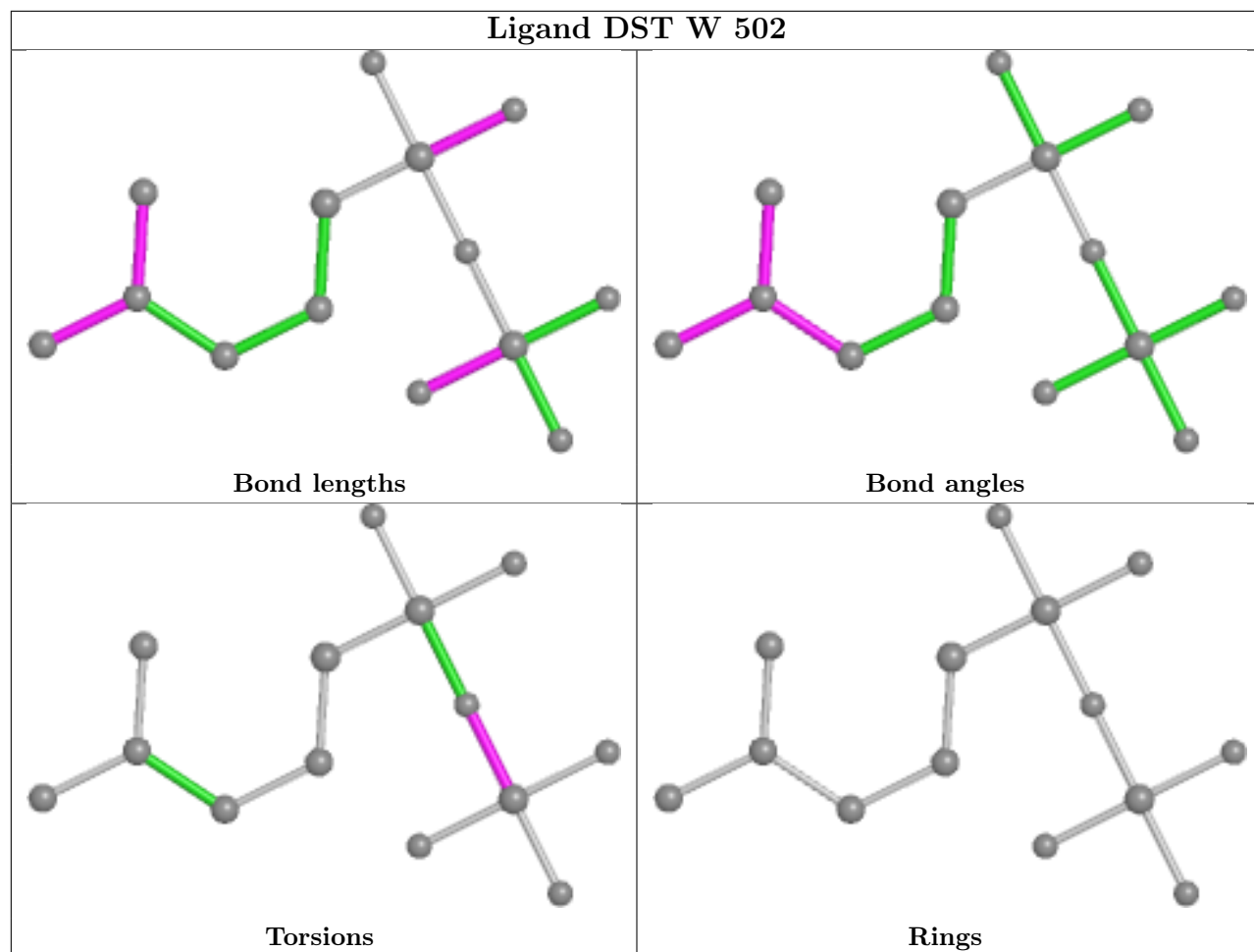


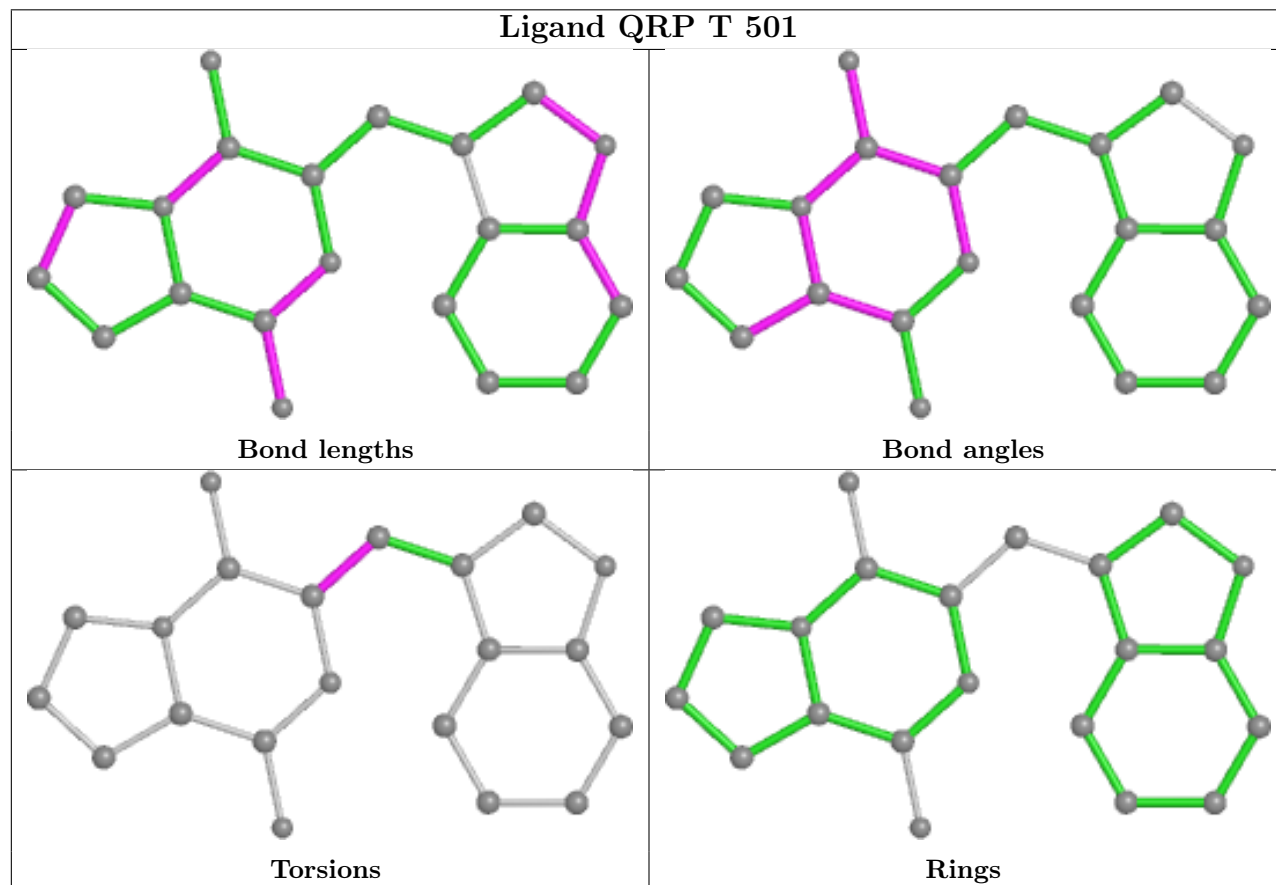
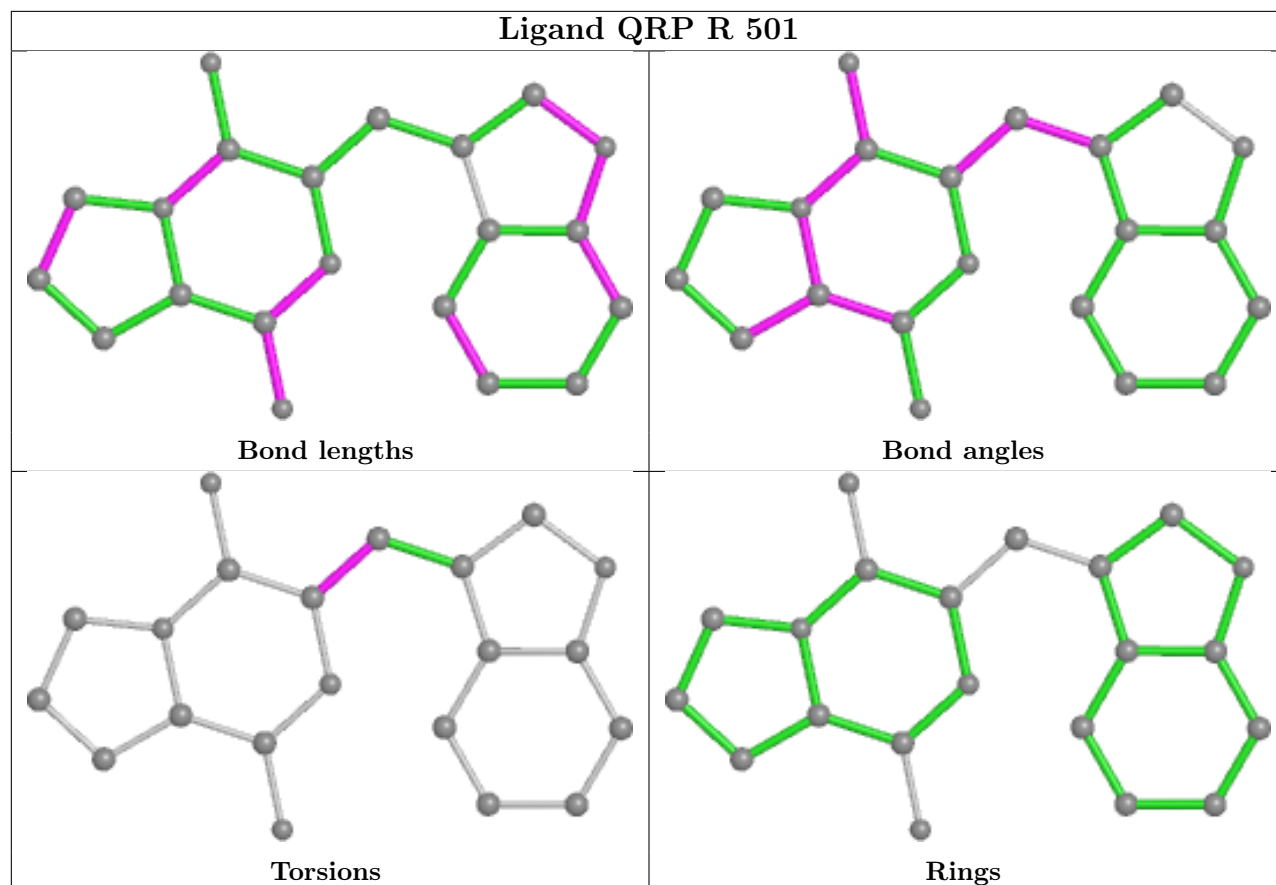


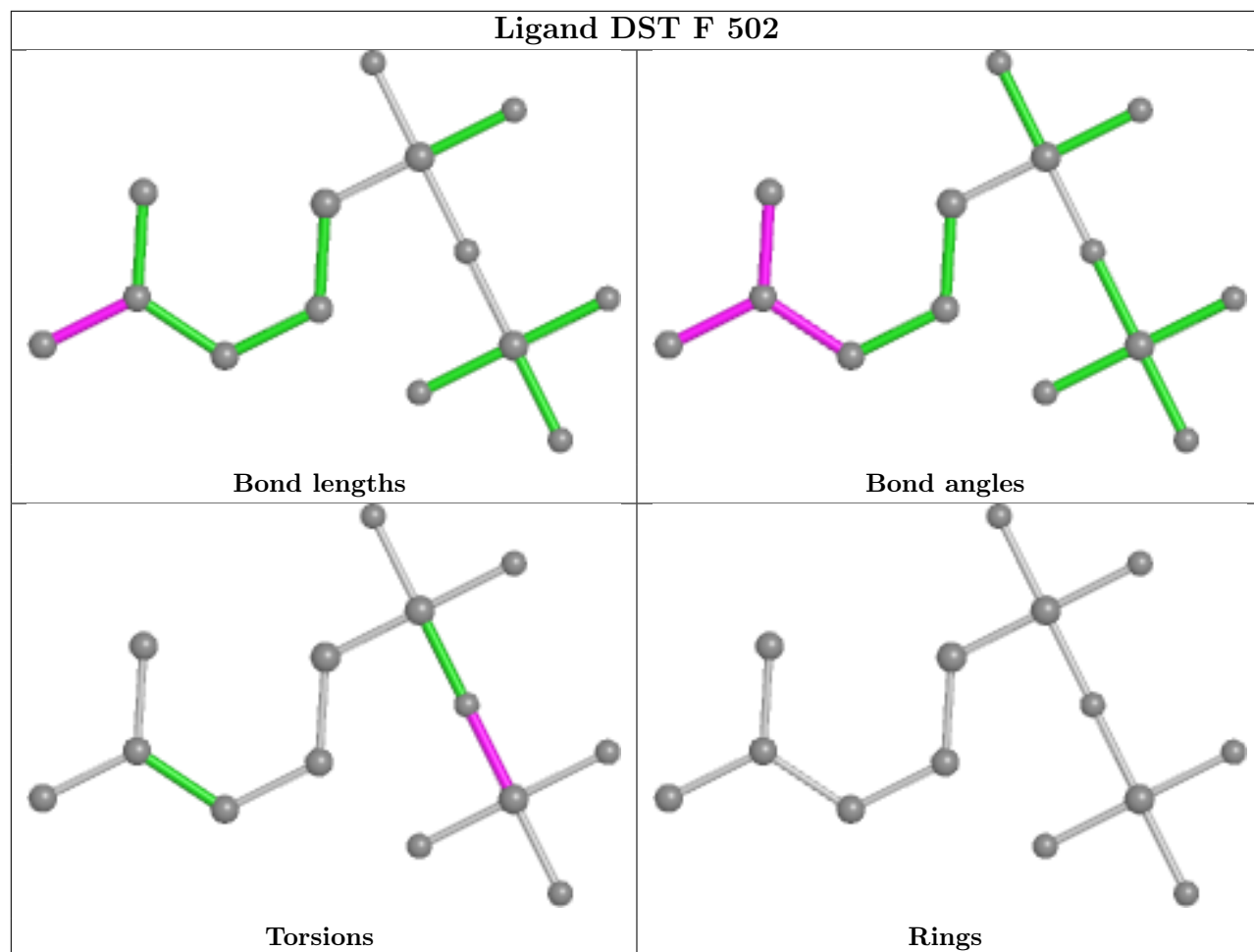


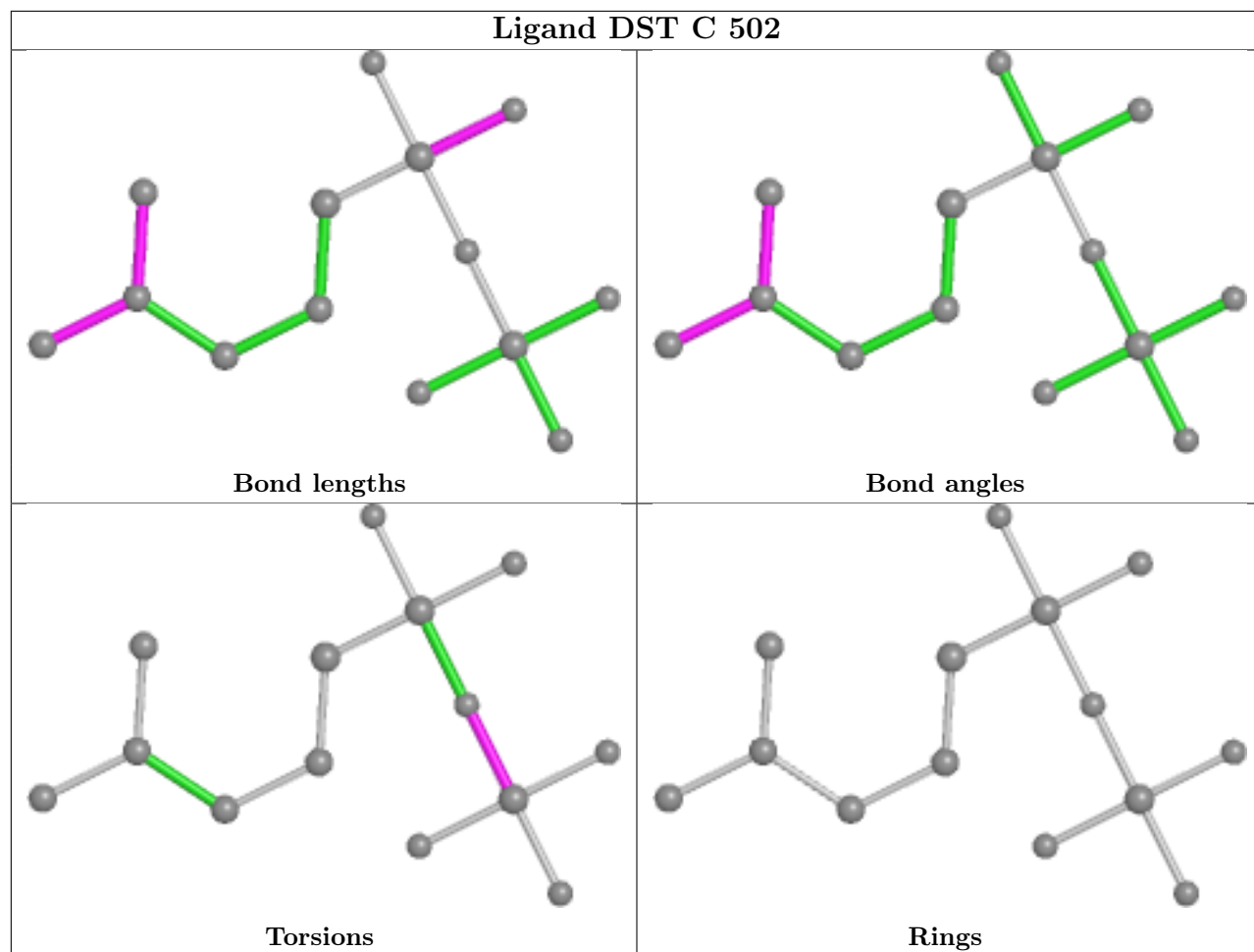


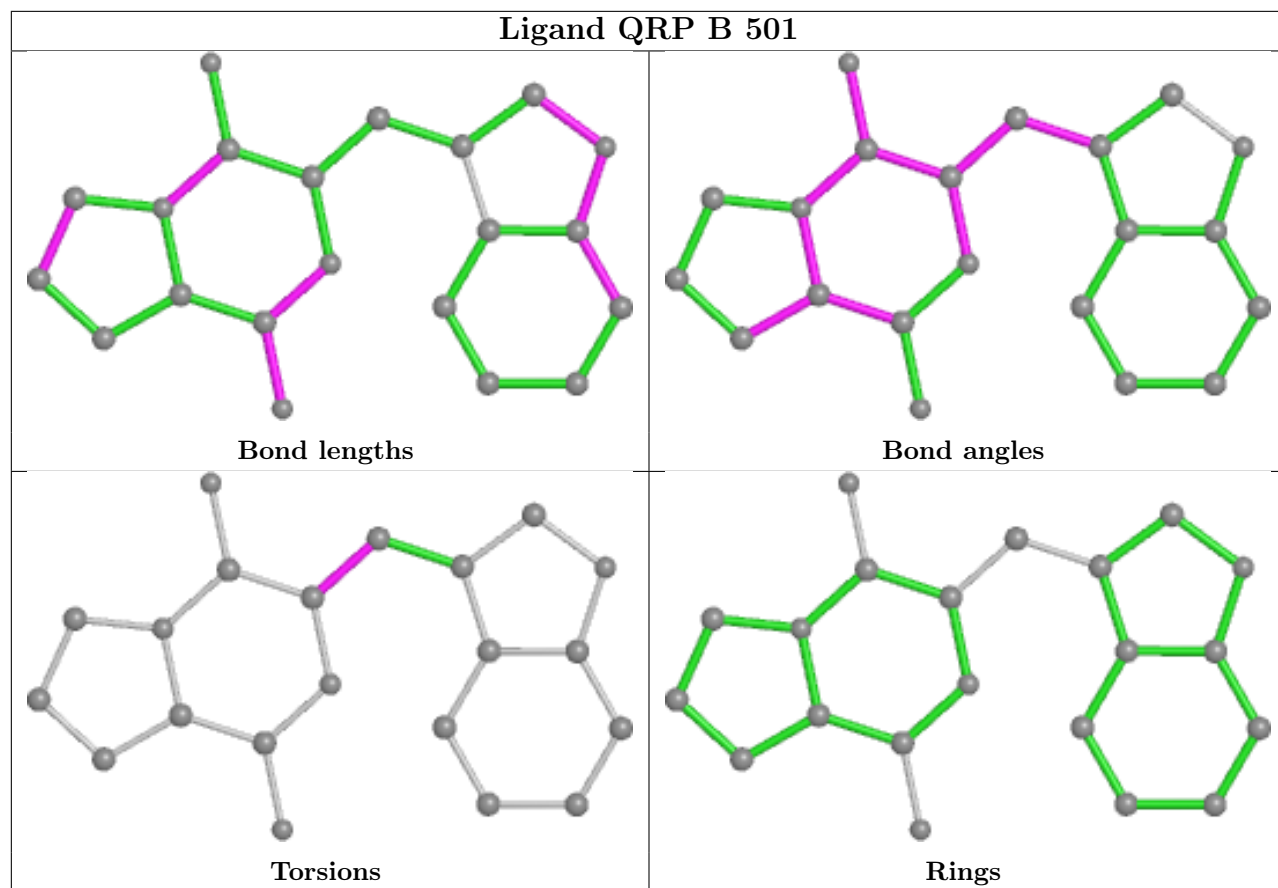


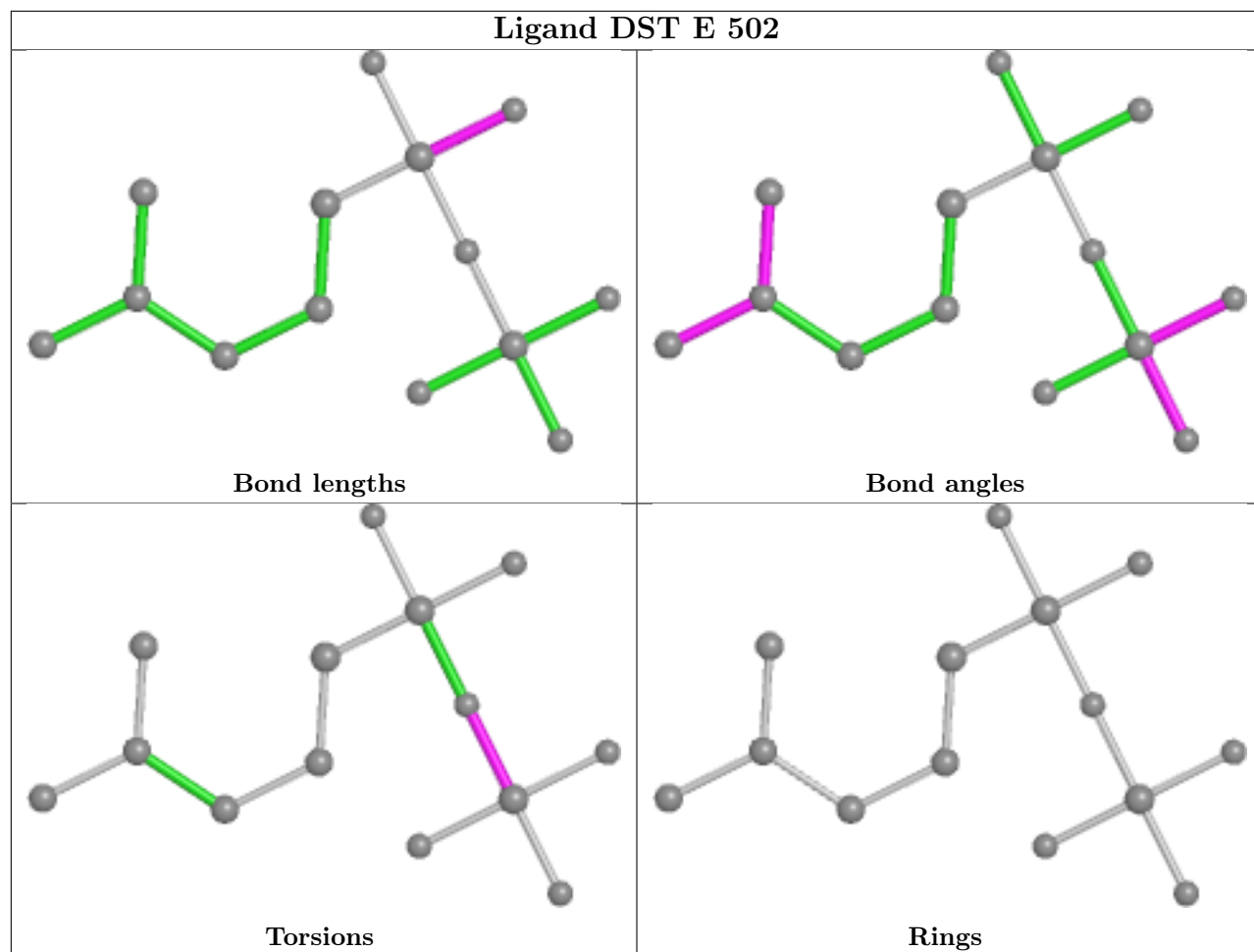


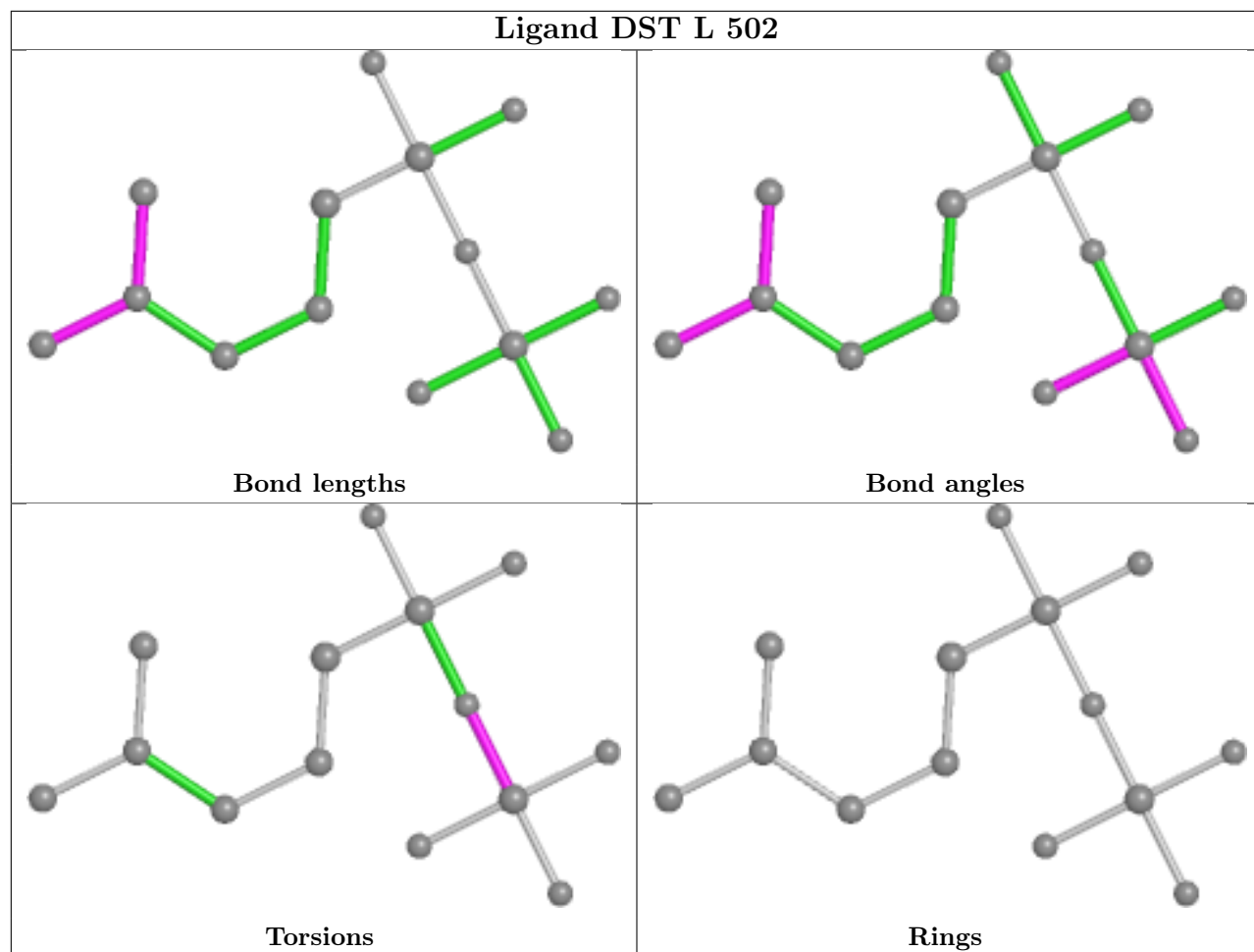


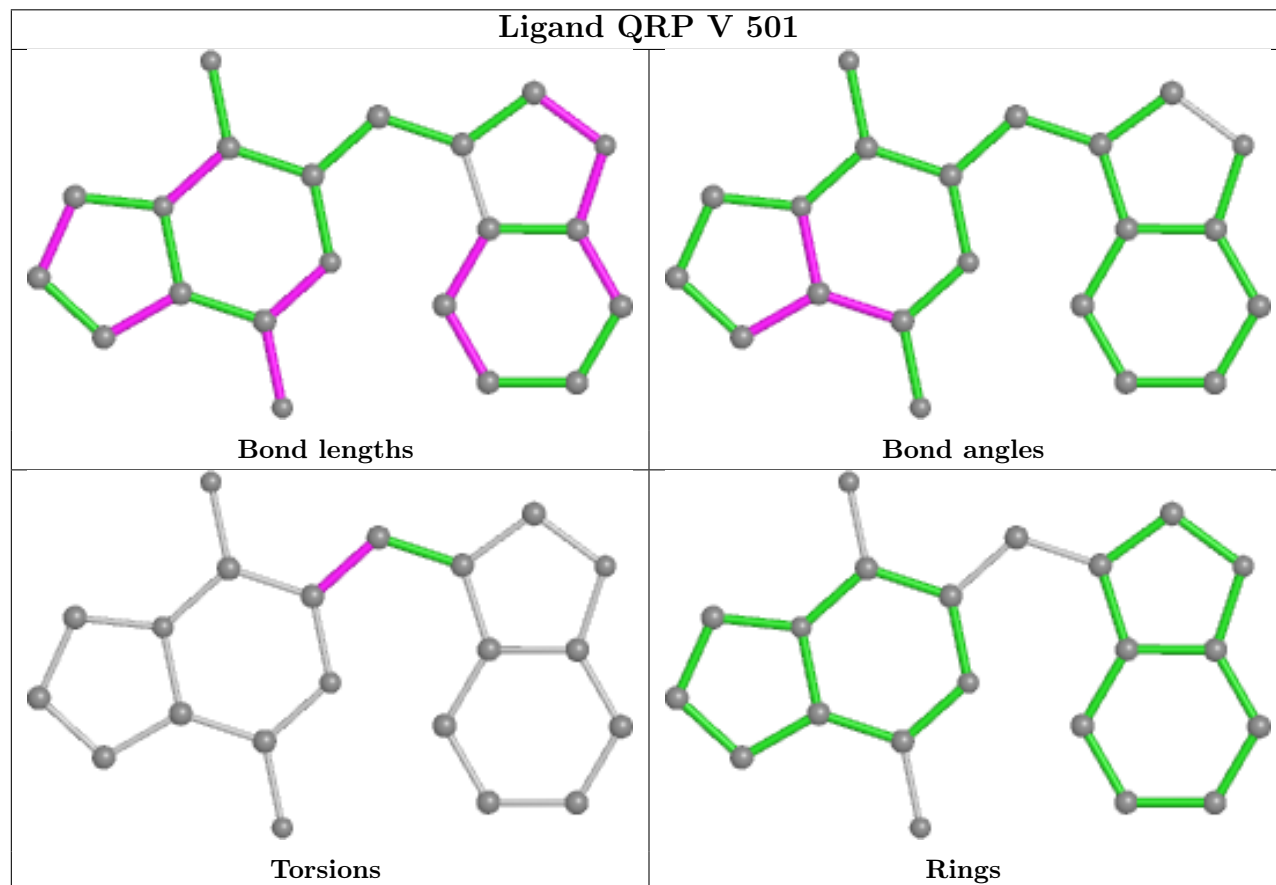
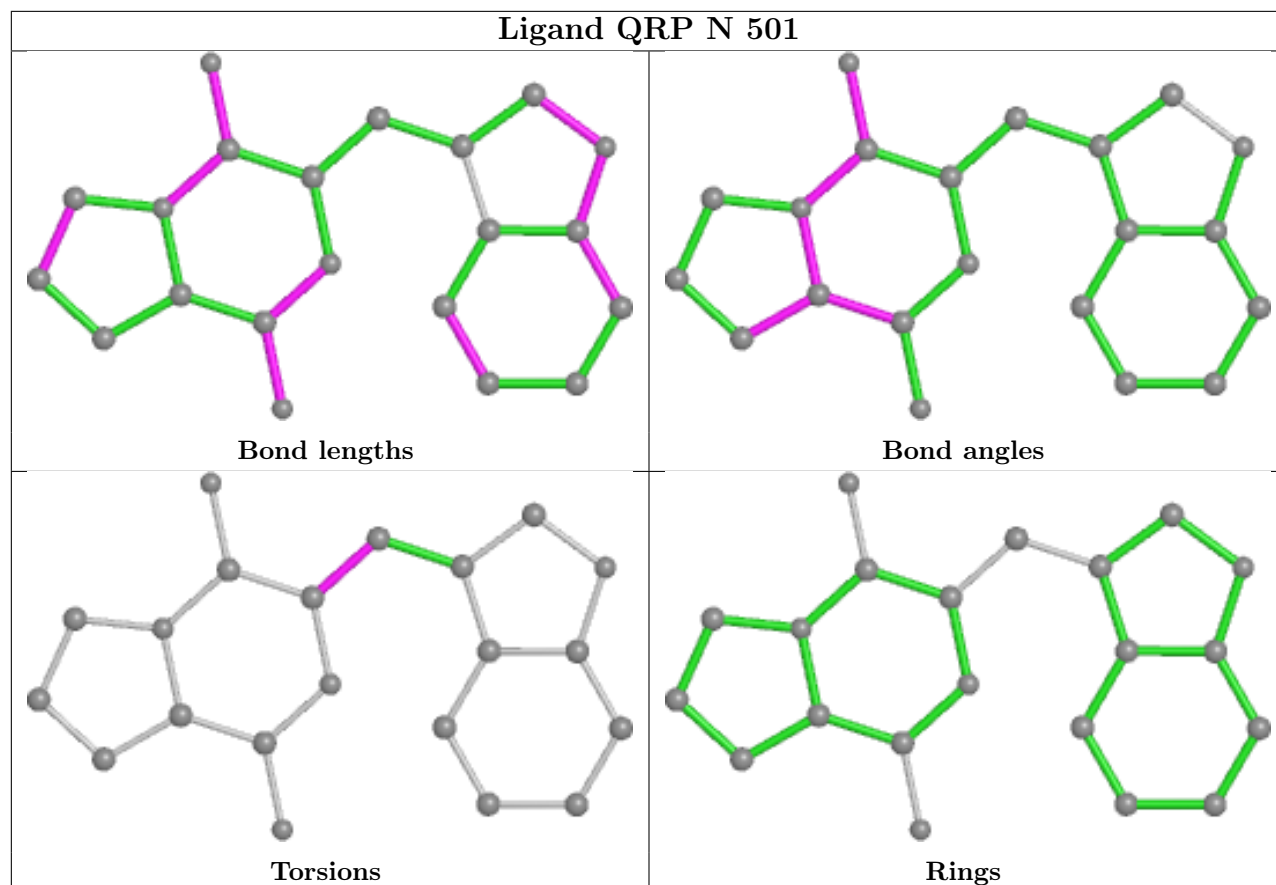


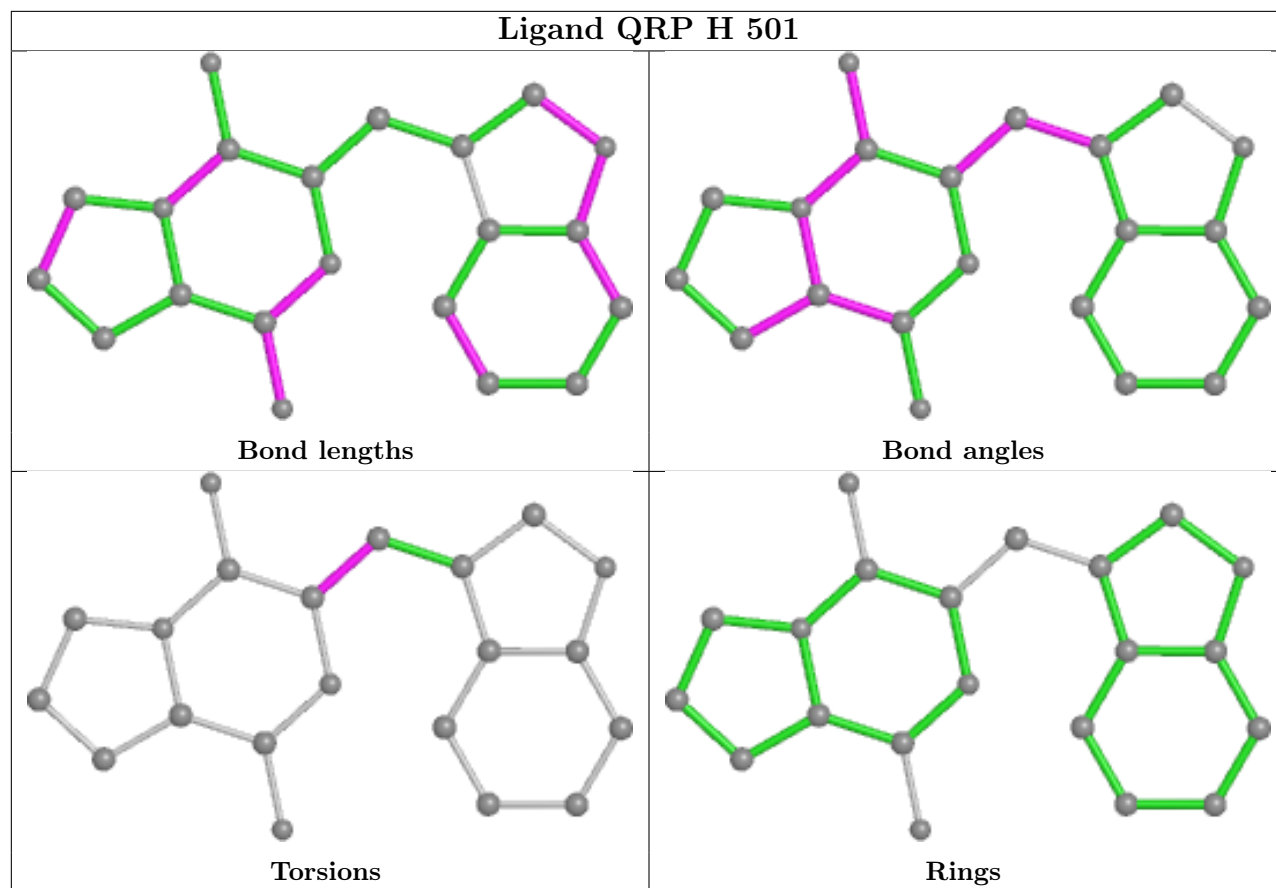


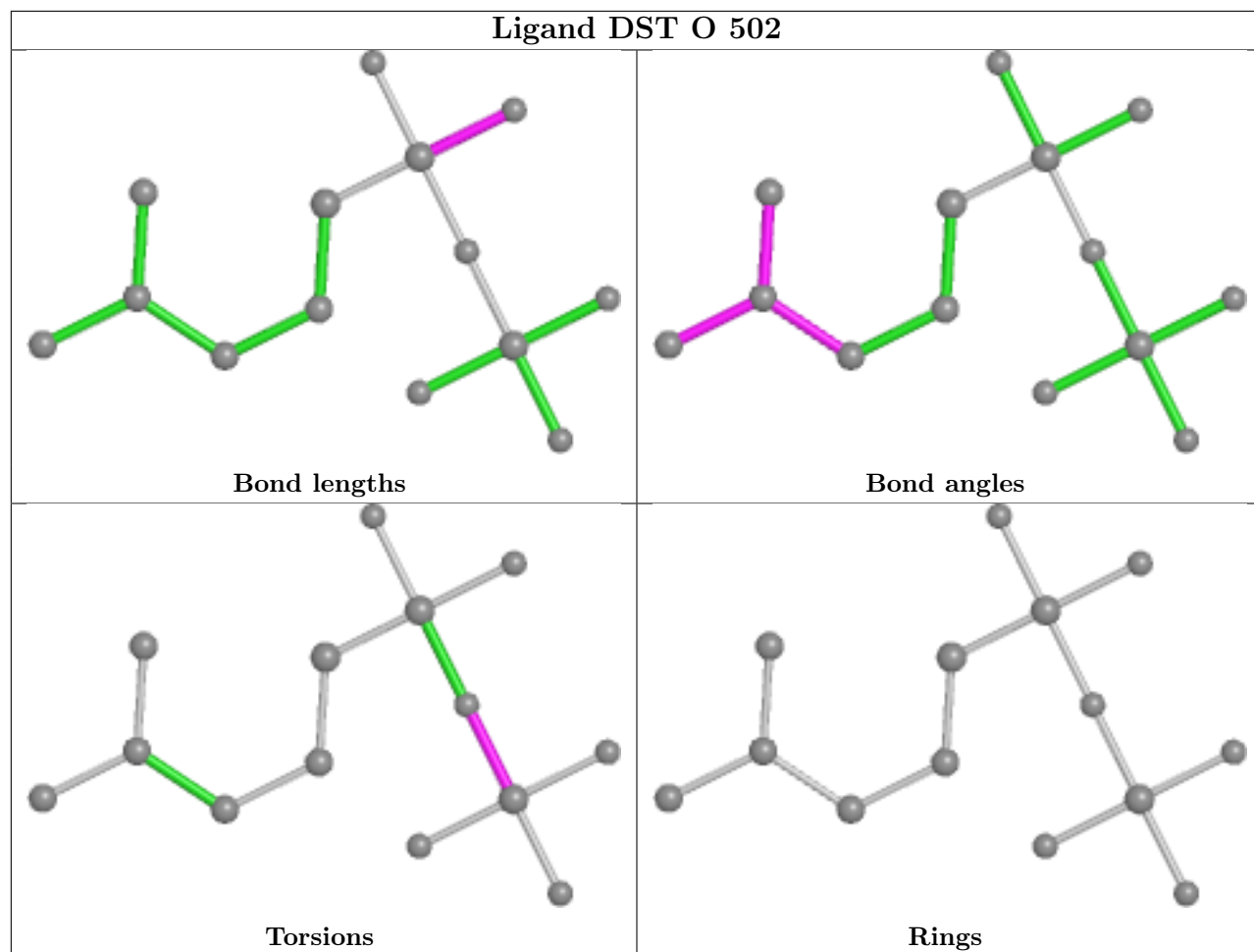


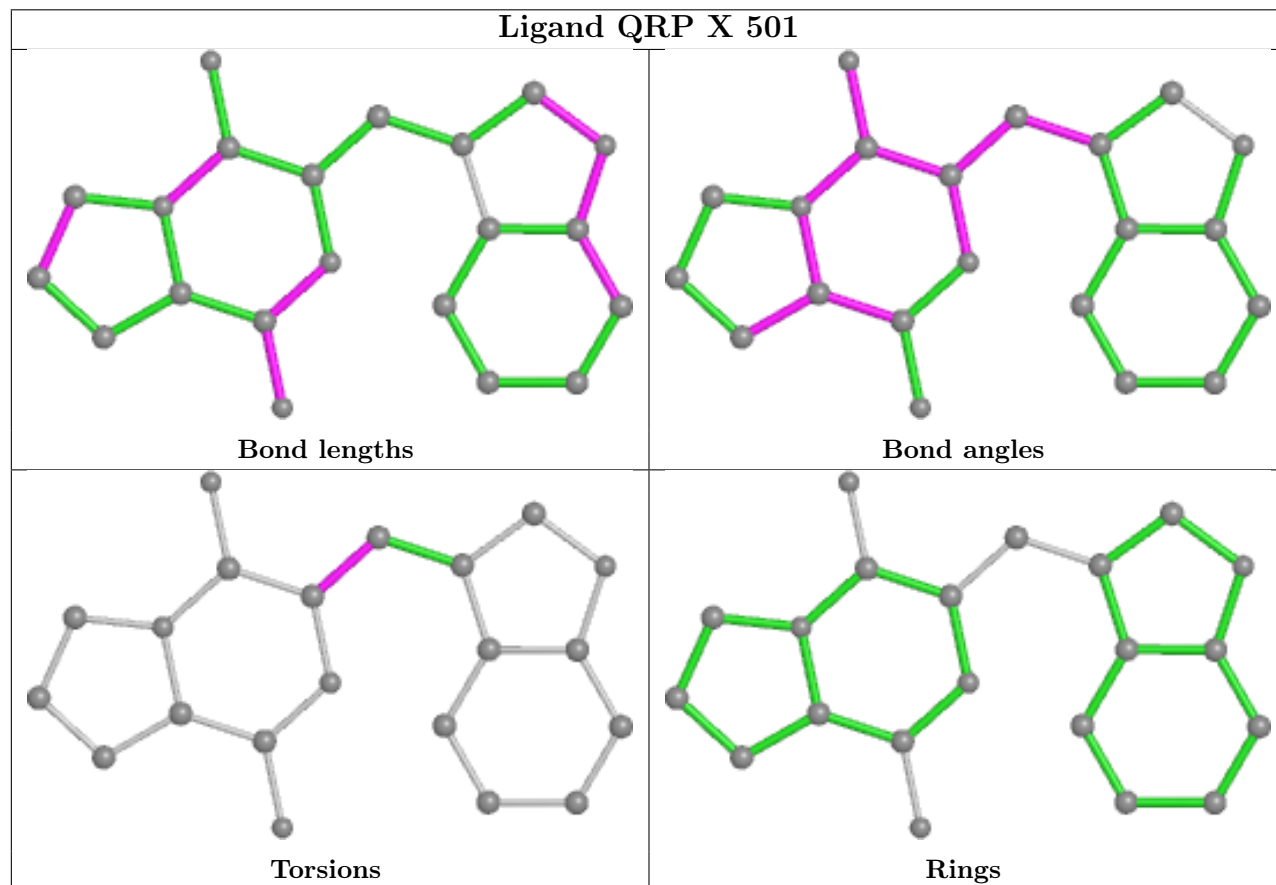
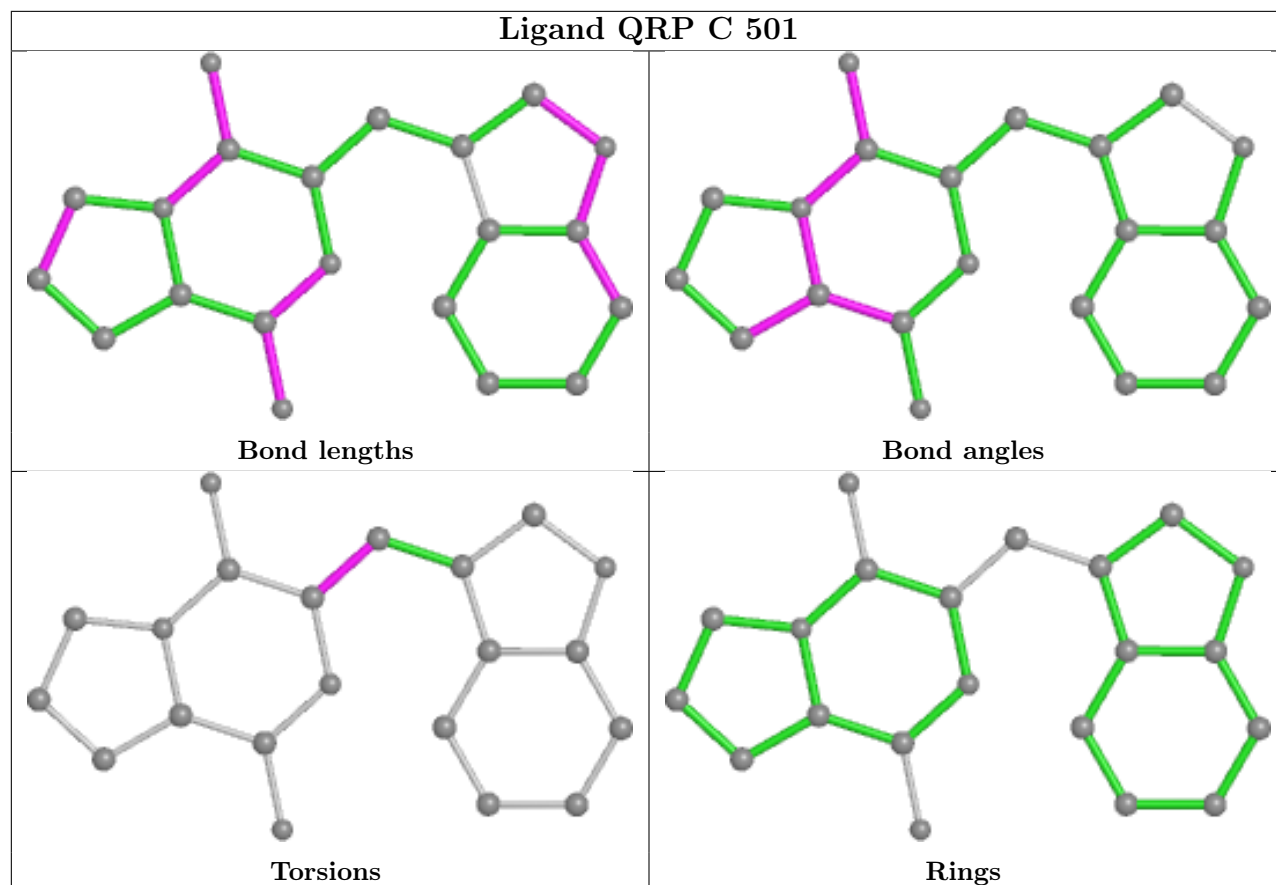


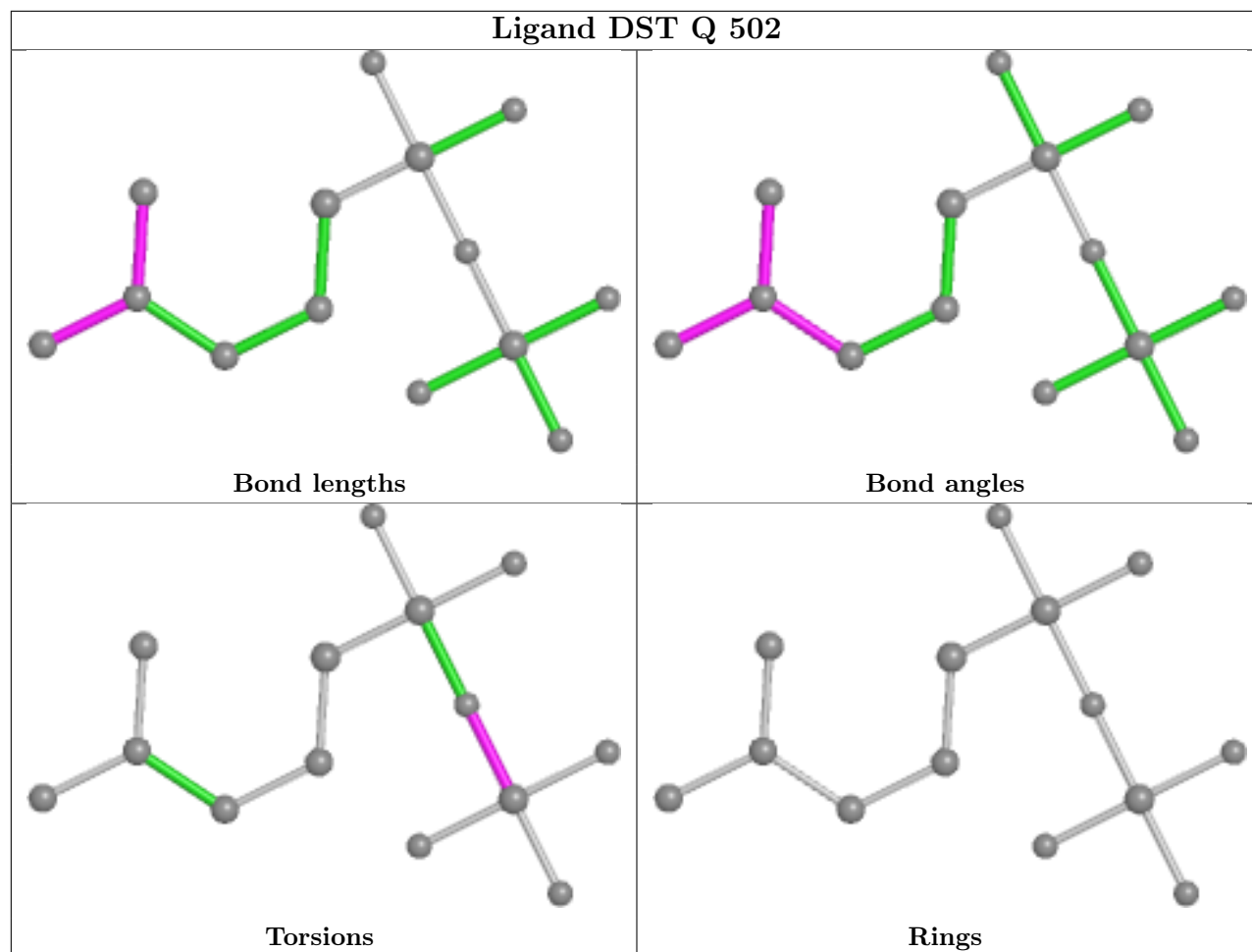


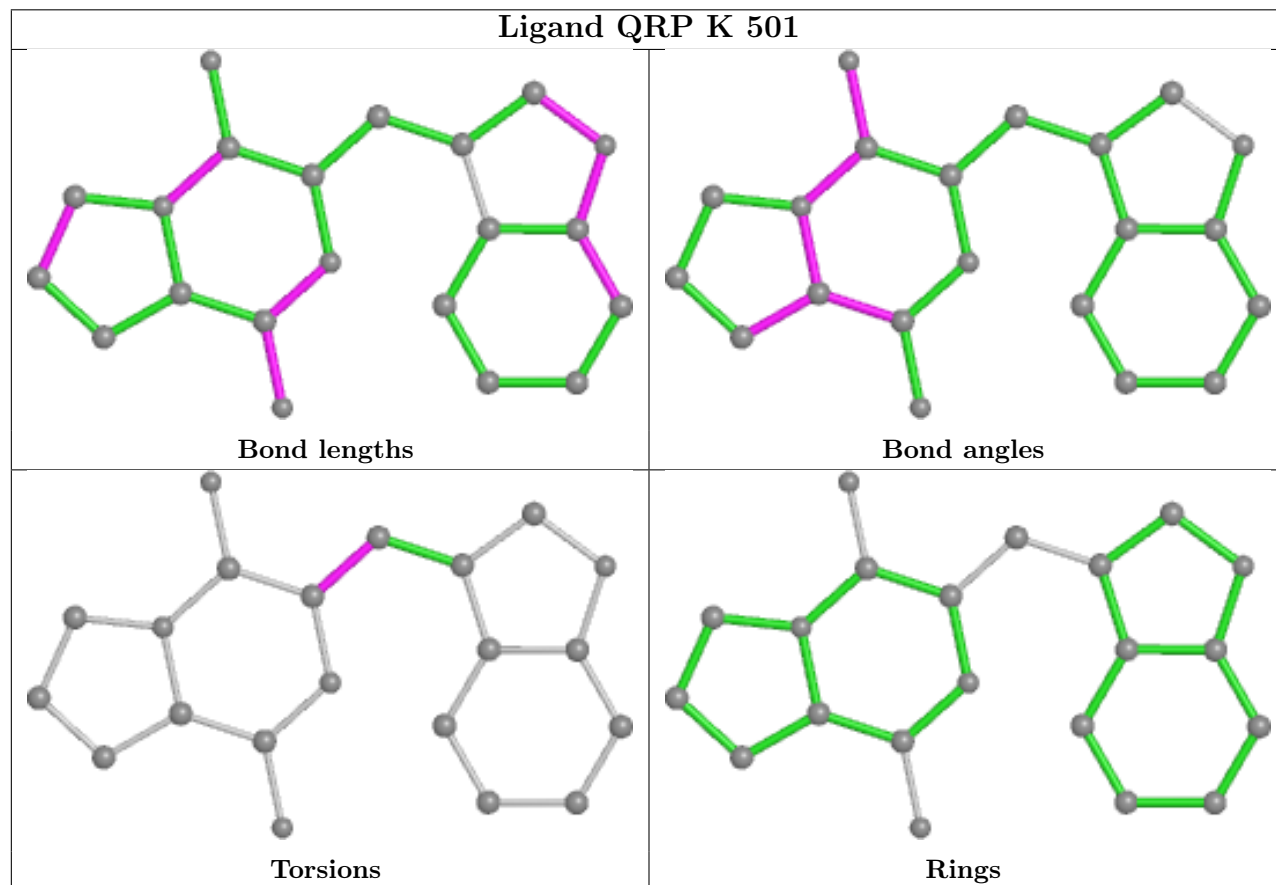
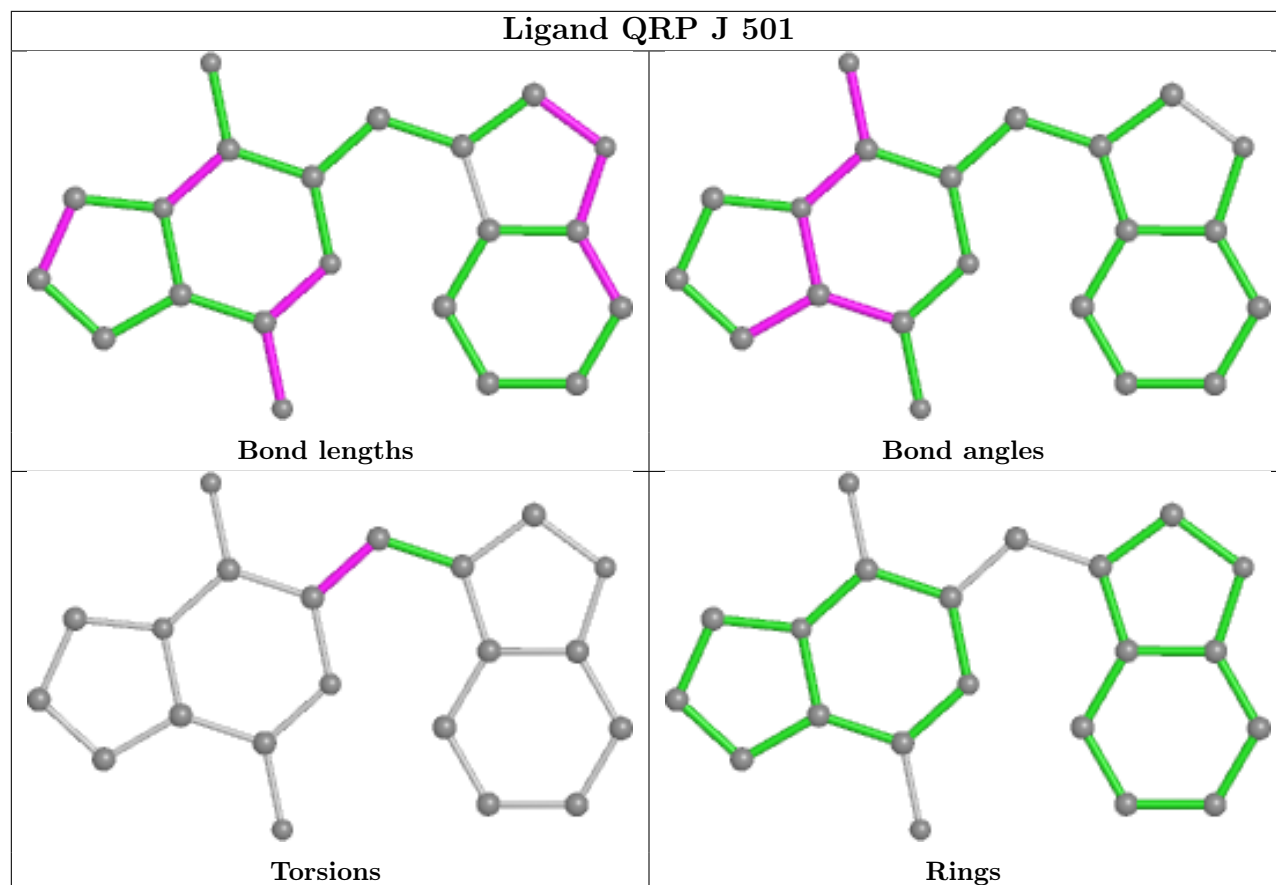


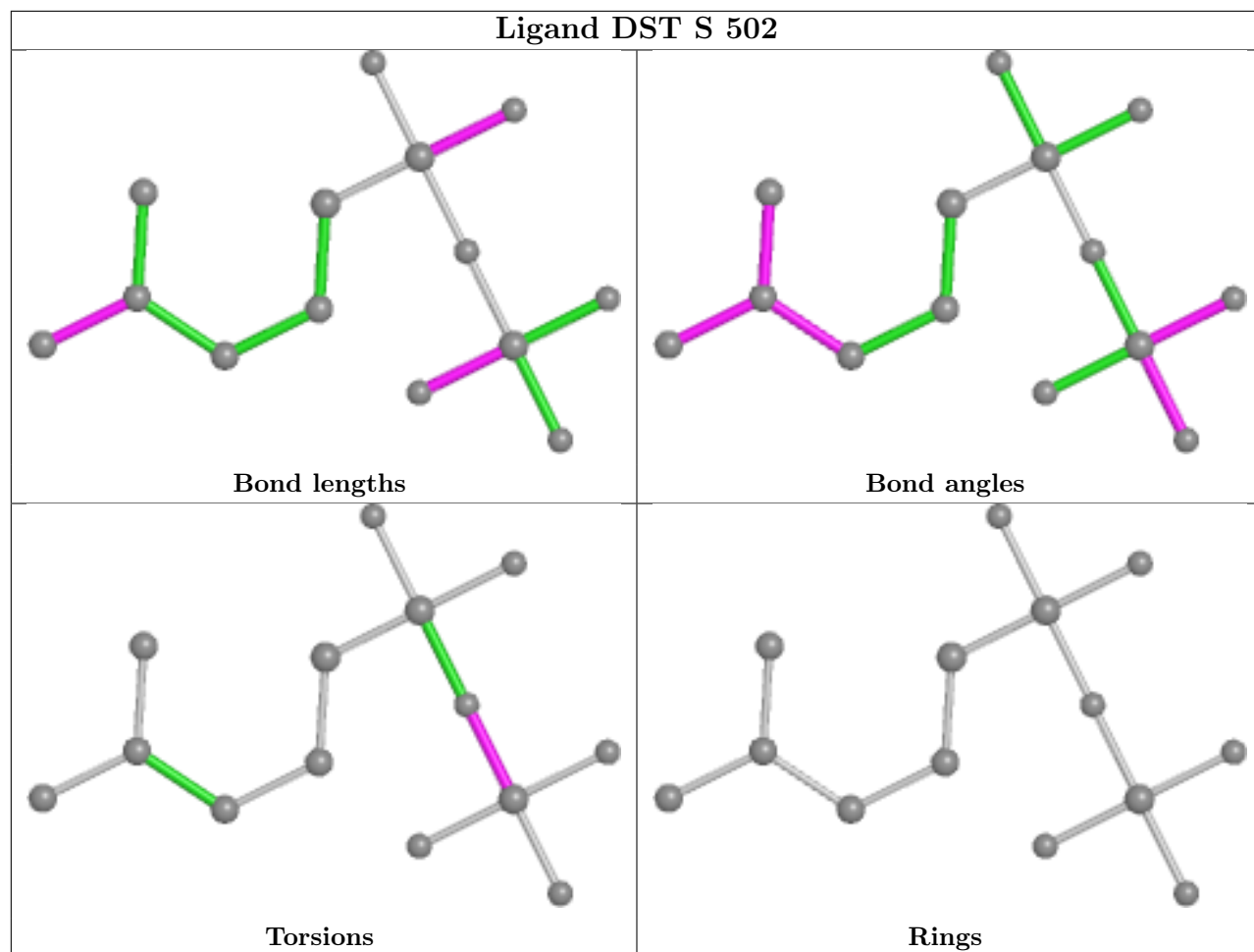


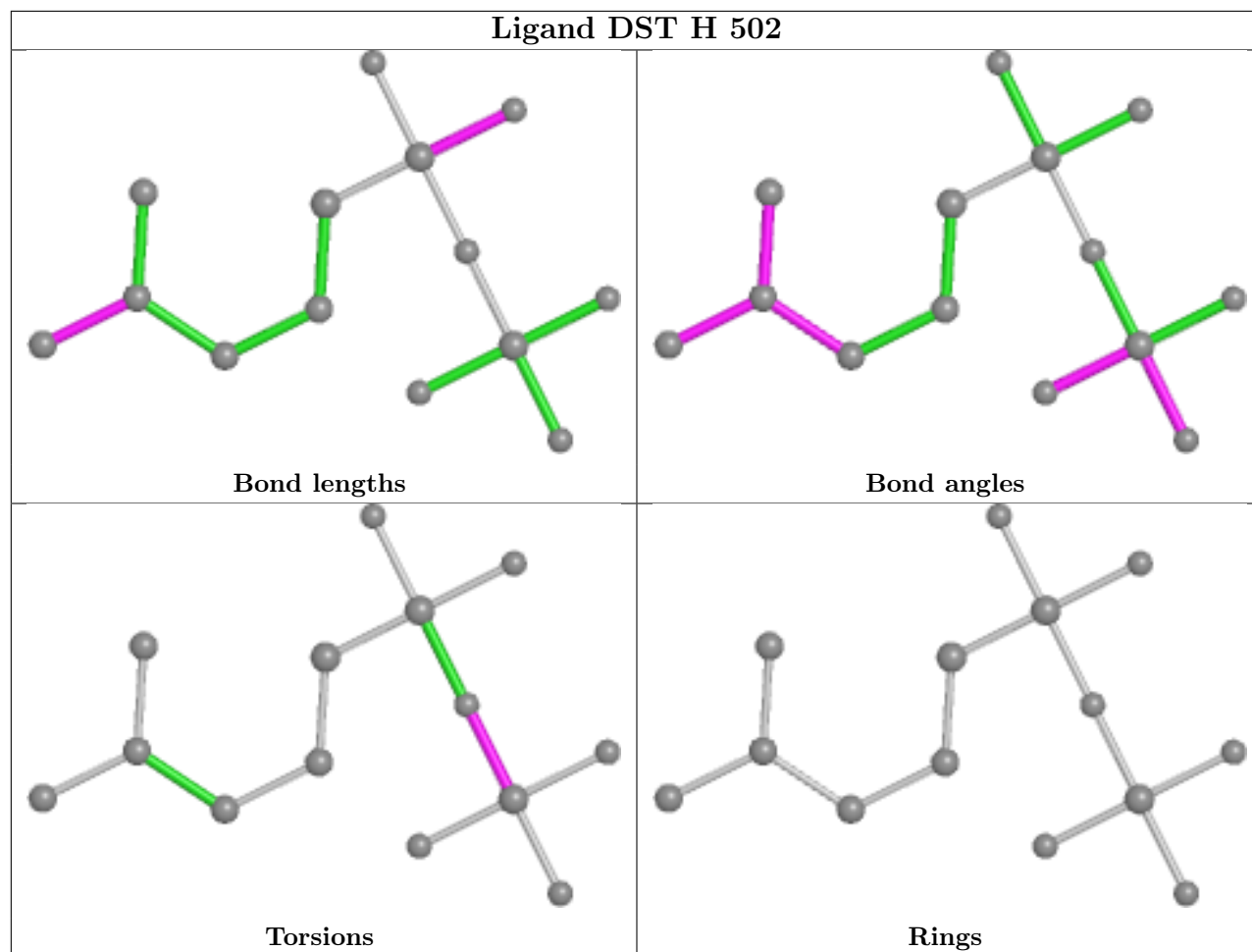












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	387/472 (81%)	-0.24	7 (1%) 68 40	67, 92, 152, 226	0
1	B	387/472 (81%)	-0.21	6 (1%) 72 44	70, 105, 156, 228	0
1	C	387/472 (81%)	-0.35	4 (1%) 82 59	67, 92, 152, 226	0
1	D	387/472 (81%)	-0.14	9 (2%) 60 31	68, 102, 158, 229	0
1	E	387/472 (81%)	-0.18	6 (1%) 72 44	69, 101, 158, 228	0
1	F	387/472 (81%)	-0.29	7 (1%) 68 40	69, 100, 157, 228	0
1	G	387/472 (81%)	-0.15	11 (2%) 53 25	66, 98, 154, 228	0
1	H	387/472 (81%)	-0.19	7 (1%) 68 40	66, 94, 154, 228	0
1	I	387/472 (81%)	-0.09	11 (2%) 53 25	78, 114, 158, 227	0
1	J	387/472 (81%)	-0.03	12 (3%) 49 21	81, 114, 160, 227	0
1	K	387/472 (81%)	-0.22	5 (1%) 77 51	74, 107, 159, 226	0
1	L	387/472 (81%)	-0.14	9 (2%) 60 31	76, 111, 158, 227	0
1	M	387/472 (81%)	-0.24	4 (1%) 82 59	67, 95, 155, 229	0
1	N	387/472 (81%)	-0.36	2 (0%) 91 75	69, 96, 155, 225	0
1	O	387/472 (81%)	-0.19	6 (1%) 72 44	71, 107, 156, 227	0
1	P	387/472 (81%)	-0.32	3 (0%) 86 65	67, 98, 154, 227	0
1	Q	387/472 (81%)	-0.16	6 (1%) 72 44	72, 106, 160, 228	0
1	R	387/472 (81%)	-0.13	10 (2%) 56 27	78, 114, 161, 227	0
1	S	387/472 (81%)	-0.07	9 (2%) 60 31	80, 117, 159, 228	0
1	T	387/472 (81%)	-0.24	6 (1%) 72 44	80, 112, 160, 229	0
1	U	387/472 (81%)	-0.16	9 (2%) 60 31	67, 99, 155, 230	0
1	V	387/472 (81%)	-0.37	2 (0%) 91 75	67, 94, 155, 226	0
1	W	387/472 (81%)	-0.04	15 (3%) 39 15	73, 110, 158, 226	0
1	X	387/472 (81%)	-0.31	8 (2%) 63 34	69, 103, 157, 228	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	9288/11328 (81%)	-0.20	174 (1%) 66 37	66, 105, 158, 230	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	PRO	14.8
1	A	351	SER	13.7
1	E	352	PRO	13.2
1	H	352	PRO	12.6
1	J	351	SER	12.3
1	J	352	PRO	12.3
1	W	351	SER	11.4
1	D	352	PRO	11.4
1	H	351	SER	9.6
1	W	349	ILE	9.6
1	L	351	SER	9.3
1	B	350	ALA	9.2
1	T	349	ILE	8.9
1	Q	351	SER	8.9
1	K	350	ALA	8.8
1	G	350	ALA	8.4
1	Q	352	PRO	8.2
1	W	350	ALA	8.2
1	L	352	PRO	8.2
1	E	351	SER	8.2
1	U	352	PRO	7.8
1	D	351	SER	7.5
1	M	352	PRO	7.5
1	L	349	ILE	7.4
1	M	349	ILE	6.8
1	X	349	ILE	6.6
1	S	349	ILE	6.5
1	H	350	ALA	6.4
1	H	349	ILE	6.1
1	E	242	GLU	6.0
1	O	349	ILE	5.8
1	J	242	GLU	5.7
1	W	32	PRO	5.7
1	C	350	ALA	5.5
1	D	243	ARG	5.3
1	D	350	ALA	5.3
1	I	349	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	349	ILE	4.9
1	K	352	PRO	4.8
1	B	351	SER	4.8
1	W	243	ARG	4.8
1	B	349	ILE	4.7
1	J	288	THR	4.6
1	K	351	SER	4.6
1	Q	350	ALA	4.5
1	F	350	ALA	4.5
1	Q	349	ILE	4.3
1	G	349	ILE	4.2
1	H	33	SER	4.2
1	C	351	SER	4.1
1	U	349	ILE	4.1
1	A	350	ALA	4.0
1	F	240	ASP	4.0
1	B	327	ILE	3.9
1	S	412	ASP	3.9
1	E	350	ALA	3.9
1	O	32	PRO	3.8
1	L	240	ASP	3.8
1	D	349	ILE	3.8
1	L	350	ALA	3.8
1	R	33	SER	3.8
1	W	242	GLU	3.8
1	P	240	ASP	3.7
1	J	350	ALA	3.7
1	D	242	GLU	3.7
1	G	352	PRO	3.7
1	J	243	ARG	3.7
1	J	240	ASP	3.7
1	W	412	ASP	3.6
1	F	351	SER	3.5
1	E	243	ARG	3.5
1	O	351	SER	3.5
1	I	92	TYR	3.4
1	A	327	ILE	3.3
1	R	361	PRO	3.3
1	L	118	HIS	3.3
1	P	349	ILE	3.3
1	T	350	ALA	3.3
1	U	350	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	398	HIS	3.2
1	W	447	TYR	3.2
1	B	352	PRO	3.2
1	M	351	SER	3.1
1	L	33	SER	3.1
1	N	349	ILE	3.1
1	R	349	ILE	3.1
1	G	363	SER	3.1
1	U	240	ASP	3.1
1	X	240	ASP	3.1
1	D	118	HIS	3.1
1	W	33	SER	3.0
1	F	243	ARG	3.0
1	S	243	ARG	2.9
1	K	243	ARG	2.9
1	U	327	ILE	2.9
1	U	351	SER	2.8
1	M	350	ALA	2.8
1	H	327	ILE	2.8
1	W	417	GLN	2.8
1	W	400	CYS	2.8
1	X	350	ALA	2.7
1	V	242	GLU	2.7
1	D	240	ASP	2.7
1	T	242	GLU	2.7
1	I	352	PRO	2.6
1	J	414	ASP	2.6
1	O	243	ARG	2.6
1	V	349	ILE	2.6
1	T	33	SER	2.6
1	T	240	ASP	2.6
1	S	32	PRO	2.6
1	C	352	PRO	2.6
1	X	327	ILE	2.6
1	I	245	GLN	2.6
1	I	180	GLN	2.6
1	A	33	SER	2.5
1	U	397	GLU	2.5
1	X	32	PRO	2.5
1	I	243	ARG	2.5
1	F	288	THR	2.5
1	H	240	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	S	33	SER	2.5
1	D	400	CYS	2.5
1	W	240	ASP	2.5
1	S	443	SER	2.5
1	R	242	GLU	2.5
1	S	414	ASP	2.4
1	I	361	PRO	2.4
1	I	327	ILE	2.4
1	W	352	PRO	2.4
1	J	412	ASP	2.4
1	I	350	ALA	2.4
1	S	351	SER	2.4
1	G	245	GLN	2.4
1	U	412	ASP	2.3
1	G	243	ARG	2.3
1	R	436	TYR	2.3
1	P	364	ARG	2.3
1	W	404	ASP	2.3
1	I	360	HIS	2.3
1	J	305	LEU	2.2
1	R	32	PRO	2.2
1	J	289	GLU	2.2
1	E	117	SER	2.2
1	W	250	PHE	2.2
1	R	448	LEU	2.2
1	G	327	ILE	2.2
1	G	361	PRO	2.2
1	C	243	ARG	2.2
1	G	351	SER	2.2
1	X	33	SER	2.2
1	F	180	GLN	2.2
1	S	364	ARG	2.2
1	X	242	GLU	2.2
1	T	414	ASP	2.2
1	I	364	ARG	2.2
1	F	196	GLN	2.2
1	A	399	ALA	2.1
1	U	33	SER	2.1
1	G	362	GLY	2.1
1	R	433	ARG	2.1
1	K	349	ILE	2.1
1	L	117	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	412	ASP	2.1
1	L	399	ALA	2.1
1	X	304	ARG	2.1
1	Q	230	THR	2.1
1	G	364	ARG	2.1
1	J	417	GLN	2.1
1	R	240	ASP	2.1
1	Q	436	TYR	2.0
1	O	350	ALA	2.0
1	N	240	ASP	2.0
1	R	397	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DST	B	502	14/14	0.79	0.44	125,150,163,166	0
3	DST	I	502	14/14	0.80	0.27	117,142,166,166	0
3	DST	G	502	14/14	0.81	0.29	110,139,155,175	0
2	QRP	F	501	21/21	0.82	0.36	90,124,157,164	0
3	DST	C	502	14/14	0.84	0.25	89,130,149,168	0
2	QRP	L	501	21/21	0.84	0.34	105,130,167,168	0
3	DST	T	502	14/14	0.84	0.27	122,147,176,178	0
3	DST	W	502	14/14	0.84	0.32	116,145,156,172	0
2	QRP	C	501	21/21	0.85	0.35	86,117,143,151	0
2	QRP	B	501	21/21	0.85	0.51	107,145,180,182	0
3	DST	F	502	14/14	0.86	0.26	106,143,159,182	0
2	QRP	Q	501	21/21	0.86	0.25	101,126,157,163	0

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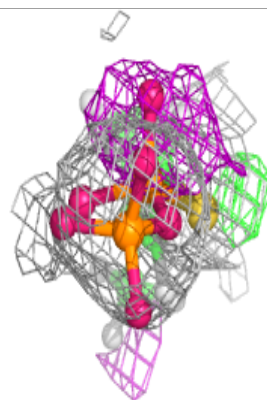
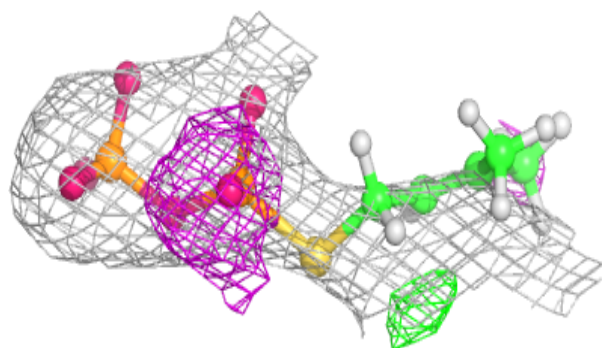
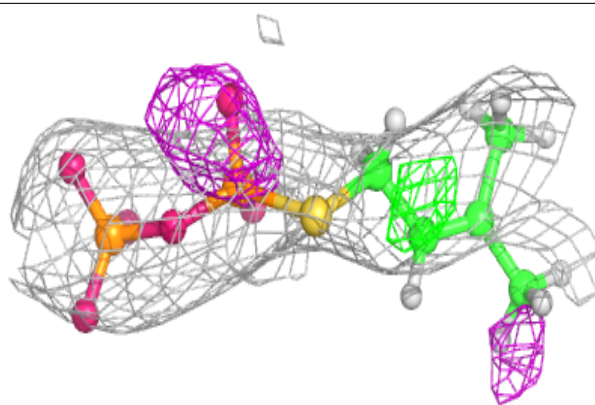
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	QRP	N	501	21/21	0.87	0.34	88,113,142,145	0
2	QRP	E	501	21/21	0.87	0.38	88,113,141,157	0
2	QRP	S	501	21/21	0.87	0.37	101,130,163,170	0
3	DST	L	502	14/14	0.87	0.20	115,139,159,169	0
2	QRP	J	501	21/21	0.87	0.45	106,134,159,168	0
2	QRP	D	501	21/21	0.87	0.39	86,120,147,150	0
2	QRP	K	501	21/21	0.88	0.42	103,134,169,172	0
2	QRP	R	501	21/21	0.88	0.28	88,124,148,163	0
2	QRP	H	501	21/21	0.88	0.29	93,115,147,147	0
3	DST	J	502	14/14	0.88	0.31	101,145,174,175	0
3	DST	K	502	14/14	0.88	0.31	125,152,174,182	0
2	QRP	G	501	21/21	0.88	0.36	109,131,156,169	0
3	DST	R	502	14/14	0.88	0.22	123,148,158,175	0
3	DST	S	502	14/14	0.88	0.24	107,137,163,188	0
3	DST	A	502	14/14	0.88	0.22	103,124,153,153	0
2	QRP	P	501	21/21	0.88	0.22	87,112,141,141	0
3	DST	X	502	14/14	0.88	0.19	91,123,171,171	0
2	QRP	U	501	21/21	0.89	0.25	88,118,158,160	0
3	DST	O	502	14/14	0.89	0.31	106,133,157,159	0
2	QRP	W	501	21/21	0.89	0.32	103,130,161,167	0
3	DST	H	502	14/14	0.89	0.20	85,125,134,155	0
2	QRP	M	501	21/21	0.89	0.24	97,118,153,155	0
3	DST	U	502	14/14	0.89	0.28	98,121,141,151	0
2	QRP	V	501	21/21	0.89	0.24	88,110,132,141	0
2	QRP	A	501	21/21	0.89	0.27	92,113,141,145	0
3	DST	V	502	14/14	0.90	0.23	96,126,148,152	0
3	DST	P	502	14/14	0.90	0.19	93,124,151,151	0
2	QRP	I	501	21/21	0.90	0.36	108,134,166,174	0
2	QRP	T	501	21/21	0.90	0.21	108,130,159,164	0
3	DST	N	502	14/14	0.91	0.19	96,125,140,163	0
3	DST	D	502	14/14	0.91	0.25	107,129,166,166	0
3	DST	M	502	14/14	0.91	0.24	93,121,143,164	0
3	DST	E	502	14/14	0.92	0.23	98,122,161,161	0
3	DST	Q	502	14/14	0.92	0.25	106,144,159,160	0
2	QRP	O	501	21/21	0.93	0.23	86,123,150,157	0
2	QRP	X	501	21/21	0.94	0.21	99,117,139,142	0

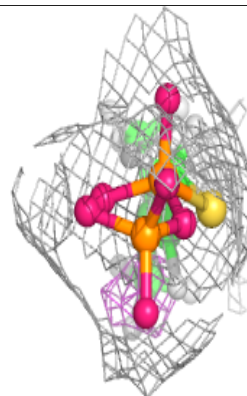
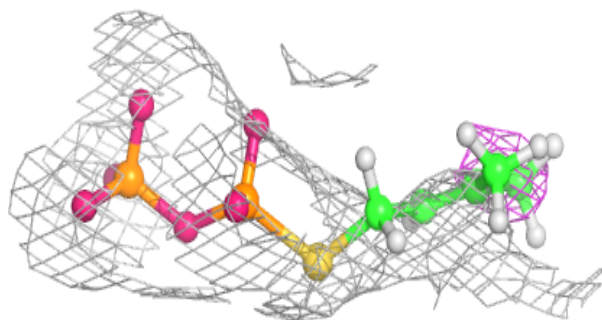
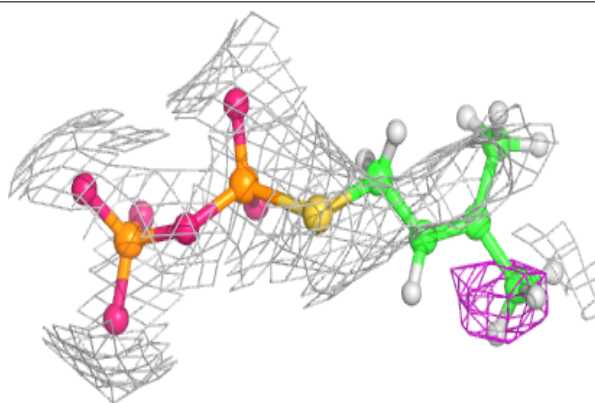
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DST B 502:

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

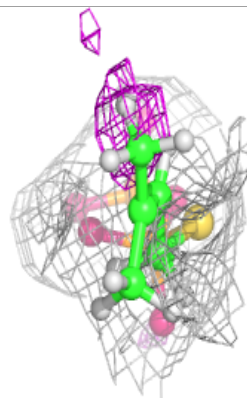
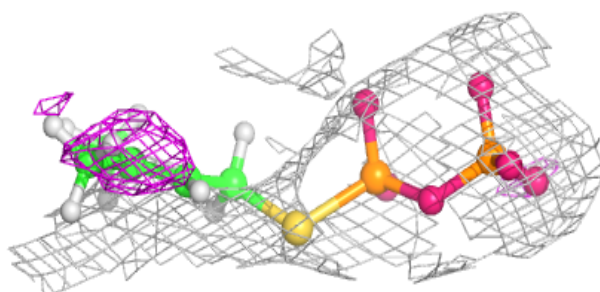
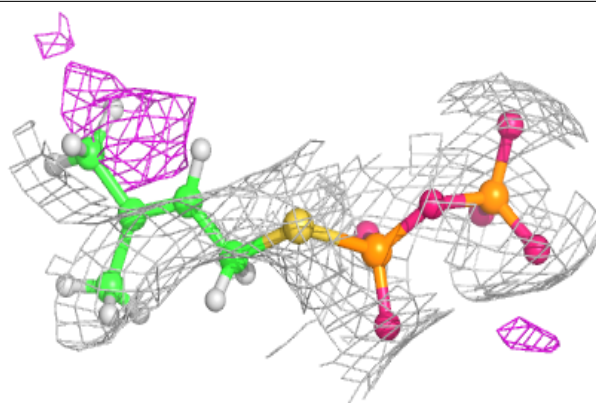
**Electron density around DST I 502:**

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

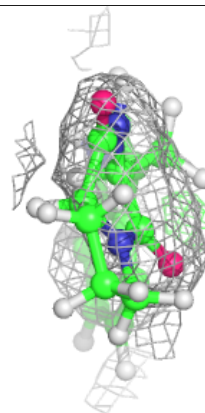
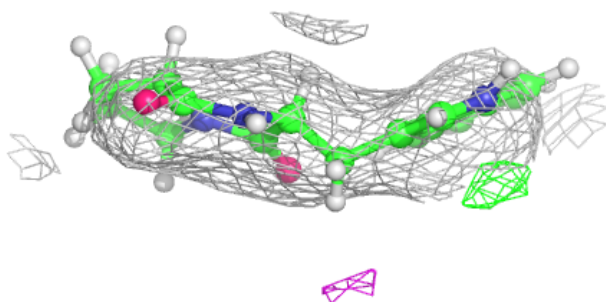
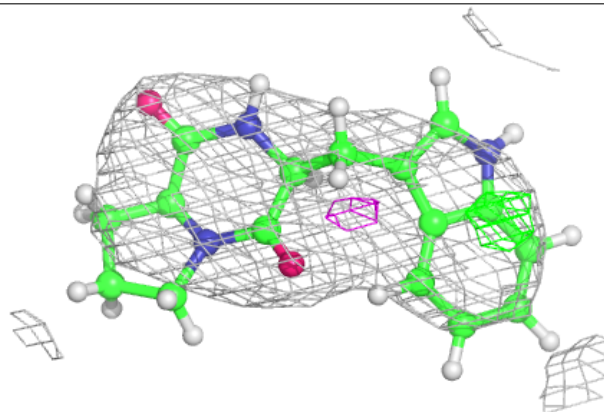


Electron density around DST G 502:

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

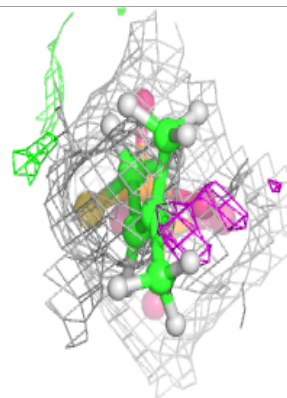
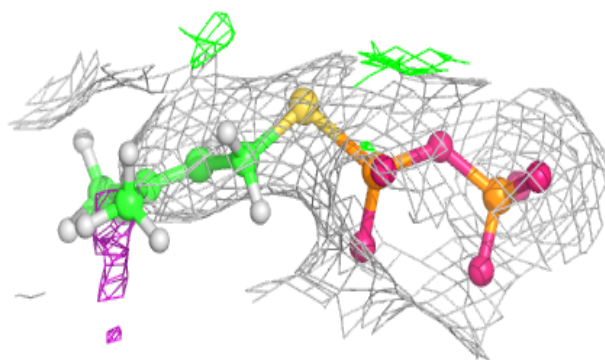
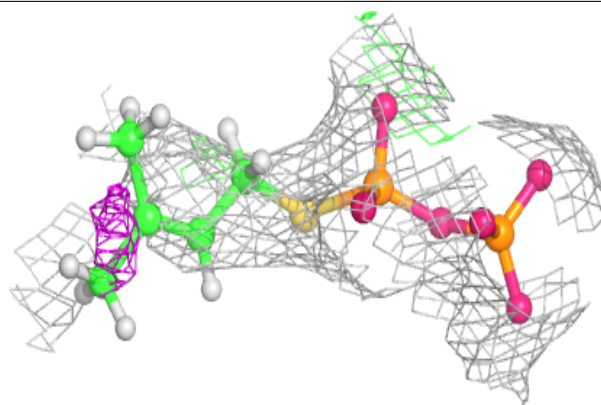
**Electron density around QRP F 501:**

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

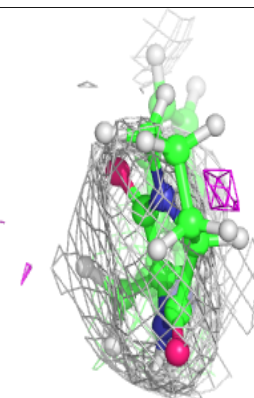
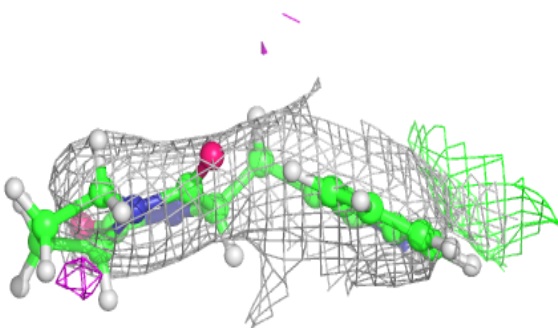
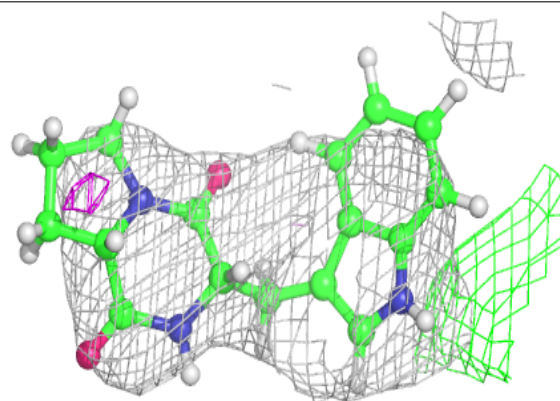


Electron density around DST C 502:

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

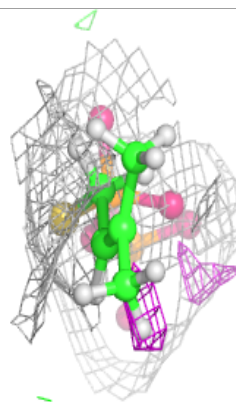
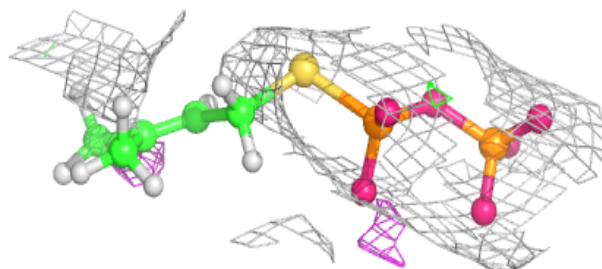
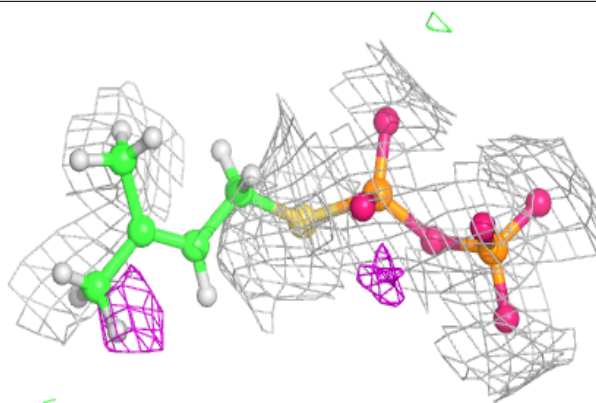
**Electron density around QRP L 501:**

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

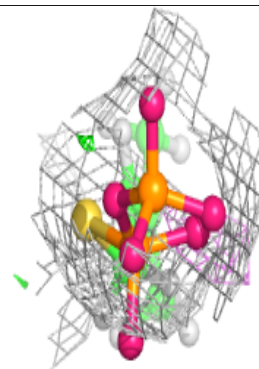
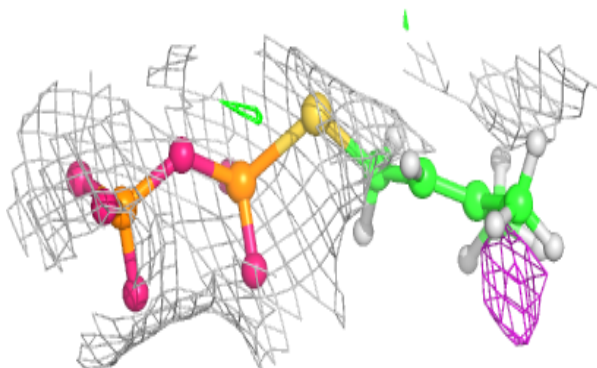
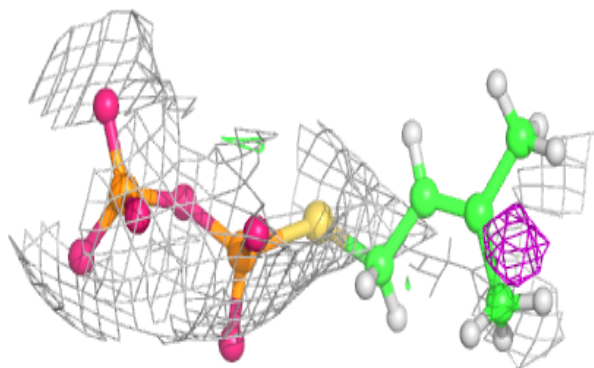


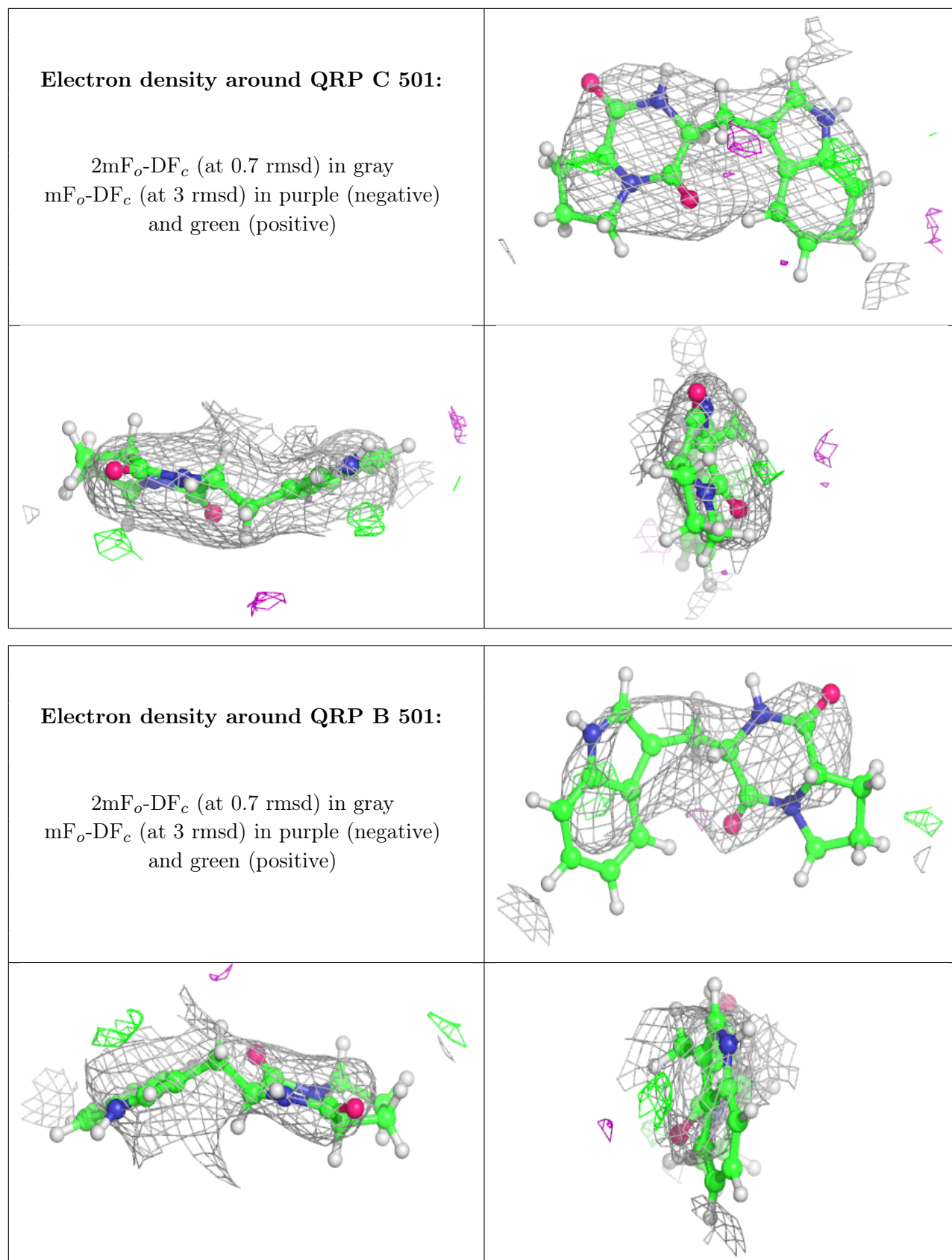
Electron density around DST T 502:

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

**Electron density around DST W 502:**

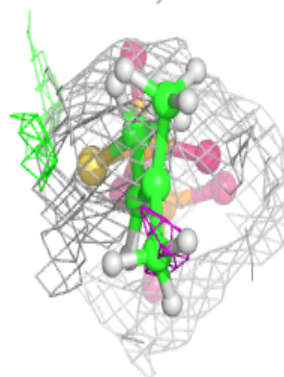
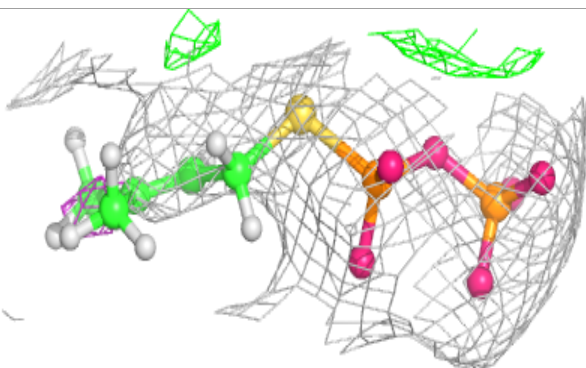
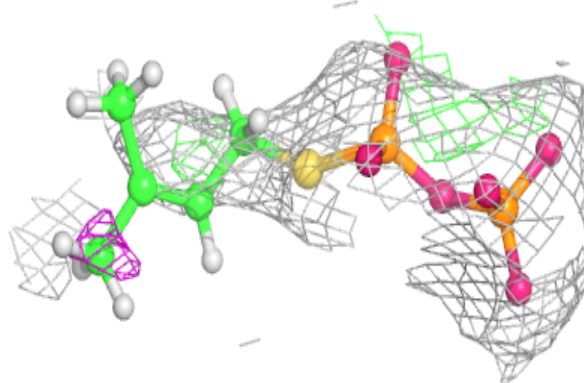
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



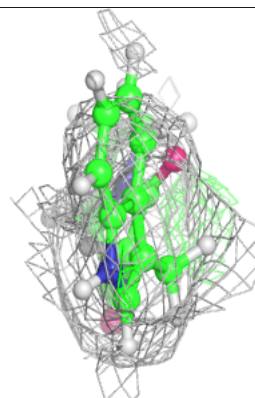
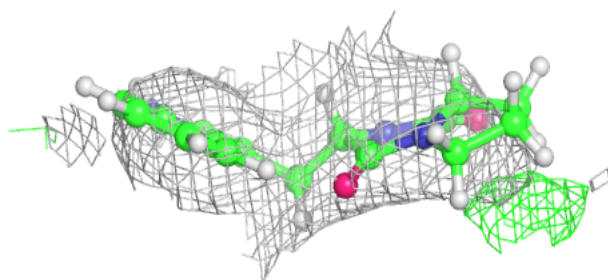
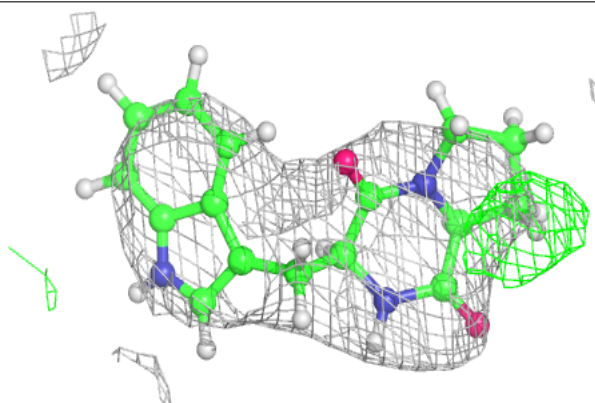


Electron density around DST F 502:

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

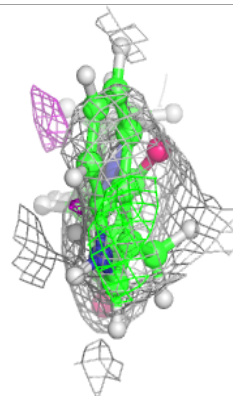
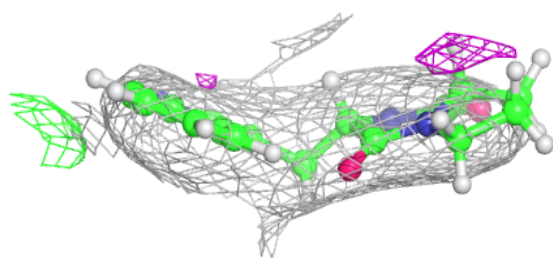
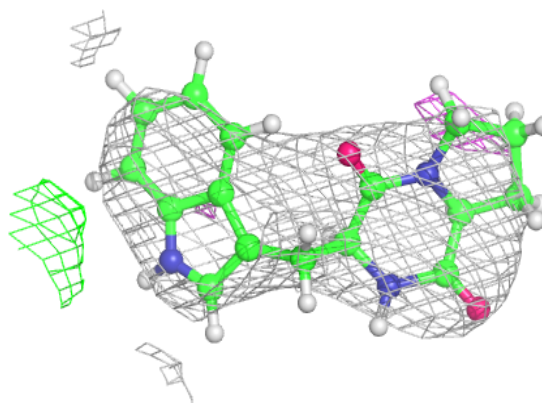
**Electron density around QRP Q 501:**

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

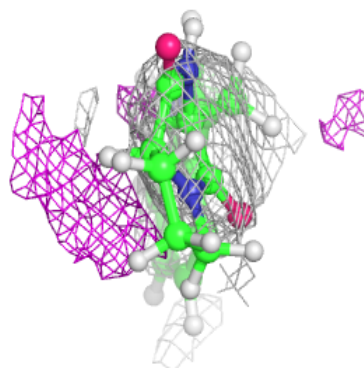
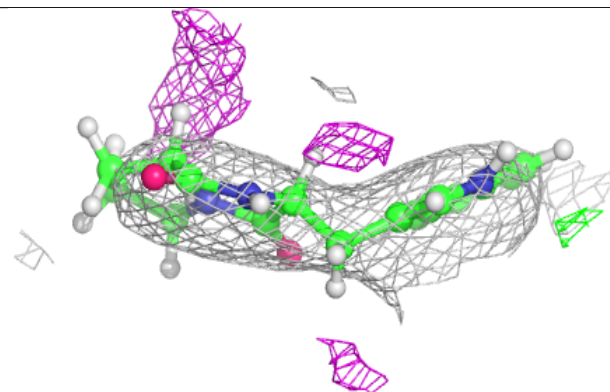
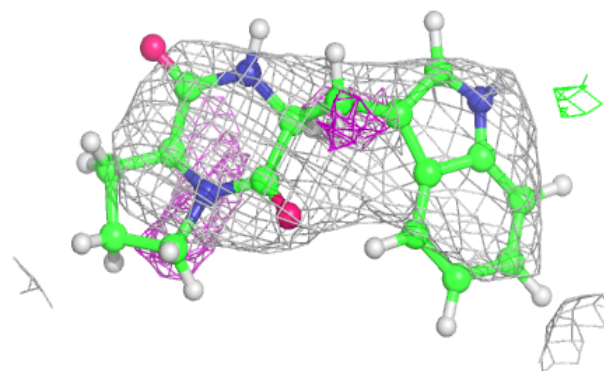


Electron density around QRP N 501:

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

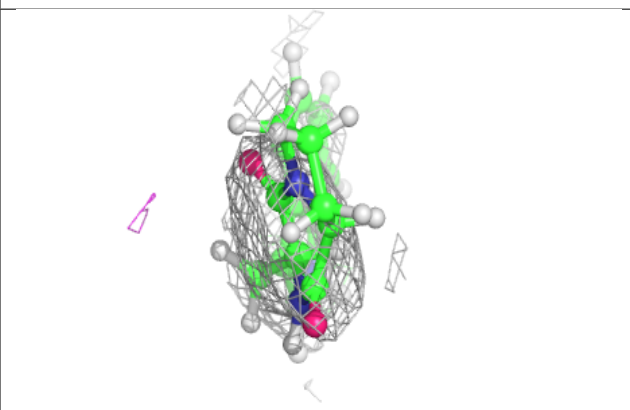
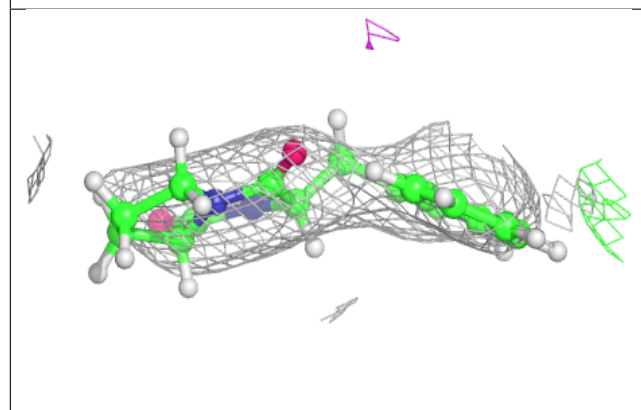
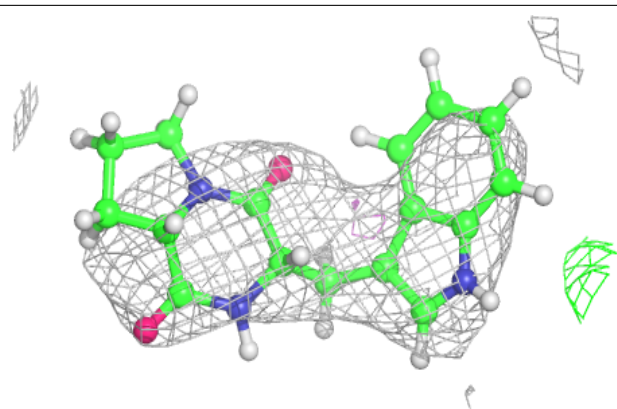
**Electron density around QRP E 501:**

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

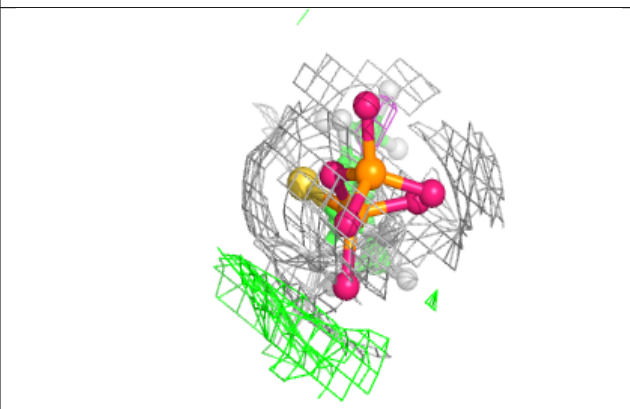
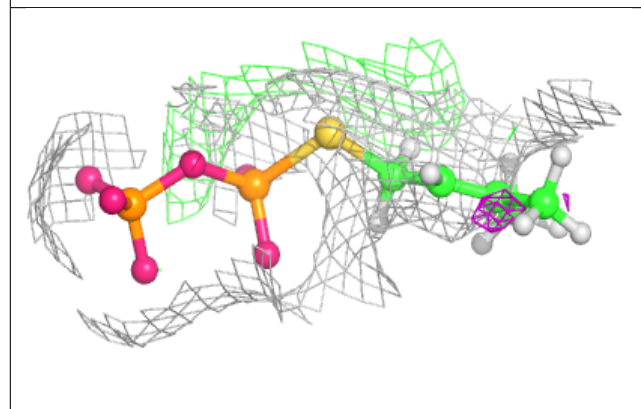
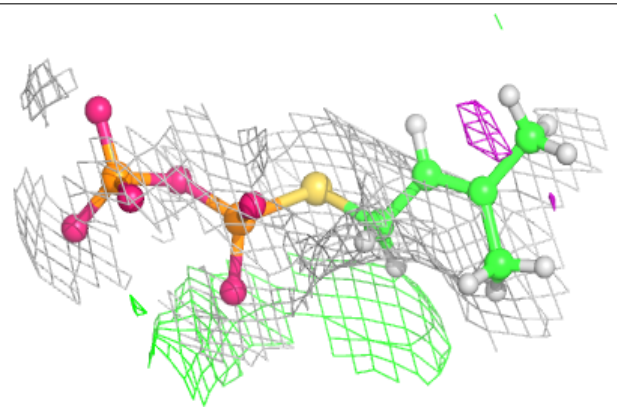


Electron density around QRP S 501:

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

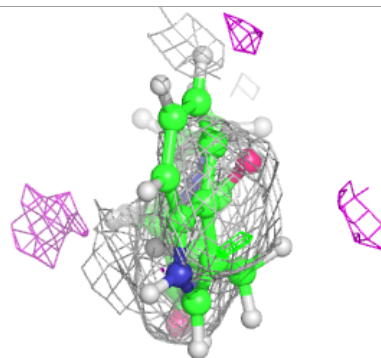
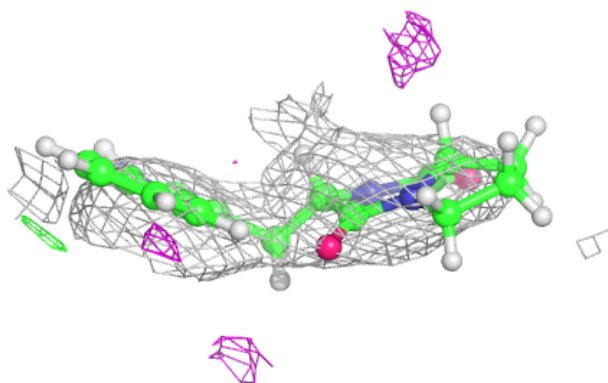
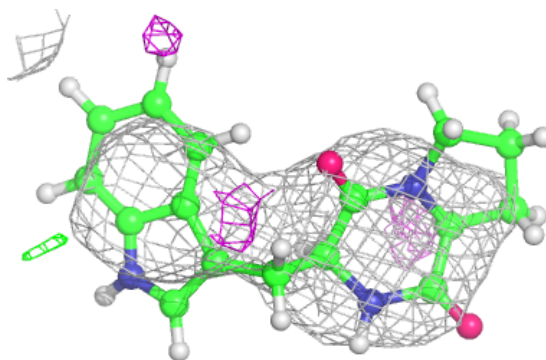
**Electron density around DST L 502:**

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

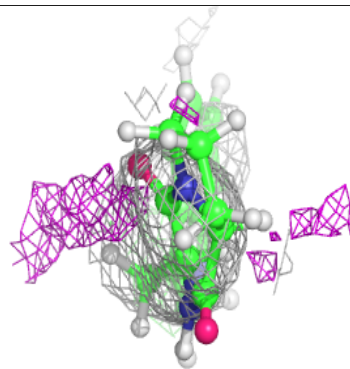
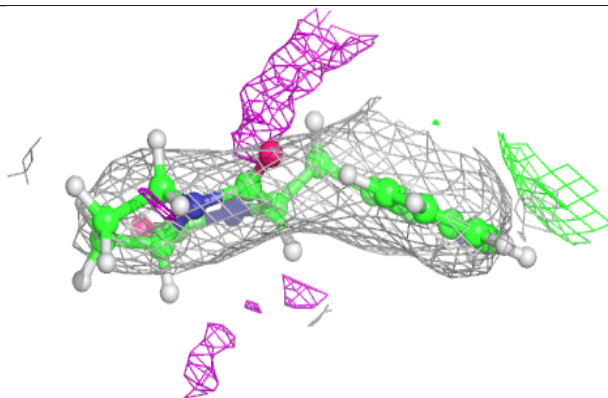
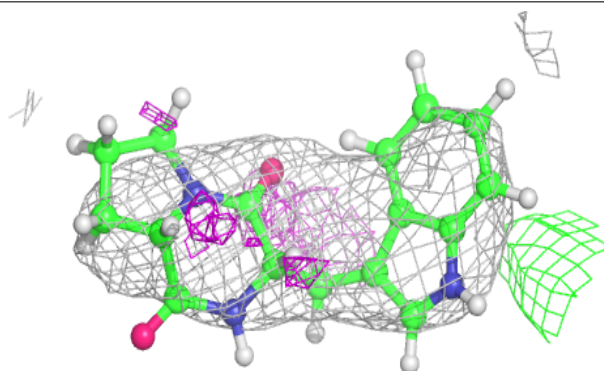


Electron density around QRP J 501:

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

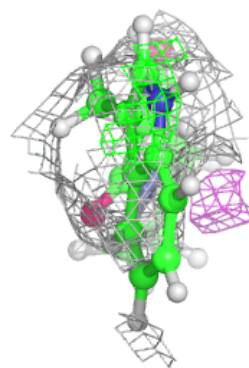
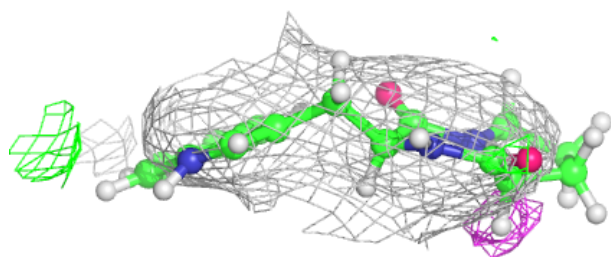
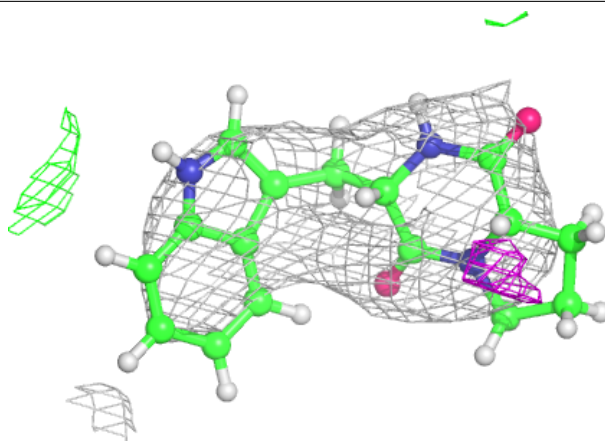
**Electron density around QRP D 501:**

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

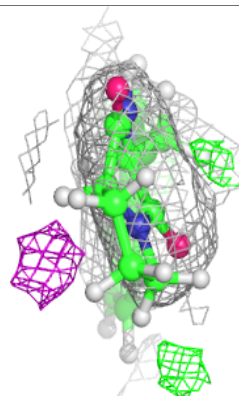
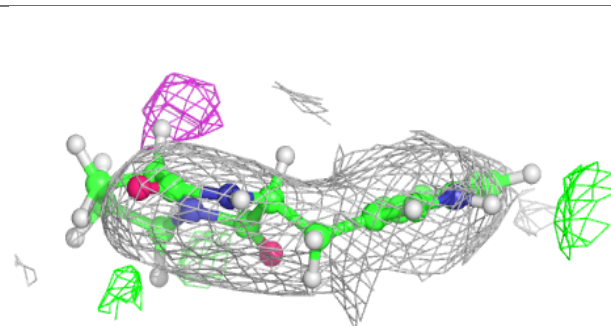
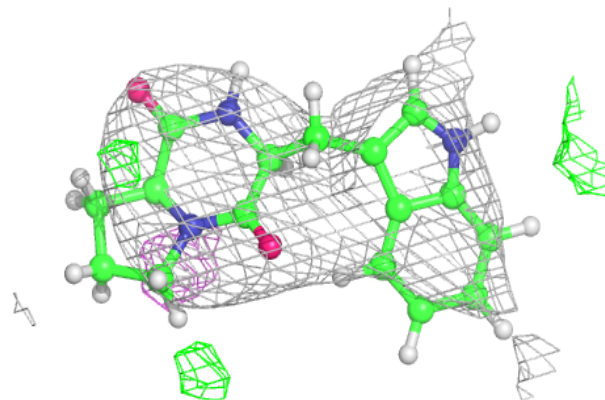


Electron density around QRP K 501:

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

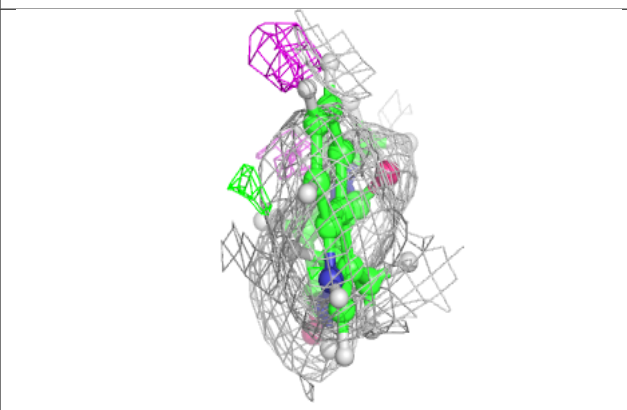
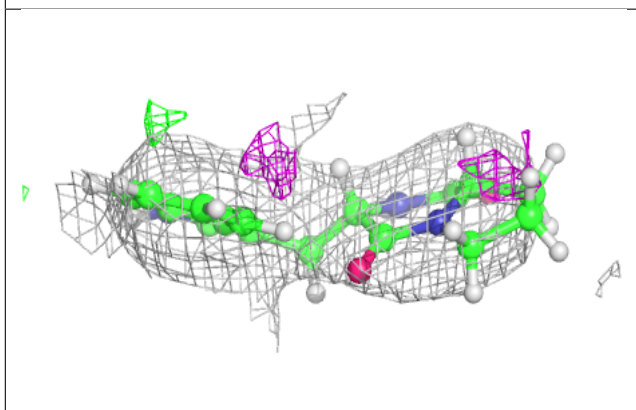
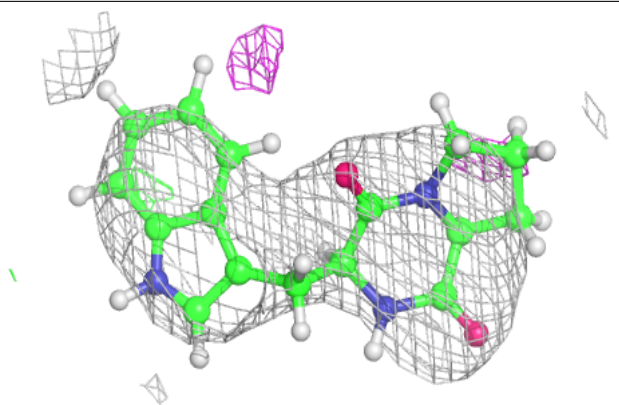
**Electron density around QRP R 501:**

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

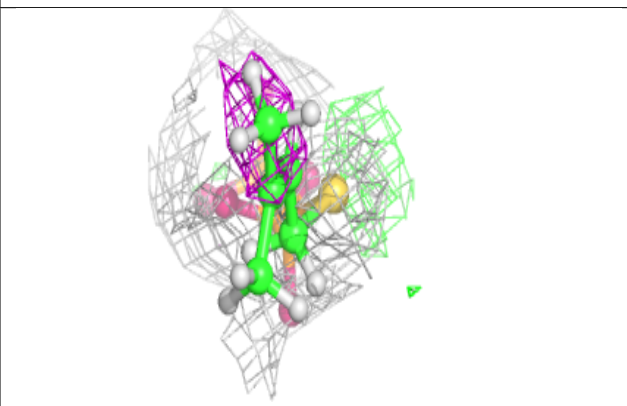
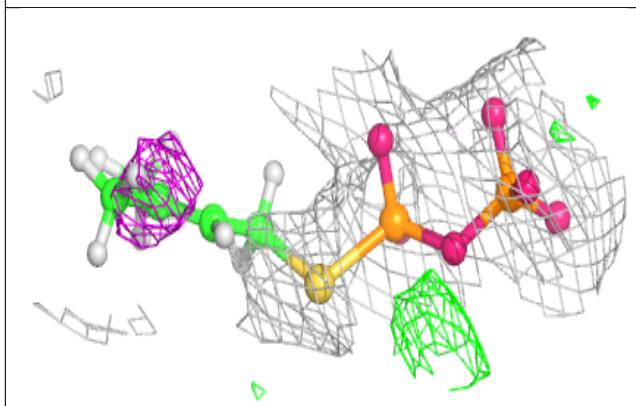
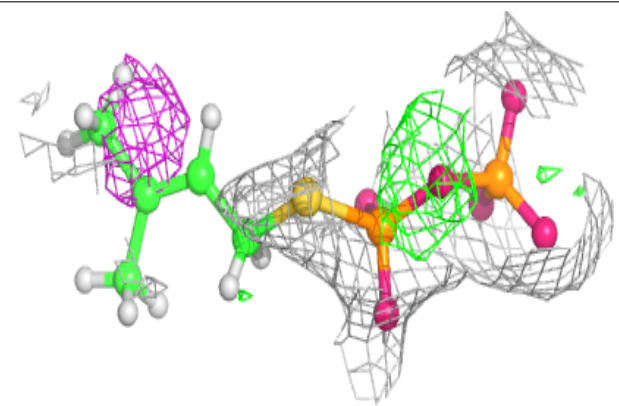


Electron density around QRP H 501:

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

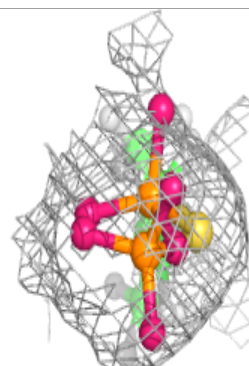
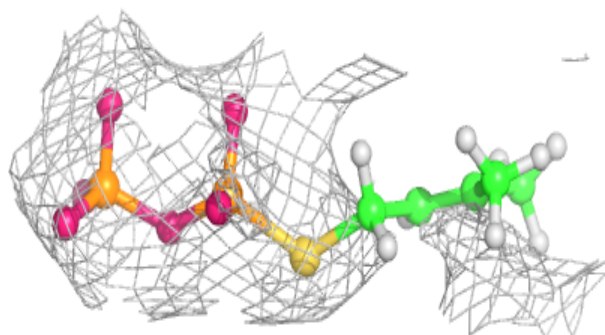
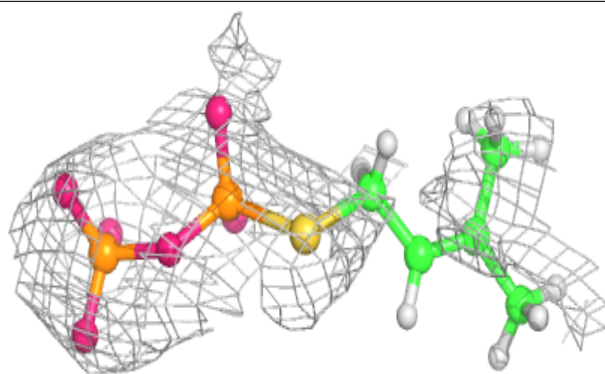
**Electron density around DST J 502:**

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

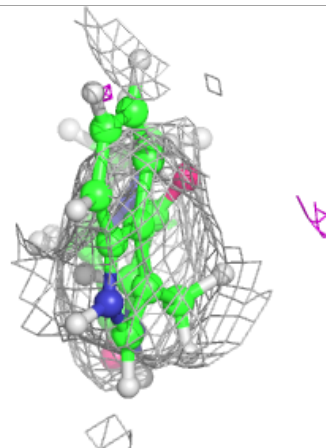
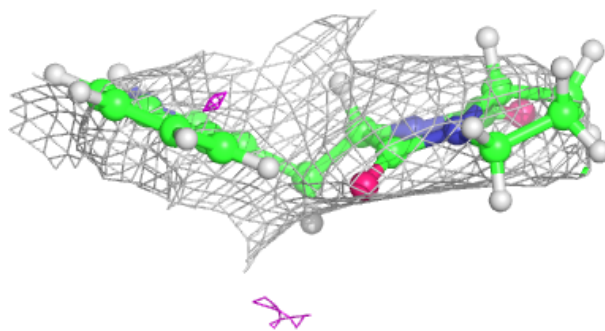
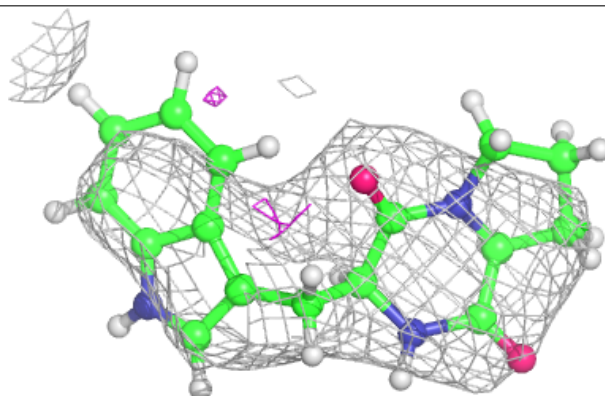


Electron density around DST K 502:

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

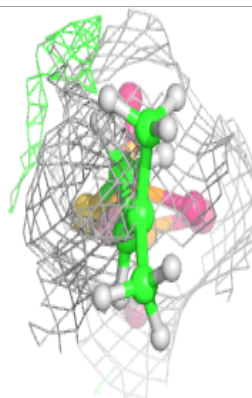
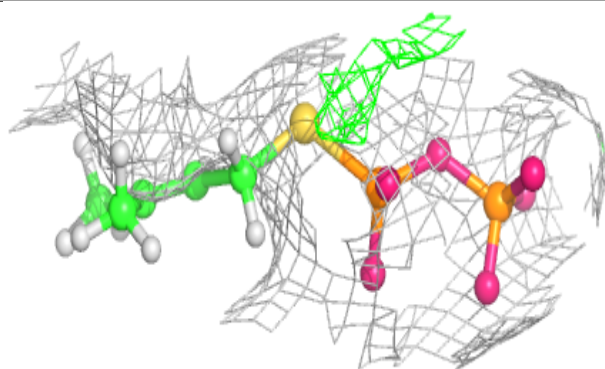
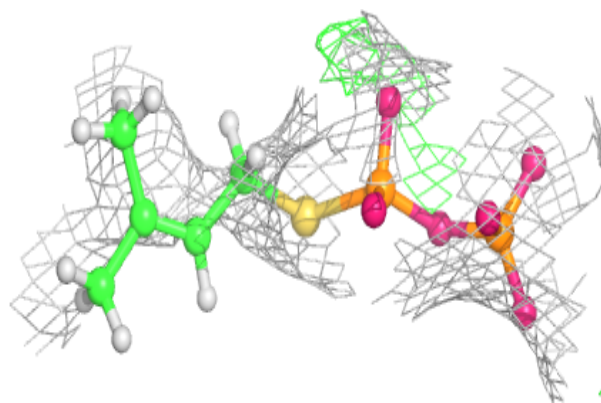
**Electron density around QRP G 501:**

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

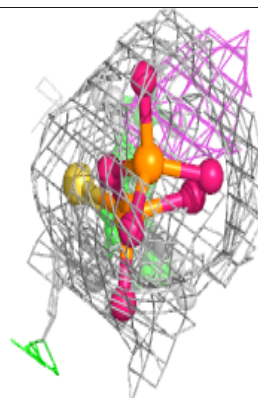
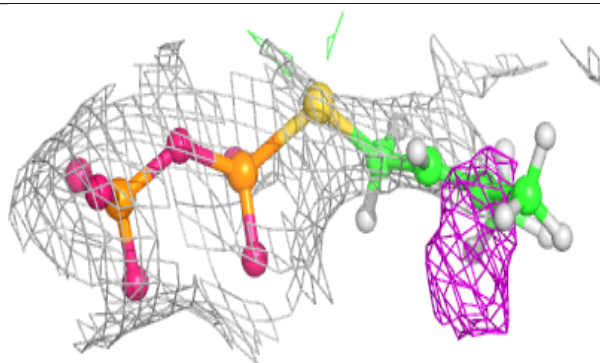
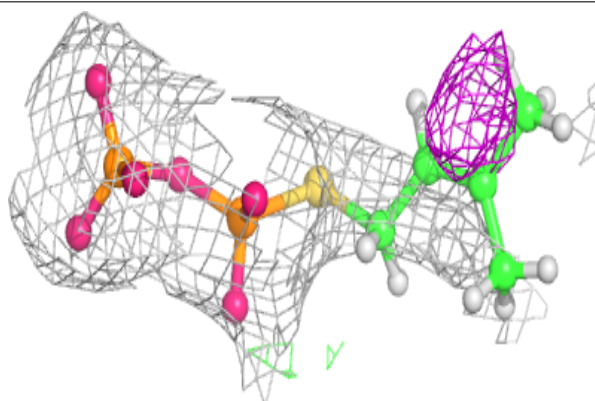


Electron density around DST R 502:

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

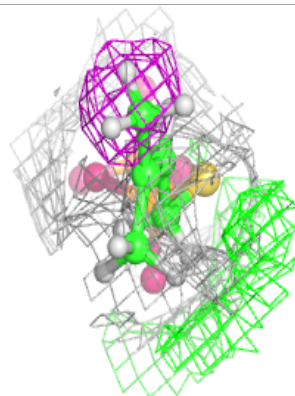
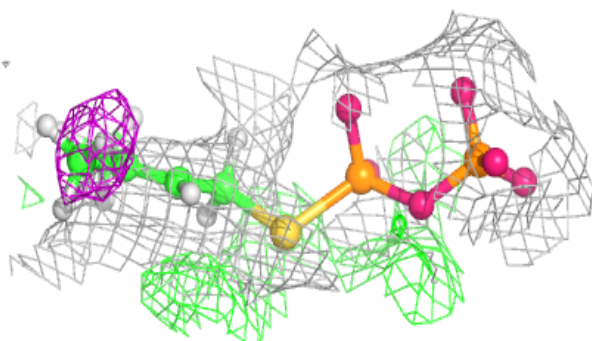
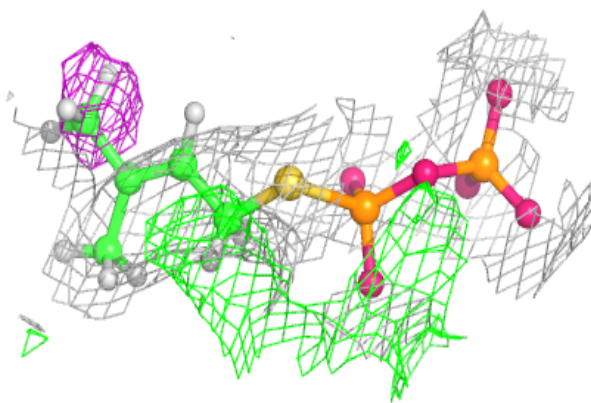
**Electron density around DST S 502:**

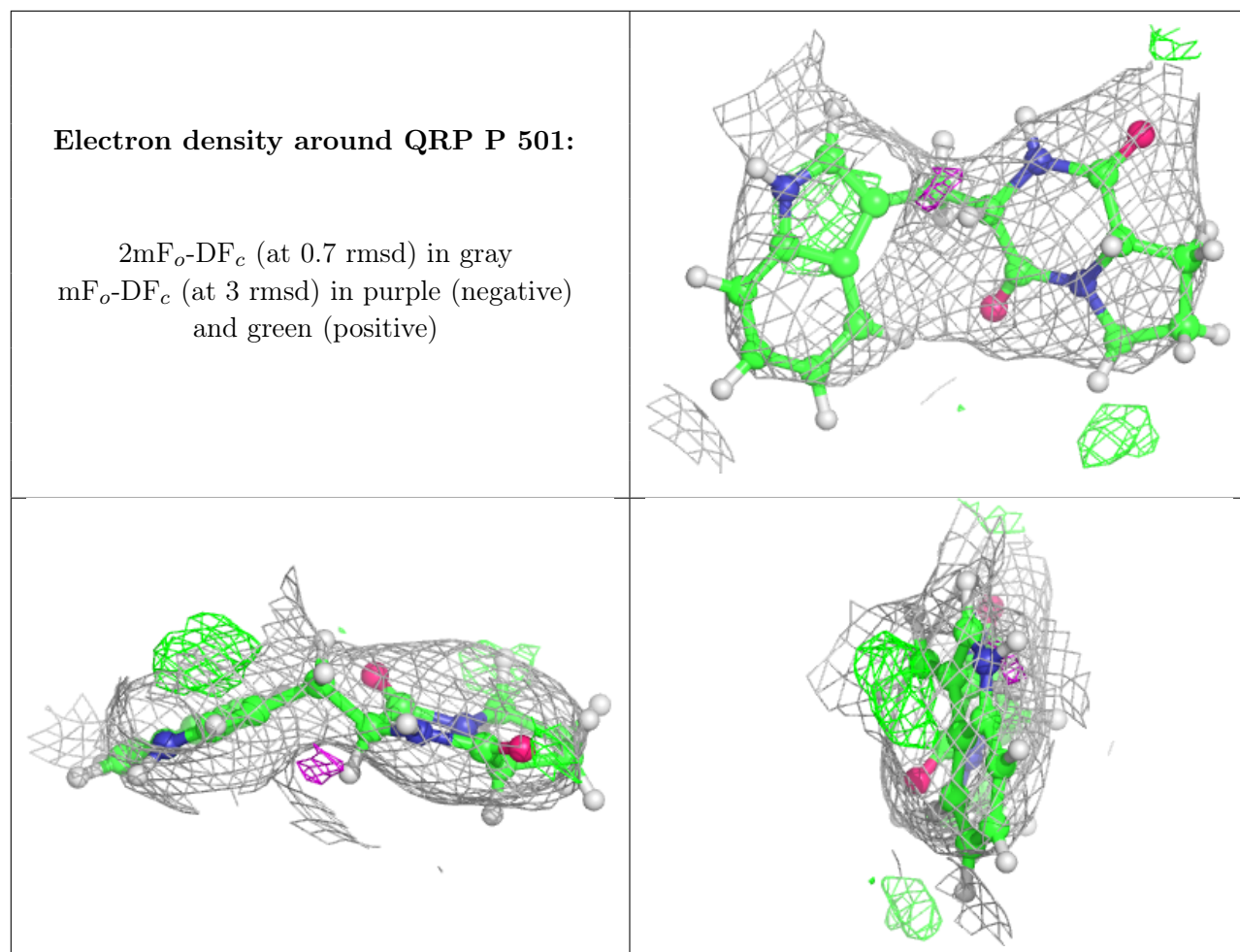
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DST A 502:

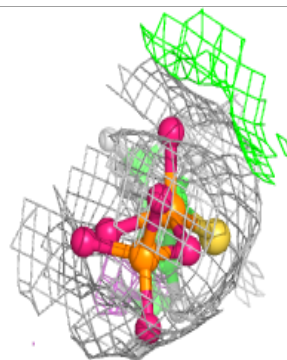
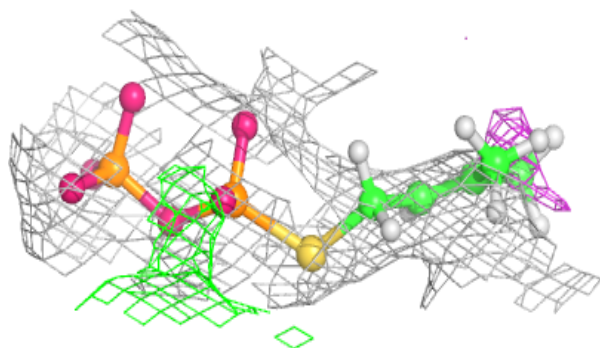
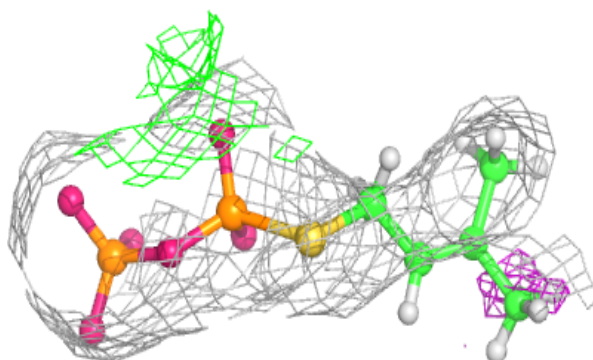
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



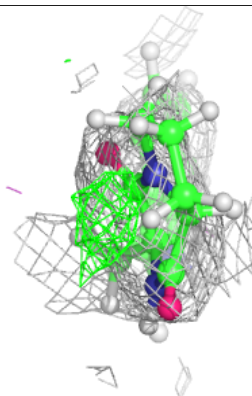
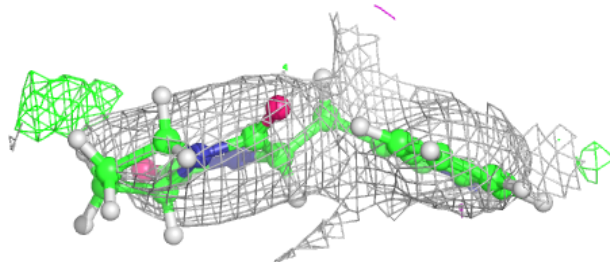
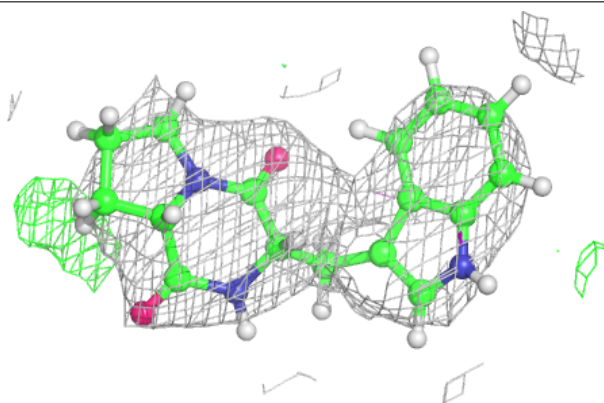


Electron density around DST X 502:

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

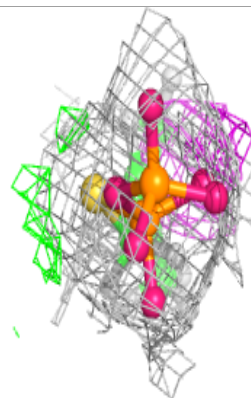
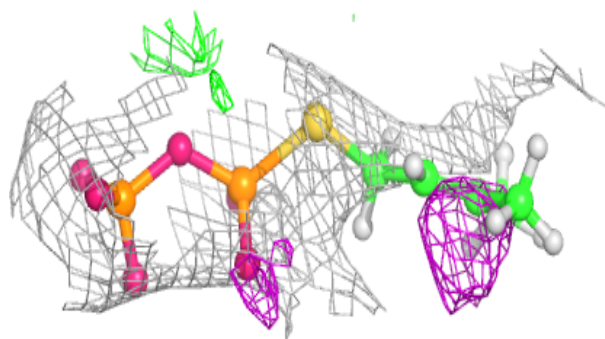
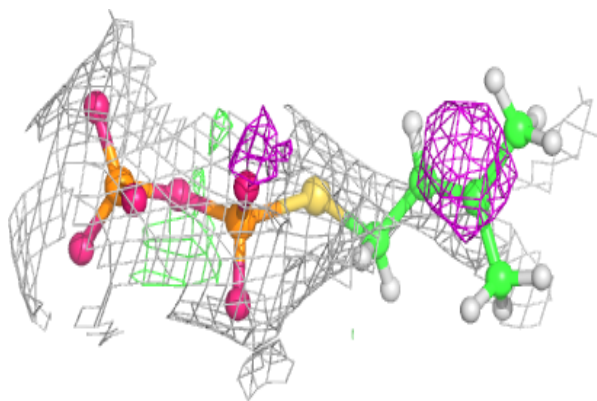
**Electron density around QRP U 501:**

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

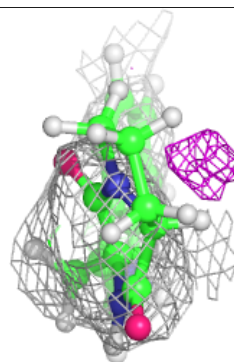
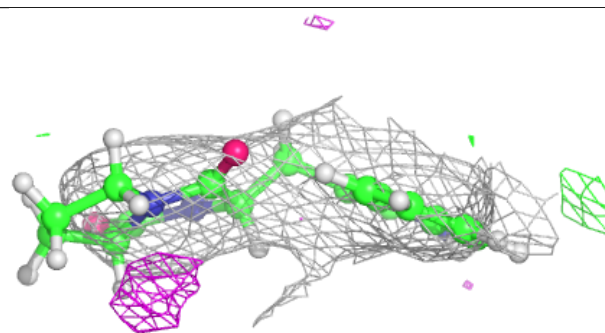
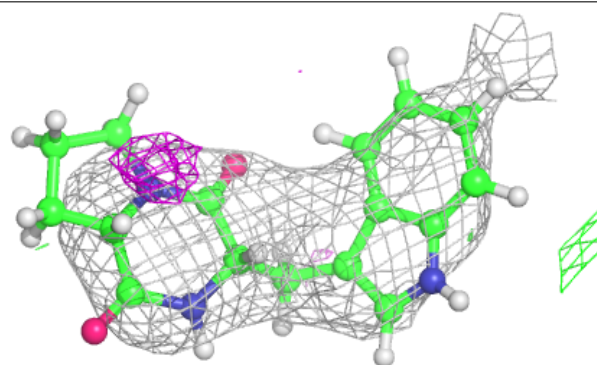


Electron density around DST O 502:

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

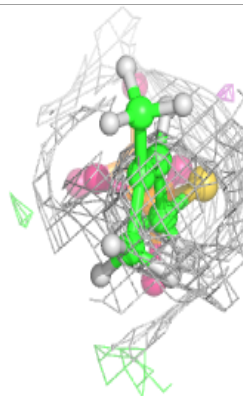
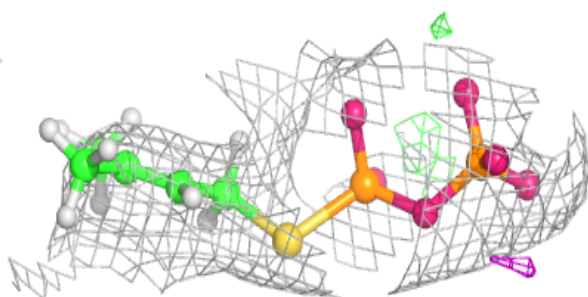
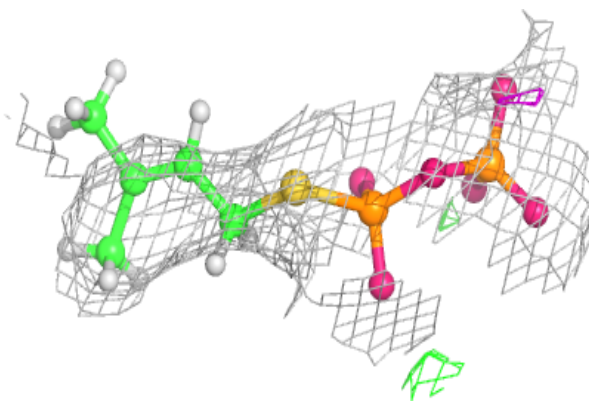
**Electron density around QRP W 501:**

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

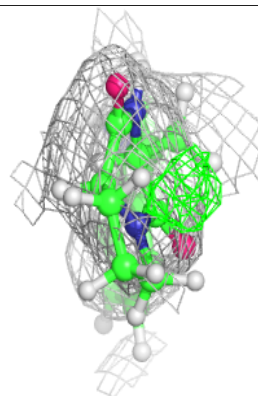
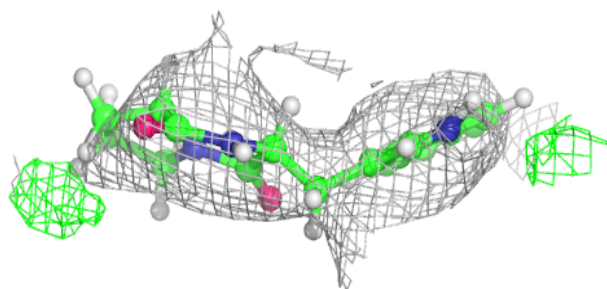
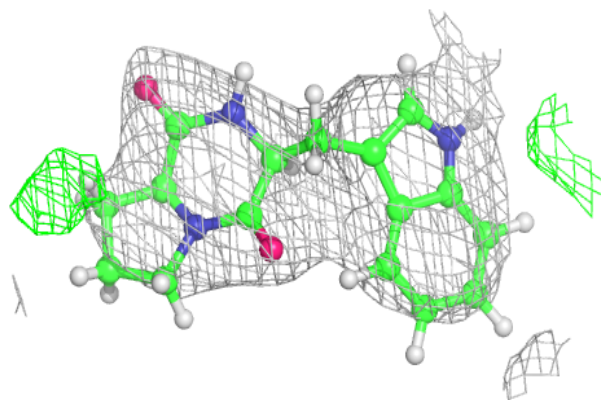


Electron density around DST H 502:

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

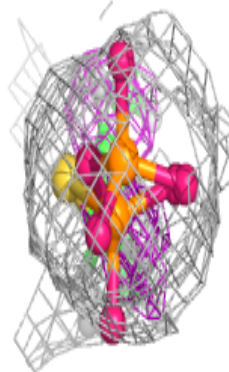
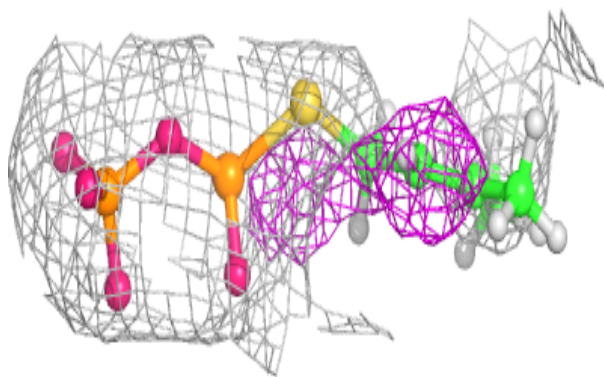
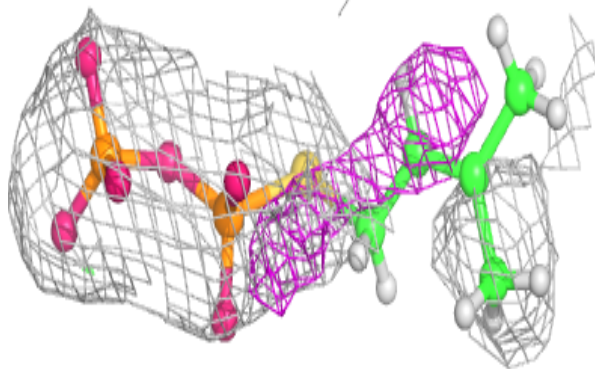
**Electron density around QRP M 501:**

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

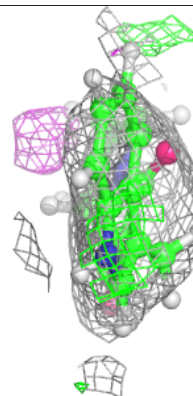
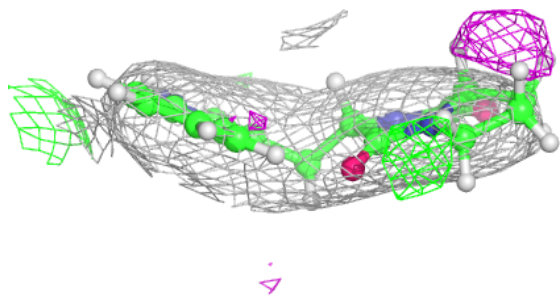
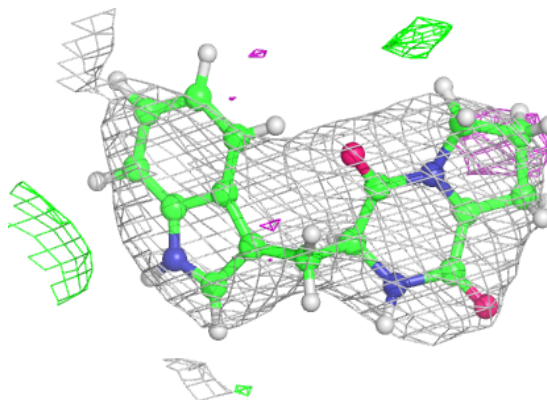


Electron density around DST U 502:

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

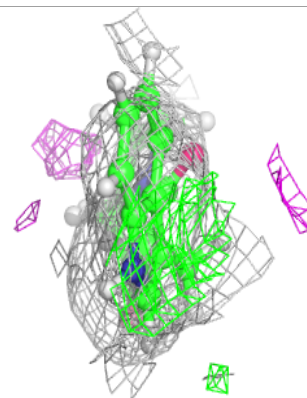
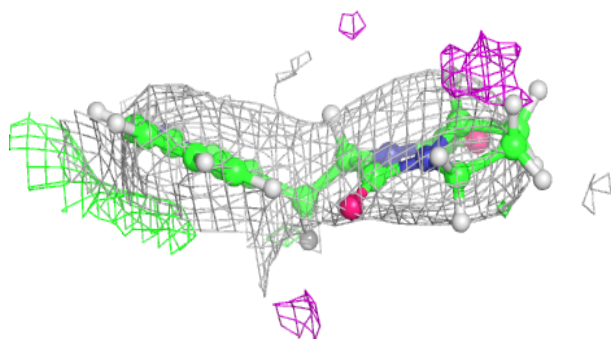
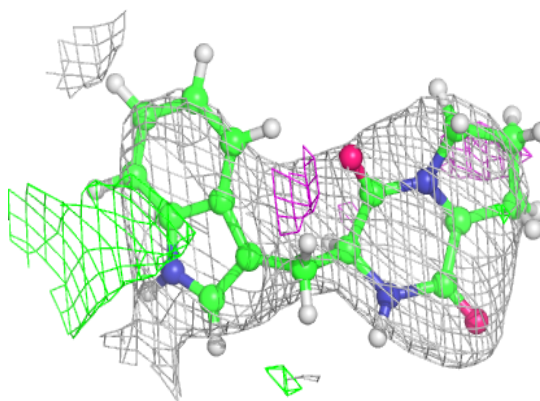
**Electron density around QRP V 501:**

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

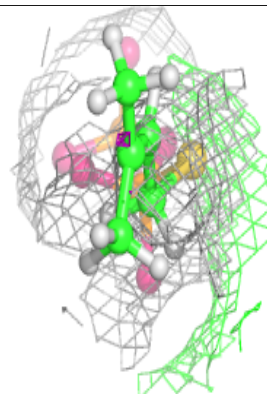
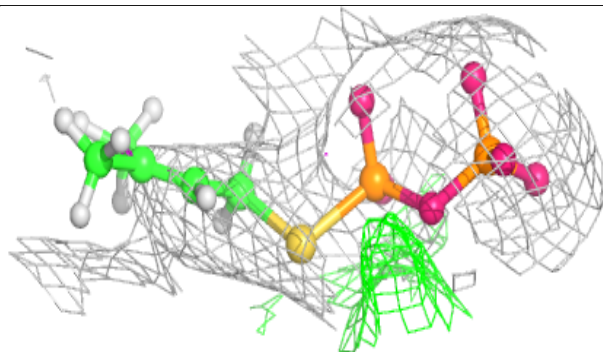
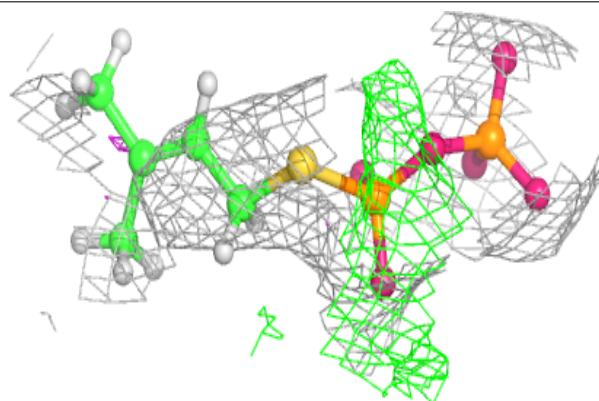


Electron density around QRP A 501:

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

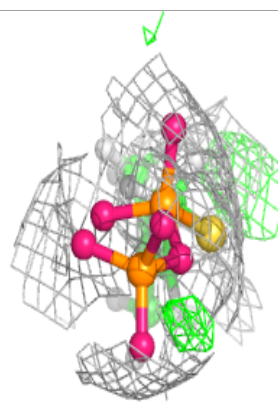
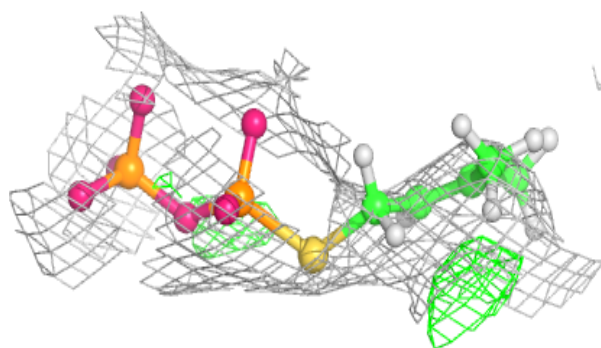
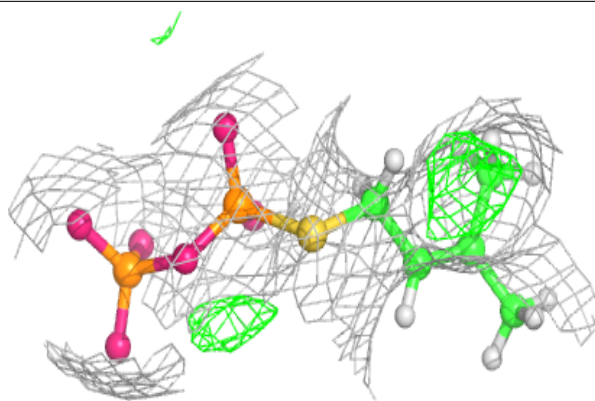
**Electron density around DST V 502:**

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

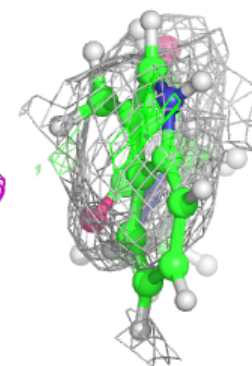
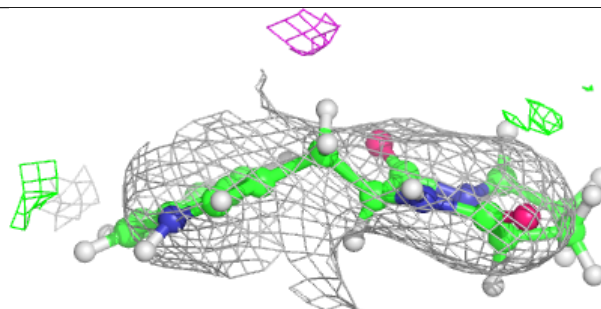
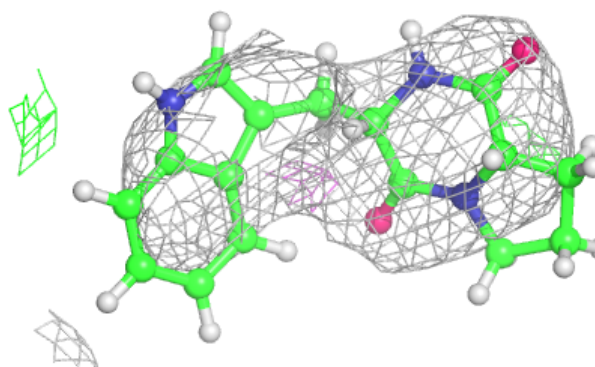


Electron density around DST P 502:

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

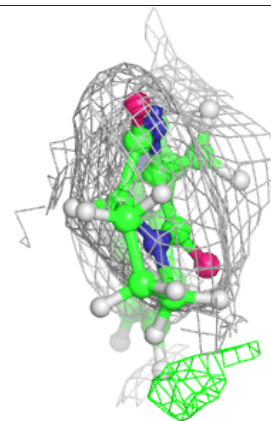
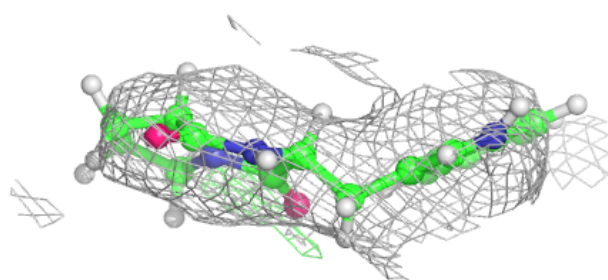
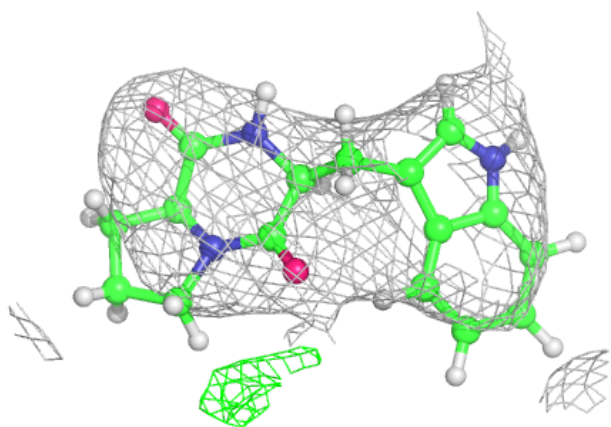
**Electron density around QRP I 501:**

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

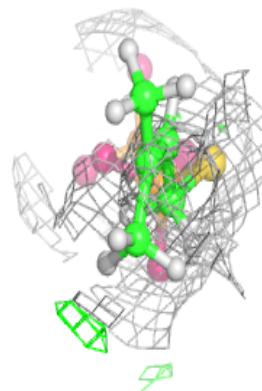
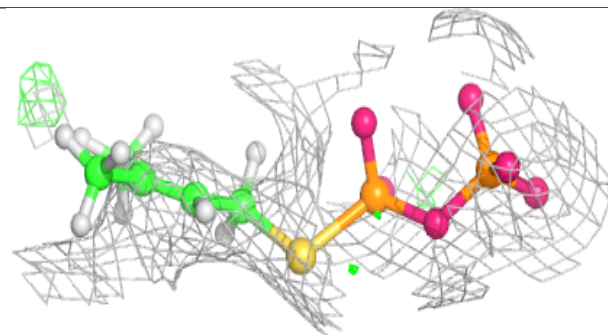
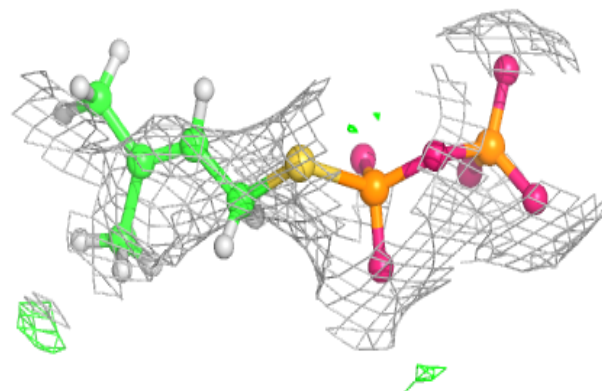


Electron density around QRP T 501:

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

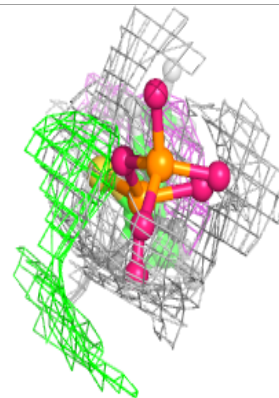
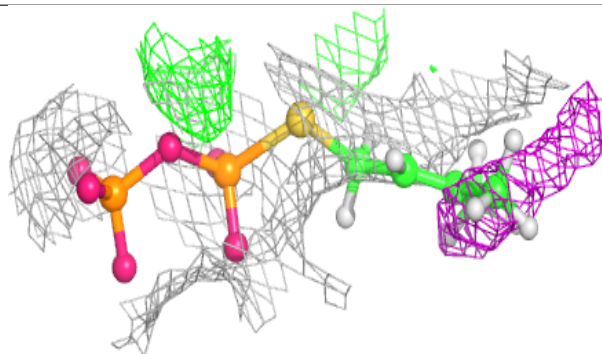
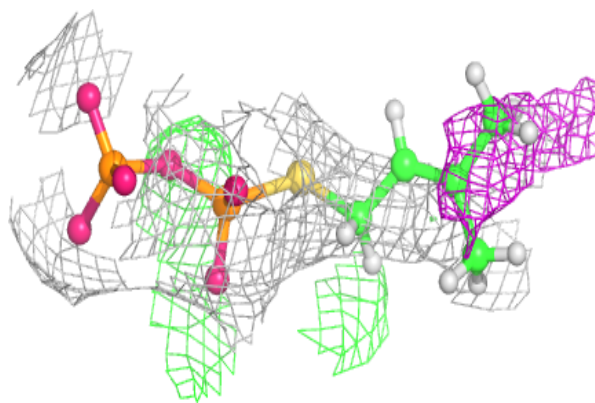
**Electron density around DST N 502:**

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

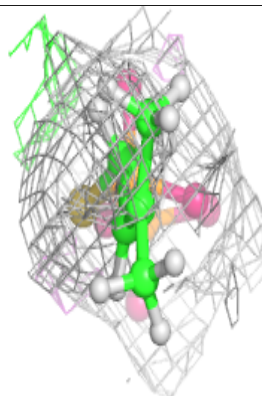
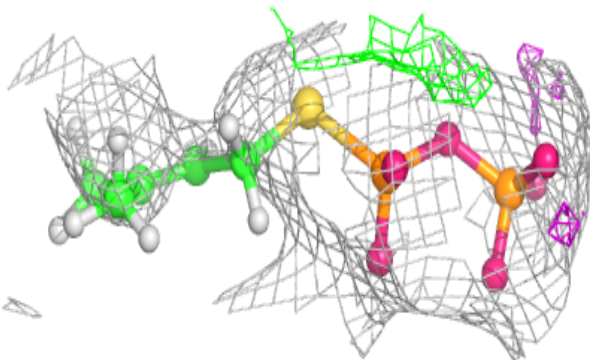
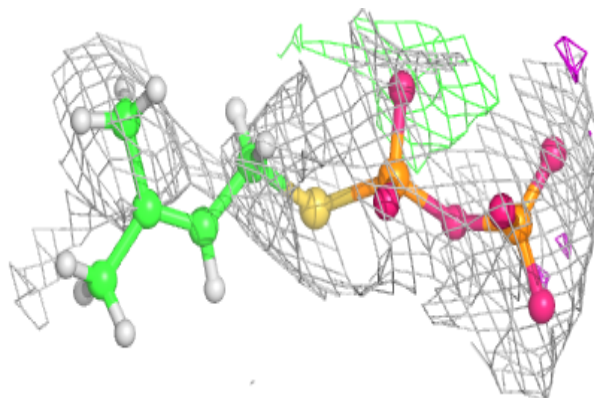


Electron density around DST D 502:

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

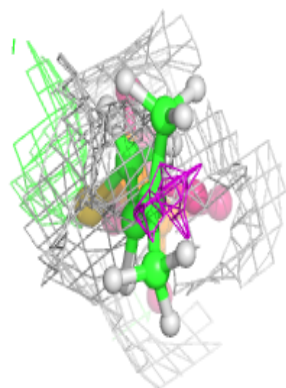
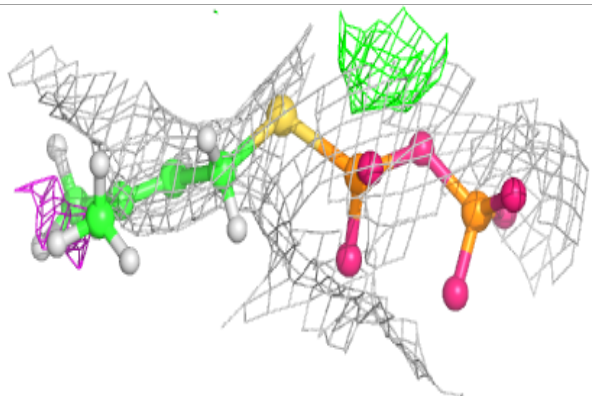
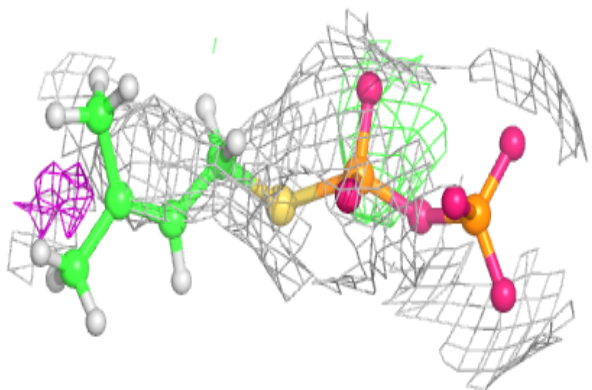
**Electron density around DST M 502:**

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

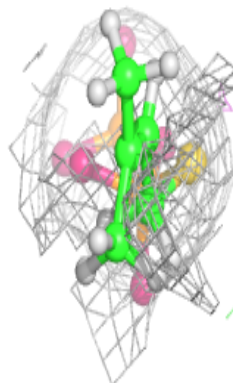
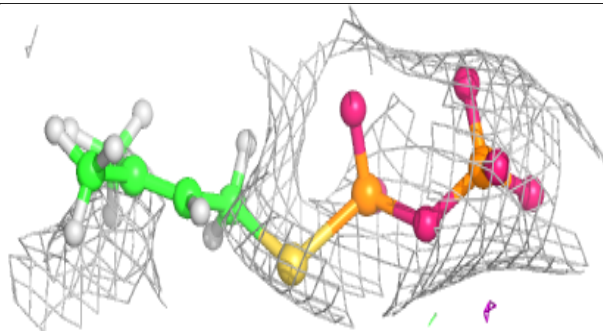
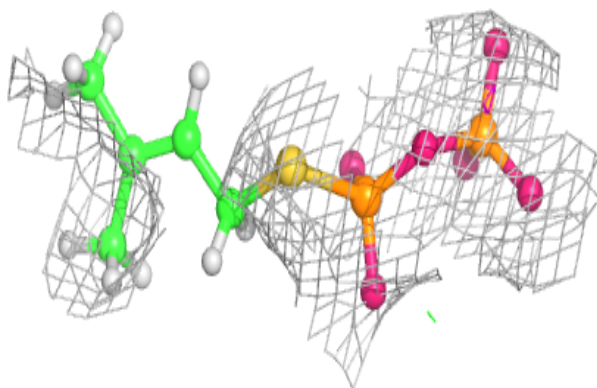


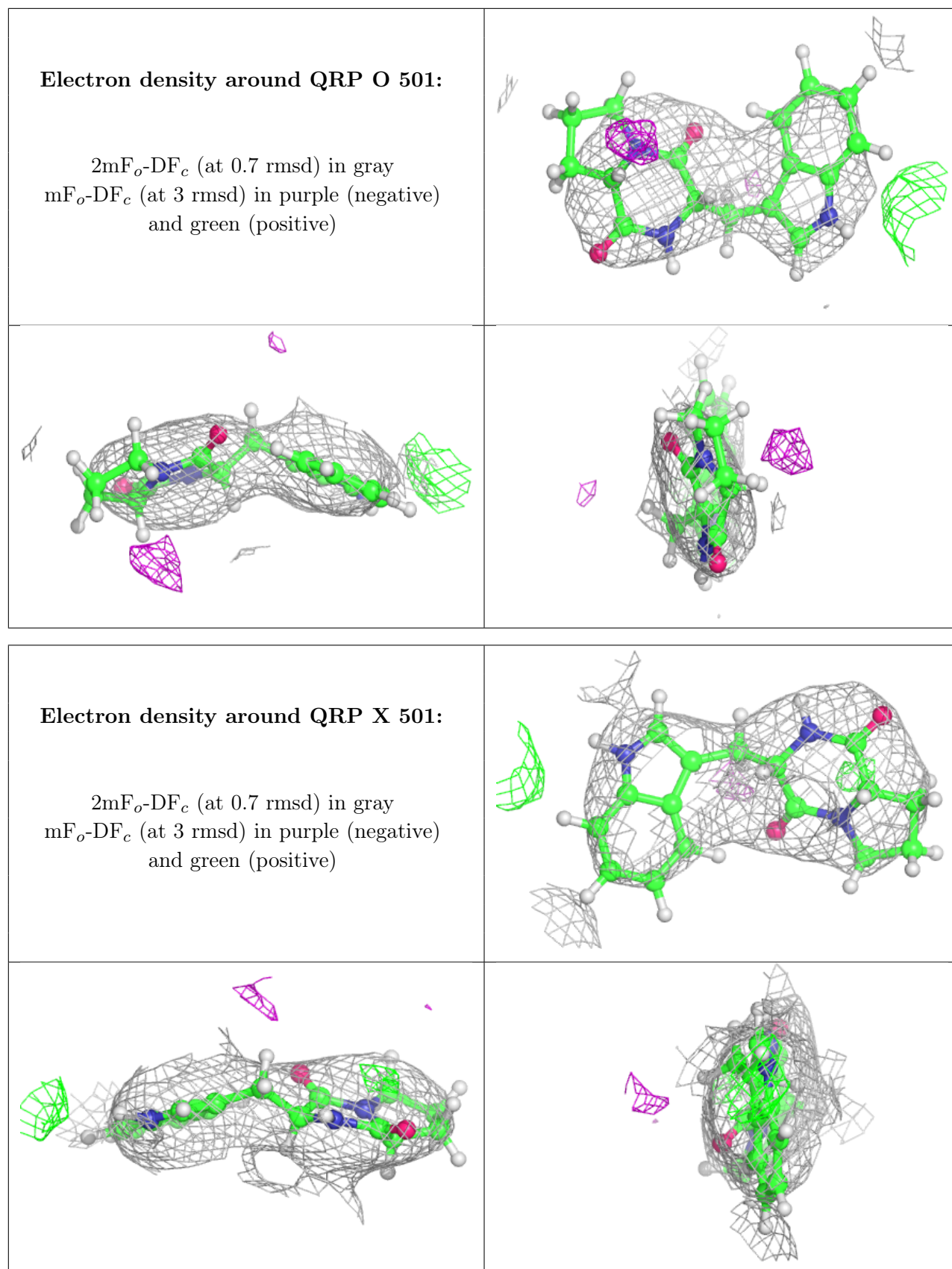
Electron density around DST E 502:

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

**Electron density around DST Q 502:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.