



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:24 AM UTC

PDB ID : 4V4C / pdb_00004v4c
Title : Crystal Structure of Pyrogallol-Phloroglucinol Transhydroxylase from *Pelobacter acidigallici*
Authors : Messerschmidt, A.; Niessen, H.; Abt, D.; Einsle, O.; Schink, B.; Kroneck, P.M.H.
Deposited on : 2004-06-02
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

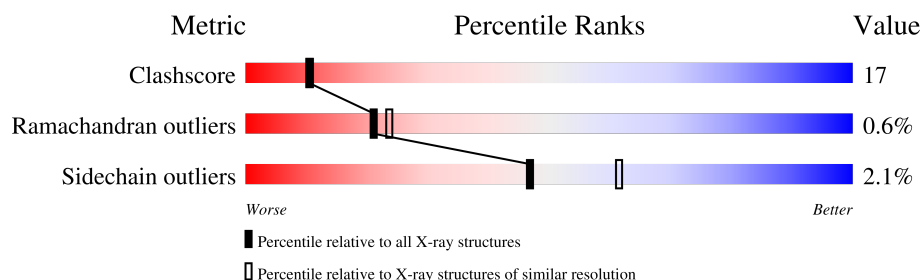
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

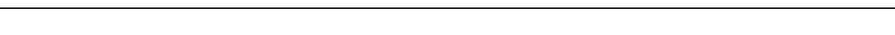
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	875	70% 27% .
1	C	875	66% 32% .
1	E	875	71% 27% .
1	G	875	69% 28% .
1	I	875	69% 29% .
1	K	875	70% 27% .
1	M	875	69% 28% .
1	O	875	68% 30% .

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Mol	Chain	Length	Quality of chain
1	Q	875	 70% 28% .
1	S	875	 69% 29% .
1	U	875	 67% 31% .
1	W	875	 64% 33% .
2	B	274	 64% 32% .
2	D	274	 63% 32% .
2	F	274	 64% 33% .
2	H	274	 62% 34% .
2	J	274	 65% 32% .
2	L	274	 56% 41% .
2	N	274	 65% 32% ..
2	P	274	 59% 38% .
2	R	274	 68% 29% .
2	T	274	 58% 38% .
2	V	274	 62% 35% .
2	X	274	 48% 48% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	C	901	-	-	X	-
3	ACT	E	901	-	-	X	-
3	ACT	G	901	-	-	X	-
3	ACT	I	901	-	-	X	-
3	ACT	K	901	-	-	X	-
3	ACT	O	901	-	-	X	-
3	ACT	W	901	-	-	X	-
7	SF4	B	303	-	-	X	-
7	SF4	D	303	-	-	X	-
7	SF4	D	304	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	F	303	-	-	X	-
7	SF4	H	303	-	-	X	-
7	SF4	H	304	-	-	X	-
7	SF4	J	303	-	-	X	-
7	SF4	L	303	-	-	X	-
7	SF4	L	304	-	-	X	-
7	SF4	N	303	-	-	X	-
7	SF4	P	302	-	-	X	-
7	SF4	P	303	-	-	X	-
7	SF4	P	304	-	-	X	-
7	SF4	R	303	-	-	X	-
7	SF4	R	304	-	-	X	-
7	SF4	T	303	-	-	X	-
7	SF4	T	304	-	-	X	-
7	SF4	V	303	-	-	X	-
7	SF4	X	302	-	-	X	-
7	SF4	X	303	-	-	X	-
7	SF4	X	304	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 122057 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pyrogallol hydroxytransferase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	C	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	E	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	G	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	I	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	K	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	M	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	O	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	Q	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	S	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	U	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	W	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P80563
C	1	MET	-	initiating methionine	UNP P80563
E	1	MET	-	initiating methionine	UNP P80563
G	1	MET	-	initiating methionine	UNP P80563
I	1	MET	-	initiating methionine	UNP P80563

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	MET	-	initiating methionine	UNP P80563
M	1	MET	-	initiating methionine	UNP P80563
O	1	MET	-	initiating methionine	UNP P80563
Q	1	MET	-	initiating methionine	UNP P80563
S	1	MET	-	initiating methionine	UNP P80563
U	1	MET	-	initiating methionine	UNP P80563
W	1	MET	-	initiating methionine	UNP P80563

- Molecule 2 is a protein called Pyrogallol hydroxytransferase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	D	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	F	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	H	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	J	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	L	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	N	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	P	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	R	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	T	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	V	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	X	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		
3	M	1	Total	C	O	0	0
			4	2	2		
3	O	1	Total	C	O	0	0
			4	2	2		
3	Q	1	Total	C	O	0	0
			4	2	2		
3	S	1	Total	C	O	0	0
			4	2	2		
3	U	1	Total	C	O	0	0
			4	2	2		
3	W	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

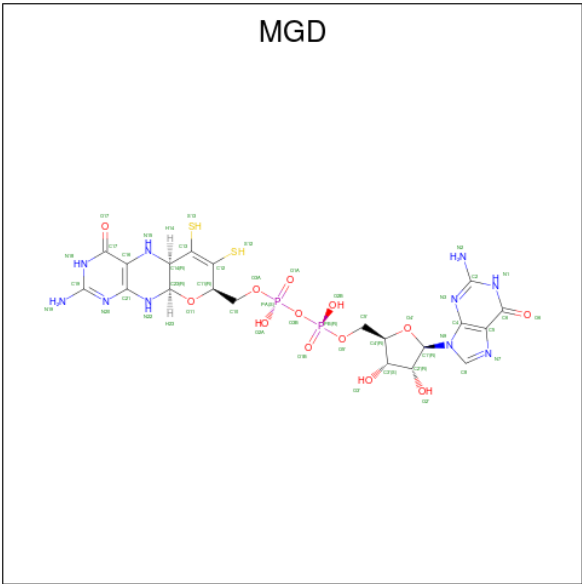
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	E	1	Total Ca 1 1	0	0
4	F	1	Total Ca 1 1	0	0
4	G	1	Total Ca 1 1	0	0
4	H	1	Total Ca 1 1	0	0
4	I	1	Total Ca 1 1	0	0
4	J	1	Total Ca 1 1	0	0
4	K	1	Total Ca 1 1	0	0
4	L	1	Total Ca 1 1	0	0
4	M	1	Total Ca 1 1	0	0
4	N	1	Total Ca 1 1	0	0
4	O	1	Total Ca 1 1	0	0
4	P	1	Total Ca 1 1	0	0
4	Q	1	Total Ca 1 1	0	0
4	R	1	Total Ca 1 1	0	0
4	S	1	Total Ca 1 1	0	0
4	T	1	Total Ca 1 1	0	0
4	U	1	Total Ca 1 1	0	0
4	V	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	W	1	Total	Ca	0	0
			1	1		
4	X	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	I	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	I	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	M	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	M	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	O	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	O	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	Q	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	Q	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	S	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	S	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	U	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	U	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	W	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	W	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo).

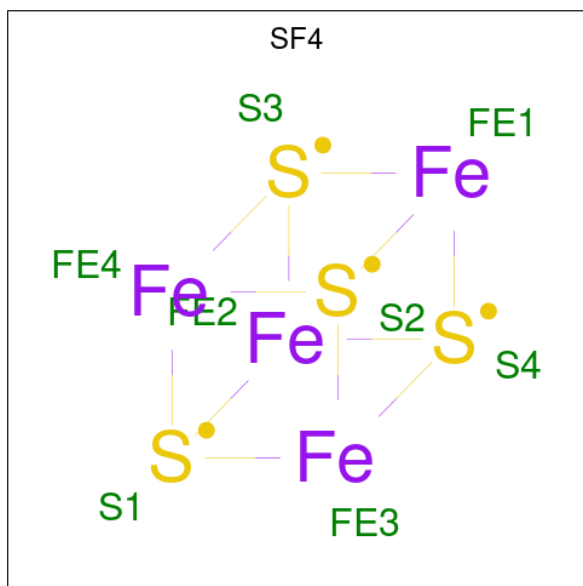
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		
6	C	1	Total	Mo	0	0
			1	1		
6	E	1	Total	Mo	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mo	0	0
			1	1		
6	I	1	Total	Mo	0	0
			1	1		
6	K	1	Total	Mo	0	0
			1	1		
6	M	1	Total	Mo	0	0
			1	1		
6	O	1	Total	Mo	0	0
			1	1		
6	Q	1	Total	Mo	0	0
			1	1		
6	S	1	Total	Mo	0	0
			1	1		
6	U	1	Total	Mo	0	0
			1	1		
6	W	1	Total	Mo	0	0
			1	1		

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 8	Fe 4	S 4	0	0
7	D	1	Total 8	Fe 4	S 4	0	0
7	D	1	Total 8	Fe 4	S 4	0	0
7	D	1	Total 8	Fe 4	S 4	0	0
7	F	1	Total 8	Fe 4	S 4	0	0
7	F	1	Total 8	Fe 4	S 4	0	0
7	F	1	Total 8	Fe 4	S 4	0	0
7	H	1	Total 8	Fe 4	S 4	0	0
7	H	1	Total 8	Fe 4	S 4	0	0
7	H	1	Total 8	Fe 4	S 4	0	0
7	J	1	Total 8	Fe 4	S 4	0	0
7	J	1	Total 8	Fe 4	S 4	0	0
7	J	1	Total 8	Fe 4	S 4	0	0
7	L	1	Total 8	Fe 4	S 4	0	0
7	L	1	Total 8	Fe 4	S 4	0	0
7	L	1	Total 8	Fe 4	S 4	0	0
7	N	1	Total 8	Fe 4	S 4	0	0
7	N	1	Total 8	Fe 4	S 4	0	0
7	N	1	Total 8	Fe 4	S 4	0	0
7	P	1	Total 8	Fe 4	S 4	0	0
7	P	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	P	1	Total 8	Fe 4	S 4	0	0
7	R	1	Total 8	Fe 4	S 4	0	0
7	R	1	Total 8	Fe 4	S 4	0	0
7	R	1	Total 8	Fe 4	S 4	0	0
7	T	1	Total 8	Fe 4	S 4	0	0
7	T	1	Total 8	Fe 4	S 4	0	0
7	T	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	V	1	Total 8	Fe 4	S 4	0	0
7	X	1	Total 8	Fe 4	S 4	0	0
7	X	1	Total 8	Fe 4	S 4	0	0
7	X	1	Total 8	Fe 4	S 4	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	688	Total 688	O 688	0	0
8	B	167	Total 167	O 167	0	0
8	C	684	Total 684	O 684	0	0
8	D	167	Total 167	O 167	0	0
8	E	684	Total 684	O 684	0	0
8	F	167	Total 167	O 167	0	0

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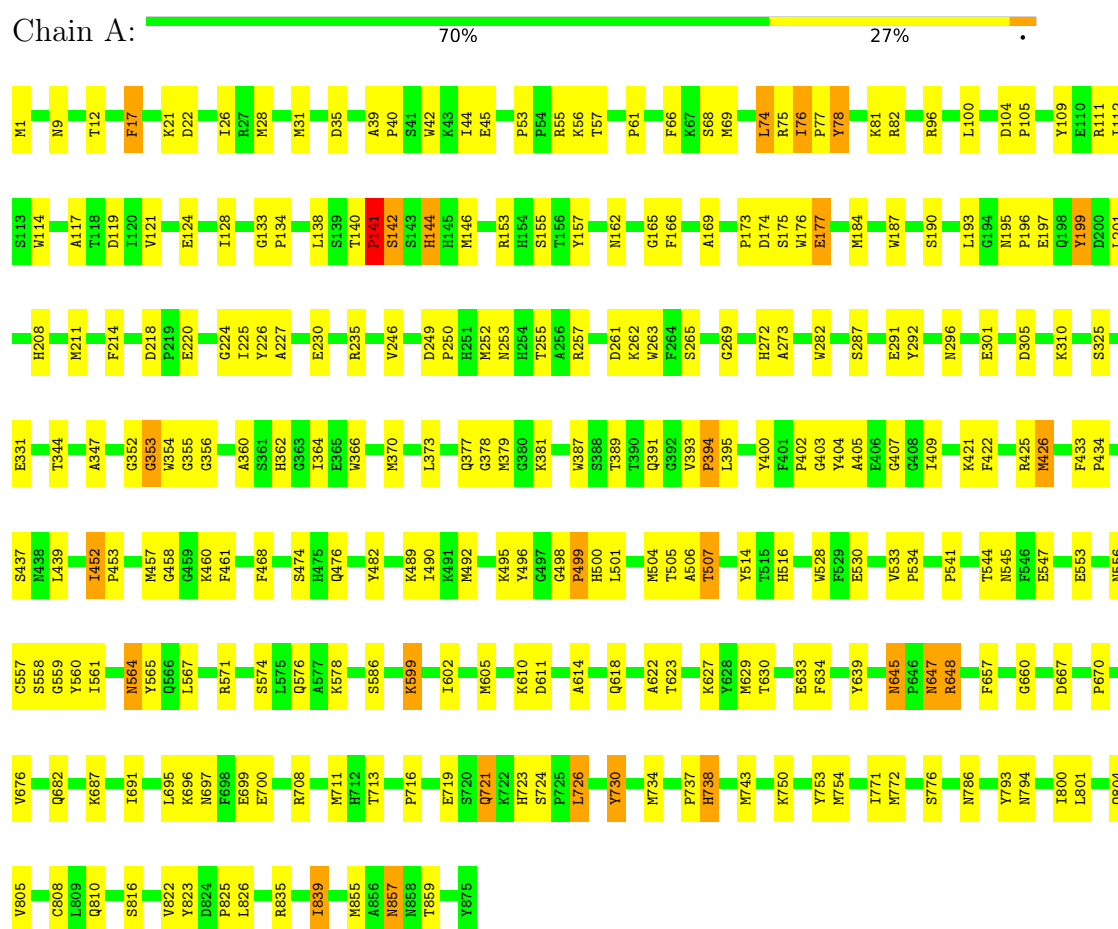
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	689	Total 689	O 689	0	0
8	H	162	Total 162	O 162	0	0
8	I	675	Total 675	O 675	0	0
8	J	170	Total 170	O 170	0	0
8	K	684	Total 684	O 684	0	0
8	L	168	Total 168	O 168	0	0
8	M	683	Total 683	O 683	0	0
8	N	163	Total 163	O 163	0	0
8	O	679	Total 679	O 679	0	0
8	P	163	Total 163	O 163	0	0
8	Q	692	Total 692	O 692	0	0
8	R	166	Total 166	O 166	0	0
8	S	675	Total 675	O 675	0	0
8	T	159	Total 159	O 159	0	0
8	U	667	Total 667	O 667	0	0
8	V	163	Total 163	O 163	0	0
8	W	677	Total 677	O 677	0	0
8	X	165	Total 165	O 165	0	0

3 Residue-property plots

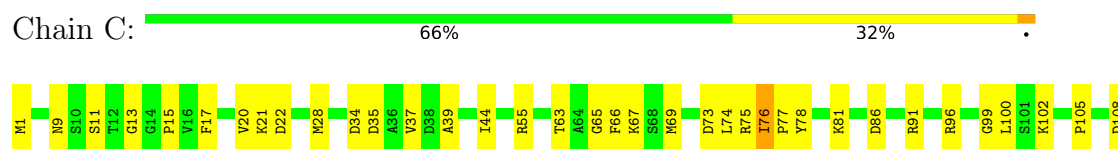
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

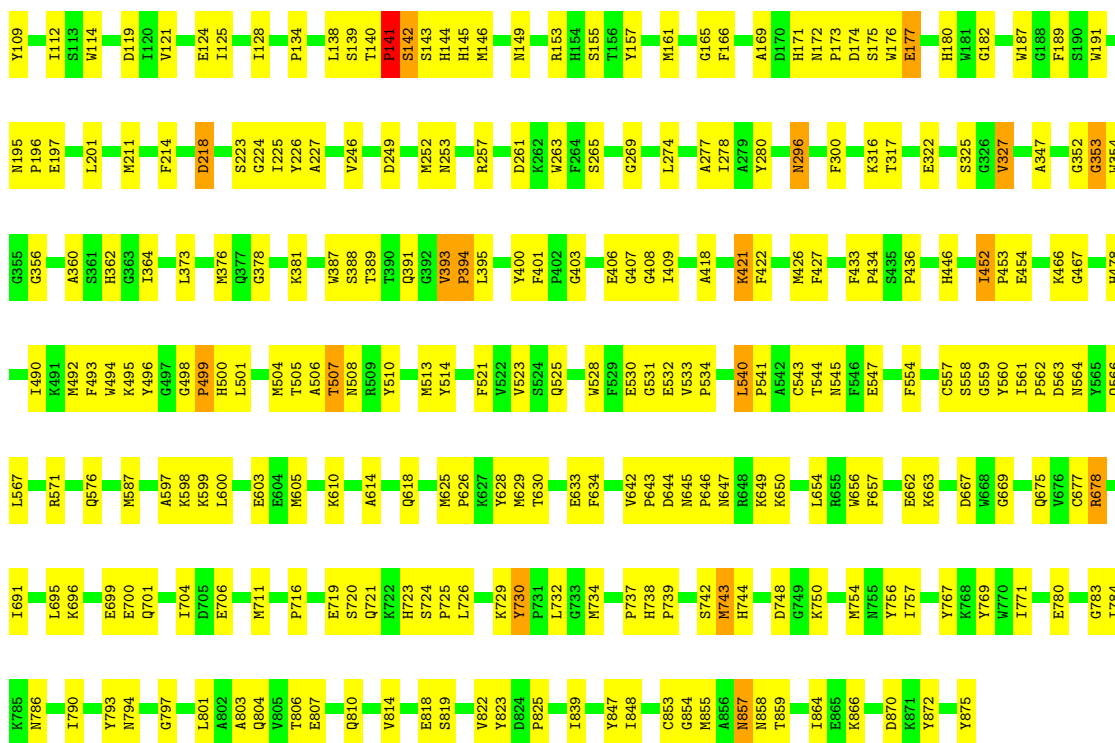
Note EDS was not executed.

• Molecule 1: Pyrogallol hydroxytransferase large subunit

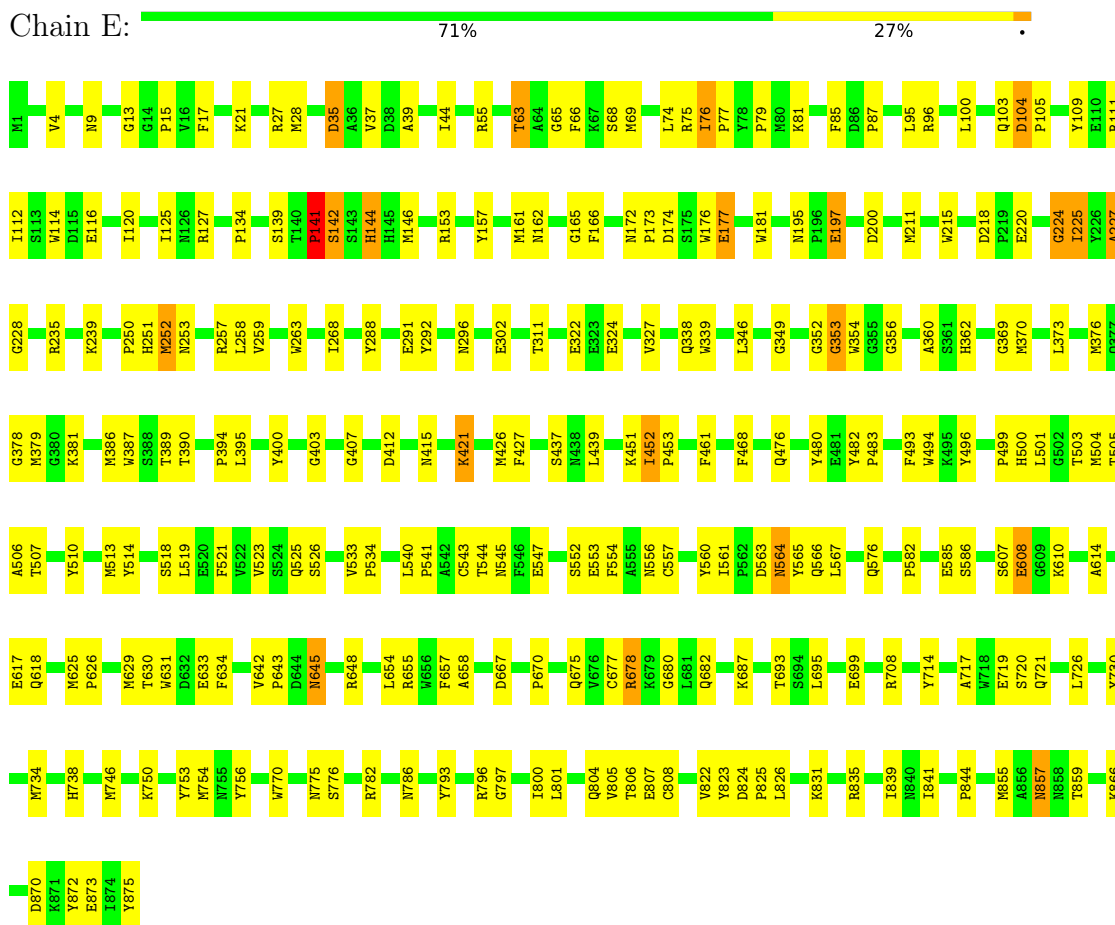


• Molecule 1: Pyrogallol hydroxytransferase large subunit

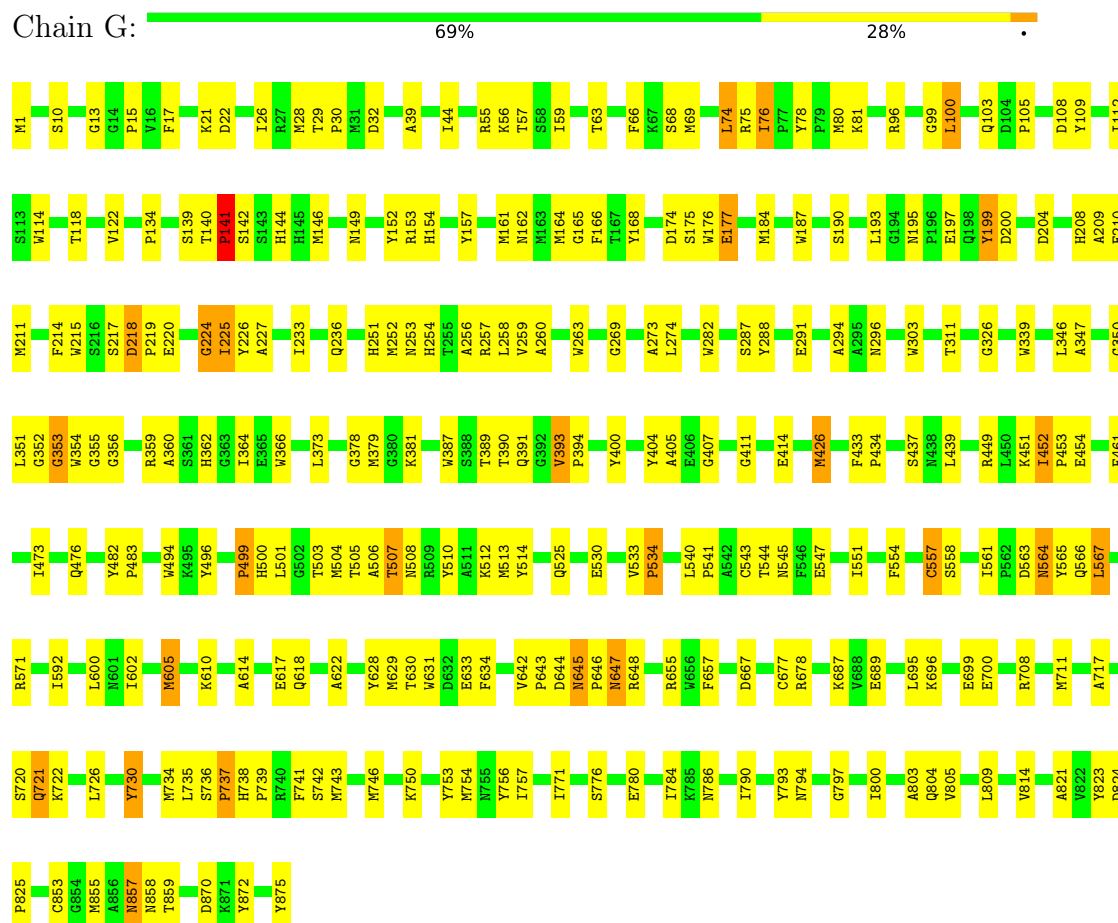




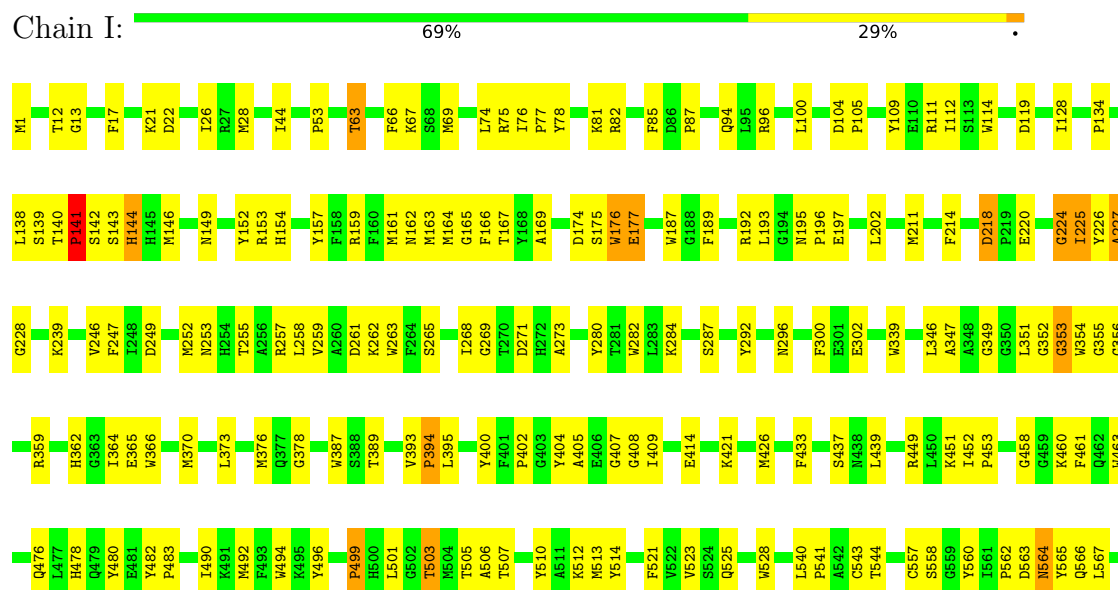
- Molecule 1: Pyrogallol hydroxytransferase large subunit

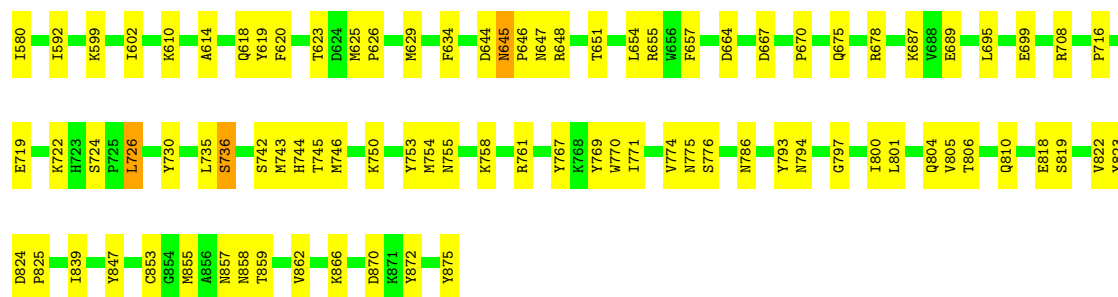


● Molecule 1: Pyrogallol hydroxytransferase large subunit



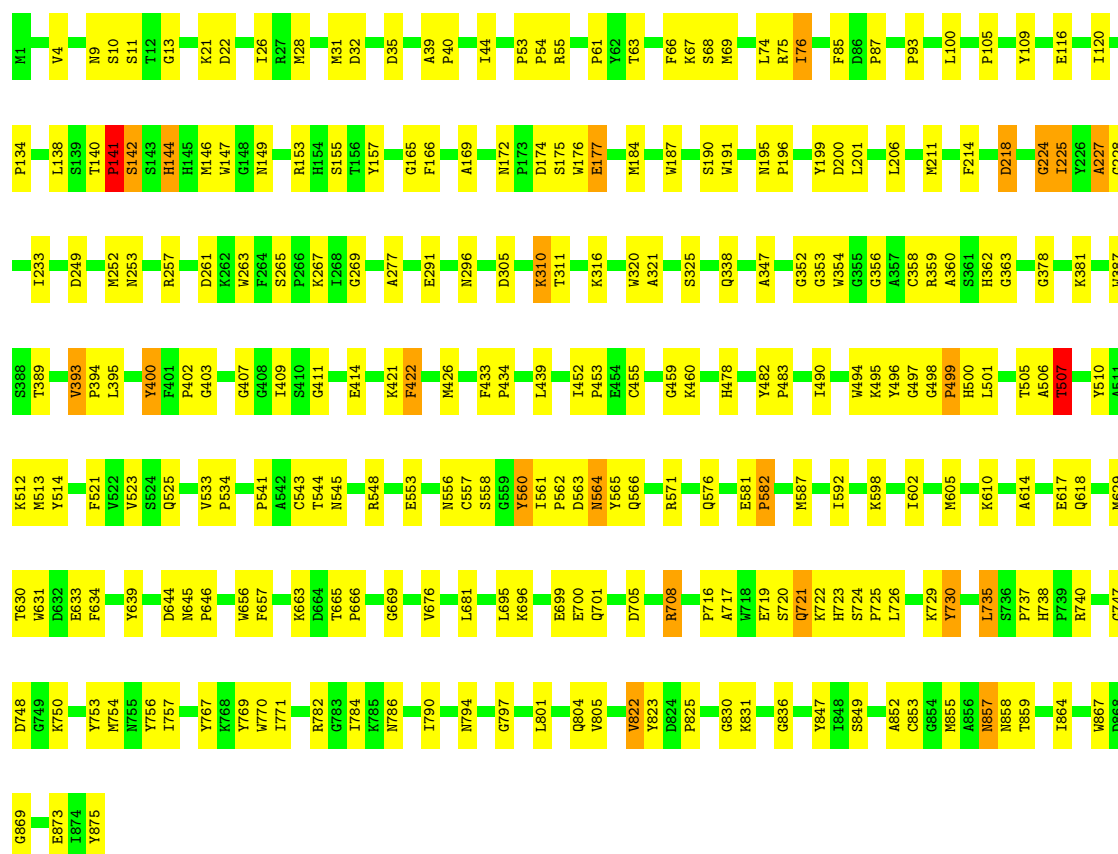
● Molecule 1: Pyrogallol hydroxytransferase large subunit





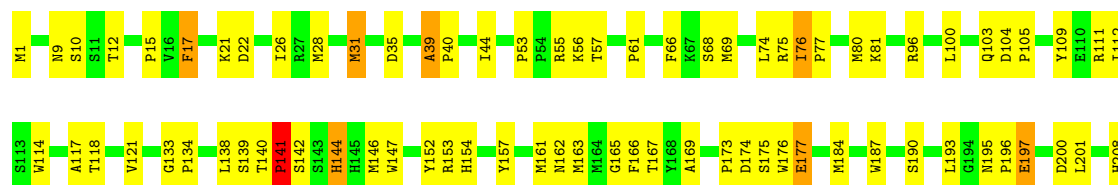
• Molecule 1: Pyrogallol hydroxytransferase large subunit

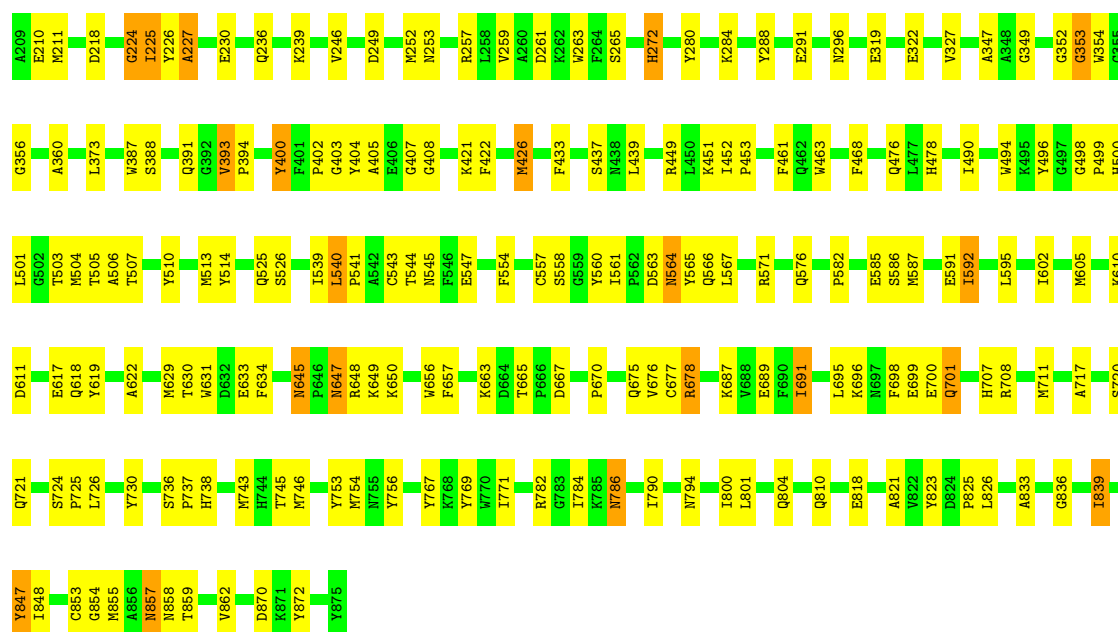
Chain K: 70% 27% .



• Molecule 1: Pyrogallol hydroxytransferase large subunit

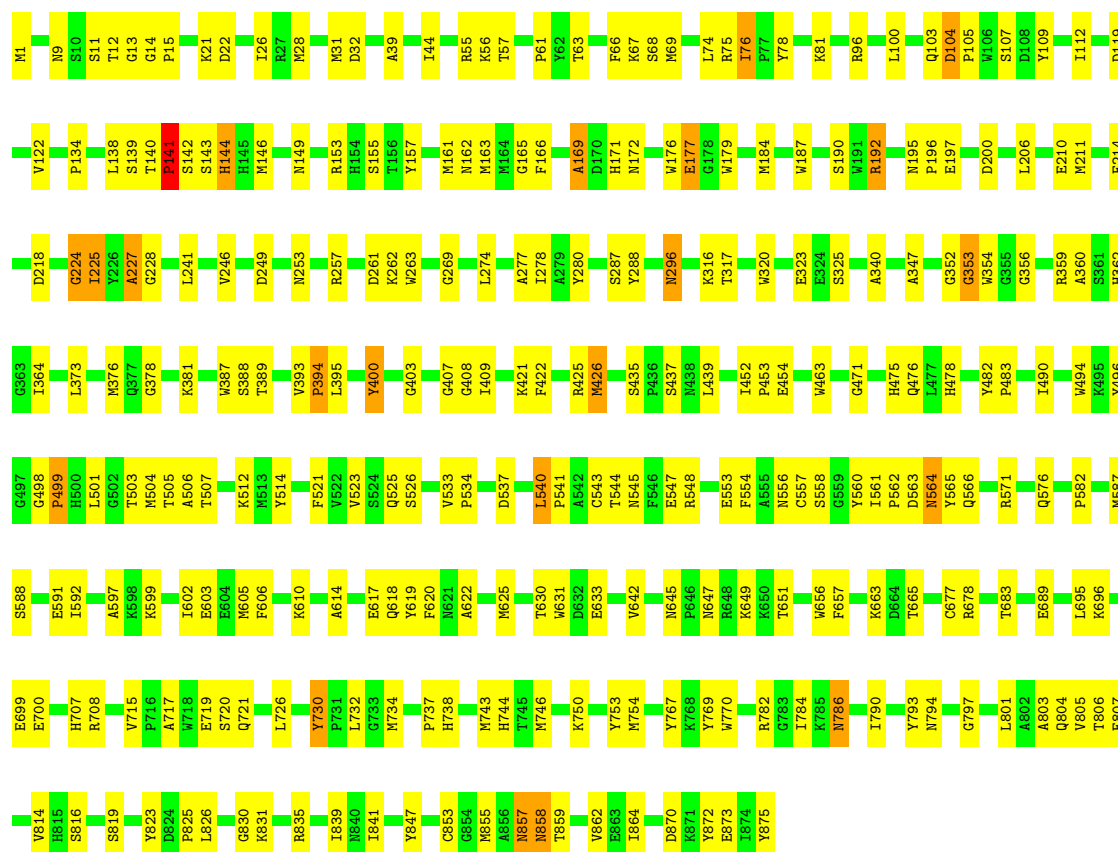
Chain M: 69% 28% .





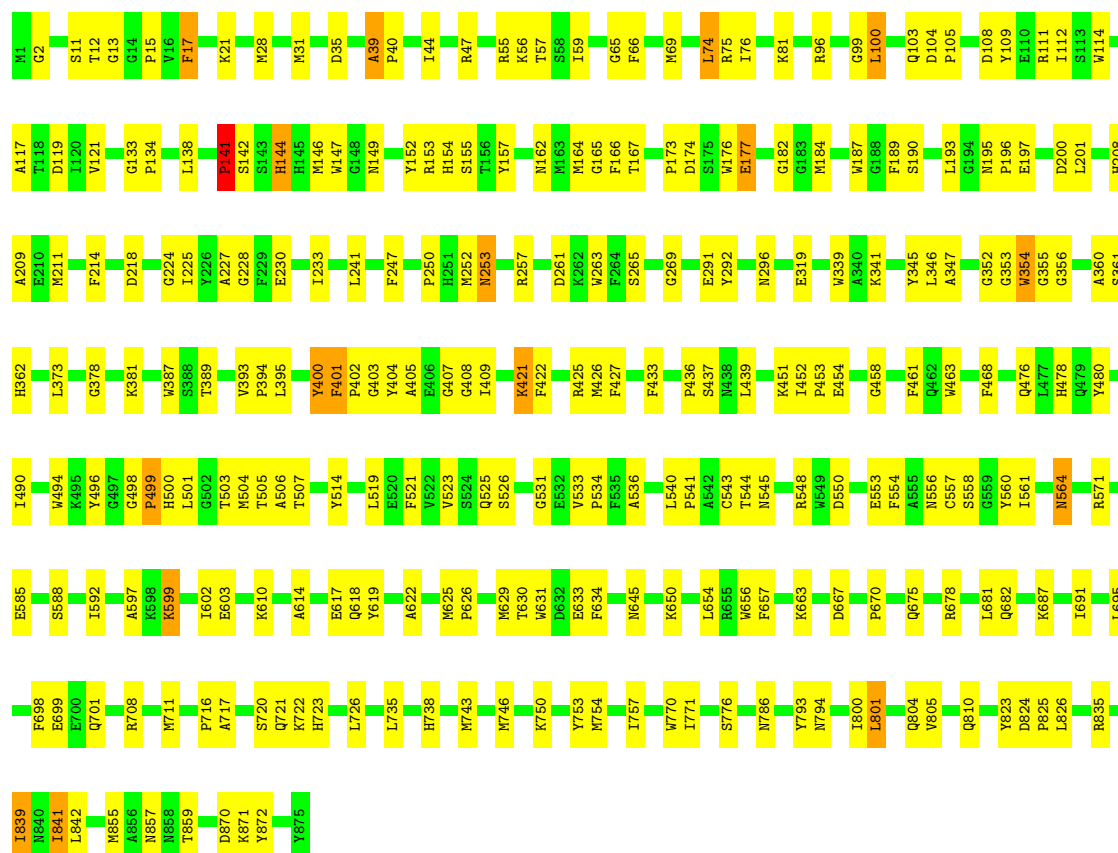
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain O: 68% 30%



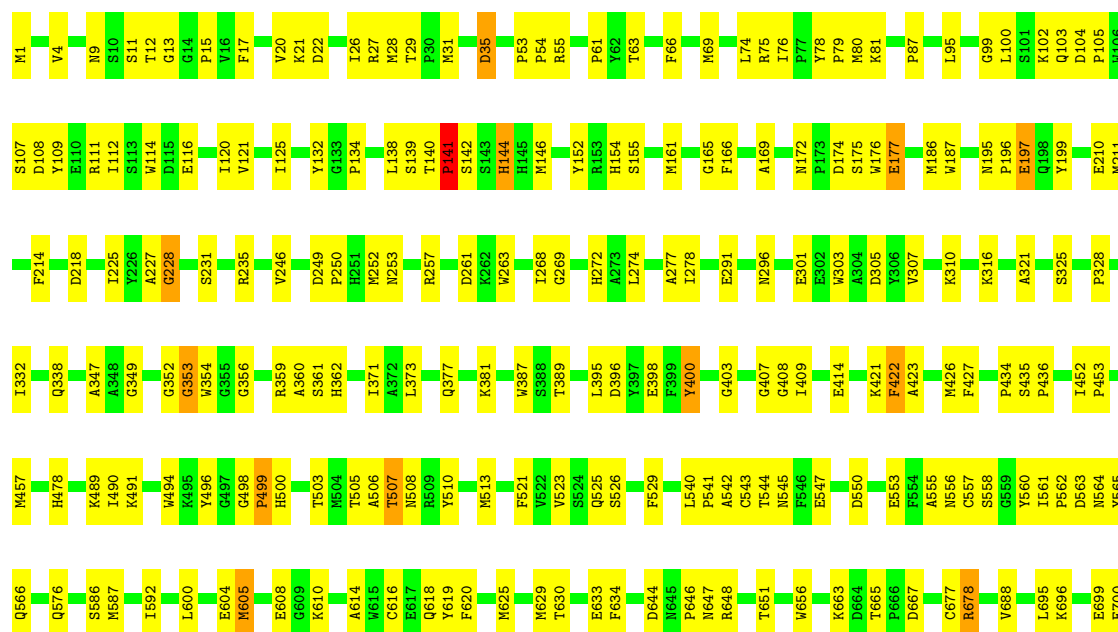
• Molecule 1: Pyrogallol hydroxytransferase large subunit

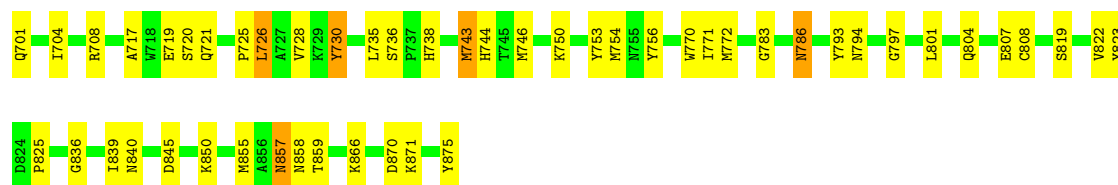
Chain Q:



- Molecule 1: Pyrogallol hydroxytransferase large subunit

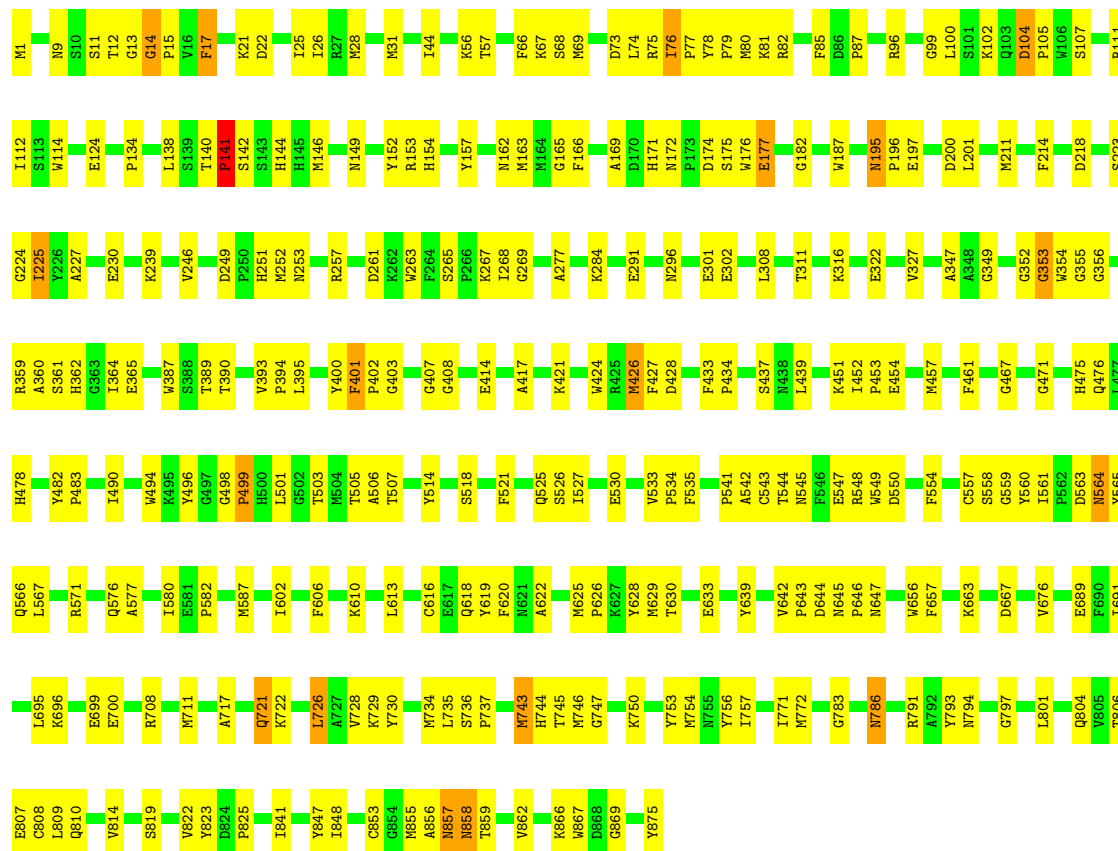
Chain S:





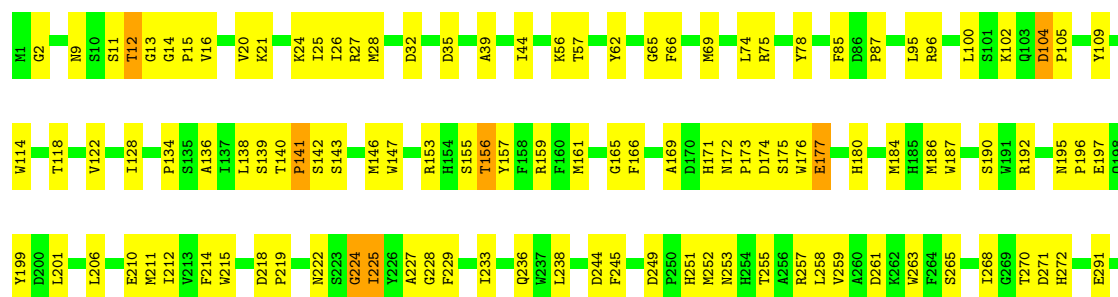
• Molecule 1: Pyrogallol hydroxytransferase large subunit

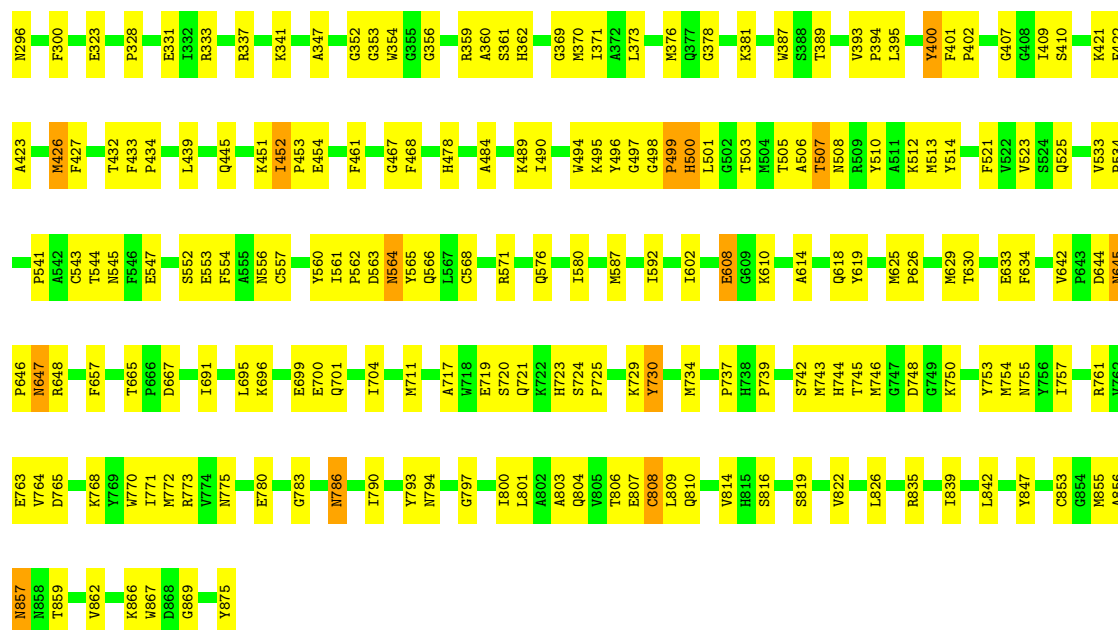
Chain U: 67% 31% .



• Molecule 1: Pyrogallol hydroxytransferase large subunit

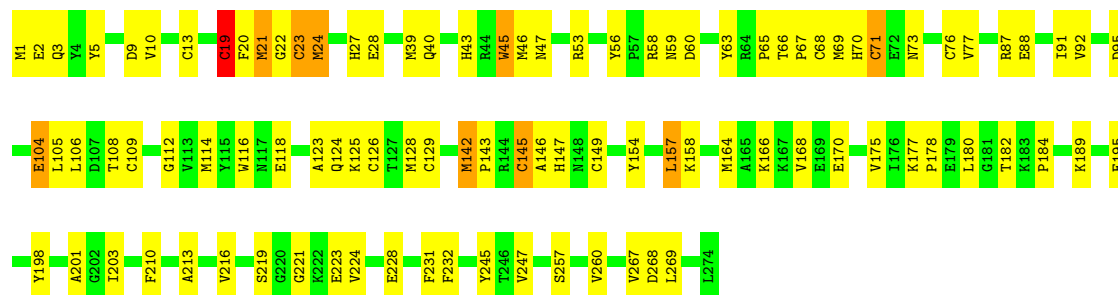
Chain W: 64% 33% .





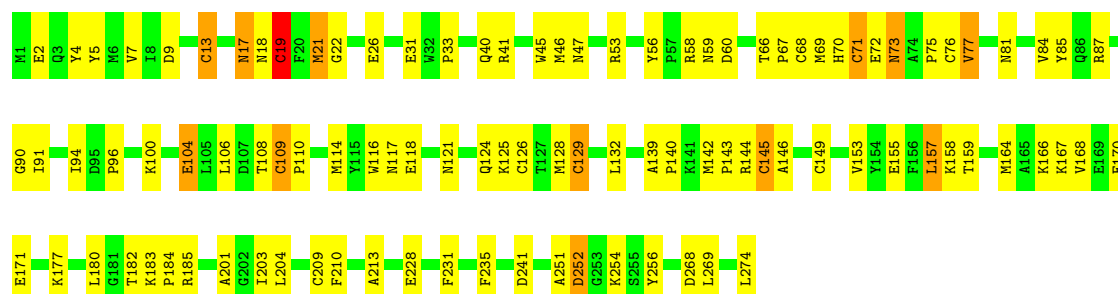
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain B: 64% 32% .



• Molecule 2: Pyrogallol hydroxytransferase small subunit

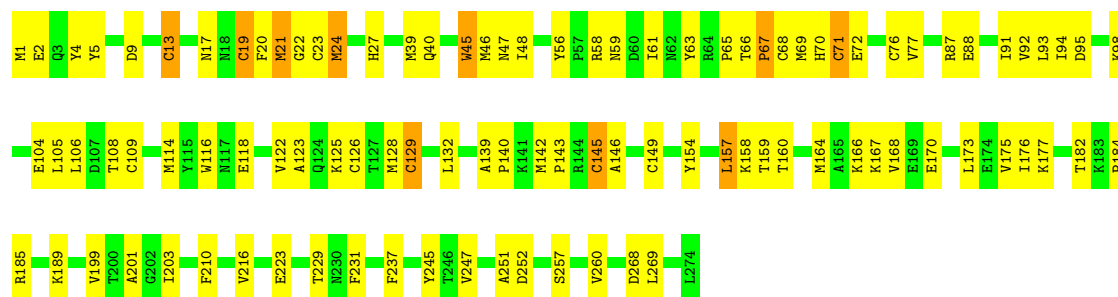
Chain D: 63% 32% .



• Molecule 2: Pyrogallol hydroxytransferase small subunit

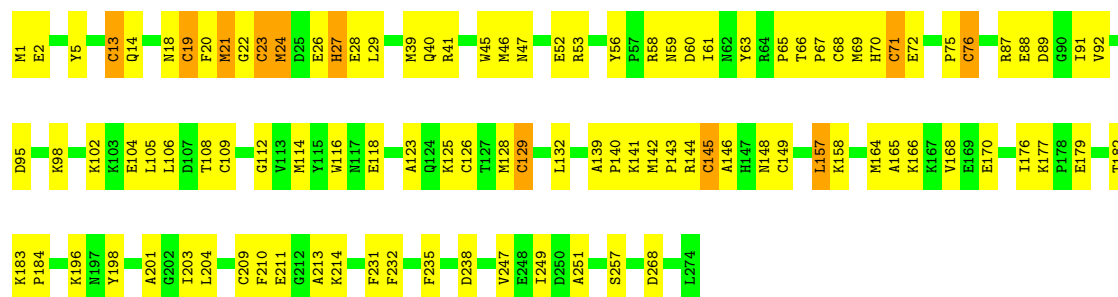
Chain F: 64% 33% .





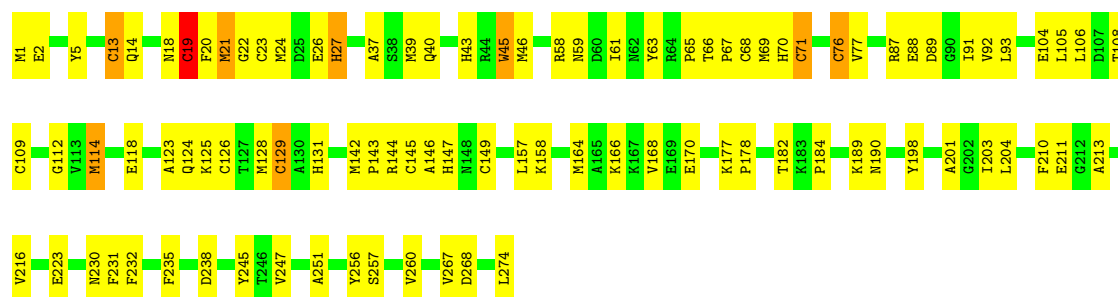
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain H: 62% 34%



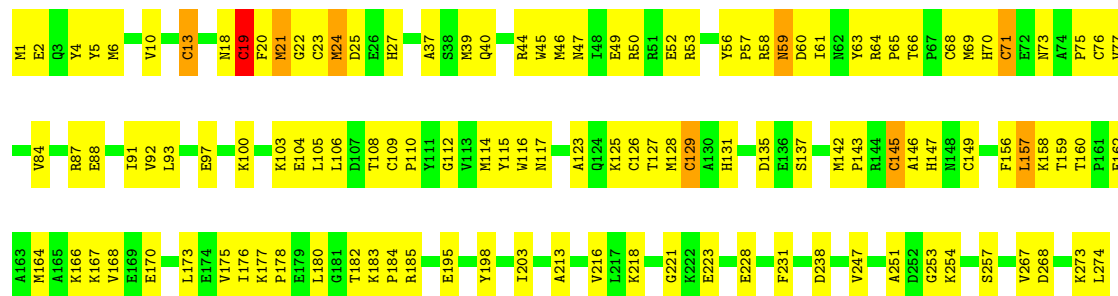
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain J: 65% 32%



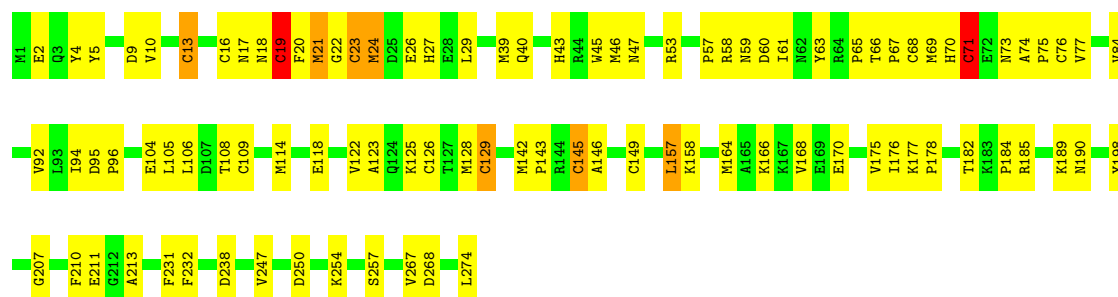
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain L: 56% 41%



- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain N:  65% 32% . .



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain P:  59% 38% .



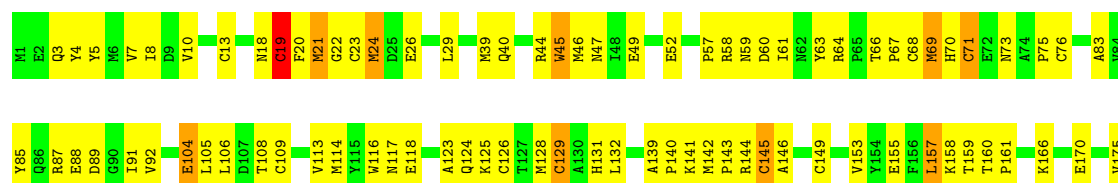
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain R:  68% 29% .



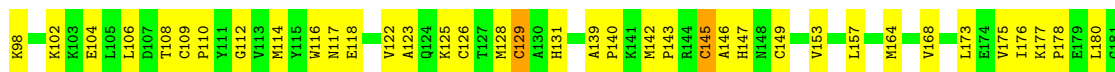
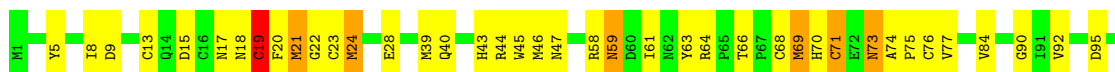
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain T:  58% 38% .

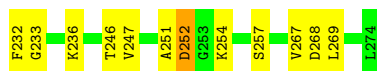
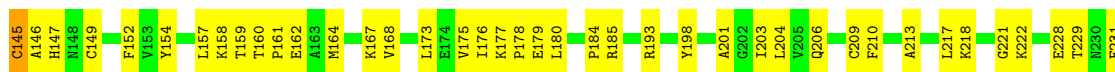
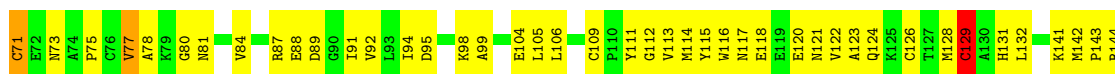




• Molecule 2: Pyrogallol hydroxytransferase small subunit



• Molecule 2: Pyrogallol hydroxytransferase small subunit



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	174.02Å 179.64Å 181.22Å 63.69° 63.98° 64.90°	Depositor
Resolution (Å)	24.98 – 2.35	Depositor
% Data completeness (in resolution range)	86.0 (24.98-2.35)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	122057	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 4MO, CA, MGD, SF4, ACT

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	0.41	0/7240	0.98	47/9815 (0.5%)
1	C	0.39	0/7240	0.97	44/9815 (0.4%)
1	E	0.39	0/7240	0.97	34/9815 (0.3%)
1	G	0.40	0/7240	0.97	46/9815 (0.5%)
1	I	0.40	0/7240	0.96	39/9815 (0.4%)
1	K	0.41	0/7240	0.97	35/9815 (0.4%)
1	M	0.41	0/7240	0.98	51/9815 (0.5%)
1	O	0.40	0/7240	0.97	44/9815 (0.4%)
1	Q	0.41	0/7240	0.98	44/9815 (0.4%)
1	S	0.39	0/7240	0.96	34/9815 (0.3%)
1	U	0.39	0/7240	0.96	38/9815 (0.4%)
1	W	0.37	0/7240	0.95	32/9815 (0.3%)
2	B	0.45	1/2231 (0.0%)	0.97	10/3009 (0.3%)
2	D	0.37	0/2231	0.90	5/3009 (0.2%)
2	F	0.41	0/2231	0.91	5/3009 (0.2%)
2	H	0.41	0/2231	0.93	4/3009 (0.1%)
2	J	0.45	0/2231	0.94	6/3009 (0.2%)
2	L	0.40	0/2231	0.89	5/3009 (0.2%)
2	N	0.45	0/2231	0.96	10/3009 (0.3%)
2	P	0.40	0/2231	0.92	4/3009 (0.1%)
2	R	0.45	0/2231	0.98	9/3009 (0.3%)
2	T	0.37	0/2231	0.89	5/3009 (0.2%)
2	V	0.38	0/2231	0.92	7/3009 (0.2%)
2	X	0.34	0/2231	0.90	6/3009 (0.2%)
All	All	0.40	1/113652 (0.0%)	0.96	564/153888 (0.4%)

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	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	142	MET	SD-CE	-5.90	1.64	1.79

All (564) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	353	GLY	N-CA-C	-9.95	99.91	111.85
1	Q	76	ILE	CA-C-N	9.88	129.52	119.24
1	Q	76	ILE	C-N-CA	9.88	129.52	119.24
2	P	77	VAL	N-CA-C	-9.37	102.73	111.45
1	C	353	GLY	N-CA-C	-9.33	100.66	111.85
1	Q	507	THR	N-CA-C	9.27	123.99	112.87
1	M	507	THR	N-CA-C	9.16	123.86	112.87
1	A	507	THR	N-CA-C	8.97	123.64	112.87
1	U	352	GLY	N-CA-C	-8.96	91.94	113.18
1	S	721	GLN	N-CA-C	8.88	120.96	111.28
1	O	352	GLY	N-CA-C	-8.85	92.21	113.18
1	E	507	THR	N-CA-C	8.80	123.78	112.34
1	K	261	ASP	N-CA-C	-8.79	102.72	113.97
1	A	352	GLY	N-CA-C	-8.73	92.48	113.18
1	S	261	ASP	N-CA-C	-8.66	102.88	113.97
1	U	507	THR	N-CA-C	8.60	123.52	112.34
1	E	352	GLY	N-CA-C	-8.54	92.94	113.18
1	Q	352	GLY	N-CA-C	-8.48	93.08	113.18
1	M	857	ASN	N-CA-C	8.46	121.26	111.11
1	W	352	GLY	N-CA-C	-8.40	93.28	113.18
1	M	352	GLY	N-CA-C	-8.38	93.31	113.18
1	K	507	THR	N-CA-C	8.26	123.08	112.34
1	W	353	GLY	N-CA-C	-8.23	100.00	111.76
1	M	104	ASP	CA-C-N	8.19	128.14	119.05
1	M	104	ASP	C-N-CA	8.19	128.14	119.05
1	C	76	ILE	CA-C-N	8.19	127.49	118.97
1	C	76	ILE	C-N-CA	8.19	127.49	118.97
1	S	857	ASN	N-CA-C	8.14	120.88	111.11
1	K	352	GLY	N-CA-C	-8.10	93.98	113.18
1	G	857	ASN	N-CA-C	8.09	120.82	111.11
1	Q	645	ASN	CA-C-N	8.05	127.77	119.56
1	Q	645	ASN	C-N-CA	8.05	127.77	119.56
1	W	407	GLY	N-CA-C	8.03	124.64	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	407	GLY	N-CA-C	8.03	126.00	115.40
1	O	507	THR	N-CA-C	8.03	122.77	112.34
1	C	352	GLY	N-CA-C	-7.99	94.26	113.18
1	I	352	GLY	N-CA-C	-7.96	94.31	113.18
1	I	645	ASN	CA-C-N	7.89	128.31	119.32
1	I	645	ASN	C-N-CA	7.89	128.31	119.32
1	S	352	GLY	N-CA-C	-7.88	94.52	113.18
1	S	76	ILE	CA-C-N	7.87	127.16	118.97
1	S	76	ILE	C-N-CA	7.87	127.16	118.97
1	C	401	PHE	CA-C-N	7.87	127.92	119.90
1	C	401	PHE	C-N-CA	7.87	127.92	119.90
1	C	645	ASN	CA-C-N	7.85	127.41	119.24
1	C	645	ASN	C-N-CA	7.85	127.41	119.24
2	X	77	VAL	N-CA-C	-7.79	105.17	112.96
1	A	647	ASN	N-CA-C	7.77	120.88	111.40
1	K	407	GLY	N-CA-C	7.70	124.25	115.08
1	G	352	GLY	N-CA-C	-7.69	94.95	113.18
1	K	730	TYR	CA-C-N	7.69	127.32	119.56
1	K	730	TYR	C-N-CA	7.69	127.32	119.56
2	B	77	VAL	N-CA-C	-7.68	102.63	111.00
1	O	857	ASN	N-CA-C	7.59	120.21	111.11
1	U	857	ASN	N-CA-C	7.57	119.17	111.07
1	K	353	GLY	N-CA-C	-7.56	101.61	111.52
1	C	507	THR	N-CA-C	7.51	122.10	112.34
1	W	261	ASP	N-CA-C	-7.46	104.03	113.72
1	E	76	ILE	CA-C-N	7.43	126.69	118.97
1	E	76	ILE	C-N-CA	7.43	126.69	118.97
1	W	730	TYR	CA-C-N	7.43	127.06	119.56
1	W	730	TYR	C-N-CA	7.43	127.06	119.56
1	W	104	ASP	CA-C-N	7.42	126.96	119.24
1	W	104	ASP	C-N-CA	7.42	126.96	119.24
1	E	407	GLY	N-CA-C	7.42	125.19	115.40
2	R	232	PHE	N-CA-C	-7.40	103.84	113.17
1	M	141	PRO	N-CA-C	-7.36	97.30	112.47
1	U	353	GLY	N-CA-C	-7.35	101.25	111.76
1	M	407	GLY	N-CA-C	7.20	123.61	114.25
1	G	645	ASN	CA-C-N	7.19	127.52	119.32
1	G	645	ASN	C-N-CA	7.19	127.52	119.32
1	A	141	PRO	N-CA-C	-7.11	97.82	112.47
1	M	259	VAL	N-CA-C	7.10	118.96	112.43
1	Q	227	ALA	N-CA-C	7.05	120.53	112.57
1	S	353	GLY	N-CA-C	-7.04	100.97	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	645	ASN	CA-C-N	7.01	127.61	119.47
1	E	645	ASN	C-N-CA	7.01	127.61	119.47
1	S	822	VAL	N-CA-C	6.93	118.11	107.99
1	G	500	HIS	N-CA-C	6.91	120.59	111.75
1	O	647	ASN	N-CA-C	6.90	121.53	113.18
1	G	407	GLY	N-CA-C	6.89	123.28	115.08
1	A	227	ALA	N-CA-C	6.86	120.32	112.57
1	I	353	GLY	N-CA-C	-6.85	102.55	111.52
1	W	12	THR	N-CA-C	-6.85	105.00	113.15
1	E	857	ASN	N-CA-C	6.84	119.61	111.33
1	Q	141	PRO	N-CA-C	-6.83	98.41	112.47
1	C	771	ILE	N-CA-C	6.82	118.86	108.71
1	I	104	ASP	CA-C-N	6.79	126.30	119.24
1	I	104	ASP	C-N-CA	6.79	126.30	119.24
1	M	500	HIS	N-CA-C	6.79	120.44	111.75
1	Q	407	GLY	N-CA-C	6.78	124.34	115.40
1	S	407	GLY	N-CA-C	6.76	124.00	115.21
1	G	730	TYR	CA-C-N	6.74	127.32	120.04
1	G	730	TYR	C-N-CA	6.74	127.32	120.04
2	X	45	TRP	N-CA-C	-6.73	104.17	112.38
1	A	422	PHE	N-CA-C	6.72	118.61	111.28
1	O	104	ASP	CA-C-N	6.70	126.20	119.24
1	O	104	ASP	C-N-CA	6.70	126.20	119.24
1	E	104	ASP	CA-C-N	6.69	128.20	119.84
1	E	104	ASP	C-N-CA	6.69	128.20	119.84
1	E	500	HIS	N-CA-C	6.69	121.03	112.34
1	M	353	GLY	N-CA-C	-6.68	102.77	111.52
1	W	192	ARG	N-CA-C	-6.67	103.74	112.41
1	I	141	PRO	N-CA-C	-6.66	98.75	112.47
1	Q	771	ILE	N-CA-C	6.66	118.63	108.71
1	K	141	PRO	N-CA-C	-6.64	98.79	112.47
1	C	730	TYR	CA-C-N	6.64	126.27	119.56
1	C	730	TYR	C-N-CA	6.64	126.27	119.56
1	G	17	PHE	N-CA-C	-6.63	98.43	109.24
2	T	69	MET	N-CA-C	6.62	119.33	111.71
1	G	141	PRO	N-CA-C	-6.62	98.83	112.47
1	M	133	GLY	CA-C-N	6.62	127.15	119.47
1	M	133	GLY	C-N-CA	6.62	127.15	119.47
1	U	261	ASP	N-CA-C	-6.60	105.38	113.50
1	C	793	TYR	N-CA-C	6.60	118.24	108.60
1	K	172	ASN	N-CA-C	-6.58	100.72	110.20
1	Q	393	VAL	CA-C-N	6.58	128.06	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	393	VAL	C-N-CA	6.58	128.06	119.84
1	O	261	ASP	N-CA-C	-6.57	105.56	113.97
1	S	730	TYR	CA-C-N	6.56	126.18	119.56
1	S	730	TYR	C-N-CA	6.56	126.18	119.56
2	L	45	TRP	N-CA-C	-6.55	104.17	111.71
1	E	17	PHE	N-CA-C	-6.55	99.02	109.76
1	O	422	PHE	N-CA-C	6.55	118.08	111.07
1	A	353	GLY	N-CA-C	-6.54	102.41	111.76
1	A	407	GLY	N-CA-C	6.53	124.02	115.40
1	U	400	TYR	N-CA-C	6.53	119.16	108.52
1	U	407	GLY	N-CA-C	6.53	122.85	115.08
1	C	149	ASN	N-CA-C	6.52	118.04	111.07
1	S	771	ILE	N-CA-C	6.51	118.41	108.71
2	D	45	TRP	N-CA-C	-6.49	104.25	111.71
1	S	210	GLU	N-CA-C	-6.49	105.90	113.88
1	K	149	ASN	N-CA-C	6.46	118.33	111.28
1	A	730	TYR	CA-C-N	6.46	126.09	119.56
1	A	730	TYR	C-N-CA	6.46	126.09	119.56
1	E	403	GLY	N-CA-C	-6.46	101.47	112.51
2	B	45	TRP	N-CA-C	-6.45	103.52	111.33
1	I	53	PRO	N-CA-C	6.43	118.55	110.70
2	R	27	HIS	N-CA-C	6.42	122.19	113.97
2	D	241	ASP	N-CA-C	-6.42	101.89	110.55
1	E	730	TYR	CA-C-N	6.42	126.04	119.56
1	E	730	TYR	C-N-CA	6.42	126.04	119.56
1	O	407	GLY	N-CA-C	6.41	123.87	115.40
1	I	507	THR	N-CA-C	6.41	124.45	110.80
2	X	267	VAL	N-CA-C	6.40	117.69	108.48
1	I	273	ALA	N-CA-C	-6.40	104.39	111.36
2	D	77	VAL	N-CA-C	-6.39	104.00	113.39
1	G	224	GLY	N-CA-C	-6.36	98.12	113.18
1	K	771	ILE	N-CA-C	6.34	118.16	108.71
1	O	200	ASP	N-CA-C	6.33	120.33	112.47
1	M	261	ASP	N-CA-C	-6.33	105.71	113.50
1	G	771	ILE	N-CA-C	6.32	118.48	108.87
1	E	224	GLY	N-CA-C	-6.31	98.23	113.18
1	C	857	ASN	N-CA-C	6.30	121.77	111.37
1	Q	401	PHE	CA-C-N	6.30	126.25	119.76
1	Q	401	PHE	C-N-CA	6.30	126.25	119.76
1	M	647	ASN	N-CA-C	6.28	120.14	112.23
1	A	104	ASP	CA-C-N	6.25	125.47	118.97
1	A	104	ASP	C-N-CA	6.25	125.47	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	104	ASP	CA-C-N	6.25	125.99	119.05
1	Q	104	ASP	C-N-CA	6.25	125.99	119.05
1	G	507	THR	N-CA-C	6.25	124.11	110.80
1	O	858	ASN	N-CA-C	6.25	121.99	113.37
1	I	771	ILE	N-CA-C	6.23	117.57	108.53
1	A	857	ASN	N-CA-C	6.20	121.60	111.37
1	Q	403	GLY	N-CA-C	-6.20	103.09	112.89
1	W	109	TYR	N-CA-C	6.19	119.62	109.72
1	K	857	ASN	N-CA-C	6.18	118.53	111.11
1	A	224	GLY	N-CA-C	-6.17	98.56	113.18
1	A	645	ASN	CA-C-N	6.15	126.33	119.32
1	A	645	ASN	C-N-CA	6.15	126.33	119.32
1	G	210	GLU	N-CA-C	-6.15	106.75	114.56
1	U	401	PHE	CA-C-N	6.15	126.09	119.76
1	U	401	PHE	C-N-CA	6.15	126.09	119.76
2	B	27	HIS	N-CA-C	6.15	122.24	114.31
1	Q	353	GLY	N-CA-C	-6.14	103.48	111.52
1	K	227	ALA	N-CA-C	6.13	120.36	112.26
1	M	210	GLU	N-CA-C	-6.13	106.40	114.31
1	W	771	ILE	N-CA-C	6.13	117.40	108.58
1	W	400	TYR	N-CA-C	6.13	118.40	108.41
1	G	824	ASP	CA-C-N	6.12	126.44	119.83
1	G	824	ASP	C-N-CA	6.12	126.44	119.83
1	C	224	GLY	N-CA-C	-6.12	98.69	113.18
2	J	27	HIS	N-CA-C	6.11	121.67	113.72
2	T	267	VAL	N-CA-C	6.11	117.39	108.53
2	J	45	TRP	N-CA-C	-6.11	104.62	111.28
1	O	403	GLY	N-CA-C	-6.10	102.94	112.58
1	U	403	GLY	N-CA-C	-6.10	103.25	112.89
1	O	645	ASN	CA-C-N	6.10	126.27	119.32
1	O	645	ASN	C-N-CA	6.10	126.27	119.32
1	S	688	VAL	N-CA-C	-6.09	100.80	108.84
1	O	149	ASN	N-CA-C	6.07	117.57	111.07
1	C	109	TYR	N-CA-C	6.06	119.58	109.95
1	C	393	VAL	CA-C-N	6.03	127.38	119.84
1	C	393	VAL	C-N-CA	6.03	127.38	119.84
1	O	540	LEU	CA-C-N	6.03	127.37	119.84
1	O	540	LEU	C-N-CA	6.03	127.37	119.84
1	I	393	VAL	CA-C-N	6.02	127.37	119.84
1	I	393	VAL	C-N-CA	6.02	127.37	119.84
1	C	858	ASN	N-CA-C	6.02	121.67	113.37
1	S	500	HIS	N-CA-C	6.01	119.45	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	407	GLY	N-CA-C	6.00	122.23	115.08
1	W	857	ASN	N-CA-C	6.00	118.59	111.33
1	A	822	VAL	N-CA-C	5.99	116.74	107.99
1	K	310	LYS	N-CA-C	5.99	117.81	111.28
1	M	76	ILE	CA-C-N	5.99	125.38	118.85
1	M	76	ILE	C-N-CA	5.99	125.38	118.85
1	A	199	TYR	N-CA-C	5.98	118.72	110.35
2	R	77	VAL	N-CA-C	-5.98	104.68	110.72
1	M	721	GLN	N-CA-C	5.98	118.75	111.82
1	O	325	SER	N-CA-C	5.97	120.84	113.50
1	W	452	ILE	CB-CA-C	-5.97	108.02	114.35
1	C	822	VAL	N-CA-C	5.96	116.69	107.99
2	N	45	TRP	N-CA-C	-5.94	104.81	111.28
1	A	261	ASP	N-CA-C	-5.93	106.20	113.50
1	E	822	VAL	N-CA-C	5.92	116.14	107.37
1	I	149	ASN	N-CA-C	5.92	117.74	111.28
1	Q	261	ASP	N-CA-C	-5.92	105.89	113.23
1	A	76	ILE	CA-C-N	5.92	127.23	119.84
1	A	76	ILE	C-N-CA	5.92	127.23	119.84
2	N	27	HIS	N-CA-C	5.91	121.15	113.88
1	I	261	ASP	N-CA-C	-5.91	105.16	112.90
1	Q	208	HIS	N-CA-C	5.91	121.93	114.31
2	R	154	TYR	N-CA-C	5.91	119.45	109.76
1	A	500	HIS	N-CA-C	5.91	119.31	111.75
1	Q	422	PHE	N-CA-C	5.90	117.39	111.07
1	C	218	ASP	CA-C-N	5.89	125.37	119.24
1	C	218	ASP	C-N-CA	5.89	125.37	119.24
2	J	77	VAL	N-CA-C	-5.89	104.58	111.00
1	M	224	GLY	N-CA-C	-5.89	99.23	113.18
1	E	141	PRO	N-CA-C	-5.88	100.35	112.47
1	S	422	PHE	N-CA-C	5.87	117.37	110.97
2	N	19	CYS	CB-CA-C	-5.86	98.76	110.42
1	W	507	THR	N-CA-C	5.86	123.28	110.80
2	F	27	HIS	N-CA-C	5.86	121.33	113.72
1	S	12	THR	N-CA-C	-5.86	106.18	113.15
1	S	197	GLU	N-CA-C	-5.85	102.81	110.53
1	Q	109	TYR	N-CA-C	5.84	119.19	110.14
2	L	267	VAL	N-CA-C	5.84	117.00	108.53
1	M	236	GLN	N-CA-C	-5.84	105.00	111.36
1	Q	224	GLY	N-CA-C	-5.83	99.36	113.18
1	C	296	ASN	N-CA-C	5.83	120.40	112.88
1	G	353	GLY	N-CA-C	-5.83	104.24	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	400	TYR	N-CA-C	5.83	118.02	108.52
1	O	463	TRP	N-CA-C	5.83	115.93	108.24
1	Q	17	PHE	N-CA-C	-5.83	99.79	109.46
1	S	400	TYR	N-CA-C	5.83	118.30	107.99
1	U	149	ASN	N-CA-C	5.82	117.30	111.07
2	B	195	GLU	N-CA-C	5.82	120.45	113.23
2	V	45	TRP	N-CA-C	-5.82	105.01	111.71
1	G	254	HIS	N-CA-C	5.82	118.40	111.71
1	G	311	THR	N-CA-C	5.82	118.84	111.69
1	A	793	TYR	N-CA-C	5.81	117.68	108.79
1	U	104	ASP	CA-C-N	5.81	127.10	119.84
1	U	104	ASP	C-N-CA	5.81	127.10	119.84
1	E	824	ASP	CA-C-N	5.81	125.74	119.76
1	E	824	ASP	C-N-CA	5.81	125.74	119.76
2	B	19	CYS	CB-CA-C	-5.80	98.87	110.42
1	U	518	SER	N-CA-C	-5.80	105.70	112.89
1	K	199	TYR	N-CA-C	5.77	118.43	110.35
1	A	133	GLY	CA-C-N	5.77	125.63	119.28
1	A	133	GLY	C-N-CA	5.77	125.63	119.28
1	M	400	TYR	N-CA-C	5.77	117.93	108.52
1	U	721	GLN	N-CA-C	5.77	118.52	111.82
1	G	567	LEU	N-CA-C	-5.77	106.07	113.23
1	I	400	TYR	N-CA-C	5.76	117.92	108.52
1	O	227	ALA	N-CA-C	5.76	119.53	111.30
1	M	74	LEU	N-CA-C	-5.75	105.84	112.92
1	O	192	ARG	N-CA-C	-5.75	105.58	112.59
1	E	807	GLU	N-CA-C	-5.74	106.25	113.72
1	E	109	TYR	N-CA-C	5.74	119.04	110.14
1	O	109	TYR	N-CA-C	5.74	119.04	110.14
2	V	232	PHE	N-CA-C	-5.74	105.94	113.17
1	K	403	GLY	N-CA-C	-5.73	102.71	112.51
1	W	227	ALA	N-CA-C	5.73	119.82	112.26
1	K	76	ILE	CA-C-N	5.72	125.25	119.19
1	K	76	ILE	C-N-CA	5.72	125.25	119.19
1	A	721	GLN	N-CA-C	5.71	117.59	111.36
2	R	267	VAL	N-CA-C	5.71	116.81	108.53
1	S	647	ASN	N-CA-C	5.71	120.40	113.38
1	E	452	ILE	CB-CA-C	-5.70	108.31	114.35
1	A	393	VAL	CA-C-N	5.70	126.97	119.84
1	A	393	VAL	C-N-CA	5.70	126.97	119.84
1	M	144	HIS	N-CA-C	5.70	118.98	110.14
1	Q	144	HIS	N-CA-C	5.70	118.89	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	327	VAL	CA-C-N	5.70	126.03	119.93
1	C	327	VAL	C-N-CA	5.70	126.03	119.93
1	K	721	GLN	N-CA-C	5.69	117.48	111.28
2	F	17	ASN	N-CA-C	5.69	119.52	112.24
1	K	109	TYR	N-CA-C	5.69	118.99	109.95
1	W	822	VAL	N-CA-C	5.68	116.04	107.80
1	I	109	TYR	N-CA-C	5.68	118.94	110.14
1	U	793	TYR	N-CA-C	5.67	116.89	108.60
1	W	224	GLY	N-CA-C	-5.67	99.73	113.18
1	Q	500	HIS	N-CA-C	5.67	119.01	111.75
1	O	210	GLU	N-CA-C	-5.67	107.36	114.56
1	M	227	ALA	N-CA-C	5.66	119.49	112.59
1	M	771	ILE	N-CA-C	5.66	117.14	108.71
2	J	267	VAL	N-CA-C	5.66	116.62	108.48
1	S	793	TYR	N-CA-C	5.65	116.85	108.60
1	O	721	GLN	N-CA-C	5.65	117.11	111.07
2	N	23	CYS	CB-CA-C	-5.64	102.02	110.88
1	C	721	GLN	N-CA-C	5.63	117.10	111.07
1	I	647	ASN	N-CA-C	5.63	119.87	112.89
1	A	452	ILE	CB-CA-C	-5.63	108.38	114.35
2	D	19	CYS	CB-CA-C	-5.63	102.23	110.95
1	I	824	ASP	CA-C-N	5.62	125.55	119.76
1	I	824	ASP	C-N-CA	5.62	125.55	119.76
1	O	144	HIS	N-CA-C	5.62	118.77	110.46
1	C	500	HIS	N-CA-C	5.61	119.64	112.34
1	M	31	MET	N-CA-C	5.61	118.11	109.07
2	B	224	VAL	N-CA-C	-5.61	108.03	113.53
1	K	500	HIS	N-CA-C	5.61	118.93	111.75
1	Q	39	ALA	CA-C-N	5.61	125.56	119.78
1	Q	39	ALA	C-N-CA	5.61	125.56	119.78
1	G	400	TYR	N-CA-C	5.61	117.66	108.52
2	F	154	TYR	N-CA-C	5.60	119.19	110.17
1	I	463	TRP	N-CA-C	5.60	115.51	108.45
1	U	689	GLU	N-CA-C	5.60	117.85	107.99
1	I	218	ASP	CA-C-N	5.60	125.06	119.24
1	I	218	ASP	C-N-CA	5.60	125.06	119.24
1	O	393	VAL	CA-C-N	5.60	126.83	119.84
1	O	393	VAL	C-N-CA	5.60	126.83	119.84
1	C	325	SER	N-CA-C	5.58	120.37	113.50
1	C	452	ILE	CB-CA-C	-5.58	108.43	114.35
1	E	353	GLY	N-CA-C	-5.58	104.21	111.52
1	M	109	TYR	N-CA-C	5.58	118.79	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	267	VAL	N-CA-C	5.58	116.52	108.48
2	D	13	CYS	CA-CB-SG	-5.58	101.56	114.40
1	G	592	ILE	N-CA-C	-5.57	105.07	110.42
1	A	403	GLY	N-CA-C	-5.57	102.98	112.51
1	W	210	GLU	N-CA-C	-5.57	107.12	114.31
1	S	172	ASN	N-CA-C	-5.57	102.11	110.24
2	V	267	VAL	N-CA-C	5.57	116.49	108.48
1	I	227	ALA	N-CA-C	5.56	120.38	111.81
1	O	241	LEU	N-CA-C	-5.56	106.17	113.17
1	Q	526	SER	N-CA-C	5.55	116.69	108.86
1	A	691	ILE	N-CA-C	-5.54	97.91	106.72
1	G	647	ASN	N-CA-C	5.54	119.21	112.23
2	R	45	TRP	N-CA-C	-5.54	104.62	111.33
1	O	141	PRO	N-CA-C	-5.54	101.06	112.47
1	C	227	ALA	N-CA-C	5.54	119.03	112.72
1	M	736	SER	CA-C-N	5.53	126.75	119.84
1	M	736	SER	C-N-CA	5.53	126.75	119.84
1	O	435	SER	CA-C-N	5.53	125.50	120.03
1	O	435	SER	C-N-CA	5.53	125.50	120.03
2	L	195	GLU	N-CA-C	5.53	118.49	111.69
1	K	144	HIS	N-CA-C	5.52	118.63	110.46
1	W	645	ASN	CA-C-N	5.52	125.19	119.56
1	W	645	ASN	C-N-CA	5.52	125.19	119.56
1	G	199	TYR	N-CA-C	5.51	118.01	110.24
1	S	507	THR	N-CA-C	5.51	122.54	110.80
1	K	218	ASP	CA-C-N	5.51	126.73	119.84
1	K	218	ASP	C-N-CA	5.51	126.73	119.84
2	T	19	CYS	CB-CA-C	-5.50	102.48	110.96
1	Q	463	TRP	N-CA-C	5.50	116.33	108.74
1	M	17	PHE	N-CA-C	-5.50	100.28	109.24
1	M	463	TRP	N-CA-C	5.50	116.32	108.74
1	O	296	ASN	N-CA-C	5.49	119.29	112.59
1	W	500	HIS	N-CA-C	5.49	117.97	111.33
1	K	224	GLY	N-CA-C	-5.49	100.18	113.18
2	R	19	CYS	CB-CA-C	-5.48	99.51	110.42
1	A	771	ILE	N-CA-C	5.48	116.87	108.71
1	W	647	ASN	N-CA-C	5.48	120.24	113.50
1	I	17	PHE	N-CA-C	-5.47	100.32	109.24
1	K	200	ASP	N-CA-C	5.47	118.98	111.54
1	O	169	ALA	N-CA-C	-5.47	96.95	107.57
1	U	200	ASP	N-CA-C	5.47	119.12	111.90
1	Q	200	ASP	N-CA-C	5.47	119.12	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	156	THR	N-CA-C	5.47	117.05	111.14
1	U	645	ASN	CA-C-N	5.47	125.12	119.05
1	U	645	ASN	C-N-CA	5.47	125.12	119.05
1	U	841	ILE	N-CA-C	-5.47	104.25	111.09
1	A	109	TYR	N-CA-C	5.46	118.61	110.14
1	W	14	GLY	CA-C-N	5.46	125.41	119.78
1	W	14	GLY	C-N-CA	5.46	125.41	119.78
1	K	735	LEU	N-CA-C	-5.46	100.99	109.72
1	I	793	TYR	N-CA-C	5.45	117.36	109.07
1	O	730	TYR	CA-C-N	5.45	125.27	119.28
1	O	730	TYR	C-N-CA	5.45	125.27	119.28
1	O	224	GLY	N-CA-C	-5.45	100.27	113.18
1	E	793	TYR	N-CA-C	5.45	117.35	109.07
1	S	435	SER	CA-C-N	5.44	125.42	120.03
1	S	435	SER	C-N-CA	5.44	125.42	120.03
1	E	39	ALA	CA-C-N	5.44	125.35	119.85
1	E	39	ALA	C-N-CA	5.44	125.35	119.85
1	G	208	HIS	N-CA-C	5.44	120.57	113.88
1	U	195	ASN	CA-C-N	5.44	125.64	120.31
1	U	195	ASN	C-N-CA	5.44	125.64	120.31
1	E	63	THR	N-CA-C	-5.43	106.78	113.41
1	M	540	LEU	CA-C-N	5.43	126.63	119.84
1	M	540	LEU	C-N-CA	5.43	126.63	119.84
1	E	552	SER	N-CA-C	5.43	115.53	107.88
1	U	12	THR	N-CA-C	-5.42	106.74	113.19
1	M	691	ILE	N-CA-C	-5.41	98.11	106.72
1	I	822	VAL	N-CA-C	5.41	115.89	107.99
2	X	16	CYS	N-CA-C	-5.41	106.84	113.50
2	V	17	ASN	N-CA-C	5.40	119.17	112.58
1	C	540	LEU	CA-C-N	5.40	126.59	119.84
1	C	540	LEU	C-N-CA	5.40	126.59	119.84
1	E	144	HIS	N-CA-C	5.39	118.06	110.14
1	I	409	ILE	N-CA-C	5.39	119.72	112.98
1	Q	74	LEU	N-CA-C	-5.39	106.29	112.92
1	W	199	TYR	N-CA-C	5.39	117.84	110.24
1	C	261	ASP	N-CA-C	-5.38	106.77	113.38
2	F	45	TRP	N-CA-C	-5.38	105.42	111.28
2	R	23	CYS	CB-CA-C	-5.38	102.68	110.96
2	N	71	CYS	N-CA-C	5.37	118.02	110.23
2	N	95	ASP	CA-C-N	5.37	126.55	119.84
2	N	95	ASP	C-N-CA	5.37	126.55	119.84
1	A	738	HIS	CA-C-N	5.36	125.62	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	HIS	C-N-CA	5.36	125.62	119.83
1	G	721	GLN	N-CA-C	5.35	118.02	111.82
1	G	557	CYS	N-CA-C	-5.35	106.81	113.55
2	P	150	GLY	N-CA-C	-5.35	106.50	115.80
1	S	144	HIS	N-CA-C	5.35	118.43	110.14
1	S	403	GLY	N-CA-C	-5.34	104.52	113.02
1	U	76	ILE	CA-C-N	5.34	124.67	118.85
1	U	76	ILE	C-N-CA	5.34	124.67	118.85
1	M	836	GLY	N-CA-C	-5.34	105.93	112.77
1	W	172	ASN	N-CA-C	-5.34	102.72	110.08
1	M	393	VAL	CA-C-N	5.33	126.51	119.84
1	M	393	VAL	C-N-CA	5.33	126.51	119.84
1	E	197	GLU	N-CA-C	-5.33	102.99	110.50
1	U	141	PRO	N-CA-C	-5.33	101.49	112.47
1	I	689	GLU	N-CA-C	5.33	117.37	107.99
1	C	647	ASN	N-CA-C	5.32	119.49	112.89
1	Q	536	ALA	N-CA-C	5.32	117.73	110.55
1	U	647	ASN	N-CA-C	5.32	119.03	112.54
1	G	473	ILE	N-CA-C	5.31	116.68	110.62
2	R	37	ALA	N-CA-C	-5.31	103.68	110.53
1	C	145	HIS	N-CA-CB	-5.31	103.49	111.56
1	G	793	TYR	N-CA-C	5.31	117.14	109.07
2	L	19	CYS	CB-CA-C	-5.31	99.85	110.42
1	E	678	ARG	N-CA-C	5.31	118.52	111.30
1	K	497	GLY	N-CA-C	-5.30	104.96	112.81
1	A	144	HIS	N-CA-C	5.30	118.64	110.42
1	K	422	PHE	N-CA-C	5.30	116.74	111.07
1	U	17	PHE	N-CA-C	-5.29	100.61	109.24
2	V	74	ALA	CA-C-N	5.29	124.47	118.97
2	V	74	ALA	C-N-CA	5.29	124.47	118.97
1	Q	341	LYS	N-CA-C	5.29	119.58	113.18
1	S	109	TYR	N-CA-C	5.29	118.34	110.14
2	X	232	PHE	N-CA-C	-5.28	106.68	113.02
1	I	224	GLY	N-CA-C	-5.28	100.67	113.18
1	G	452	ILE	CB-CA-C	-5.28	108.69	113.70
1	U	822	VAL	N-CA-C	5.27	115.68	107.99
2	J	19	CYS	CB-CA-C	-5.27	99.94	110.42
1	G	74	LEU	N-CA-C	-5.26	106.45	112.92
2	F	77	VAL	N-CA-C	-5.25	105.28	111.00
1	M	53	PRO	N-CA-C	5.25	117.10	110.70
2	T	45	TRP	N-CA-C	-5.24	105.57	111.28
2	B	23	CYS	CB-CA-C	-5.24	102.66	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	218	ASP	CA-C-N	5.24	125.29	119.32
1	G	218	ASP	C-N-CA	5.24	125.29	119.32
1	U	227	ALA	N-CA-C	5.23	119.63	112.88
1	Q	400	TYR	N-CA-C	5.23	117.05	108.52
1	Q	133	GLY	CA-C-N	5.23	125.28	119.32
1	Q	133	GLY	C-N-CA	5.23	125.28	119.32
1	M	645	ASN	CA-C-N	5.22	126.37	119.84
1	M	645	ASN	C-N-CA	5.22	126.37	119.84
1	M	526	SER	N-CA-C	5.22	116.60	109.18
1	K	822	VAL	N-CA-C	5.22	115.29	107.51
2	H	27	HIS	N-CA-C	5.22	120.30	113.88
1	M	39	ALA	CA-C-N	5.22	125.15	119.78
1	M	39	ALA	C-N-CA	5.22	125.15	119.78
1	S	141	PRO	N-CA-C	-5.21	101.74	112.47
1	A	230	GLU	N-CA-C	5.21	117.63	111.33
2	L	37	ALA	N-CA-C	-5.21	103.04	110.59
1	W	426	MET	N-CA-C	5.20	117.03	111.36
2	J	37	ALA	N-CA-C	-5.20	103.17	110.35
1	G	393	VAL	CA-C-N	5.19	126.33	119.84
1	G	393	VAL	C-N-CA	5.19	126.33	119.84
1	A	325	SER	N-CA-C	5.19	119.88	113.50
1	U	14	GLY	CA-C-N	5.18	125.09	119.85
1	U	14	GLY	C-N-CA	5.18	125.09	119.85
1	K	645	ASN	CA-C-N	5.18	126.32	119.84
1	K	645	ASN	C-N-CA	5.18	126.32	119.84
1	G	273	ALA	N-CA-C	-5.18	105.32	111.69
2	H	232	PHE	N-CA-C	-5.18	106.64	113.17
1	A	74	LEU	N-CA-C	-5.17	106.75	113.16
1	A	208	HIS	N-CA-C	5.17	120.98	114.31
1	I	63	THR	N-CA-C	-5.17	105.27	112.45
1	M	611	ASP	N-CA-C	-5.17	102.37	110.17
1	C	141	PRO	N-CA-C	-5.17	101.83	112.47
1	O	793	TYR	N-CA-C	5.16	116.14	108.60
1	U	858	ASN	N-CA-C	5.16	121.80	110.80
1	A	273	ALA	N-CA-C	-5.16	105.73	111.36
1	C	172	ASN	N-CA-C	-5.16	102.70	110.24
1	O	537	ASP	N-CA-C	-5.16	107.11	113.41
1	I	592	ILE	N-CA-C	-5.16	105.68	110.53
1	Q	354	TRP	CB-CA-C	-5.16	109.08	115.89
1	G	76	ILE	CA-C-N	5.15	124.47	118.85
1	G	76	ILE	C-N-CA	5.15	124.47	118.85
1	M	689	GLU	N-CA-C	5.15	117.06	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	16	VAL	N-CA-C	5.15	116.07	108.45
1	Q	824	ASP	CA-C-N	5.15	125.06	119.76
1	Q	824	ASP	C-N-CA	5.15	125.06	119.76
1	E	227	ALA	N-CA-C	5.14	119.12	111.87
1	I	144	HIS	N-CA-C	5.14	118.39	110.42
1	G	227	ALA	N-CA-C	5.14	119.05	112.26
1	G	109	TYR	N-CA-C	5.14	118.11	110.14
1	A	255	THR	N-CA-C	-5.14	105.76	111.36
1	G	678	ARG	N-CA-C	5.13	118.28	111.30
1	C	403	GLY	N-CA-C	-5.13	103.73	112.51
1	S	199	TYR	N-CA-C	5.13	117.33	110.35
1	G	326	GLY	N-CA-C	-5.12	108.26	114.92
1	M	197	GLU	N-CA-C	-5.12	103.28	110.50
1	U	736	SER	CA-C-N	5.11	126.23	119.84
1	U	736	SER	C-N-CA	5.11	126.23	119.84
1	I	858	ASN	N-CA-C	5.11	120.42	113.37
1	K	393	VAL	CA-C-N	5.11	126.23	119.84
1	K	393	VAL	C-N-CA	5.11	126.23	119.84
1	M	208	HIS	N-CA-C	5.11	120.90	114.31
1	A	474	SER	N-CA-C	5.11	119.49	113.16
1	I	176	TRP	N-CA-C	5.10	119.65	113.38
1	G	689	GLU	N-CA-C	5.10	116.96	107.99
1	Q	841	ILE	N-CA-C	-5.10	105.41	112.50
2	P	232	PHE	N-CA-C	-5.09	106.75	113.17
1	Q	793	TYR	N-CA-C	5.09	116.81	109.07
2	V	69	MET	N-CA-C	5.09	118.75	112.54
1	G	858	ASN	N-CA-C	5.09	121.64	110.80
2	T	232	PHE	N-CA-C	-5.09	106.76	113.17
1	C	86	ASP	CA-C-N	5.09	125.12	119.32
1	C	86	ASP	C-N-CA	5.09	125.12	119.32
1	C	17	PHE	N-CA-C	-5.08	100.95	109.24
1	O	172	ASN	N-CA-C	-5.08	103.06	110.08
1	S	296	ASN	N-CA-C	5.08	119.44	112.88
2	B	95	ASP	CA-C-N	5.08	125.11	119.32
2	B	95	ASP	C-N-CA	5.08	125.11	119.32
2	N	232	PHE	N-CA-C	-5.08	106.78	113.17
1	M	678	ARG	N-CA-C	5.07	118.44	111.54
1	M	592	ILE	N-CA-C	-5.07	105.76	110.53
1	A	574	SER	N-CA-C	5.07	117.50	109.50
1	O	63	THR	N-CA-C	-5.07	107.23	113.41
2	P	241	ASP	N-CA-C	-5.06	103.25	110.59
1	Q	230	GLU	N-CA-C	5.06	116.80	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	325	SER	N-CA-C	5.06	119.53	112.90
1	U	172	ASN	N-CA-C	-5.05	103.11	110.08
1	S	807	GLU	N-CA-C	-5.05	107.15	113.72
2	H	45	TRP	N-CA-C	-5.05	105.22	111.33
1	M	701	GLN	N-CA-C	-5.05	107.09	113.20
1	G	853	CYS	N-CA-C	5.04	117.69	110.68
1	E	608	GLU	N-CA-C	-5.04	106.71	112.86
1	A	17	PHE	N-CA-C	-5.04	101.03	109.24
1	G	209	ALA	N-CA-C	5.04	117.34	110.24
1	M	403	GLY	N-CA-C	-5.04	103.90	112.51
2	H	23	CYS	CB-CA-C	-5.02	103.22	110.96
1	K	400	TYR	N-CA-C	5.02	117.43	109.24
1	W	793	TYR	N-CA-C	5.02	115.16	108.38
1	I	503	THR	N-CA-C	5.02	121.09	114.12
1	A	578	LYS	N-CA-C	-5.01	99.61	108.23
2	N	267	VAL	N-CA-C	5.01	115.70	108.48
1	U	230	GLU	N-CA-C	5.01	116.75	111.28
1	C	678	ARG	N-CA-C	5.01	118.36	111.54
2	N	74	ALA	N-CA-C	5.01	118.51	109.44
1	I	736	SER	CA-C-N	5.01	126.10	119.84
1	I	736	SER	C-N-CA	5.01	126.10	119.84
1	Q	149	ASN	N-CA-C	5.01	116.55	111.14
1	S	836	GLY	N-CA-C	-5.01	106.69	112.50
2	X	27	HIS	N-CA-C	5.01	119.86	113.55
1	A	611	ASP	N-CA-C	-5.00	102.62	110.17
1	O	76	ILE	CA-C-N	5.00	124.30	118.85
1	O	76	ILE	C-N-CA	5.00	124.30	118.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	847	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7018	0	6645	201	0
1	C	7018	0	6645	217	0
1	E	7018	0	6645	188	0
1	G	7018	0	6645	216	0
1	I	7018	0	6645	199	0
1	K	7018	0	6645	208	0
1	M	7018	0	6645	203	0
1	O	7018	0	6645	215	0
1	Q	7018	0	6645	195	0
1	S	7018	0	6645	223	0
1	U	7018	0	6645	251	0
1	W	7018	0	6645	254	0
2	B	2182	0	2077	85	0
2	D	2182	0	2077	96	0
2	F	2182	0	2077	88	0
2	H	2182	0	2077	97	0
2	J	2182	0	2077	87	0
2	L	2182	0	2077	108	0
2	N	2182	0	2077	88	0
2	P	2182	0	2077	114	0
2	R	2182	0	2077	80	0
2	T	2182	0	2077	110	0
2	V	2182	0	2077	96	0
2	X	2182	0	2077	146	0
3	A	4	0	3	1	0
3	C	4	0	3	3	0
3	E	4	0	3	2	0
3	G	4	0	3	3	0
3	I	4	0	3	3	0
3	K	4	0	3	3	0
3	M	4	0	3	1	0
3	O	4	0	3	2	0
3	Q	4	0	3	1	0
3	S	4	0	3	1	0
3	U	4	0	3	1	0
3	W	4	0	3	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
4	X	1	0	0	0	0
5	A	94	0	44	12	0
5	C	94	0	44	11	0
5	E	94	0	44	8	0
5	G	94	0	44	10	0
5	I	94	0	44	12	0
5	K	94	0	44	10	0
5	M	94	0	44	11	0
5	O	94	0	44	10	0
5	Q	94	0	44	9	0
5	S	94	0	44	11	0
5	U	94	0	44	14	0
5	W	94	0	44	13	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
6	M	1	0	0	0	0
6	O	1	0	0	0	0
6	Q	1	0	0	0	0
6	S	1	0	0	0	0
6	U	1	0	0	0	0
6	W	1	0	0	0	0
7	B	24	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	24	0	0	5	0
7	F	24	0	0	3	0
7	H	24	0	0	5	0
7	J	24	0	0	3	0
7	L	24	0	0	6	0
7	N	24	0	0	4	0
7	P	24	0	0	6	0
7	R	24	0	0	5	0
7	T	24	0	0	7	0
7	V	24	0	0	4	0
7	X	24	0	0	7	0
8	A	688	0	0	20	0
8	B	167	0	0	5	0
8	C	684	0	0	18	0
8	D	167	0	0	4	0
8	E	684	0	0	22	0
8	F	167	0	0	1	0
8	G	689	0	0	19	0
8	H	162	0	0	6	0
8	I	675	0	0	20	0
8	J	170	0	0	3	0
8	K	684	0	0	25	0
8	L	168	0	0	9	0
8	M	683	0	0	16	0
8	N	163	0	0	6	0
8	O	679	0	0	21	0
8	P	163	0	0	6	0
8	Q	692	0	0	20	0
8	R	166	0	0	3	0
8	S	675	0	0	21	0
8	T	159	0	0	4	0
8	U	667	0	0	26	0
8	V	163	0	0	6	0
8	W	677	0	0	27	0
8	X	165	0	0	12	0
All	All	122057	0	105228	3673	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 17.

All (3673) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:19:CYS:HB3	2:L:145:CYS:HB3	1.19	1.09
2:T:19:CYS:HB3	2:T:145:CYS:HB3	1.37	1.03
2:N:2:GLU:HG2	2:N:158:LYS:HG2	1.40	1.02
1:A:557:CYS:H	1:A:564:ASN:HD21	1.07	1.02
2:P:19:CYS:HB3	2:P:145:CYS:HB3	1.40	1.01
1:U:753:TYR:HB3	2:V:24:MET:HE3	1.41	1.01
1:Q:557:CYS:H	1:Q:564:ASN:HD21	1.01	1.00
2:X:69:MET:HB3	2:X:184:PRO:HB3	1.43	1.00
1:A:66:PHE:HA	1:A:69:MET:HE3	1.44	1.00
2:P:143:PRO:HB3	7:P:303:SF4:S1	2.03	0.99
2:N:207:GLY:HA2	1:S:728:VAL:HG12	1.40	0.99
2:R:207:GLY:HA2	1:U:728:VAL:HG12	1.42	0.99
2:V:69:MET:HB3	2:V:184:PRO:HB3	1.42	0.99
1:S:557:CYS:H	1:S:564:ASN:HD21	1.01	0.99
1:S:604:GLU:HB3	1:S:605:MET:HE3	1.45	0.99
2:L:143:PRO:HB3	7:L:303:SF4:S1	2.03	0.98
2:L:59:ASN:HD22	2:L:59:ASN:H	1.11	0.98
2:D:143:PRO:HB3	7:D:303:SF4:S1	2.04	0.97
1:W:69:MET:HE2	1:W:754:MET:HE1	1.46	0.97
2:X:143:PRO:HB3	7:X:303:SF4:S1	2.05	0.97
2:T:128:MET:HA	7:T:303:SF4:S1	2.06	0.96
1:C:66:PHE:HZ	1:C:146:MET:HE1	1.29	0.95
1:I:356:GLY:N	5:I:904:MGD:O1B	1.99	0.95
1:M:360:ALA:HB1	1:M:859:THR:HG23	1.48	0.95
2:R:46:MET:HE1	2:R:66:THR:N	1.82	0.95
1:Q:610:LYS:NZ	1:Q:618:GLN:HE22	1.65	0.94
1:E:557:CYS:H	1:E:564:ASN:HD21	1.01	0.94
2:D:69:MET:HB3	2:D:184:PRO:HB3	1.49	0.94
1:W:360:ALA:HB1	1:W:859:THR:HG23	1.49	0.94
1:U:557:CYS:H	1:U:564:ASN:HD21	1.01	0.94
1:M:28:MET:HE1	1:M:66:PHE:HB3	1.51	0.93
1:G:629:MET:HE2	1:G:634:PHE:HA	1.49	0.93
1:I:557:CYS:H	1:I:564:ASN:HD21	0.94	0.93
1:Q:28:MET:HE1	1:Q:66:PHE:HB3	1.51	0.92
2:N:19:CYS:HB3	2:N:145:CYS:HB3	1.49	0.92
2:T:143:PRO:HB3	7:T:303:SF4:S1	2.10	0.92
1:G:557:CYS:H	1:G:564:ASN:HD21	1.06	0.91
1:I:426:MET:HE1	1:I:618:GLN:HG2	1.50	0.91
1:Q:66:PHE:HZ	1:Q:146:MET:HE1	1.36	0.91
1:G:66:PHE:HA	1:G:69:MET:HE3	1.50	0.91
2:P:128:MET:HA	7:P:303:SF4:S1	2.10	0.90
2:H:143:PRO:HB3	7:H:303:SF4:S1	2.10	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:PRO:HB3	7:B:303:SF4:S1	2.11	0.90
2:H:19:CYS:HB3	2:H:145:CYS:HB3	1.54	0.90
2:V:128:MET:HA	7:V:303:SF4:S1	2.12	0.90
1:S:211:MET:HE1	2:T:231:PHE:HZ	1.35	0.90
1:C:66:PHE:HA	1:C:69:MET:HE3	1.54	0.90
2:J:128:MET:HA	7:J:303:SF4:S1	2.11	0.90
1:Q:211:MET:HE1	2:R:231:PHE:CZ	2.07	0.90
1:G:165:GLY:HA3	1:G:166:PHE:HB3	1.54	0.89
2:X:40:GLN:NE2	2:X:117:ASN:HA	1.87	0.89
1:W:28:MET:HE1	1:W:66:PHE:HB3	1.51	0.89
1:A:426:MET:HE1	1:A:618:GLN:HG2	1.55	0.89
2:J:256:TYR:HB2	2:J:274:LEU:HD21	1.53	0.89
1:I:66:PHE:HZ	1:I:146:MET:HE1	1.38	0.89
1:M:557:CYS:H	1:M:564:ASN:HD21	1.14	0.89
1:W:561:ILE:HG22	1:W:564:ASN:HB3	1.55	0.89
1:S:561:ILE:HG22	1:S:564:ASN:HB3	1.55	0.89
2:D:128:MET:HA	7:D:303:SF4:S1	2.13	0.89
1:K:146:MET:HE3	1:K:545:ASN:OD1	1.72	0.89
1:W:645:ASN:ND2	1:W:648:ARG:HB3	1.88	0.89
2:F:46:MET:HE1	2:F:66:THR:N	1.88	0.88
1:K:557:CYS:H	1:K:564:ASN:HD21	1.18	0.88
1:O:557:CYS:H	1:O:564:ASN:HD21	1.21	0.88
2:P:70:HIS:HD2	2:P:92:VAL:H	1.20	0.88
1:U:66:PHE:HZ	1:U:146:MET:HE1	1.36	0.88
2:X:129:CYS:HB3	2:X:131:HIS:CE1	2.08	0.88
1:K:66:PHE:CZ	1:K:146:MET:HE1	2.08	0.88
1:Q:165:GLY:HA3	1:Q:166:PHE:HB3	1.55	0.88
1:A:69:MET:HE2	1:A:754:MET:HE1	1.55	0.88
1:U:610:LYS:NZ	1:U:618:GLN:HE22	1.70	0.87
1:A:426:MET:CE	1:A:618:GLN:HG2	2.04	0.87
1:I:753:TYR:HB3	2:J:21:MET:HE2	1.56	0.87
2:F:19:CYS:HB3	2:F:145:CYS:HB3	1.56	0.87
1:S:28:MET:HE1	1:S:66:PHE:HB3	1.54	0.87
1:E:218:ASP:OD2	1:E:253:ASN:HB2	1.74	0.87
1:G:360:ALA:HB1	1:G:859:THR:HG23	1.57	0.87
1:Q:610:LYS:HZ3	1:Q:618:GLN:HE22	1.19	0.87
1:C:557:CYS:H	1:C:564:ASN:HD21	1.16	0.86
1:K:146:MET:HE2	1:K:544:THR:HB	1.56	0.86
1:S:610:LYS:NZ	1:S:618:GLN:HE22	1.71	0.86
2:L:128:MET:HA	7:L:303:SF4:S1	2.15	0.86
1:U:165:GLY:HA3	1:U:166:PHE:HB3	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:19:CYS:HB2	2:X:46:MET:HG2	1.55	0.86
1:K:753:TYR:HB3	2:L:24:MET:HE3	1.58	0.86
2:B:128:MET:HA	7:B:303:SF4:S1	2.15	0.85
1:K:610:LYS:NZ	1:K:618:GLN:HE22	1.74	0.85
1:K:629:MET:HE2	1:K:634:PHE:HA	1.58	0.85
1:K:66:PHE:HZ	1:K:146:MET:HE1	1.40	0.85
1:K:28:MET:HE1	1:K:66:PHE:HB3	1.58	0.85
2:P:46:MET:HE1	2:P:66:THR:N	1.92	0.85
2:D:19:CYS:HB3	2:D:145:CYS:HB3	1.56	0.85
2:R:70:HIS:HD2	2:R:92:VAL:H	1.23	0.84
1:A:141:PRO:HA	1:A:496:TYR:HB3	1.56	0.84
1:E:645:ASN:ND2	1:E:648:ARG:HB3	1.92	0.84
1:K:165:GLY:HA3	1:K:166:PHE:HB3	1.59	0.84
1:A:695:LEU:O	1:A:699:GLU:HG2	1.78	0.84
1:M:165:GLY:HA3	1:M:166:PHE:HB3	1.58	0.84
2:P:73:ASN:OD1	1:S:648:ARG:HA	1.78	0.84
2:V:143:PRO:HB3	7:V:303:SF4:S1	2.18	0.84
2:H:114:MET:HE3	2:H:123:ALA:HB1	1.59	0.83
2:X:201:ALA:HB2	2:X:269:LEU:HB2	1.58	0.83
1:A:28:MET:HE1	1:A:66:PHE:HB3	1.58	0.83
1:C:211:MET:HE1	2:D:231:PHE:CZ	2.14	0.83
2:B:76:CYS:HB3	2:B:108:THR:OG1	1.78	0.83
2:H:128:MET:HA	7:H:303:SF4:S1	2.18	0.83
2:N:128:MET:HA	7:N:303:SF4:S1	2.18	0.83
1:O:66:PHE:HA	1:O:69:MET:HE3	1.60	0.83
1:K:849:SER:HB3	1:K:852:ALA:HB3	1.59	0.83
1:O:610:LYS:NZ	1:O:618:GLN:HE22	1.77	0.83
1:A:184:MET:HE2	1:A:190:SER:HA	1.60	0.83
2:X:19:CYS:HB3	2:X:145:CYS:HB3	1.59	0.83
2:N:70:HIS:HD2	2:N:92:VAL:H	1.25	0.83
2:R:128:MET:HA	7:R:303:SF4:S1	2.18	0.83
1:Q:66:PHE:CZ	1:Q:146:MET:HE1	2.14	0.82
1:W:258:LEU:HG	1:W:259:VAL:HG13	1.61	0.82
1:W:783:GLY:O	1:W:866:LYS:HD2	1.79	0.82
1:A:66:PHE:HZ	1:A:146:MET:HE1	1.44	0.82
2:J:143:PRO:HB3	7:J:303:SF4:S1	2.19	0.82
1:M:426:MET:HA	1:M:426:MET:HE3	1.61	0.82
1:I:426:MET:CE	1:I:618:GLN:HG2	2.08	0.82
1:M:66:PHE:HA	1:M:69:MET:HE3	1.60	0.82
1:O:138:LEU:HB2	1:O:490:ILE:HD12	1.61	0.82
1:E:69:MET:HE2	1:E:754:MET:HE3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:503:THR:HG21	5:I:903:MGD:O2A	1.80	0.82
2:P:27:HIS:HB2	2:P:39:MET:HE3	1.59	0.82
1:W:610:LYS:NZ	1:W:618:GLN:HE22	1.78	0.82
1:K:426:MET:HE3	1:K:426:MET:HA	1.62	0.82
1:M:211:MET:HE1	2:N:231:PHE:HZ	1.44	0.82
2:N:46:MET:HE1	2:N:66:THR:N	1.95	0.82
1:Q:503:THR:HG21	5:Q:903:MGD:O2A	1.80	0.82
1:S:211:MET:HE1	2:T:231:PHE:CZ	2.15	0.81
1:A:360:ALA:HB1	1:A:859:THR:HG23	1.60	0.81
1:A:426:MET:HA	1:A:426:MET:HE3	1.61	0.81
1:A:823:TYR:CZ	1:A:825:PRO:HG3	2.15	0.81
1:C:360:ALA:HB1	1:C:859:THR:HG23	1.60	0.81
1:E:165:GLY:HA3	1:E:166:PHE:HB3	1.62	0.81
1:U:66:PHE:CZ	1:U:146:MET:HE1	2.16	0.81
1:W:32:ASP:OD2	8:W:1659:HOH:O	1.97	0.81
1:K:561:ILE:HG22	1:K:564:ASN:HB3	1.62	0.81
2:F:69:MET:HB3	2:F:184:PRO:HB3	1.61	0.81
2:J:2:GLU:HG2	2:J:158:LYS:HG2	1.61	0.81
1:O:561:ILE:HG22	1:O:564:ASN:HB3	1.63	0.81
1:S:753:TYR:HB3	2:T:24:MET:HE3	1.63	0.81
1:S:426:MET:CE	1:S:618:GLN:HG2	2.11	0.81
1:M:138:LEU:HB2	1:M:490:ILE:HD12	1.63	0.81
1:S:360:ALA:HB1	1:S:859:THR:HG23	1.61	0.81
2:B:70:HIS:HD2	2:B:92:VAL:H	1.25	0.80
1:I:629:MET:HE2	1:I:634:PHE:HA	1.61	0.80
1:M:211:MET:HE1	2:N:231:PHE:CZ	2.16	0.80
1:Q:146:MET:HE2	1:Q:544:THR:HB	1.63	0.80
1:Q:146:MET:HE3	1:Q:545:ASN:OD1	1.79	0.80
1:W:165:GLY:HA3	1:W:166:PHE:HB3	1.62	0.80
1:C:69:MET:HE2	1:C:754:MET:HE1	1.64	0.80
2:F:68:CYS:HB2	2:F:126:CYS:HB3	1.63	0.80
2:F:128:MET:HA	7:F:303:SF4:S1	2.22	0.80
1:G:561:ILE:HG22	1:G:564:ASN:HB3	1.63	0.80
1:Q:69:MET:HE2	1:Q:754:MET:HE1	1.63	0.80
1:W:557:CYS:H	1:W:564:ASN:HD21	1.29	0.80
2:H:46:MET:HE1	2:H:66:THR:N	1.96	0.80
1:O:794:ASN:HD22	1:O:862:VAL:HG12	1.47	0.80
2:F:76:CYS:HB3	2:F:108:THR:OG1	1.82	0.80
1:M:66:PHE:HZ	1:M:146:MET:HE1	1.46	0.80
1:A:629:MET:HE2	1:A:634:PHE:HA	1.62	0.80
1:K:252:MET:HE3	1:K:263:TRP:CE3	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:66:PHE:CZ	1:M:146:MET:HE1	2.17	0.80
1:M:146:MET:HE3	1:M:545:ASN:OD1	1.80	0.80
1:O:211:MET:HE1	2:P:231:PHE:CZ	2.17	0.80
1:S:557:CYS:N	1:S:564:ASN:HD21	1.80	0.80
2:D:46:MET:HE1	2:D:66:THR:N	1.98	0.79
1:I:610:LYS:NZ	1:I:618:GLN:HE22	1.80	0.79
2:J:76:CYS:HB3	2:J:108:THR:OG1	1.82	0.79
1:O:28:MET:HE1	1:O:66:PHE:HB3	1.63	0.79
1:G:211:MET:HE1	2:H:231:PHE:CZ	2.16	0.79
1:Q:44:ILE:HD11	1:Q:394:PRO:HG2	1.65	0.79
1:O:66:PHE:HZ	1:O:146:MET:HE1	1.47	0.79
2:T:175:VAL:HG23	2:T:178:PRO:HG3	1.65	0.79
1:W:146:MET:HE2	1:W:544:THR:HB	1.65	0.79
2:B:40:GLN:HE22	2:B:118:GLU:H	1.30	0.79
1:Q:426:MET:HA	1:Q:426:MET:HE3	1.64	0.79
1:Q:691:ILE:HD11	1:Q:711:MET:HE3	1.65	0.79
1:W:138:LEU:HB2	1:W:490:ILE:HD12	1.63	0.79
1:I:557:CYS:H	1:I:564:ASN:ND2	1.78	0.78
1:O:69:MET:HE2	1:O:754:MET:CE	2.14	0.78
2:X:128:MET:HA	7:X:303:SF4:S1	2.22	0.78
1:G:69:MET:HE2	1:G:754:MET:HE1	1.65	0.78
1:S:69:MET:HE2	1:S:754:MET:CE	2.14	0.78
1:U:695:LEU:O	1:U:699:GLU:HG2	1.83	0.78
1:S:823:TYR:CZ	1:S:825:PRO:HG3	2.18	0.78
2:J:105:LEU:HB3	2:J:114:MET:HE1	1.65	0.78
1:S:457:MET:HE3	8:S:1002:HOH:O	1.84	0.78
1:U:138:LEU:HB2	1:U:490:ILE:HD12	1.66	0.78
1:G:645:ASN:ND2	1:G:648:ARG:HB3	1.99	0.78
1:G:141:PRO:HA	1:G:496:TYR:HB3	1.66	0.78
1:Q:360:ALA:HB1	1:Q:859:THR:HG23	1.63	0.77
1:C:69:MET:HE2	1:C:754:MET:CE	2.14	0.77
1:C:426:MET:HE3	1:C:426:MET:HA	1.66	0.77
1:Q:319:GLU:HG2	1:U:726:LEU:HD13	1.66	0.77
1:U:426:MET:CE	1:U:618:GLN:HG2	2.14	0.77
1:E:211:MET:HE1	2:F:231:PHE:CZ	2.19	0.77
2:B:68:CYS:HB2	2:B:126:CYS:HB3	1.66	0.77
1:C:66:PHE:CZ	1:C:146:MET:HE1	2.18	0.77
1:I:557:CYS:N	1:I:564:ASN:HD21	1.78	0.77
1:C:561:ILE:HG22	1:C:564:ASN:HB3	1.65	0.77
1:E:66:PHE:HZ	1:E:146:MET:HE1	1.49	0.77
2:J:46:MET:HE1	2:J:66:THR:N	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MET:HE2	1:A:754:MET:CE	2.14	0.77
1:E:557:CYS:H	1:E:564:ASN:ND2	1.79	0.77
1:W:645:ASN:HD21	1:W:648:ARG:HB3	1.49	0.77
2:B:68:CYS:CB	2:B:126:CYS:HB3	2.14	0.77
1:E:610:LYS:HZ1	1:E:618:GLN:HE22	1.32	0.77
1:M:691:ILE:HD11	1:M:711:MET:HE3	1.67	0.77
1:W:69:MET:HE2	1:W:754:MET:CE	2.15	0.77
1:O:360:ALA:HB1	1:O:859:THR:HG23	1.67	0.76
2:L:53:ARG:HB2	2:L:60:ASP:OD1	1.86	0.76
1:U:557:CYS:N	1:U:564:ASN:HD21	1.80	0.76
1:I:28:MET:HE1	1:I:66:PHE:HB3	1.68	0.76
2:H:23:CYS:HB3	2:H:39:MET:HE1	1.67	0.76
2:N:142:MET:HE2	2:N:146:ALA:HB1	1.65	0.76
2:P:70:HIS:CD2	2:P:92:VAL:H	2.04	0.76
1:U:81:LYS:HB2	1:U:112:ILE:HD13	1.67	0.76
1:G:28:MET:HE1	1:G:66:PHE:HB3	1.65	0.76
2:L:23:CYS:HB3	2:L:39:MET:HE1	1.68	0.76
2:F:143:PRO:HB3	7:F:303:SF4:S1	2.25	0.76
2:D:201:ALA:HB2	2:D:269:LEU:HB2	1.68	0.76
1:M:426:MET:CE	1:M:618:GLN:HG2	2.15	0.76
2:P:68:CYS:HB3	2:P:126:CYS:HB3	1.67	0.76
1:E:100:LEU:HD12	1:E:105:PRO:HG3	1.69	0.76
1:A:66:PHE:CZ	1:A:146:MET:HE1	2.20	0.75
1:U:426:MET:HA	1:U:426:MET:HE3	1.68	0.75
1:U:426:MET:HE1	1:U:618:GLN:HG2	1.68	0.75
1:G:426:MET:CE	1:G:618:GLN:HG2	2.16	0.75
1:K:211:MET:HE1	1:K:338:GLN:HG2	1.67	0.75
1:E:69:MET:HE2	1:E:754:MET:CE	2.15	0.75
1:G:69:MET:HE2	1:G:754:MET:CE	2.15	0.75
1:C:394:PRO:HG3	8:C:1324:HOH:O	1.86	0.75
2:D:56:TYR:HA	2:D:59:ASN:HD22	1.52	0.75
1:C:211:MET:HE1	2:D:231:PHE:HZ	1.48	0.75
1:C:426:MET:HE1	1:C:618:GLN:HG2	1.68	0.75
1:M:146:MET:HE2	1:M:544:THR:HB	1.69	0.75
1:O:61:PRO:HB3	8:P:563:HOH:O	1.87	0.75
1:O:69:MET:HE2	1:O:754:MET:HE1	1.66	0.75
1:S:786:ASN:HD21	1:S:804:GLN:HA	1.49	0.75
1:U:360:ALA:HB1	1:U:859:THR:HG23	1.67	0.75
1:I:69:MET:HE2	1:I:754:MET:HE1	1.68	0.75
2:J:23:CYS:HB3	2:J:39:MET:HE1	1.69	0.75
2:R:143:PRO:HB3	7:R:303:SF4:S1	2.27	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:503:THR:HG21	5:G:903:MGD:O2A	1.86	0.74
1:E:146:MET:HE3	1:E:545:ASN:OD1	1.86	0.74
1:I:165:GLY:HA3	1:I:166:PHE:HB3	1.68	0.74
1:O:719:GLU:HG2	1:O:859:THR:O	1.86	0.74
2:F:46:MET:HE1	2:F:66:THR:H	1.51	0.74
2:T:68:CYS:HB3	2:T:126:CYS:HB3	1.67	0.74
1:W:629:MET:HE2	1:W:634:PHE:HA	1.70	0.74
1:A:719:GLU:HG2	1:A:859:THR:O	1.87	0.74
1:O:823:TYR:CZ	1:O:825:PRO:HG3	2.21	0.74
2:V:70:HIS:HD2	2:V:92:VAL:H	1.36	0.74
1:A:211:MET:HE1	2:B:231:PHE:CZ	2.21	0.74
1:K:823:TYR:CZ	1:K:825:PRO:HG3	2.22	0.74
2:N:143:PRO:HB3	7:N:303:SF4:S1	2.28	0.74
1:O:253:ASN:O	1:O:257:ARG:HG3	1.86	0.74
2:F:68:CYS:CB	2:F:126:CYS:HB3	2.18	0.74
2:X:95:ASP:HB3	2:X:98:LYS:HB2	1.69	0.74
2:V:68:CYS:HB3	2:V:126:CYS:HB3	1.70	0.74
1:C:141:PRO:HA	1:C:496:TYR:HB3	1.69	0.74
1:O:695:LEU:O	1:O:699:GLU:HG2	1.87	0.74
1:K:426:MET:CE	1:K:618:GLN:HG2	2.18	0.73
1:S:786:ASN:ND2	1:S:804:GLN:HA	2.02	0.73
2:T:40:GLN:HE22	2:T:118:GLU:H	1.36	0.73
2:X:84:VAL:HG22	2:X:94:ILE:HG12	1.69	0.73
1:G:823:TYR:CZ	1:G:825:PRO:HG3	2.23	0.73
1:G:74:LEU:HD12	1:G:750:LYS:HA	1.69	0.73
1:O:753:TYR:HB3	2:P:24:MET:HE3	1.70	0.73
1:G:162:ASN:HA	8:G:1369:HOH:O	1.87	0.73
1:C:426:MET:CE	1:C:618:GLN:HG2	2.18	0.73
1:I:69:MET:HE2	1:I:754:MET:CE	2.18	0.73
1:O:165:GLY:HA3	1:O:166:PHE:HB3	1.68	0.73
1:A:561:ILE:HG22	1:A:564:ASN:HB3	1.71	0.73
1:E:503:THR:HG21	5:E:903:MGD:O2A	1.89	0.73
2:N:5:TYR:HB2	2:N:157:LEU:CD1	2.18	0.73
1:E:610:LYS:NZ	1:E:618:GLN:HE22	1.86	0.73
1:G:426:MET:HA	1:G:426:MET:HE3	1.69	0.73
2:L:40:GLN:NE2	2:L:117:ASN:HA	2.02	0.73
1:U:44:ILE:HD11	1:U:394:PRO:HG2	1.70	0.73
1:C:610:LYS:NZ	1:C:618:GLN:HE22	1.86	0.73
2:L:142:MET:HE2	2:L:146:ALA:C	2.14	0.73
1:S:426:MET:HE1	1:S:618:GLN:HG2	1.69	0.73
1:I:644:ASP:O	1:I:646:PRO:HD3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:68:CYS:HB2	2:R:126:CYS:HB3	1.70	0.72
2:D:76:CYS:HB3	2:D:108:THR:OG1	1.90	0.72
1:I:66:PHE:HA	1:I:69:MET:HE3	1.71	0.72
2:L:19:CYS:HB3	2:L:145:CYS:CB	2.10	0.72
1:M:629:MET:HE2	1:M:634:PHE:HA	1.70	0.72
1:Q:252:MET:HE3	1:Q:263:TRP:CE3	2.25	0.72
2:V:19:CYS:HB3	2:V:145:CYS:HB3	1.70	0.72
2:V:76:CYS:HB3	2:V:108:THR:OG1	1.89	0.72
1:W:328:PRO:HB2	1:W:331:GLU:HG3	1.70	0.72
1:G:356:GLY:H	5:G:904:MGD:H5'2	1.54	0.72
2:J:70:HIS:HD2	2:J:92:VAL:H	1.36	0.72
1:U:146:MET:HE3	1:U:545:ASN:OD1	1.89	0.72
2:X:142:MET:HE2	2:X:146:ALA:C	2.14	0.72
2:X:23:CYS:HB3	2:X:39:MET:HE1	1.70	0.72
2:R:40:GLN:HE22	2:R:118:GLU:H	1.35	0.72
1:S:66:PHE:HZ	1:S:146:MET:HE1	1.55	0.72
2:T:64:ARG:HD2	2:T:176:ILE:HD11	1.71	0.72
2:B:105:LEU:HB3	2:B:114:MET:HE1	1.70	0.72
1:I:426:MET:HA	1:I:426:MET:HE3	1.70	0.72
2:J:40:GLN:HE22	2:J:118:GLU:H	1.37	0.72
2:L:59:ASN:H	2:L:59:ASN:ND2	1.86	0.72
1:Q:100:LEU:HD12	1:Q:105:PRO:HG3	1.70	0.72
2:R:19:CYS:HB3	2:R:145:CYS:HB3	1.70	0.72
2:R:68:CYS:CB	2:R:126:CYS:HB3	2.20	0.72
1:S:753:TYR:HB3	2:T:21:MET:HE2	1.69	0.72
1:U:691:ILE:HD11	1:U:711:MET:HE3	1.70	0.72
1:C:143:SER:HB3	3:C:901:ACT:H3	1.70	0.72
1:I:44:ILE:HD11	1:I:394:PRO:HG2	1.72	0.72
2:J:21:MET:CE	2:J:24:MET:HE3	2.19	0.72
2:R:23:CYS:HB3	2:R:39:MET:HE1	1.72	0.72
2:T:40:GLN:NE2	2:T:118:GLU:H	1.88	0.72
1:A:356:GLY:H	5:A:904:MGD:H5'2	1.55	0.71
2:J:21:MET:HA	2:J:21:MET:HE3	1.72	0.71
1:C:823:TYR:CZ	1:C:825:PRO:HG3	2.24	0.71
1:M:61:PRO:HB3	8:N:563:HOH:O	1.88	0.71
1:O:503:THR:HG21	5:O:903:MGD:O2A	1.89	0.71
1:S:146:MET:HE2	1:S:544:THR:HB	1.72	0.71
1:I:141:PRO:HA	1:I:496:TYR:HB3	1.73	0.71
2:L:166:LYS:O	2:L:170:GLU:HG3	1.90	0.71
1:O:74:LEU:HD12	1:O:750:LYS:HA	1.71	0.71
1:O:146:MET:HE3	1:O:545:ASN:OD1	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:256:TYR:HB2	2:T:274:LEU:HD21	1.72	0.71
1:K:610:LYS:HZ2	1:K:618:GLN:HE22	1.35	0.71
1:Q:184:MET:HE2	1:Q:190:SER:HA	1.72	0.71
2:R:142:MET:HE2	2:R:146:ALA:C	2.15	0.71
1:G:449:ARG:HD2	8:G:1038:HOH:O	1.91	0.71
1:M:69:MET:HE2	1:M:754:MET:HE1	1.73	0.71
1:Q:610:LYS:HB3	1:Q:614:ALA:HB3	1.70	0.71
1:M:610:LYS:NZ	1:M:618:GLN:HE22	1.89	0.71
2:N:76:CYS:HB3	2:N:108:THR:OG1	1.91	0.71
1:C:757:ILE:HG23	2:D:17:ASN:OD1	1.91	0.70
2:L:71:CYS:HA	2:L:184:PRO:HA	1.72	0.70
1:U:610:LYS:HZ3	1:U:618:GLN:HE22	1.39	0.70
1:W:691:ILE:HD11	1:W:711:MET:HE3	1.73	0.70
1:A:146:MET:HE2	1:A:544:THR:HB	1.73	0.70
1:E:379:MET:HE3	1:E:654:LEU:HD13	1.71	0.70
2:H:46:MET:HE1	2:H:66:THR:H	1.54	0.70
1:I:823:TYR:CZ	1:I:825:PRO:HG3	2.26	0.70
2:B:142:MET:HE2	2:B:147:HIS:N	2.07	0.70
2:F:23:CYS:HB3	2:F:39:MET:HE1	1.72	0.70
1:O:146:MET:HG2	5:O:903:MGD:N7	2.06	0.70
1:C:165:GLY:HA3	1:C:166:PHE:HB3	1.72	0.70
2:N:207:GLY:HA2	1:S:728:VAL:CG1	2.18	0.70
1:O:96:ARG:HD2	1:O:514:TYR:O	1.91	0.70
1:A:165:GLY:HA3	1:A:166:PHE:HB3	1.72	0.70
2:H:68:CYS:HB3	2:H:126:CYS:HB3	1.72	0.70
2:N:114:MET:HA	2:N:125:LYS:HB3	1.72	0.70
2:B:164:MET:O	2:B:168:VAL:HG23	1.92	0.70
1:M:557:CYS:N	1:M:564:ASN:HD21	1.89	0.70
1:K:426:MET:HE1	1:K:618:GLN:HG2	1.72	0.70
2:N:46:MET:HE1	2:N:66:THR:H	1.55	0.70
1:Q:134:PRO:HB2	1:Q:439:LEU:HD11	1.74	0.70
2:F:114:MET:HE3	2:F:123:ALA:HB1	1.73	0.70
2:P:69:MET:HB3	2:P:184:PRO:HB3	1.73	0.70
2:V:18:ASN:HB2	7:V:302:SF4:S1	2.31	0.70
1:W:155:SER:OG	1:W:409:ILE:HG12	1.91	0.70
2:N:23:CYS:HB3	2:N:39:MET:HE1	1.73	0.69
2:P:72:GLU:HA	8:P:471:HOH:O	1.91	0.69
1:W:508:ASN:O	1:W:512:LYS:HG3	1.92	0.69
1:E:66:PHE:CZ	1:E:146:MET:HE1	2.26	0.69
2:F:20:PHE:CZ	2:F:24:MET:HE2	2.26	0.69
1:C:28:MET:HE1	1:C:66:PHE:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:823:TYR:CZ	1:M:825:PRO:HG3	2.27	0.69
1:K:66:PHE:CD1	1:K:69:MET:HE3	2.28	0.69
1:A:138:LEU:HB2	1:A:490:ILE:HD12	1.74	0.69
1:G:610:LYS:NZ	1:G:618:GLN:HE22	1.91	0.69
2:P:71:CYS:HA	2:P:184:PRO:HA	1.75	0.69
2:V:58:ARG:HD2	2:V:268:ASP:OD1	1.92	0.69
2:J:142:MET:HE2	2:J:146:ALA:C	2.18	0.69
2:J:142:MET:HE3	2:J:146:ALA:HB1	1.75	0.69
1:M:69:MET:HE2	1:M:754:MET:CE	2.23	0.69
2:N:106:LEU:HD22	2:N:114:MET:HG3	1.74	0.69
1:W:146:MET:HE3	1:W:545:ASN:OD1	1.92	0.69
2:V:40:GLN:HE22	2:V:118:GLU:H	1.38	0.69
1:E:427:PHE:HB3	8:E:1029:HOH:O	1.92	0.69
1:G:197:GLU:OE2	1:G:667:ASP:HB2	1.93	0.69
2:B:46:MET:HE1	2:B:66:THR:N	2.08	0.68
1:I:870:ASP:HB3	1:I:872:TYR:CE1	2.28	0.68
2:L:19:CYS:CB	2:L:145:CYS:HB3	2.11	0.68
1:M:503:THR:HG21	5:M:903:MGD:O2A	1.93	0.68
1:S:66:PHE:CD1	1:S:69:MET:HE3	2.28	0.68
1:C:644:ASP:O	1:C:646:PRO:HD3	1.93	0.68
2:F:203:ILE:HD13	2:F:229:THR:HG21	1.75	0.68
1:I:695:LEU:O	1:I:699:GLU:HG2	1.92	0.68
1:U:211:MET:HE1	2:V:231:PHE:CZ	2.28	0.68
2:X:175:VAL:HG23	2:X:178:PRO:HG3	1.74	0.68
1:A:630:THR:OG1	1:A:633:GLU:HG3	1.93	0.68
1:K:360:ALA:HB1	1:K:859:THR:HG23	1.74	0.68
1:O:746:MET:HE2	5:O:903:MGD:O1B	1.93	0.68
1:C:695:LEU:O	1:C:699:GLU:HG2	1.92	0.68
1:O:211:MET:HE1	2:P:231:PHE:HZ	1.53	0.68
1:Q:629:MET:HE2	1:Q:634:PHE:HA	1.76	0.68
1:S:610:LYS:HZ3	1:S:618:GLN:HE22	1.41	0.68
1:C:91:ARG:HH12	1:C:124:GLU:CD	2.01	0.68
2:H:40:GLN:NE2	2:H:118:GLU:H	1.91	0.68
1:K:141:PRO:HA	1:K:496:TYR:HB3	1.76	0.68
1:W:74:LEU:HD12	1:W:750:LYS:HA	1.75	0.68
2:X:10:VAL:HG13	2:X:63:TYR:O	1.92	0.68
2:H:20:PHE:CZ	2:H:24:MET:HE2	2.29	0.68
1:Q:218:ASP:OD2	1:Q:253:ASN:HB2	1.92	0.68
1:Q:599:LYS:HG3	8:Q:1671:HOH:O	1.93	0.68
1:W:757:ILE:HG23	2:X:17:ASN:OD1	1.93	0.68
1:A:610:LYS:NZ	1:A:618:GLN:HE22	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:68:CYS:CB	2:J:126:CYS:HB3	2.23	0.68
2:D:19:CYS:HB2	2:D:46:MET:HG2	1.76	0.68
1:E:695:LEU:O	1:E:699:GLU:HG2	1.93	0.68
2:N:53:ARG:HB2	2:N:60:ASP:OD1	1.94	0.68
1:G:66:PHE:HZ	1:G:146:MET:HE1	1.59	0.68
1:G:100:LEU:HD12	1:G:105:PRO:HG3	1.76	0.68
2:L:76:CYS:HB3	2:L:108:THR:OG1	1.93	0.68
1:W:66:PHE:CZ	1:W:146:MET:HE1	2.29	0.68
1:M:356:GLY:H	5:M:904:MGD:H5'2	1.58	0.68
2:B:58:ARG:HD2	2:B:268:ASP:OD1	1.93	0.67
2:H:68:CYS:CB	2:H:126:CYS:HB3	2.24	0.67
1:K:356:GLY:H	5:K:904:MGD:H5'2	1.59	0.67
1:O:146:MET:HE2	1:O:544:THR:HB	1.74	0.67
1:U:69:MET:HE2	1:U:754:MET:CE	2.23	0.67
1:E:510:TYR:O	1:E:513:MET:HG2	1.94	0.67
1:E:360:ALA:HB1	1:E:859:THR:HG23	1.75	0.67
2:P:216:VAL:HG13	2:P:223:GLU:HG3	1.77	0.67
1:S:211:MET:HE2	1:S:246:VAL:HG23	1.76	0.67
1:S:558:SER:H	1:S:564:ASN:ND2	1.92	0.67
2:T:129:CYS:HB3	2:T:131:HIS:CE1	2.28	0.67
2:V:46:MET:HE1	2:V:66:THR:N	2.09	0.67
1:W:143:SER:HB3	3:W:901:ACT:H3	1.76	0.67
2:D:71:CYS:HA	2:D:184:PRO:HA	1.75	0.67
2:D:77:VAL:HG22	2:D:84:VAL:HG12	1.76	0.67
1:M:257:ARG:HD3	2:N:61:ILE:HG21	1.77	0.67
2:N:142:MET:HE2	2:N:146:ALA:CB	2.24	0.67
2:R:21:MET:HE2	2:R:24:MET:HE3	1.76	0.67
2:X:2:GLU:HG2	2:X:158:LYS:HG2	1.75	0.67
1:A:61:PRO:HB3	8:B:563:HOH:O	1.94	0.67
1:A:211:MET:HE1	2:B:231:PHE:HZ	1.60	0.67
2:D:53:ARG:HB2	2:D:60:ASP:OD1	1.95	0.67
2:D:142:MET:HE1	8:D:430:HOH:O	1.94	0.67
1:G:530:GLU:OE1	1:G:821:ALA:HB1	1.94	0.67
1:S:604:GLU:HB3	1:S:605:MET:CE	2.22	0.67
2:X:87:ARG:HG3	2:X:91:ILE:O	1.94	0.67
1:A:100:LEU:HD12	1:A:105:PRO:HG3	1.76	0.67
2:D:104:GLU:CD	2:D:104:GLU:H	2.03	0.67
1:G:610:LYS:HB3	1:G:614:ALA:HB3	1.75	0.67
2:H:114:MET:HA	2:H:125:LYS:HB3	1.77	0.67
1:K:138:LEU:HB2	1:K:490:ILE:HD12	1.76	0.67
1:W:141:PRO:HA	1:W:496:TYR:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:PRO:HA	1:E:496:TYR:HB3	1.77	0.67
1:K:756:TYR:HD1	2:L:24:MET:HE1	1.59	0.67
2:L:69:MET:HB3	2:L:184:PRO:HB3	1.77	0.67
2:N:68:CYS:CB	2:N:126:CYS:HB3	2.25	0.67
2:N:71:CYS:HB2	2:N:182:THR:O	1.95	0.67
1:Q:426:MET:CE	1:Q:618:GLN:HG2	2.24	0.67
1:U:610:LYS:HZ2	1:U:618:GLN:HE22	1.40	0.67
1:C:558:SER:H	1:C:564:ASN:ND2	1.92	0.67
1:I:394:PRO:HG3	8:I:1324:HOH:O	1.94	0.67
2:L:106:LEU:HD11	2:L:116:TRP:HB2	1.77	0.67
1:O:141:PRO:HA	1:O:496:TYR:HB3	1.77	0.67
1:U:142:SER:HB2	5:U:903:MGD:H5'2	1.77	0.67
1:G:870:ASP:HB3	1:G:872:TYR:CE1	2.30	0.67
1:O:66:PHE:CZ	1:O:146:MET:HE1	2.29	0.67
2:T:49:GLU:HG3	2:T:64:ARG:NH2	2.10	0.67
1:W:184:MET:HE2	1:W:190:SER:HA	1.75	0.67
1:U:211:MET:HE1	2:V:231:PHE:HZ	1.60	0.66
3:C:901:ACT:H1	8:C:1044:HOH:O	1.94	0.66
1:W:75:ARG:HH22	1:W:547:GLU:CD	2.01	0.66
1:C:629:MET:HE2	1:C:634:PHE:HA	1.77	0.66
1:I:211:MET:HE1	2:J:231:PHE:CZ	2.31	0.66
1:M:786:ASN:ND2	1:M:804:GLN:HA	2.10	0.66
1:A:855:MET:HB2	1:A:857:ASN:OD1	1.95	0.66
1:C:74:LEU:HD12	1:C:750:LYS:HA	1.76	0.66
1:G:746:MET:HE2	5:G:903:MGD:O1B	1.96	0.66
2:P:205:VAL:HG13	2:P:254:LYS:NZ	2.10	0.66
1:Q:870:ASP:HB3	1:Q:872:TYR:CE1	2.31	0.66
2:B:104:GLU:CD	2:B:104:GLU:H	2.03	0.66
2:J:68:CYS:HB2	2:J:126:CYS:HB3	1.77	0.66
1:W:695:LEU:O	1:W:699:GLU:HG2	1.96	0.66
1:E:177:GLU:HA	1:E:177:GLU:OE2	1.96	0.66
2:F:56:TYR:HA	2:F:59:ASN:HD22	1.61	0.66
1:K:69:MET:SD	1:K:747:GLY:HA2	2.36	0.66
1:Q:319:GLU:HG2	1:U:726:LEU:CD1	2.26	0.66
1:S:75:ARG:HH21	1:S:543:CYS:HA	1.61	0.66
2:T:23:CYS:HB3	2:T:39:MET:HE1	1.77	0.66
2:B:2:GLU:HG2	2:B:158:LYS:HG2	1.76	0.66
1:U:746:MET:HE2	5:U:903:MGD:O1B	1.96	0.66
2:D:73:ASN:HB3	2:D:182:THR:HA	1.78	0.66
2:J:20:PHE:CZ	2:J:24:MET:HE2	2.30	0.66
2:P:142:MET:HE2	2:P:146:ALA:C	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:211:MET:HE1	2:R:231:PHE:HZ	1.59	0.66
1:U:561:ILE:HG22	1:U:564:ASN:HB3	1.78	0.66
2:X:18:ASN:HB2	7:X:302:SF4:S1	2.36	0.66
2:X:40:GLN:HE21	2:X:117:ASN:HA	1.60	0.66
1:S:610:LYS:HZ2	1:S:618:GLN:HE22	1.43	0.65
1:S:695:LEU:O	1:S:699:GLU:HG2	1.95	0.65
2:B:43:HIS:ND1	8:B:403:HOH:O	2.29	0.65
1:E:677:CYS:SG	8:E:1662:HOH:O	2.54	0.65
1:M:426:MET:HE1	1:M:618:GLN:HG2	1.78	0.65
2:P:23:CYS:HB3	2:P:39:MET:HE1	1.78	0.65
2:X:21:MET:HE3	8:X:565:HOH:O	1.97	0.65
1:A:74:LEU:HD12	1:A:750:LYS:HA	1.78	0.65
1:A:146:MET:HG2	5:A:903:MGD:N7	2.11	0.65
2:H:2:GLU:HG2	2:H:158:LYS:HG2	1.78	0.65
2:N:70:HIS:CD2	2:N:92:VAL:H	2.12	0.65
1:O:426:MET:HE1	1:O:618:GLN:O	1.95	0.65
2:R:46:MET:CE	2:R:66:THR:N	2.60	0.65
1:O:558:SER:H	1:O:564:ASN:ND2	1.94	0.65
1:Q:356:GLY:H	5:Q:904:MGD:H5'2	1.60	0.65
1:U:823:TYR:CZ	1:U:825:PRO:HG3	2.31	0.65
2:X:71:CYS:HB3	2:X:184:PRO:HA	1.77	0.65
2:X:164:MET:O	2:X:168:VAL:HG23	1.97	0.65
1:A:387:TRP:CE2	1:A:389:THR:HA	2.32	0.65
1:E:66:PHE:HA	1:E:69:MET:HE3	1.77	0.65
2:F:21:MET:CE	2:F:24:MET:HE3	2.27	0.65
2:H:69:MET:HB3	2:H:184:PRO:HB3	1.79	0.65
2:R:40:GLN:NE2	2:R:118:GLU:H	1.93	0.65
1:W:201:LEU:HD13	1:W:387:TRP:HB2	1.78	0.65
1:S:426:MET:HE2	1:S:618:GLN:HG2	1.79	0.65
2:X:105:LEU:HB3	2:X:114:MET:HE1	1.79	0.65
1:A:629:MET:HE2	1:A:634:PHE:CA	2.27	0.65
2:L:49:GLU:HG3	2:L:64:ARG:NH2	2.12	0.65
2:R:70:HIS:CD2	2:R:92:VAL:H	2.10	0.65
2:V:19:CYS:O	2:V:22:GLY:N	2.28	0.65
2:F:71:CYS:HB2	2:F:182:THR:O	1.97	0.65
1:O:395:LEU:HD12	1:O:566:GLN:HA	1.78	0.65
2:P:68:CYS:CB	2:P:126:CYS:HB3	2.26	0.65
1:W:610:LYS:HZ3	1:W:618:GLN:NE2	1.95	0.65
3:E:901:ACT:H1	8:E:1044:HOH:O	1.96	0.65
1:M:1:MET:H3	1:M:22:ASP:CG	2.05	0.65
2:N:125:LYS:HD2	2:N:126:CYS:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:2:GLU:HG2	2:P:158:LYS:HG2	1.77	0.65
2:T:69:MET:HB3	2:T:184:PRO:HB3	1.79	0.65
2:X:71:CYS:HA	2:X:184:PRO:HA	1.78	0.65
2:H:1:MET:HE2	2:H:88:GLU:OE2	1.97	0.64
1:W:175:SER:HA	1:W:359:ARG:HH21	1.61	0.64
2:F:68:CYS:HB3	2:F:70:HIS:CE1	2.32	0.64
1:O:790:ILE:HD13	1:O:803:ALA:HB2	1.77	0.64
1:S:630:THR:OG1	1:S:633:GLU:HG3	1.97	0.64
1:W:610:LYS:HZ3	1:W:618:GLN:HE22	1.44	0.64
1:C:99:GLY:HA2	1:C:102:LYS:HE2	1.78	0.64
1:E:195:ASN:HD21	1:E:354:TRP:CD1	2.15	0.64
1:G:695:LEU:O	1:G:699:GLU:HG2	1.96	0.64
1:Q:31:MET:O	1:Q:56:LYS:HG3	1.98	0.64
1:S:146:MET:CE	1:S:544:THR:HB	2.26	0.64
3:M:901:ACT:H1	8:M:1043:HOH:O	1.97	0.64
2:R:56:TYR:HA	2:R:59:ASN:HD22	1.62	0.64
2:V:142:MET:HE2	2:V:146:ALA:C	2.22	0.64
2:V:229:THR:HB	2:V:233:GLY:HA2	1.79	0.64
1:A:291:GLU:CD	1:A:291:GLU:H	2.05	0.64
1:C:855:MET:HB2	1:C:857:ASN:OD1	1.97	0.64
1:Q:69:MET:HE2	1:Q:754:MET:CE	2.28	0.64
1:O:187:TRP:CH2	1:O:196:PRO:HB3	2.32	0.64
1:O:770:TRP:HB3	1:O:801:LEU:HD23	1.80	0.64
1:S:81:LYS:HB2	1:S:112:ILE:HD13	1.78	0.64
2:V:75:PRO:HD2	7:V:304:SF4:S4	2.38	0.64
1:W:610:LYS:NZ	1:W:618:GLN:NE2	2.45	0.64
1:M:753:TYR:HB3	2:N:24:MET:HE3	1.80	0.64
2:T:106:LEU:HD23	2:T:114:MET:HE2	1.80	0.64
2:X:71:CYS:HB3	2:X:184:PRO:CA	2.27	0.64
2:B:68:CYS:HB3	2:B:70:HIS:CE1	2.33	0.64
1:C:356:GLY:H	5:C:904:MGD:C5'	2.11	0.64
1:G:426:MET:HE1	1:G:618:GLN:HG2	1.79	0.64
2:L:68:CYS:HB3	2:L:126:CYS:HB3	1.78	0.64
2:V:5:TYR:CD2	2:V:164:MET:HG2	2.33	0.64
2:V:71:CYS:HA	2:V:184:PRO:HA	1.80	0.64
2:B:68:CYS:HB2	2:B:126:CYS:CB	2.27	0.64
1:I:66:PHE:CZ	1:I:146:MET:HE1	2.26	0.64
1:C:146:MET:HE3	1:C:545:ASN:OD1	1.98	0.63
1:E:557:CYS:N	1:E:564:ASN:HD21	1.85	0.63
1:M:319:GLU:HG2	1:S:726:LEU:CD1	2.27	0.63
1:O:610:LYS:HZ3	1:O:618:GLN:HE22	1.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:15:PRO:HD3	1:W:554:PHE:CE1	2.33	0.63
1:A:96:ARG:HD2	1:A:514:TYR:O	1.99	0.63
1:K:356:GLY:H	5:K:904:MGD:C5'	2.11	0.63
2:P:21:MET:HA	2:P:21:MET:CE	2.27	0.63
2:V:125:LYS:HD2	2:V:126:CYS:O	1.99	0.63
2:D:68:CYS:HB3	2:D:126:CYS:HB3	1.78	0.63
2:L:5:TYR:HB2	2:L:157:LEU:CD1	2.29	0.63
1:O:563:ASP:O	1:O:566:GLN:HG2	1.97	0.63
1:W:100:LEU:HD12	1:W:105:PRO:HG3	1.80	0.63
1:E:134:PRO:HB2	1:E:439:LEU:HD11	1.79	0.63
1:I:387:TRP:CE2	1:I:389:THR:HA	2.34	0.63
1:W:801:LEU:HD11	1:W:839:ILE:HD11	1.80	0.63
2:F:203:ILE:HD12	2:F:203:ILE:N	2.13	0.63
2:N:207:GLY:CA	1:S:728:VAL:HG12	2.22	0.63
1:Q:66:PHE:CD1	1:Q:69:MET:HE3	2.34	0.63
1:I:211:MET:HE1	2:J:231:PHE:HZ	1.63	0.63
1:M:870:ASP:HB3	1:M:872:TYR:CE1	2.34	0.63
2:N:40:GLN:NE2	2:N:118:GLU:H	1.96	0.63
1:U:729:LYS:HD2	8:U:1139:HOH:O	1.99	0.63
1:W:369:GLY:O	1:W:373:LEU:HD13	1.98	0.63
1:W:630:THR:OG1	1:W:633:GLU:HG3	1.99	0.63
1:E:146:MET:HE2	1:E:544:THR:HB	1.80	0.63
1:E:746:MET:HE2	5:E:903:MGD:O1B	1.98	0.63
1:G:177:GLU:HA	1:G:177:GLU:OE2	1.99	0.63
1:I:21:LYS:HB3	1:I:26:ILE:HD11	1.79	0.63
1:O:146:MET:CE	1:O:544:THR:HB	2.28	0.63
2:R:76:CYS:HB3	2:R:108:THR:OG1	1.98	0.63
1:W:186:MET:HE2	1:W:371:ILE:HG22	1.80	0.63
2:X:19:CYS:CB	2:X:145:CYS:HB3	2.29	0.63
1:C:356:GLY:H	5:C:904:MGD:H5'2	1.64	0.63
2:F:114:MET:HA	2:F:125:LYS:HB3	1.81	0.63
1:I:13:GLY:HA3	1:I:63:THR:OG1	1.99	0.63
2:P:40:GLN:HE22	2:P:118:GLU:H	1.45	0.63
1:Q:557:CYS:H	1:Q:564:ASN:ND2	1.86	0.63
2:R:21:MET:HE2	2:R:21:MET:HA	1.81	0.63
2:X:177:LYS:N	2:X:178:PRO:HD3	2.14	0.63
1:G:630:THR:OG1	1:G:633:GLU:HG3	1.99	0.63
1:K:495:LYS:HD2	1:K:514:TYR:OH	1.99	0.63
2:R:142:MET:HE1	8:R:428:HOH:O	1.97	0.63
1:U:457:MET:HE3	8:U:1002:HOH:O	1.98	0.63
2:V:71:CYS:HB2	2:V:182:THR:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:ARG:HB2	1:C:642:VAL:HB	1.81	0.62
1:E:823:TYR:CZ	1:E:825:PRO:HG3	2.34	0.62
2:N:40:GLN:HE22	2:N:118:GLU:H	1.47	0.62
2:R:68:CYS:HB2	2:R:126:CYS:CB	2.29	0.62
2:T:76:CYS:HB3	2:T:108:THR:OG1	1.98	0.62
1:G:610:LYS:HZ2	1:G:618:GLN:HE22	1.47	0.62
2:J:104:GLU:CD	2:J:104:GLU:H	2.07	0.62
1:O:100:LEU:HD12	1:O:105:PRO:HG3	1.81	0.62
1:S:66:PHE:CZ	1:S:146:MET:HE1	2.33	0.62
2:V:95:ASP:HB3	2:V:98:LYS:HB2	1.80	0.62
1:M:541:PRO:HB2	1:M:586:SER:HA	1.81	0.62
1:S:426:MET:HE3	1:S:426:MET:HA	1.80	0.62
1:S:801:LEU:HD11	1:S:839:ILE:HD11	1.81	0.62
1:W:218:ASP:OD2	1:W:253:ASN:HB2	1.99	0.62
2:B:40:GLN:NE2	2:B:118:GLU:H	1.98	0.62
1:E:74:LEU:HD12	1:E:750:LYS:HA	1.82	0.62
1:G:677:CYS:SG	8:G:1667:HOH:O	2.56	0.62
1:M:610:LYS:HZ1	1:M:618:GLN:HE22	1.45	0.62
1:M:146:MET:CE	1:M:544:THR:HB	2.30	0.62
2:T:125:LYS:HD2	2:T:126:CYS:O	1.99	0.62
2:B:70:HIS:CD2	2:B:92:VAL:H	2.13	0.62
2:D:17:ASN:HD22	2:D:17:ASN:N	1.97	0.62
2:N:21:MET:HA	2:N:21:MET:CE	2.29	0.62
1:O:394:PRO:HG3	8:O:1329:HOH:O	1.99	0.62
2:P:185:ARG:CZ	2:P:185:ARG:HB3	2.29	0.62
1:Q:153:ARG:O	1:Q:157:TYR:HB3	2.00	0.62
2:X:56:TYR:HA	2:X:59:ASN:HD22	1.63	0.62
1:E:44:ILE:HD11	1:E:394:PRO:HG2	1.82	0.62
1:Q:141:PRO:HA	1:Q:496:TYR:HB3	1.81	0.62
1:S:165:GLY:HA3	1:S:166:PHE:HB3	1.81	0.62
1:S:553:GLU:HG2	1:S:556:ASN:HB2	1.82	0.62
1:U:786:ASN:HD21	1:U:804:GLN:HA	1.64	0.62
1:W:503:THR:HG21	5:W:903:MGD:O2A	2.00	0.62
1:C:177:GLU:OE2	1:C:177:GLU:HA	2.00	0.62
1:G:378:GLY:O	1:G:381:LYS:HG2	1.99	0.62
1:I:140:THR:HB	1:I:169:ALA:HB3	1.82	0.62
2:L:114:MET:HB3	2:L:125:LYS:HB3	1.80	0.62
2:P:114:MET:HB3	2:P:125:LYS:HB3	1.81	0.62
1:U:140:THR:HB	1:U:169:ALA:HB3	1.82	0.62
2:V:142:MET:HE2	2:V:147:HIS:N	2.15	0.62
2:X:1:MET:HE2	2:X:88:GLU:OE2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:PRO:HG3	8:A:1324:HOH:O	1.99	0.62
1:C:81:LYS:HB2	1:C:112:ILE:HD13	1.81	0.62
2:J:5:TYR:HB2	2:J:157:LEU:CD1	2.30	0.62
1:K:201:LEU:HD13	1:K:387:TRP:HB2	1.82	0.62
1:K:786:ASN:ND2	1:K:804:GLN:HA	2.14	0.62
1:U:478:HIS:HD2	8:U:1210:HOH:O	1.82	0.62
2:L:70:HIS:HD2	2:L:92:VAL:H	1.48	0.62
2:N:68:CYS:HB2	2:N:126:CYS:HB3	1.81	0.62
1:Q:81:LYS:HB2	1:Q:112:ILE:HD13	1.82	0.62
2:R:71:CYS:HB2	2:R:182:THR:O	2.00	0.62
1:W:212:ILE:HD11	1:W:238:LEU:HD13	1.82	0.62
2:B:114:MET:HA	2:B:125:LYS:HB3	1.81	0.61
1:C:100:LEU:HD12	1:C:105:PRO:HG3	1.80	0.61
1:O:426:MET:HA	1:O:426:MET:HE3	1.82	0.61
1:U:134:PRO:HB2	1:U:439:LEU:HD11	1.82	0.61
1:U:166:PHE:N	1:U:439:LEU:HD12	2.15	0.61
2:V:40:GLN:NE2	2:V:117:ASN:HA	2.15	0.61
1:W:66:PHE:HZ	1:W:146:MET:HE1	1.63	0.61
1:K:146:MET:CE	1:K:544:THR:HB	2.30	0.61
1:K:756:TYR:CD1	2:L:24:MET:HE1	2.35	0.61
1:O:452:ILE:HB	1:O:453:PRO:HD3	1.82	0.61
2:P:19:CYS:HB2	2:P:46:MET:HG2	1.82	0.61
1:Q:201:LEU:HD13	1:Q:387:TRP:HB2	1.82	0.61
1:W:610:LYS:HZ2	1:W:618:GLN:HE22	1.48	0.61
2:X:77:VAL:HG22	2:X:84:VAL:HG12	1.81	0.61
1:K:362:HIS:HB3	1:K:717:ALA:HB2	1.82	0.61
2:R:19:CYS:O	2:R:22:GLY:N	2.33	0.61
1:W:187:TRP:CH2	1:W:196:PRO:HB3	2.35	0.61
2:X:118:GLU:HG2	8:X:549:HOH:O	2.00	0.61
1:A:128:ILE:CD1	1:A:492:MET:HB2	2.30	0.61
1:C:644:ASP:C	1:C:646:PRO:HD3	2.25	0.61
1:E:252:MET:HE3	1:E:263:TRP:CE3	2.34	0.61
2:J:46:MET:HE1	2:J:65:PRO:C	2.25	0.61
1:O:356:GLY:H	5:O:904:MGD:H5'2	1.65	0.61
1:W:561:ILE:CG2	1:W:564:ASN:HB3	2.29	0.61
2:L:164:MET:O	2:L:168:VAL:HG23	2.01	0.61
1:Q:426:MET:HE1	1:Q:618:GLN:HG2	1.81	0.61
1:E:28:MET:HE1	1:E:66:PHE:HB3	1.83	0.61
1:K:786:ASN:HD22	1:K:805:VAL:H	1.47	0.61
1:Q:610:LYS:HZ3	1:Q:618:GLN:NE2	1.93	0.61
1:U:100:LEU:HD12	1:U:105:PRO:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:855:MET:HB2	1:E:857:ASN:OD1	2.01	0.61
2:H:166:LYS:HG2	2:H:170:GLU:OE2	2.01	0.61
1:U:696:LYS:O	1:U:700:GLU:HG3	1.99	0.61
1:W:39:ALA:HB1	8:W:1275:HOH:O	2.00	0.61
1:E:356:GLY:H	5:E:904:MGD:H5'2	1.65	0.61
1:E:395:LEU:HD12	1:E:566:GLN:HA	1.82	0.61
1:K:144:HIS:HB2	5:K:903:MGD:O1B	2.00	0.61
2:R:104:GLU:CD	2:R:104:GLU:H	2.09	0.61
1:K:195:ASN:HD21	1:K:354:TRP:CD1	2.19	0.61
1:K:452:ILE:HB	1:K:453:PRO:HD3	1.82	0.61
2:L:58:ARG:HD2	2:L:268:ASP:OD1	1.99	0.61
2:N:142:MET:CE	2:N:146:ALA:HB1	2.29	0.61
1:S:629:MET:HE2	1:S:634:PHE:HA	1.83	0.61
1:U:76:ILE:HG22	1:U:541:PRO:HG3	1.82	0.61
2:V:218:LYS:HG2	2:V:223:GLU:HA	1.83	0.61
1:I:134:PRO:HB2	1:I:439:LEU:HD11	1.83	0.61
1:M:746:MET:HE2	5:M:903:MGD:O1B	2.01	0.61
2:P:76:CYS:HB3	2:P:108:THR:OG1	2.00	0.61
2:T:46:MET:HE1	2:T:66:THR:N	2.15	0.61
1:U:557:CYS:H	1:U:564:ASN:ND2	1.86	0.61
1:W:15:PRO:HD2	8:W:1003:HOH:O	2.00	0.61
2:X:94:ILE:HG22	2:X:95:ASP:N	2.15	0.61
2:X:217:LEU:HD12	2:X:246:THR:O	2.01	0.61
1:A:541:PRO:HB2	1:A:586:SER:HA	1.81	0.60
2:F:142:MET:HE2	2:F:146:ALA:CB	2.31	0.60
1:O:794:ASN:ND2	1:O:862:VAL:HG12	2.14	0.60
1:U:195:ASN:HD21	1:U:354:TRP:CD1	2.19	0.60
2:X:19:CYS:HA	2:X:145:CYS:HB3	1.83	0.60
2:X:40:GLN:HE22	2:X:117:ASN:HA	1.66	0.60
1:C:146:MET:HE2	1:C:544:THR:HB	1.83	0.60
2:D:19:CYS:HB3	2:D:145:CYS:CB	2.29	0.60
2:F:13:CYS:HB3	2:F:63:TYR:HB2	1.83	0.60
2:J:40:GLN:NE2	2:J:118:GLU:H	1.99	0.60
2:P:5:TYR:CD2	2:P:164:MET:HG2	2.36	0.60
2:H:46:MET:HE3	2:H:47:ASN:N	2.16	0.60
1:I:239:LYS:HE2	8:I:1602:HOH:O	2.00	0.60
1:K:61:PRO:HB3	8:L:567:HOH:O	2.00	0.60
2:P:58:ARG:HD2	2:P:268:ASP:OD1	2.00	0.60
1:U:356:GLY:H	5:U:904:MGD:H5'2	1.67	0.60
1:M:426:MET:HE1	1:M:618:GLN:O	2.00	0.60
1:S:75:ARG:NH2	1:S:543:CYS:HA	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:CYS:HB3	2:B:39:MET:HE1	1.83	0.60
1:C:13:GLY:HA3	1:C:63:THR:OG1	2.02	0.60
2:D:72:GLU:OE1	2:D:183:LYS:HB3	2.01	0.60
2:N:68:CYS:HB3	2:N:70:HIS:CE1	2.37	0.60
2:R:43:HIS:ND1	8:R:402:HOH:O	2.31	0.60
1:U:602:ILE:HG23	8:U:1079:HOH:O	2.02	0.60
1:G:66:PHE:CZ	1:G:146:MET:HE1	2.35	0.60
1:I:177:GLU:HA	1:I:177:GLU:OE2	2.01	0.60
2:J:68:CYS:HB2	2:J:126:CYS:CB	2.31	0.60
2:P:19:CYS:O	2:P:22:GLY:N	2.34	0.60
1:U:311:THR:HG21	8:U:1503:HOH:O	2.02	0.60
1:W:426:MET:HE2	1:W:618:GLN:OE1	2.01	0.60
1:W:510:TYR:O	1:W:513:MET:HG2	2.01	0.60
1:C:528:TRP:CD2	1:C:750:LYS:HD3	2.37	0.60
1:C:786:ASN:ND2	1:C:804:GLN:HA	2.16	0.60
1:M:645:ASN:ND2	1:M:648:ARG:HB3	2.17	0.60
1:O:195:ASN:HD21	1:O:354:TRP:CD1	2.19	0.60
1:Q:74:LEU:HD12	1:Q:750:LYS:HA	1.84	0.60
1:S:356:GLY:H	5:S:904:MGD:H5'2	1.66	0.60
1:U:163:MET:HE1	1:U:606:PHE:HA	1.83	0.60
1:K:32:ASP:HB2	8:K:1663:HOH:O	2.01	0.60
1:M:66:PHE:CD1	1:M:69:MET:HE3	2.37	0.60
2:R:21:MET:HA	2:R:21:MET:CE	2.32	0.60
1:S:557:CYS:H	1:S:564:ASN:ND2	1.86	0.60
2:T:10:VAL:HG13	2:T:63:TYR:O	2.02	0.60
2:T:19:CYS:HB2	2:T:46:MET:HG2	1.84	0.60
2:V:23:CYS:HB3	2:V:39:MET:HE1	1.83	0.60
1:W:296:ASN:HB3	1:W:657:PHE:CZ	2.36	0.60
1:A:100:LEU:CD1	1:A:105:PRO:HG3	2.32	0.60
1:I:77:PRO:HB2	1:I:78:TYR:CD2	2.36	0.60
1:K:426:MET:HE1	1:K:618:GLN:O	2.02	0.60
1:O:738:HIS:HE2	5:O:903:MGD:H15	1.50	0.60
2:X:58:ARG:HD2	2:X:268:ASP:OD1	2.02	0.60
2:L:46:MET:HE3	2:L:47:ASN:N	2.17	0.60
1:M:146:MET:HE2	1:M:544:THR:CB	2.32	0.60
1:M:602:ILE:HG21	8:M:1074:HOH:O	2.01	0.60
1:G:1:MET:H3	1:G:22:ASP:CG	2.10	0.59
1:Q:214:PHE:HA	1:Q:347:ALA:HB3	1.84	0.59
1:G:10:SER:HA	1:G:15:PRO:HA	1.83	0.59
1:G:756:TYR:HD1	2:H:24:MET:HE1	1.65	0.59
1:O:557:CYS:N	1:O:564:ASN:HD21	1.97	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:494:TRP:HE1	1:Q:525:GLN:HE21	1.50	0.59
2:V:5:TYR:HB2	2:V:157:LEU:CD1	2.32	0.59
2:V:46:MET:HE3	2:V:47:ASN:N	2.18	0.59
1:W:134:PRO:HB2	1:W:439:LEU:HD11	1.84	0.59
1:A:738:HIS:HE2	5:A:903:MGD:H15	1.50	0.59
2:B:105:LEU:HB3	2:B:114:MET:CE	2.33	0.59
2:J:164:MET:O	2:J:168:VAL:HG23	2.02	0.59
1:Q:44:ILE:HD11	1:Q:394:PRO:CG	2.31	0.59
1:Q:189:PHE:HZ	1:Q:654:LEU:HD21	1.67	0.59
1:U:503:THR:HG21	5:U:903:MGD:O2A	2.02	0.59
2:X:129:CYS:HB3	2:X:131:HIS:HE1	1.63	0.59
2:B:19:CYS:HB2	2:B:46:MET:HG2	1.85	0.59
2:B:142:MET:HE2	2:B:146:ALA:C	2.27	0.59
1:I:1:MET:H3	1:I:22:ASP:CG	2.11	0.59
1:M:394:PRO:HG3	8:M:1323:HOH:O	2.02	0.59
2:R:56:TYR:HA	2:R:59:ASN:ND2	2.18	0.59
1:S:746:MET:HE2	5:S:903:MGD:O1B	2.01	0.59
2:V:68:CYS:CB	2:V:126:CYS:HB3	2.32	0.59
1:W:356:GLY:H	5:W:904:MGD:H5'2	1.68	0.59
1:W:426:MET:HA	1:W:426:MET:HE3	1.83	0.59
1:E:211:MET:HE3	8:E:1453:HOH:O	2.01	0.59
2:P:21:MET:HA	2:P:21:MET:HE2	1.84	0.59
1:S:75:ARG:HH22	1:S:547:GLU:CD	2.10	0.59
2:T:5:TYR:HB2	2:T:157:LEU:CD1	2.31	0.59
2:H:106:LEU:HD23	2:H:114:MET:HE2	1.83	0.59
1:K:146:MET:HE2	1:K:544:THR:CB	2.32	0.59
1:S:146:MET:HE3	1:S:545:ASN:OD1	2.02	0.59
1:U:141:PRO:HA	1:U:496:TYR:HB3	1.85	0.59
1:U:257:ARG:HD3	2:V:61:ILE:HG21	1.84	0.59
1:U:644:ASP:O	1:U:646:PRO:HD3	2.02	0.59
1:U:722:LYS:HG2	8:U:1562:HOH:O	2.02	0.59
1:A:265:SER:O	1:A:810:GLN:NE2	2.34	0.59
2:D:58:ARG:HD2	2:D:268:ASP:OD1	2.02	0.59
2:P:112:GLY:HA2	8:P:516:HOH:O	2.03	0.59
1:U:395:LEU:HD12	1:U:566:GLN:HA	1.83	0.59
2:V:59:ASN:ND2	2:V:59:ASN:H	2.01	0.59
1:A:557:CYS:N	1:A:564:ASN:HD21	1.88	0.59
2:H:19:CYS:O	2:H:22:GLY:N	2.35	0.59
1:K:822:VAL:O	1:K:836:GLY:HA3	2.03	0.59
1:O:176:TRP:O	1:O:177:GLU:C	2.46	0.59
2:P:166:LYS:O	2:P:170:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:106:LEU:HD23	2:V:114:MET:HE2	1.85	0.59
1:W:177:GLU:HA	1:W:177:GLU:OE2	2.02	0.59
1:W:765:ASP:HB2	8:W:1169:HOH:O	2.01	0.59
2:D:106:LEU:HD22	2:D:114:MET:HG3	1.85	0.59
1:I:143:SER:HB3	3:I:901:ACT:H3	1.85	0.59
1:M:100:LEU:HD12	1:M:105:PRO:HG3	1.83	0.59
1:M:494:TRP:HE1	1:M:525:GLN:HE21	1.51	0.59
2:T:166:LYS:HE2	2:T:170:GLU:OE2	2.02	0.59
1:A:610:LYS:HZ1	1:A:618:GLN:HE22	1.51	0.59
1:G:426:MET:HE1	1:G:618:GLN:O	2.02	0.59
1:G:558:SER:H	1:G:564:ASN:ND2	2.01	0.59
2:H:76:CYS:HB3	2:H:108:THR:OG1	2.02	0.59
3:I:901:ACT:H1	8:I:1043:HOH:O	2.03	0.59
1:Q:629:MET:HE2	1:Q:634:PHE:CA	2.33	0.59
1:S:400:TYR:CZ	1:S:421:LYS:HD2	2.37	0.59
2:V:102:LYS:HB3	2:V:104:GLU:OE2	2.02	0.59
1:A:146:MET:HE3	1:A:545:ASN:OD1	2.02	0.58
1:G:756:TYR:CD1	2:H:24:MET:HE1	2.38	0.58
1:I:100:LEU:HD12	1:I:105:PRO:HG3	1.85	0.58
1:K:176:TRP:O	1:K:177:GLU:C	2.45	0.58
1:Q:746:MET:HE2	5:Q:903:MGD:O1B	2.03	0.58
1:U:848:ILE:HG12	1:U:856:ALA:HB2	1.85	0.58
2:X:53:ARG:HB2	2:X:60:ASP:OD1	2.02	0.58
1:G:218:ASP:OD2	1:G:253:ASN:HB2	2.04	0.58
1:G:296:ASN:O	1:G:687:LYS:HB3	2.03	0.58
2:J:71:CYS:HB2	2:J:182:THR:O	2.04	0.58
1:K:478:HIS:HD2	8:K:1207:HOH:O	1.85	0.58
2:L:105:LEU:HB3	2:L:114:MET:HE1	1.85	0.58
2:L:114:MET:CB	2:L:125:LYS:HB3	2.33	0.58
2:D:142:MET:HE2	2:D:146:ALA:C	2.29	0.58
1:E:100:LEU:CD1	1:E:105:PRO:HG3	2.33	0.58
2:L:19:CYS:O	2:L:22:GLY:N	2.35	0.58
1:M:44:ILE:HD11	1:M:394:PRO:HG2	1.85	0.58
1:Q:610:LYS:NZ	1:Q:618:GLN:NE2	2.44	0.58
2:R:21:MET:CE	2:R:24:MET:HE3	2.34	0.58
2:R:207:GLY:HA2	1:U:728:VAL:CG1	2.27	0.58
1:U:408:GLY:HA2	1:U:619:TYR:HE1	1.69	0.58
2:X:105:LEU:HD12	8:X:498:HOH:O	2.03	0.58
1:C:387:TRP:CE2	1:C:389:THR:HA	2.39	0.58
1:C:719:GLU:HG2	1:C:859:THR:O	2.04	0.58
1:C:786:ASN:HD21	1:C:804:GLN:HA	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:146:MET:HG2	5:M:903:MGD:N7	2.18	0.58
1:Q:356:GLY:H	5:Q:904:MGD:C5'	2.17	0.58
1:U:104:ASP:OD2	1:U:107:SER:HB3	2.03	0.58
1:U:166:PHE:H	1:U:439:LEU:HD12	1.68	0.58
1:W:753:TYR:HB3	2:X:24:MET:HE3	1.85	0.58
2:D:106:LEU:HD23	2:D:114:MET:HE2	1.85	0.58
1:K:695:LEU:O	1:K:699:GLU:HG2	2.04	0.58
2:L:218:LYS:HG2	2:L:223:GLU:HA	1.85	0.58
1:Q:561:ILE:HG22	1:Q:564:ASN:HB3	1.86	0.58
2:T:70:HIS:HD2	2:T:92:VAL:H	1.50	0.58
1:W:146:MET:CE	1:W:544:THR:HB	2.32	0.58
1:W:147:TRP:CD1	1:W:552:SER:HG	2.21	0.58
1:K:849:SER:HB3	1:K:852:ALA:CB	2.33	0.58
2:L:75:PRO:HD2	7:L:304:SF4:S4	2.43	0.58
1:O:197:GLU:OE2	1:O:665:THR:OG1	2.20	0.58
2:V:5:TYR:HB2	2:V:157:LEU:HD11	1.85	0.58
2:V:256:TYR:HB2	2:V:274:LEU:HD21	1.85	0.58
1:A:826:LEU:HD21	1:A:835:ARG:HD3	1.86	0.58
2:B:114:MET:HE3	2:B:123:ALA:HB1	1.85	0.58
1:C:494:TRP:HE1	1:C:525:GLN:HE21	1.50	0.58
2:D:46:MET:HE1	2:D:66:THR:H	1.69	0.58
2:D:46:MET:HE3	2:D:47:ASN:N	2.19	0.58
2:F:5:TYR:HB2	2:F:157:LEU:CD1	2.33	0.58
1:K:558:SER:H	1:K:564:ASN:ND2	2.01	0.58
1:O:364:ILE:HD13	1:O:708:ARG:HG3	1.86	0.58
1:Q:823:TYR:CZ	1:Q:825:PRO:HG3	2.38	0.58
1:U:28:MET:HE1	1:U:67:LYS:N	2.19	0.58
1:A:1:MET:H3	1:A:22:ASP:CG	2.11	0.58
1:E:81:LYS:HB2	1:E:112:ILE:HD13	1.84	0.58
2:J:46:MET:CE	2:J:66:THR:N	2.66	0.58
1:M:81:LYS:HB2	1:M:112:ILE:HD13	1.86	0.58
2:N:46:MET:CE	2:N:66:THR:H	2.17	0.58
2:R:46:MET:CE	2:R:66:THR:H	2.17	0.58
2:T:19:CYS:O	2:T:22:GLY:N	2.36	0.58
2:T:46:MET:HE3	2:T:47:ASN:N	2.17	0.58
2:V:106:LEU:HD11	2:V:116:TRP:HB2	1.84	0.58
2:B:68:CYS:HB3	2:B:126:CYS:HB3	1.85	0.58
1:C:140:THR:HB	1:C:169:ALA:HB3	1.86	0.58
1:E:339:TRP:CH2	1:E:346:LEU:HD13	2.39	0.58
1:E:870:ASP:HB3	1:E:872:TYR:CE1	2.39	0.58
2:L:4:TYR:CE2	2:L:158:LYS:HD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:503:THR:HG21	5:S:903:MGD:O2A	2.04	0.58
2:T:68:CYS:SG	2:T:113:VAL:HG21	2.44	0.58
1:W:174:ASP:O	1:W:177:GLU:HG2	2.03	0.58
1:C:630:THR:OG1	1:C:633:GLU:HG3	2.03	0.58
1:O:67:LYS:HE3	2:P:29:LEU:HD12	1.86	0.58
1:U:610:LYS:NZ	1:U:618:GLN:NE2	2.47	0.58
3:U:901:ACT:H1	8:U:1047:HOH:O	2.03	0.58
1:W:211:MET:HE1	2:X:231:PHE:CZ	2.39	0.58
2:J:1:MET:HE2	2:J:88:GLU:OE2	2.03	0.57
1:O:356:GLY:H	5:O:904:MGD:C5'	2.17	0.57
2:P:18:ASN:HB2	7:P:302:SF4:S1	2.44	0.57
1:S:644:ASP:C	1:S:646:PRO:HD3	2.28	0.57
1:W:20:VAL:HG13	1:W:24:LYS:O	2.04	0.57
2:X:19:CYS:CB	2:X:46:MET:HG2	2.33	0.57
2:X:71:CYS:CA	2:X:184:PRO:HA	2.34	0.57
2:X:106:LEU:HD11	2:X:116:TRP:HB2	1.85	0.57
1:I:629:MET:HE2	1:I:634:PHE:CA	2.33	0.57
2:J:112:GLY:HA2	8:J:519:HOH:O	2.03	0.57
1:K:610:LYS:NZ	1:K:618:GLN:NE2	2.49	0.57
1:M:676:VAL:HG13	8:M:1053:HOH:O	2.03	0.57
2:N:19:CYS:O	2:N:22:GLY:N	2.35	0.57
2:N:58:ARG:HD2	2:N:268:ASP:OD1	2.05	0.57
1:U:28:MET:HE1	1:U:66:PHE:HB3	1.87	0.57
2:X:19:CYS:HB3	2:X:145:CYS:CB	2.31	0.57
2:H:40:GLN:HE22	2:H:118:GLU:H	1.52	0.57
1:M:134:PRO:HB2	1:M:439:LEU:HD11	1.85	0.57
2:T:75:PRO:HD2	7:T:304:SF4:S4	2.45	0.57
1:E:146:MET:CE	1:E:544:THR:HB	2.35	0.57
2:H:210:PHE:HD2	2:H:213:ALA:HB2	1.70	0.57
1:S:35:ASP:OD1	1:S:55:ARG:HD3	2.04	0.57
1:S:744:HIS:HA	1:S:819:SER:HB3	1.86	0.57
1:U:75:ARG:HH22	1:U:547:GLU:CD	2.13	0.57
1:U:265:SER:O	1:U:810:GLN:NE2	2.37	0.57
2:X:19:CYS:CA	2:X:145:CYS:HB3	2.35	0.57
2:X:73:ASN:O	2:X:75:PRO:HD3	2.04	0.57
1:A:146:MET:CE	1:A:544:THR:HB	2.33	0.57
1:C:197:GLU:OE2	1:C:667:ASP:HB2	2.04	0.57
1:G:356:GLY:H	5:G:904:MGD:C5'	2.15	0.57
1:I:645:ASN:ND2	1:I:648:ARG:HB3	2.18	0.57
2:L:216:VAL:HG13	2:L:223:GLU:HG3	1.86	0.57
1:S:400:TYR:CE1	1:S:421:LYS:HD2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:296:ASN:O	1:M:687:LYS:HB3	2.04	0.57
1:O:134:PRO:HB2	1:O:439:LEU:HD11	1.86	0.57
2:R:46:MET:HE1	2:R:65:PRO:C	2.28	0.57
1:S:140:THR:HB	1:S:169:ALA:HB3	1.85	0.57
1:U:547:GLU:OE1	1:U:582:PRO:HA	2.04	0.57
1:U:825:PRO:HD2	8:U:1341:HOH:O	2.04	0.57
1:G:44:ILE:HD11	1:G:394:PRO:HG2	1.86	0.57
1:G:146:MET:HE2	1:G:544:THR:HA	1.86	0.57
1:G:184:MET:HE2	1:G:190:SER:HA	1.87	0.57
1:I:146:MET:CE	1:I:544:THR:HB	2.35	0.57
1:I:351:LEU:HD12	1:I:567:LEU:HD21	1.87	0.57
1:I:510:TYR:O	1:I:513:MET:HG2	2.05	0.57
2:J:21:MET:HE1	2:J:24:MET:HE3	1.87	0.57
1:S:104:ASP:OD2	1:S:107:SER:HB3	2.03	0.57
2:T:18:ASN:HB2	7:T:302:SF4:S1	2.44	0.57
2:V:176:ILE:HG22	2:V:177:LYS:HG3	1.87	0.57
2:B:166:LYS:HG2	2:B:170:GLU:OE2	2.05	0.57
1:E:153:ARG:O	1:E:157:TYR:HB3	2.05	0.57
1:O:786:ASN:ND2	1:O:804:GLN:HA	2.20	0.57
2:P:201:ALA:HB2	2:P:269:LEU:HB2	1.86	0.57
2:R:203:ILE:N	2:R:203:ILE:HD12	2.19	0.57
2:T:114:MET:HA	2:T:125:LYS:HB3	1.86	0.57
1:W:557:CYS:N	1:W:564:ASN:HD21	2.02	0.57
2:X:4:TYR:CD1	2:X:89:ASP:HB2	2.40	0.57
1:M:252:MET:HE3	1:M:263:TRP:CE3	2.40	0.57
1:M:650:LYS:HE3	8:M:1227:HOH:O	2.05	0.57
2:N:69:MET:HB3	2:N:184:PRO:HB3	1.86	0.57
1:O:378:GLY:O	1:O:381:LYS:HG2	2.05	0.57
1:Q:695:LEU:O	1:Q:699:GLU:HG2	2.05	0.57
1:S:69:MET:HE2	1:S:754:MET:HE1	1.85	0.57
1:U:177:GLU:HA	1:U:177:GLU:OE2	2.05	0.57
2:D:56:TYR:HA	2:D:59:ASN:ND2	2.18	0.57
1:K:85:PHE:CE2	1:K:87:PRO:HG3	2.40	0.57
1:Q:400:TYR:CZ	1:Q:421:LYS:HD2	2.39	0.57
2:R:114:MET:HA	2:R:125:LYS:HB3	1.86	0.57
1:U:786:ASN:ND2	1:U:804:GLN:HA	2.19	0.57
2:V:177:LYS:N	2:V:178:PRO:HD3	2.19	0.57
1:W:186:MET:HE2	1:W:371:ILE:CG2	2.35	0.57
2:H:139:ALA:HB3	2:H:140:PRO:HD3	1.87	0.56
1:Q:291:GLU:CD	1:Q:291:GLU:H	2.13	0.56
1:U:176:TRP:O	1:U:177:GLU:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:746:MET:HE2	5:W:903:MGD:O1B	2.05	0.56
1:G:146:MET:HE3	1:G:545:ASN:OD1	2.04	0.56
1:I:249:ASP:CG	5:I:904:MGD:H1'	2.30	0.56
2:J:142:MET:HE2	2:J:147:HIS:N	2.20	0.56
1:K:257:ARG:HD3	2:L:61:ILE:HG21	1.87	0.56
1:K:610:LYS:HZ3	1:K:618:GLN:HE22	1.51	0.56
1:O:69:MET:HE2	1:O:754:MET:HE3	1.87	0.56
2:X:17:ASN:N	2:X:17:ASN:HD22	2.01	0.56
1:A:377:GLN:O	1:A:381:LYS:HE2	2.06	0.56
1:C:823:TYR:CE2	1:C:825:PRO:HG3	2.40	0.56
2:D:68:CYS:CB	2:D:126:CYS:HB3	2.35	0.56
1:G:510:TYR:O	1:G:513:MET:HG2	2.06	0.56
1:I:494:TRP:HE1	1:I:525:GLN:HE21	1.52	0.56
1:K:134:PRO:HB2	1:K:439:LEU:HD11	1.86	0.56
1:K:233:ILE:HG22	8:K:1331:HOH:O	2.04	0.56
2:L:40:GLN:HE21	2:L:117:ASN:HA	1.69	0.56
2:L:77:VAL:HG22	2:L:84:VAL:HG12	1.87	0.56
1:M:319:GLU:HG2	1:S:726:LEU:HD13	1.87	0.56
2:P:106:LEU:HD11	2:P:116:TRP:HB2	1.87	0.56
2:R:68:CYS:HB3	2:R:70:HIS:CE1	2.40	0.56
1:S:4:VAL:HG22	1:S:21:LYS:HB2	1.87	0.56
1:S:144:HIS:CG	1:S:743:MET:HE1	2.40	0.56
1:S:291:GLU:H	1:S:291:GLU:CD	2.13	0.56
2:T:71:CYS:HB2	2:T:182:THR:O	2.05	0.56
2:V:75:PRO:HG2	2:V:110:PRO:HG2	1.87	0.56
2:V:112:GLY:HA2	8:V:516:HOH:O	2.05	0.56
2:X:112:GLY:HA2	8:X:520:HOH:O	2.05	0.56
1:A:35:ASP:OD1	1:A:55:ARG:HD3	2.06	0.56
1:C:146:MET:CE	1:C:544:THR:HB	2.35	0.56
1:G:364:ILE:HD13	1:G:708:ARG:HG3	1.88	0.56
1:W:66:PHE:CD1	1:W:69:MET:HE3	2.41	0.56
1:W:387:TRP:CE2	1:W:389:THR:HA	2.41	0.56
2:F:105:LEU:HB3	2:F:114:MET:HE1	1.87	0.56
1:M:218:ASP:OD2	1:M:253:ASN:HB2	2.06	0.56
2:N:254:LYS:HD2	2:N:274:LEU:OXT	2.06	0.56
1:S:176:TRP:O	1:S:177:GLU:C	2.47	0.56
1:A:66:PHE:HA	1:A:69:MET:CE	2.26	0.56
1:A:140:THR:HB	1:A:169:ALA:HB3	1.87	0.56
1:G:146:MET:HE3	1:G:545:ASN:H	1.71	0.56
1:G:252:MET:HE3	1:G:263:TRP:CE3	2.41	0.56
1:G:494:TRP:HE1	1:G:525:GLN:HE21	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:696:LYS:O	1:G:700:GLU:HG3	2.05	0.56
1:I:563:ASP:O	1:I:566:GLN:HG2	2.06	0.56
1:M:141:PRO:HA	1:M:496:TYR:HB3	1.87	0.56
1:W:647:ASN:HB2	8:W:1448:HOH:O	2.04	0.56
2:F:1:MET:HE2	2:F:88:GLU:OE2	2.06	0.56
1:G:565:TYR:C	1:G:567:LEU:H	2.13	0.56
1:Q:15:PRO:HD2	8:Q:1003:HOH:O	2.06	0.56
1:W:146:MET:HG2	5:W:903:MGD:N7	2.19	0.56
1:W:494:TRP:HE1	1:W:525:GLN:HE21	1.54	0.56
1:C:738:HIS:HE2	5:C:903:MGD:H15	1.54	0.56
2:H:70:HIS:HD2	2:H:92:VAL:H	1.52	0.56
1:K:75:ARG:NH2	1:K:543:CYS:HA	2.21	0.56
1:K:729:LYS:HD2	8:K:1134:HOH:O	2.05	0.56
2:L:114:MET:HE3	2:L:123:ALA:HB1	1.86	0.56
2:N:104:GLU:H	2:N:104:GLU:CD	2.13	0.56
2:N:142:MET:HE2	2:N:146:ALA:C	2.31	0.56
1:O:100:LEU:CD1	1:O:105:PRO:HG3	2.36	0.56
1:Q:871:LYS:HG2	8:Q:1236:HOH:O	2.06	0.56
1:U:558:SER:H	1:U:564:ASN:ND2	2.03	0.56
1:U:610:LYS:HA	8:U:1475:HOH:O	2.05	0.56
1:W:719:GLU:HG2	1:W:859:THR:O	2.05	0.56
2:X:40:GLN:HB3	2:X:43:HIS:CE1	2.41	0.56
2:X:55:THR:HG22	8:X:537:HOH:O	2.04	0.56
2:X:92:VAL:HG21	7:X:304:SF4:S1	2.45	0.56
2:D:203:ILE:N	2:D:203:ILE:HD12	2.21	0.56
1:E:165:GLY:CA	1:E:166:PHE:HB3	2.35	0.56
2:F:56:TYR:HA	2:F:59:ASN:ND2	2.20	0.56
1:G:855:MET:HB2	1:G:857:ASN:OD1	2.05	0.56
2:H:166:LYS:HE2	2:H:170:GLU:OE2	2.05	0.56
1:I:77:PRO:HB2	1:I:78:TYR:CE2	2.41	0.56
1:I:775:ASN:HA	1:I:806:THR:O	2.06	0.56
1:K:9:ASN:HA	1:K:576:GLN:HA	1.88	0.56
1:K:563:ASP:O	1:K:566:GLN:HG2	2.05	0.56
1:K:719:GLU:HG2	1:K:859:THR:O	2.05	0.56
2:N:21:MET:HA	2:N:21:MET:HE3	1.88	0.56
1:O:602:ILE:HG23	8:O:1075:HOH:O	2.06	0.56
1:Q:35:ASP:OD1	1:Q:55:ARG:HD3	2.05	0.56
1:U:56:LYS:HG2	1:U:57:THR:N	2.21	0.56
1:U:165:GLY:HA3	1:U:166:PHE:CB	2.26	0.56
1:C:121:VAL:O	1:C:125:ILE:HG13	2.07	0.56
2:D:166:LYS:HG2	2:D:170:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:TYR:HA	2:H:59:ASN:HD22	1.71	0.56
1:I:610:LYS:HZ2	1:I:618:GLN:HE22	1.52	0.56
2:L:135:ASP:OD1	2:L:137:SER:HB2	2.06	0.56
2:P:40:GLN:NE2	2:P:118:GLU:H	2.04	0.56
1:Q:146:MET:CE	1:Q:544:THR:HB	2.33	0.56
1:S:725:PRO:HD2	8:S:1201:HOH:O	2.06	0.56
1:U:426:MET:HE2	1:U:618:GLN:HG2	1.87	0.56
1:W:495:LYS:HD2	1:W:514:TYR:OH	2.06	0.56
1:W:770:TRP:HB3	1:W:801:LEU:HD22	1.88	0.56
2:B:19:CYS:O	2:B:22:GLY:N	2.39	0.55
1:E:258:LEU:HG	1:E:259:VAL:HG13	1.88	0.55
2:F:91:ILE:HG22	2:F:93:LEU:HG	1.88	0.55
1:K:561:ILE:CG2	1:K:564:ASN:HB3	2.36	0.55
2:L:73:ASN:HB3	2:L:182:THR:HA	1.88	0.55
1:O:426:MET:HE3	1:O:622:ALA:HB2	1.87	0.55
2:P:205:VAL:HG13	2:P:254:LYS:HZ2	1.68	0.55
1:Q:146:MET:HE2	1:Q:544:THR:CB	2.34	0.55
1:U:476:GLN:OE1	1:U:708:ARG:NH2	2.39	0.55
1:A:505:THR:HG22	1:A:857:ASN:ND2	2.21	0.55
2:D:71:CYS:CA	2:D:184:PRO:HA	2.36	0.55
1:G:730:TYR:CE1	1:G:794:ASN:HA	2.41	0.55
1:G:797:GLY:HA2	1:G:875:TYR:CE2	2.40	0.55
2:H:142:MET:HE2	2:H:146:ALA:CB	2.36	0.55
2:J:210:PHE:HD2	2:J:213:ALA:HB2	1.71	0.55
2:P:71:CYS:HB2	2:P:182:THR:O	2.06	0.55
2:P:185:ARG:NH1	2:P:185:ARG:CB	2.69	0.55
2:P:219:SER:C	2:P:221:GLY:H	2.14	0.55
1:W:85:PHE:CE2	1:W:87:PRO:HG3	2.41	0.55
1:G:291:GLU:CD	1:G:291:GLU:H	2.14	0.55
1:O:649:LYS:HE3	1:O:651:THR:CG2	2.37	0.55
2:P:19:CYS:CB	2:P:145:CYS:HB3	2.26	0.55
2:P:114:MET:HA	2:P:125:LYS:HB3	1.89	0.55
1:Q:461:PHE:HA	8:Q:1500:HOH:O	2.05	0.55
1:S:134:PRO:HB3	1:S:165:GLY:HA2	1.89	0.55
2:T:52:GLU:HG3	2:T:61:ILE:HD12	1.87	0.55
2:T:114:MET:CB	2:T:125:LYS:HB3	2.35	0.55
1:W:174:ASP:OD1	1:W:175:SER:N	2.38	0.55
2:D:19:CYS:CB	2:D:145:CYS:HB3	2.31	0.55
1:K:426:MET:HE2	1:K:618:GLN:HG2	1.88	0.55
1:O:296:ASN:HB3	1:O:657:PHE:CZ	2.41	0.55
1:S:61:PRO:HB3	8:T:559:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:44:ILE:HD11	1:U:394:PRO:CG	2.35	0.55
1:A:426:MET:HE2	1:A:618:GLN:HG2	1.87	0.55
1:A:553:GLU:HG2	1:A:556:ASN:HB2	1.89	0.55
1:C:704:ILE:HG23	8:C:1650:HOH:O	2.07	0.55
1:I:797:GLY:HA2	1:I:875:TYR:CE2	2.41	0.55
2:T:142:MET:HE2	2:T:146:ALA:C	2.31	0.55
1:U:69:MET:HE2	1:U:754:MET:HE1	1.89	0.55
2:X:204:LEU:HD23	2:X:209:CYS:HA	1.89	0.55
2:B:71:CYS:HB2	2:B:182:THR:O	2.06	0.55
1:E:324:GLU:OE1	1:E:714:TYR:OH	2.22	0.55
1:E:753:TYR:HB3	2:F:21:MET:HE2	1.88	0.55
2:F:19:CYS:HB2	2:F:46:MET:HG2	1.87	0.55
2:F:210:PHE:CE2	2:F:251:ALA:HB1	2.42	0.55
1:K:69:MET:HE2	1:K:754:MET:CE	2.36	0.55
1:K:134:PRO:HD2	8:K:1361:HOH:O	2.06	0.55
2:L:114:MET:HA	2:L:125:LYS:HB3	1.89	0.55
1:M:96:ARG:HD2	1:M:514:TYR:O	2.07	0.55
1:M:426:MET:HE3	1:M:622:ALA:HB2	1.89	0.55
1:M:707:HIS:HD2	8:M:1386:HOH:O	1.89	0.55
1:S:719:GLU:HG2	1:S:859:THR:O	2.06	0.55
2:V:40:GLN:HB3	2:V:43:HIS:CE1	2.42	0.55
1:C:296:ASN:HB3	1:C:657:PHE:CZ	2.42	0.55
2:F:166:LYS:HG2	2:F:170:GLU:OE2	2.06	0.55
1:I:722:LYS:HG2	8:I:1016:HOH:O	2.06	0.55
2:L:46:MET:HE1	2:L:66:THR:N	2.21	0.55
1:M:504:MET:HE3	8:M:1038:HOH:O	2.05	0.55
1:M:587:MET:HE2	1:M:591:GLU:HB3	1.88	0.55
1:G:134:PRO:HB2	1:G:439:LEU:HD11	1.88	0.55
2:R:58:ARG:HD2	2:R:268:ASP:OD1	2.06	0.55
2:T:58:ARG:HD2	2:T:268:ASP:OD1	2.06	0.55
1:U:153:ARG:O	1:U:157:TYR:HB3	2.07	0.55
1:W:587:MET:HE2	1:W:592:ILE:HA	1.89	0.55
1:C:452:ILE:HB	1:C:453:PRO:HD3	1.89	0.55
2:D:19:CYS:O	2:D:22:GLY:N	2.39	0.55
2:D:40:GLN:NE2	2:D:117:ASN:HA	2.22	0.55
1:K:155:SER:OG	1:K:409:ILE:HG12	2.07	0.55
1:M:66:PHE:HA	1:M:69:MET:CE	2.32	0.55
1:M:738:HIS:HE2	5:M:903:MGD:H15	1.55	0.55
1:O:287:SER:HB2	1:O:340:ALA:HB1	1.89	0.55
1:O:630:THR:OG1	1:O:633:GLU:HG3	2.07	0.55
1:W:32:ASP:HB2	8:W:1659:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:720:SER:OG	1:W:723:HIS:HB2	2.07	0.55
1:C:187:TRP:CH2	1:C:196:PRO:HB3	2.42	0.55
1:E:96:ARG:HD2	1:E:514:TYR:O	2.07	0.55
2:J:5:TYR:HB2	2:J:157:LEU:HD11	1.88	0.55
2:J:21:MET:CE	2:J:21:MET:HA	2.37	0.55
1:O:78:TYR:C	1:O:541:PRO:HG2	2.31	0.55
1:Q:387:TRP:CE2	1:Q:389:THR:HA	2.42	0.55
3:Q:901:ACT:H1	8:Q:1043:HOH:O	2.07	0.55
1:S:187:TRP:CH2	1:S:196:PRO:HB3	2.42	0.55
1:E:356:GLY:H	5:E:904:MGD:C5'	2.20	0.54
1:G:351:LEU:HD12	1:G:567:LEU:HD21	1.88	0.54
2:H:68:CYS:HB3	2:H:70:HIS:CE1	2.43	0.54
1:K:211:MET:HE3	8:K:1452:HOH:O	2.06	0.54
1:O:610:LYS:HZ2	1:O:618:GLN:HE22	1.53	0.54
1:Q:165:GLY:CA	1:Q:166:PHE:HB3	2.34	0.54
2:T:92:VAL:HG11	7:T:304:SF4:S1	2.48	0.54
1:U:526:SER:HB3	8:U:1120:HOH:O	2.06	0.54
1:U:735:LEU:HD23	1:U:735:LEU:H	1.71	0.54
1:A:296:ASN:O	1:A:687:LYS:HB3	2.06	0.54
1:C:44:ILE:HD11	1:C:394:PRO:HG2	1.89	0.54
1:C:730:TYR:CE1	1:C:794:ASN:HA	2.41	0.54
1:C:734:MET:HB2	1:C:814:VAL:HG23	1.88	0.54
1:C:870:ASP:HB3	1:C:872:TYR:CE1	2.43	0.54
1:I:21:LYS:CB	1:I:26:ILE:HD11	2.36	0.54
2:J:69:MET:HB3	2:J:184:PRO:HB3	1.90	0.54
1:M:144:HIS:NE2	5:M:904:MGD:S13	2.80	0.54
2:P:23:CYS:O	2:P:27:HIS:N	2.41	0.54
1:S:15:PRO:HD2	8:S:1007:HOH:O	2.06	0.54
1:W:146:MET:HE2	1:W:544:THR:CB	2.35	0.54
1:C:391:GLN:HG2	1:C:567:LEU:HD23	1.89	0.54
1:E:476:GLN:OE1	1:E:708:ARG:NH2	2.40	0.54
2:H:139:ALA:O	2:H:141:LYS:HG3	2.08	0.54
2:J:203:ILE:HD12	2:J:203:ILE:N	2.23	0.54
1:K:557:CYS:N	1:K:564:ASN:HD21	1.96	0.54
1:O:75:ARG:HH22	1:O:547:GLU:CD	2.14	0.54
2:R:39:MET:HE2	2:R:45:TRP:CD2	2.43	0.54
1:W:786:ASN:ND2	1:W:804:GLN:HA	2.23	0.54
1:M:21:LYS:HB3	1:M:26:ILE:HD11	1.88	0.54
1:M:691:ILE:CD1	1:M:711:MET:HE3	2.35	0.54
1:M:696:LYS:O	1:M:700:GLU:HG3	2.08	0.54
2:T:114:MET:HB3	2:T:125:LYS:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:229:PHE:HA	8:W:1340:HOH:O	2.06	0.54
2:X:19:CYS:O	2:X:22:GLY:N	2.40	0.54
1:A:201:LEU:HD13	1:A:387:TRP:HB2	1.89	0.54
1:C:100:LEU:CD1	1:C:105:PRO:HG3	2.38	0.54
1:C:146:MET:HG2	5:C:903:MGD:N7	2.22	0.54
1:G:561:ILE:CG2	1:G:564:ASN:HB3	2.35	0.54
1:I:349:GLY:HA3	1:I:353:GLY:O	2.07	0.54
1:K:76:ILE:HG22	1:K:541:PRO:HG3	1.89	0.54
1:K:598:LYS:HG3	8:K:1261:HOH:O	2.07	0.54
2:L:10:VAL:HG13	2:L:63:TYR:O	2.08	0.54
1:Q:155:SER:OG	1:Q:409:ILE:HG12	2.07	0.54
2:T:142:MET:HE1	8:T:429:HOH:O	2.06	0.54
1:U:533:VAL:HB	1:U:534:PRO:HD3	1.89	0.54
1:W:44:ILE:HD11	1:W:394:PRO:HG2	1.89	0.54
1:A:262:LYS:HG2	2:B:232:PHE:CE1	2.43	0.54
1:C:252:MET:HE3	1:C:263:TRP:CE3	2.43	0.54
2:D:90:GLY:HA3	2:D:185:ARG:NH2	2.23	0.54
1:G:100:LEU:CD1	1:G:105:PRO:HG3	2.37	0.54
1:G:146:MET:HG2	5:G:903:MGD:N7	2.21	0.54
2:J:68:CYS:HB3	2:J:70:HIS:CE1	2.42	0.54
1:M:558:SER:H	1:M:564:ASN:ND2	2.04	0.54
1:M:730:TYR:CZ	1:M:794:ASN:HA	2.42	0.54
2:P:46:MET:HE1	2:P:66:THR:H	1.72	0.54
2:P:72:GLU:HG2	2:P:185:ARG:NH2	2.23	0.54
2:X:4:TYR:HD1	2:X:89:ASP:HB2	1.73	0.54
2:B:5:TYR:HB2	2:B:157:LEU:CD1	2.38	0.54
1:C:610:LYS:HZ2	1:C:618:GLN:HE22	1.53	0.54
1:E:114:TRP:CZ2	1:E:541:PRO:HD2	2.42	0.54
1:O:426:MET:CE	1:O:618:GLN:HG2	2.37	0.54
1:Q:166:PHE:N	1:Q:439:LEU:HD12	2.23	0.54
1:S:146:MET:HE2	1:S:544:THR:CB	2.37	0.54
1:E:162:ASN:HA	8:E:1368:HOH:O	2.07	0.54
1:E:541:PRO:HB2	1:E:586:SER:HA	1.89	0.54
1:I:75:ARG:NH2	1:I:543:CYS:HA	2.23	0.54
1:I:195:ASN:HD21	1:I:354:TRP:CD1	2.25	0.54
1:O:119:ASP:OD1	1:O:599:LYS:HE2	2.07	0.54
1:O:717:ALA:HB3	1:O:720:SER:HB3	1.88	0.54
1:U:15:PRO:HD3	1:U:554:PHE:CD1	2.43	0.54
1:U:253:ASN:O	1:U:257:ARG:HG3	2.08	0.54
1:U:628:TYR:CE2	1:U:643:PRO:HG2	2.43	0.54
2:X:39:MET:HE2	2:X:45:TRP:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:GLY:HA2	8:A:1207:HOH:O	2.08	0.54
2:B:166:LYS:HE2	2:B:170:GLU:OE2	2.08	0.54
1:C:629:MET:HE2	1:C:634:PHE:CA	2.37	0.54
1:I:753:TYR:CB	2:J:21:MET:HE2	2.34	0.54
1:K:738:HIS:HE2	5:K:903:MGD:H15	1.55	0.54
3:K:901:ACT:H1	8:K:1043:HOH:O	2.06	0.54
2:T:21:MET:HE3	2:T:21:MET:HA	1.90	0.54
1:U:211:MET:HE2	1:U:246:VAL:CG2	2.38	0.54
1:U:610:LYS:HZ3	1:U:618:GLN:NE2	2.02	0.54
1:W:195:ASN:HD21	1:W:354:TRP:CD1	2.25	0.54
1:W:772:MET:HB2	1:W:801:LEU:HD13	1.89	0.54
1:A:356:GLY:H	5:A:904:MGD:C5'	2.21	0.54
1:A:501:LEU:HD13	1:A:823:TYR:CG	2.43	0.54
2:F:46:MET:HE1	2:F:65:PRO:C	2.33	0.54
2:F:72:GLU:HG2	2:F:185:ARG:NH2	2.23	0.54
2:J:68:CYS:HB3	2:J:126:CYS:HB3	1.88	0.54
2:J:70:HIS:CD2	2:J:92:VAL:H	2.22	0.54
1:K:75:ARG:HH21	1:K:543:CYS:HA	1.72	0.54
1:O:66:PHE:CD1	1:O:69:MET:HE3	2.43	0.54
1:O:257:ARG:HD3	2:P:61:ILE:HG21	1.89	0.54
2:P:157:LEU:HD12	2:P:157:LEU:O	2.08	0.54
1:Q:2:GLY:O	1:Q:21:LYS:HE3	2.07	0.54
2:V:106:LEU:CD2	2:V:114:MET:HG3	2.38	0.54
2:B:203:ILE:HD12	2:B:203:ILE:N	2.23	0.53
1:C:818:GLU:O	1:C:819:SER:HB2	2.07	0.53
1:G:76:ILE:HG22	1:G:541:PRO:HG3	1.91	0.53
2:L:52:GLU:HG3	2:L:61:ILE:HD12	1.89	0.53
1:O:146:MET:HE2	1:O:544:THR:CB	2.39	0.53
2:R:68:CYS:HB3	2:R:126:CYS:HB3	1.90	0.53
2:T:198:TYR:HB3	2:T:238:ASP:HA	1.90	0.53
2:V:59:ASN:H	2:V:59:ASN:HD22	1.54	0.53
1:W:28:MET:HE1	1:W:66:PHE:CB	2.31	0.53
2:X:26:GLU:OE2	2:X:132:LEU:HD21	2.07	0.53
1:A:134:PRO:HB2	1:A:439:LEU:HD11	1.89	0.53
1:M:174:ASP:OD1	1:M:175:SER:N	2.40	0.53
1:M:288:TYR:HA	8:M:1503:HOH:O	2.08	0.53
1:Q:66:PHE:HA	1:Q:69:MET:HE3	1.91	0.53
2:V:21:MET:HA	2:V:21:MET:HE2	1.90	0.53
2:X:179:GLU:HG2	2:X:180:LEU:N	2.24	0.53
1:A:21:LYS:HB3	1:A:26:ILE:HD11	1.90	0.53
1:K:533:VAL:HB	1:K:534:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:100:LEU:CD1	1:M:105:PRO:HG3	2.39	0.53
1:M:197:GLU:OE2	1:M:667:ASP:HB2	2.08	0.53
2:N:166:LYS:O	2:N:170:GLU:HG3	2.07	0.53
2:P:185:ARG:HB3	2:P:185:ARG:NH1	2.24	0.53
1:Q:233:ILE:HD11	8:Q:1184:HOH:O	2.08	0.53
1:Q:400:TYR:HA	8:Q:1458:HOH:O	2.07	0.53
1:Q:826:LEU:HD21	1:Q:835:ARG:HD3	1.90	0.53
2:T:71:CYS:HA	2:T:184:PRO:HA	1.89	0.53
1:U:28:MET:HE2	1:U:67:LYS:HB2	1.89	0.53
1:U:165:GLY:CA	1:U:166:PHE:HB3	2.31	0.53
1:U:772:MET:HB2	1:U:801:LEU:HD13	1.90	0.53
1:W:610:LYS:HB3	1:W:614:ALA:HB3	1.91	0.53
1:A:489:LYS:HD3	8:A:1020:HOH:O	2.08	0.53
2:F:46:MET:HE2	2:F:48:ILE:HG12	1.91	0.53
1:G:195:ASN:HD21	1:G:354:TRP:CD1	2.26	0.53
1:G:426:MET:HE3	1:G:622:ALA:HB2	1.89	0.53
1:G:628:TYR:CE2	1:G:643:PRO:HG2	2.43	0.53
1:K:44:ILE:HG21	1:K:206:LEU:HD12	1.90	0.53
1:Q:855:MET:HB2	1:Q:857:ASN:OD1	2.09	0.53
2:R:142:MET:HE3	2:R:146:ALA:HB1	1.90	0.53
1:U:356:GLY:HA2	1:U:359:ARG:NH1	2.23	0.53
1:U:644:ASP:C	1:U:646:PRO:HD3	2.33	0.53
2:V:9:ASP:HA	2:V:189:LYS:HB3	1.90	0.53
2:V:104:GLU:H	2:V:104:GLU:CD	2.15	0.53
2:L:59:ASN:HD22	2:L:59:ASN:N	1.92	0.53
1:M:12:THR:O	1:M:226:TYR:HA	2.09	0.53
2:N:175:VAL:HG23	2:N:178:PRO:HG3	1.91	0.53
1:Q:610:LYS:HZ1	1:Q:618:GLN:HE22	1.52	0.53
2:R:2:GLU:HG2	2:R:158:LYS:HG2	1.89	0.53
2:R:18:ASN:HB2	7:R:302:SF4:S1	2.48	0.53
1:S:69:MET:HE2	1:S:754:MET:HE3	1.89	0.53
1:U:11:SER:C	1:U:13:GLY:H	2.15	0.53
1:U:214:PHE:HA	1:U:347:ALA:HB3	1.91	0.53
1:U:249:ASP:CG	5:U:904:MGD:H1'	2.34	0.53
2:V:19:CYS:HB2	2:V:46:MET:HG2	1.89	0.53
1:A:716:PRO:HB3	1:A:723:HIS:CD2	2.44	0.53
1:E:79:PRO:HB2	1:E:112:ILE:O	2.07	0.53
2:F:70:HIS:HD2	2:F:92:VAL:H	1.55	0.53
1:I:224:GLY:O	1:I:225:ILE:HB	2.09	0.53
2:L:168:VAL:HA	2:L:173:LEU:HD12	1.89	0.53
1:M:162:ASN:CG	1:M:437:SER:HB2	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:177:GLU:HA	1:M:177:GLU:OE2	2.09	0.53
1:O:826:LEU:HD21	1:O:835:ARG:HD3	1.91	0.53
1:S:197:GLU:OE2	1:S:667:ASP:HB2	2.09	0.53
1:S:218:ASP:OD2	1:S:253:ASN:HB2	2.07	0.53
1:A:218:ASP:OD2	1:A:253:ASN:HB2	2.09	0.53
2:B:201:ALA:HB2	2:B:269:LEU:HB2	1.90	0.53
1:E:394:PRO:HG3	8:E:1325:HOH:O	2.08	0.53
2:L:19:CYS:HB2	2:L:46:MET:HG2	1.90	0.53
2:L:68:CYS:CB	2:L:126:CYS:HB3	2.38	0.53
1:M:138:LEU:HD12	1:M:167:THR:O	2.07	0.53
1:O:274:LEU:O	1:O:278:ILE:HG13	2.09	0.53
1:O:323:GLU:HB2	8:O:1578:HOH:O	2.09	0.53
1:O:478:HIS:HD2	8:O:1210:HOH:O	1.92	0.53
1:Q:504:MET:HE3	8:Q:1038:HOH:O	2.08	0.53
1:W:800:ILE:HD12	1:W:800:ILE:N	2.24	0.53
1:A:645:ASN:ND2	1:A:648:ARG:HB3	2.24	0.53
1:G:426:MET:HE2	1:G:618:GLN:HG2	1.89	0.53
1:I:176:TRP:CE2	1:I:193:LEU:HD12	2.44	0.53
1:M:114:TRP:CZ2	1:M:541:PRO:HD2	2.44	0.53
1:O:526:SER:HB3	8:O:1116:HOH:O	2.09	0.53
1:O:553:GLU:HB3	1:O:556:ASN:CB	2.38	0.53
1:S:735:LEU:HD23	1:S:735:LEU:H	1.73	0.53
1:U:218:ASP:OD2	1:U:253:ASN:HB2	2.09	0.53
2:V:19:CYS:CB	2:V:145:CYS:HB3	2.39	0.53
1:A:44:ILE:HD11	1:A:394:PRO:HG2	1.90	0.53
1:E:547:GLU:OE1	1:E:582:PRO:HA	2.08	0.53
1:I:176:TRP:O	1:I:177:GLU:C	2.51	0.53
1:K:35:ASP:OD1	1:K:55:ARG:HD3	2.09	0.53
1:M:501:LEU:HD13	1:M:823:TYR:CD2	2.44	0.53
2:N:68:CYS:HB3	2:N:126:CYS:HB3	1.89	0.53
2:T:204:LEU:HD23	2:T:209:CYS:HA	1.90	0.53
1:U:96:ARG:HD3	1:U:535:PHE:O	2.09	0.53
1:U:301:GLU:H	1:U:301:GLU:CD	2.17	0.53
1:U:563:ASP:HA	1:U:565:TYR:CE1	2.44	0.53
1:W:165:GLY:CA	1:W:166:PHE:HB3	2.36	0.53
1:A:378:GLY:O	1:A:381:LYS:HG2	2.09	0.53
1:A:504:MET:HE3	8:A:1038:HOH:O	2.08	0.53
2:B:177:LYS:N	2:B:178:PRO:HD3	2.24	0.53
1:C:263:TRP:CZ2	1:C:265:SER:HB2	2.44	0.53
2:F:166:LYS:O	2:F:170:GLU:HG3	2.08	0.53
1:G:99:GLY:N	1:G:108:ASP:OD2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:670:PRO:HG2	1:I:675:GLN:CD	2.34	0.53
1:I:746:MET:HE2	5:I:903:MGD:O1B	2.09	0.53
1:M:319:GLU:HG2	1:S:726:LEU:HD12	1.90	0.53
2:R:13:CYS:HB3	2:R:63:TYR:HB2	1.89	0.53
1:S:195:ASN:HD21	1:S:354:TRP:CD1	2.26	0.53
2:T:40:GLN:HB2	2:T:117:ASN:ND2	2.24	0.53
1:U:68:SER:HB3	1:U:753:TYR:CE2	2.44	0.53
2:X:167:LYS:HZ2	2:X:173:LEU:HD11	1.74	0.53
1:C:353:GLY:O	1:C:354:TRP:HB2	2.08	0.52
1:E:563:ASP:O	1:E:566:GLN:HG2	2.09	0.52
2:F:5:TYR:HB2	2:F:157:LEU:HD13	1.91	0.52
1:I:146:MET:HG2	5:I:903:MGD:N7	2.23	0.52
1:I:758:LYS:HG3	8:J:401:HOH:O	2.10	0.52
1:M:767:TYR:HB3	1:M:769:TYR:CE1	2.44	0.52
1:O:44:ILE:HD11	1:O:394:PRO:HG2	1.90	0.52
1:A:364:ILE:HD13	1:A:708:ARG:HG3	1.90	0.52
1:A:400:TYR:CE1	1:A:421:LYS:HD2	2.45	0.52
2:D:71:CYS:HB2	2:D:182:THR:O	2.10	0.52
1:E:369:GLY:O	1:E:373:LEU:HD13	2.09	0.52
1:E:494:TRP:HE1	1:E:525:GLN:HE21	1.57	0.52
1:E:505:THR:O	1:E:506:ALA:C	2.53	0.52
2:F:142:MET:HE2	2:F:146:ALA:C	2.33	0.52
1:G:165:GLY:CA	1:G:166:PHE:HB3	2.36	0.52
2:H:19:CYS:CB	2:H:145:CYS:HB3	2.34	0.52
2:J:87:ARG:HD3	2:J:93:LEU:HD12	1.91	0.52
1:K:825:PRO:HD2	8:K:1337:HOH:O	2.09	0.52
2:L:97:GLU:OE2	2:L:100:LYS:HD2	2.09	0.52
1:M:211:MET:HE2	1:M:246:VAL:HG23	1.91	0.52
2:P:164:MET:O	2:P:168:VAL:HG23	2.09	0.52
1:S:11:SER:C	1:S:13:GLY:H	2.17	0.52
1:S:395:LEU:HD12	1:S:566:GLN:HA	1.91	0.52
2:D:18:ASN:HB2	7:D:302:SF4:S1	2.49	0.52
2:D:26:GLU:HB2	2:D:144:ARG:HH11	1.74	0.52
1:G:32:ASP:HB2	8:G:1669:HOH:O	2.09	0.52
1:I:366:TRP:NE1	1:I:370:MET:HE3	2.24	0.52
1:K:191:TRP:CE2	1:K:669:GLY:HA3	2.44	0.52
1:K:757:ILE:HD13	8:L:567:HOH:O	2.09	0.52
2:P:216:VAL:CG1	2:P:223:GLU:HG3	2.40	0.52
1:W:645:ASN:HD22	1:W:648:ARG:HD3	1.73	0.52
1:A:269:GLY:HA2	1:A:362:HIS:CG	2.44	0.52
1:A:647:ASN:O	1:A:648:ARG:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:296:ASN:HB3	1:K:657:PHE:CZ	2.44	0.52
1:K:387:TRP:CE2	1:K:389:THR:HA	2.44	0.52
2:L:253:GLY:N	2:T:88:GLU:OE2	2.43	0.52
1:O:177:GLU:HA	1:O:177:GLU:OE2	2.09	0.52
2:P:141:LYS:HA	8:P:498:HOH:O	2.09	0.52
1:S:21:LYS:HB3	1:S:26:ILE:HD11	1.92	0.52
1:S:214:PHE:HA	1:S:347:ALA:HB3	1.91	0.52
1:S:414:GLU:HG3	8:S:1443:HOH:O	2.10	0.52
2:X:185:ARG:CZ	2:X:185:ARG:HB3	2.39	0.52
1:A:177:GLU:HA	1:A:177:GLU:OE2	2.09	0.52
2:B:21:MET:HE2	2:B:21:MET:HA	1.89	0.52
2:D:96:PRO:O	2:D:100:LYS:HG3	2.09	0.52
1:K:100:LEU:HD12	1:K:105:PRO:HG3	1.90	0.52
1:M:118:THR:HG21	1:M:595:LEU:HD23	1.90	0.52
1:M:565:TYR:C	1:M:567:LEU:H	2.16	0.52
1:M:784:ILE:HD13	1:M:790:ILE:HG21	1.92	0.52
2:P:46:MET:HE3	2:P:47:ASN:N	2.25	0.52
1:Q:426:MET:HE2	1:Q:618:GLN:HG2	1.91	0.52
1:S:396:ASP:OD2	1:S:398:GLU:HB2	2.09	0.52
2:V:19:CYS:HA	2:V:145:CYS:HB3	1.92	0.52
1:W:197:GLU:OE2	1:W:667:ASP:HB2	2.10	0.52
2:X:68:CYS:HB3	2:X:126:CYS:HB3	1.91	0.52
2:X:122:VAL:HG22	2:X:123:ALA:N	2.24	0.52
1:A:753:TYR:HB3	2:B:24:MET:HE3	1.90	0.52
1:C:9:ASN:HA	1:C:576:GLN:HA	1.91	0.52
1:C:189:PHE:HZ	1:C:654:LEU:HD21	1.75	0.52
2:D:5:TYR:HB2	2:D:157:LEU:CD1	2.39	0.52
2:D:252:ASP:HB3	2:D:254:LYS:CE	2.40	0.52
2:H:198:TYR:HB3	2:H:238:ASP:HA	1.91	0.52
2:J:142:MET:CE	2:J:146:ALA:HB1	2.38	0.52
2:N:19:CYS:HB2	2:N:46:MET:HG2	1.89	0.52
1:O:786:ASN:HD21	1:O:804:GLN:HA	1.75	0.52
2:R:20:PHE:CZ	2:R:24:MET:HE2	2.44	0.52
1:W:142:SER:HB3	5:W:903:MGD:O1A	2.09	0.52
1:W:564:ASN:HD22	1:W:564:ASN:N	2.06	0.52
1:A:301:GLU:CD	1:A:301:GLU:H	2.18	0.52
1:C:155:SER:OG	1:C:409:ILE:HG12	2.09	0.52
1:E:75:ARG:NH2	1:E:543:CYS:HA	2.25	0.52
1:E:426:MET:HE2	1:E:618:GLN:OE1	2.09	0.52
2:L:21:MET:CE	2:L:21:MET:HA	2.40	0.52
1:M:356:GLY:H	5:M:904:MGD:C5'	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:211:MET:HE2	1:S:246:VAL:CG2	2.38	0.52
2:T:4:TYR:CE2	2:T:158:LYS:HD2	2.44	0.52
1:U:14:GLY:HA2	1:U:554:PHE:CE1	2.44	0.52
1:U:74:LEU:HD12	1:U:750:LYS:HA	1.91	0.52
2:D:106:LEU:CD2	2:D:114:MET:HG3	2.40	0.52
1:E:66:PHE:CD1	1:E:69:MET:HE3	2.45	0.52
1:I:175:SER:HA	1:I:359:ARG:HH21	1.75	0.52
1:K:387:TRP:CZ2	1:K:389:THR:HA	2.44	0.52
1:M:561:ILE:HG22	1:M:564:ASN:HB3	1.92	0.52
2:N:13:CYS:HB3	2:N:63:TYR:HB2	1.90	0.52
1:O:28:MET:HE1	1:O:67:LYS:N	2.25	0.52
2:P:70:HIS:HD2	2:P:92:VAL:N	2.00	0.52
1:U:162:ASN:HD22	1:U:166:PHE:HE2	1.56	0.52
1:G:68:SER:HB3	1:G:753:TYR:CE2	2.44	0.52
1:G:204:ASP:OD2	1:G:655:ARG:NH2	2.42	0.52
1:K:177:GLU:HA	1:K:177:GLU:OE2	2.09	0.52
1:M:510:TYR:O	1:M:513:MET:HG2	2.10	0.52
1:O:9:ASN:HA	1:O:576:GLN:HA	1.92	0.52
2:P:104:GLU:H	2:P:104:GLU:CD	2.18	0.52
1:Q:708:ARG:HD2	8:Q:1046:HOH:O	2.09	0.52
1:S:252:MET:HE3	1:S:263:TRP:CE3	2.44	0.52
1:U:66:PHE:CD1	1:U:69:MET:HE3	2.44	0.52
1:W:323:GLU:HB3	8:W:1112:HOH:O	2.10	0.52
1:A:305:ASP:OD1	1:A:310:LYS:HD2	2.10	0.52
2:B:146:ALA:HA	2:B:154:TYR:CD1	2.45	0.52
1:E:610:LYS:NZ	1:E:618:GLN:NE2	2.58	0.52
1:M:153:ARG:O	1:M:157:TYR:HB3	2.10	0.52
1:Q:400:TYR:CE1	1:Q:421:LYS:HD2	2.45	0.52
2:R:166:LYS:HG2	2:R:170:GLU:OE2	2.11	0.52
1:U:141:PRO:HD3	1:U:157:TYR:CZ	2.45	0.52
1:W:100:LEU:CD1	1:W:105:PRO:HG3	2.39	0.52
1:A:176:TRP:O	1:A:177:GLU:C	2.52	0.51
1:G:69:MET:HE2	1:G:754:MET:HE3	1.91	0.51
1:G:146:MET:CE	1:G:544:THR:HB	2.39	0.51
2:H:102:LYS:HB3	2:H:104:GLU:OE2	2.10	0.51
1:K:211:MET:HE1	2:L:231:PHE:CZ	2.45	0.51
1:M:195:ASN:HD21	1:M:354:TRP:CD1	2.28	0.51
1:M:756:TYR:CD1	2:N:24:MET:HE1	2.45	0.51
2:N:77:VAL:HG22	2:N:84:VAL:HG12	1.92	0.51
1:O:103:GLN:N	1:O:103:GLN:CD	2.68	0.51
2:P:21:MET:HE2	2:P:24:MET:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:28:MET:HE1	1:S:66:PHE:CB	2.34	0.51
1:S:144:HIS:NE2	5:S:904:MGD:S13	2.83	0.51
2:T:39:MET:HE2	2:T:45:TRP:CD2	2.44	0.51
2:T:177:LYS:N	2:T:178:PRO:HD3	2.24	0.51
1:W:249:ASP:CG	5:W:904:MGD:HI'	2.35	0.51
1:W:356:GLY:H	5:W:904:MGD:C5'	2.23	0.51
2:X:71:CYS:CB	2:X:184:PRO:HA	2.39	0.51
1:C:11:SER:C	1:C:13:GLY:H	2.18	0.51
1:C:426:MET:HE1	1:C:618:GLN:O	2.10	0.51
1:E:253:ASN:O	1:E:257:ARG:HG3	2.11	0.51
1:I:162:ASN:HD22	1:I:166:PHE:HE2	1.57	0.51
1:I:258:LEU:HG	1:I:259:VAL:HG13	1.93	0.51
2:J:70:HIS:HD2	2:J:92:VAL:N	2.05	0.51
2:J:105:LEU:C	2:J:114:MET:HE2	2.35	0.51
1:M:140:THR:HB	1:M:169:ALA:HB3	1.92	0.51
1:M:677:CYS:C	1:M:678:ARG:HG2	2.34	0.51
1:O:21:LYS:HB3	1:O:26:ILE:HD11	1.92	0.51
2:P:105:LEU:HB3	2:P:114:MET:HE1	1.92	0.51
2:R:198:TYR:HB3	2:R:238:ASP:HA	1.92	0.51
1:S:87:PRO:HB3	8:S:1506:HOH:O	2.10	0.51
1:S:356:GLY:H	5:S:904:MGD:C5'	2.23	0.51
2:T:139:ALA:HB3	2:T:140:PRO:HD3	1.92	0.51
1:U:211:MET:HE2	1:U:246:VAL:HG23	1.91	0.51
1:W:387:TRP:CZ2	1:W:389:THR:HA	2.45	0.51
1:W:847:TYR:CZ	1:W:853:CYS:HB3	2.45	0.51
2:X:44:ARG:C	2:X:46:MET:N	2.67	0.51
2:D:139:ALA:HB3	2:D:140:PRO:HD3	1.92	0.51
2:D:252:ASP:C	2:D:254:LYS:H	2.19	0.51
1:E:719:GLU:HG2	1:E:859:THR:O	2.11	0.51
1:E:823:TYR:CE2	1:E:825:PRO:HG3	2.46	0.51
2:F:19:CYS:CB	2:F:145:CYS:HB3	2.36	0.51
1:G:296:ASN:HB3	1:G:657:PHE:CZ	2.46	0.51
1:K:140:THR:HB	1:K:169:ALA:HB3	1.92	0.51
1:K:740:ARG:HD2	8:K:1438:HOH:O	2.09	0.51
2:L:112:GLY:HA2	8:L:523:HOH:O	2.09	0.51
1:O:28:MET:HE2	1:O:67:LYS:HB2	1.91	0.51
1:Q:476:GLN:OE1	1:Q:708:ARG:NH2	2.44	0.51
1:Q:786:ASN:ND2	1:Q:804:GLN:HA	2.24	0.51
1:E:387:TRP:CE2	1:E:389:THR:HA	2.46	0.51
1:E:629:MET:HE2	1:E:633:GLU:C	2.35	0.51
1:I:735:LEU:HD23	1:I:735:LEU:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:426:MET:HE2	1:M:618:GLN:HG2	1.91	0.51
2:N:5:TYR:HB2	2:N:157:LEU:HD11	1.91	0.51
2:R:75:PRO:HD2	7:R:304:SF4:S4	2.50	0.51
1:A:670:PRO:HB3	1:A:682:GLN:HB2	1.90	0.51
1:E:480:TYR:HA	8:E:1178:HOH:O	2.09	0.51
1:K:10:SER:HG	1:K:147:TRP:CD1	2.28	0.51
2:T:139:ALA:O	2:T:141:LYS:HG3	2.11	0.51
2:X:99:ALA:HB1	8:X:498:HOH:O	2.10	0.51
2:X:180:LEU:HB2	8:X:521:HOH:O	2.09	0.51
2:B:157:LEU:H	2:B:157:LEU:HD12	1.75	0.51
1:C:478:HIS:HD2	8:C:1208:HOH:O	1.93	0.51
2:D:164:MET:O	2:D:168:VAL:HG23	2.10	0.51
1:E:9:ASN:HA	1:E:576:GLN:HA	1.91	0.51
1:E:629:MET:HE2	1:E:634:PHE:N	2.26	0.51
1:G:78:TYR:O	1:G:80:MET:HG3	2.10	0.51
2:J:23:CYS:O	2:J:27:HIS:N	2.38	0.51
1:K:786:ASN:HD21	1:K:804:GLN:HA	1.75	0.51
2:L:254:LYS:HD2	2:L:274:LEU:OXT	2.10	0.51
1:O:165:GLY:CA	1:O:166:PHE:HB3	2.38	0.51
1:Q:176:TRP:O	1:Q:177:GLU:C	2.54	0.51
1:S:770:TRP:HB3	1:S:801:LEU:HD23	1.92	0.51
1:W:11:SER:C	1:W:13:GLY:H	2.18	0.51
1:W:505:THR:HG22	1:W:857:ASN:ND2	2.25	0.51
1:W:563:ASP:HA	1:W:565:TYR:CE1	2.45	0.51
1:W:797:GLY:HA2	1:W:875:TYR:CE2	2.45	0.51
2:B:20:PHE:CZ	2:B:24:MET:HE2	2.46	0.51
1:C:143:SER:CB	3:C:901:ACT:H3	2.40	0.51
1:E:617:GLU:HG3	1:E:631:TRP:CG	2.45	0.51
2:F:68:CYS:HB2	2:F:126:CYS:CB	2.36	0.51
1:G:629:MET:HE2	1:G:634:PHE:CA	2.32	0.51
2:J:114:MET:HA	2:J:125:LYS:HB3	1.92	0.51
1:K:495:LYS:HD3	8:K:1109:HOH:O	2.11	0.51
1:K:722:LYS:HG2	8:K:1562:HOH:O	2.11	0.51
1:O:55:ARG:HD2	8:O:1646:HOH:O	2.10	0.51
1:O:81:LYS:HB2	1:O:112:ILE:HD13	1.93	0.51
1:O:214:PHE:HA	1:O:347:ALA:HB3	1.93	0.51
1:Q:738:HIS:HE2	5:Q:903:MGD:H15	1.57	0.51
1:S:252:MET:HB3	1:S:808:CYS:HB3	1.91	0.51
1:S:349:GLY:HA3	1:S:353:GLY:O	2.11	0.51
1:U:322:GLU:HG3	1:U:327:VAL:O	2.11	0.51
1:U:393:VAL:HG12	1:U:395:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:21:MET:HA	2:V:21:MET:CE	2.41	0.51
1:W:95:LEU:HA	8:W:1539:HOH:O	2.09	0.51
2:B:46:MET:HE1	2:B:65:PRO:C	2.35	0.51
2:B:69:MET:HB2	7:B:304:SF4:S2	2.51	0.51
1:E:561:ILE:HG22	1:E:564:ASN:HB3	1.93	0.51
1:G:387:TRP:CE2	1:G:389:THR:HA	2.46	0.51
1:I:452:ILE:N	1:I:453:PRO:CD	2.74	0.51
1:M:28:MET:HE1	1:M:66:PHE:CB	2.32	0.51
1:M:647:ASN:HB2	8:M:1446:HOH:O	2.10	0.51
1:Q:533:VAL:HB	1:Q:534:PRO:HD3	1.93	0.51
2:R:69:MET:HB2	7:R:304:SF4:S2	2.51	0.51
1:S:756:TYR:HD1	2:T:24:MET:HE1	1.74	0.51
1:U:499:PRO:HB2	1:U:745:THR:HG21	1.93	0.51
1:C:119:ASP:OD1	1:C:599:LYS:NZ	2.43	0.51
1:C:557:CYS:N	1:C:564:ASN:HD21	1.96	0.51
1:G:174:ASP:OD1	1:G:175:SER:N	2.44	0.51
2:H:179:GLU:N	2:H:179:GLU:OE1	2.41	0.51
1:S:301:GLU:H	1:S:301:GLU:CD	2.19	0.51
1:U:174:ASP:OD1	1:U:175:SER:N	2.44	0.51
1:W:251:HIS:HA	1:W:809:LEU:HD23	1.92	0.51
2:X:69:MET:HG3	2:X:111:TYR:CE2	2.46	0.51
2:X:106:LEU:HD23	2:X:114:MET:HE2	1.93	0.51
1:A:214:PHE:HA	1:A:347:ALA:HB3	1.93	0.51
2:F:40:GLN:HE22	2:F:118:GLU:H	1.59	0.51
2:F:125:LYS:HD2	2:F:126:CYS:O	2.11	0.51
1:O:855:MET:HB2	1:O:857:ASN:OD1	2.10	0.51
1:S:303:TRP:O	1:S:307:VAL:HG23	2.11	0.51
1:U:356:GLY:H	5:U:904:MGD:C5'	2.23	0.51
2:V:77:VAL:HG22	2:V:84:VAL:HG12	1.92	0.51
1:E:378:GLY:O	1:E:381:LYS:HG2	2.11	0.50
1:E:452:ILE:HB	1:E:453:PRO:HD3	1.92	0.50
2:F:139:ALA:HB3	2:F:140:PRO:HD3	1.93	0.50
1:I:114:TRP:CZ2	1:I:541:PRO:HD2	2.46	0.50
1:M:118:THR:HG21	1:M:595:LEU:CD2	2.41	0.50
2:N:40:GLN:HB3	2:N:43:HIS:CE1	2.46	0.50
2:X:49:GLU:HG3	2:X:64:ARG:NH2	2.26	0.50
2:B:142:MET:HE1	8:B:429:HOH:O	2.11	0.50
1:C:65:GLY:HA3	2:D:21:MET:HG3	1.93	0.50
1:E:553:GLU:HG2	1:E:556:ASN:HB2	1.94	0.50
1:G:600:LEU:HB3	8:G:1074:HOH:O	2.10	0.50
1:K:782:ARG:HD3	1:K:864:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:786:ASN:ND2	1:K:805:VAL:H	2.09	0.50
1:S:305:ASP:OD1	1:S:310:LYS:HD2	2.11	0.50
2:T:106:LEU:HD11	2:T:116:TRP:HB2	1.93	0.50
1:U:549:TRP:CE3	1:U:577:ALA:HA	2.46	0.50
1:W:12:THR:HG23	8:W:1332:HOH:O	2.12	0.50
1:C:39:ALA:O	1:C:55:ARG:NH2	2.39	0.50
1:I:339:TRP:CH2	1:I:346:LEU:HD13	2.46	0.50
1:K:74:LEU:HD12	1:K:750:LYS:HA	1.92	0.50
1:O:587:MET:HE3	1:O:591:GLU:HB3	1.94	0.50
1:Q:452:ILE:HB	1:Q:453:PRO:HD3	1.93	0.50
1:Q:480:TYR:HA	8:Q:1178:HOH:O	2.12	0.50
1:Q:498:GLY:N	1:Q:499:PRO:HD3	2.27	0.50
1:S:269:GLY:HA2	1:S:362:HIS:CE1	2.46	0.50
2:V:213:ALA:O	2:V:228:GLU:HA	2.11	0.50
1:W:233:ILE:O	1:W:236:GLN:HB3	2.12	0.50
1:A:12:THR:O	1:A:226:TYR:HA	2.11	0.50
1:A:602:ILE:HG23	8:A:1075:HOH:O	2.10	0.50
2:B:216:VAL:HG13	2:B:223:GLU:HG3	1.94	0.50
1:G:214:PHE:HA	1:G:347:ALA:HB3	1.93	0.50
1:O:263:TRP:HZ3	2:P:59:ASN:HD21	1.59	0.50
1:S:452:ILE:HB	1:S:453:PRO:HD3	1.92	0.50
1:S:744:HIS:HA	1:S:819:SER:CB	2.40	0.50
1:U:362:HIS:HB3	1:U:717:ALA:HB2	1.93	0.50
1:W:166:PHE:N	1:W:439:LEU:HD12	2.26	0.50
1:W:501:LEU:HA	1:W:507:THR:HB	1.92	0.50
1:C:66:PHE:CD1	1:C:69:MET:HE3	2.47	0.50
1:C:96:ARG:HD2	1:C:514:TYR:O	2.12	0.50
1:C:153:ARG:O	1:C:157:TYR:HB3	2.11	0.50
1:E:797:GLY:HA2	1:E:875:TYR:CE2	2.45	0.50
1:E:826:LEU:HD21	1:E:835:ARG:HD3	1.92	0.50
1:G:215:TRP:CD1	1:G:366:TRP:HE1	2.29	0.50
3:G:901:ACT:H1	8:G:1042:HOH:O	2.12	0.50
1:I:365:GLU:HG2	8:I:1099:HOH:O	2.11	0.50
1:M:698:PHE:HA	1:M:701:GLN:NE2	2.26	0.50
1:M:725:PRO:HA	1:S:704:ILE:HG13	1.93	0.50
2:N:43:HIS:ND1	8:N:405:HOH:O	2.35	0.50
1:O:211:MET:HE2	1:O:246:VAL:HG23	1.93	0.50
1:Q:146:MET:HG2	5:Q:903:MGD:N7	2.27	0.50
1:Q:177:GLU:OE2	1:Q:177:GLU:HA	2.12	0.50
2:R:19:CYS:HB2	2:R:46:MET:HG2	1.92	0.50
1:S:155:SER:OG	1:S:409:ILE:HG12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:114:MET:HB3	2:V:125:LYS:HB3	1.93	0.50
1:C:20:VAL:HG12	1:C:21:LYS:N	2.27	0.50
1:C:218:ASP:OD2	1:C:253:ASN:HB2	2.11	0.50
1:G:756:TYR:OH	2:H:41:ARG:HD3	2.10	0.50
1:I:449:ARG:HD2	8:I:1038:HOH:O	2.12	0.50
1:I:644:ASP:C	1:I:646:PRO:HD3	2.36	0.50
1:K:630:THR:OG1	1:K:633:GLU:HG3	2.11	0.50
2:L:164:MET:HE3	2:L:167:LYS:HB3	1.93	0.50
1:O:15:PRO:HB2	1:O:31:MET:SD	2.51	0.50
1:Q:138:LEU:HB2	1:Q:490:ILE:HD12	1.94	0.50
1:Q:629:MET:HE2	1:Q:634:PHE:N	2.26	0.50
1:S:563:ASP:HA	1:S:565:TYR:CE1	2.46	0.50
1:S:756:TYR:CD1	2:T:24:MET:HE1	2.46	0.50
2:T:40:GLN:NE2	2:T:117:ASN:HA	2.27	0.50
2:X:213:ALA:O	2:X:228:GLU:HA	2.12	0.50
1:C:378:GLY:O	1:C:381:LYS:HG2	2.12	0.50
2:J:59:ASN:ND2	2:J:59:ASN:H	2.09	0.50
1:K:4:VAL:HG23	8:K:1533:HOH:O	2.12	0.50
1:K:716:PRO:HB3	1:K:723:HIS:CG	2.47	0.50
3:S:901:ACT:H1	8:S:1046:HOH:O	2.11	0.50
2:T:114:MET:HG2	8:T:515:HOH:O	2.12	0.50
1:U:144:HIS:CG	1:U:743:MET:HE1	2.47	0.50
1:W:265:SER:O	1:W:810:GLN:NE2	2.45	0.50
1:W:400:TYR:CZ	1:W:421:LYS:HD2	2.46	0.50
1:A:458:GLY:HA3	8:A:1544:HOH:O	2.12	0.50
1:C:176:TRP:O	1:C:177:GLU:C	2.54	0.50
1:C:729:LYS:NZ	8:C:1135:HOH:O	2.45	0.50
1:C:739:PRO:HG2	1:C:742:SER:O	2.10	0.50
2:D:252:ASP:HB3	2:D:254:LYS:HE2	1.94	0.50
2:H:247:VAL:O	2:H:257:SER:HA	2.12	0.50
1:K:174:ASP:OD1	1:K:175:SER:N	2.43	0.50
2:L:213:ALA:O	2:L:228:GLU:HA	2.12	0.50
1:M:347:ALA:CB	1:M:388:SER:HA	2.41	0.50
1:M:756:TYR:HD1	2:N:24:MET:HE1	1.76	0.50
1:M:847:TYR:CZ	1:M:853:CYS:HB3	2.47	0.50
1:O:505:THR:O	1:O:506:ALA:C	2.55	0.50
2:P:185:ARG:HB2	2:P:185:ARG:HH11	1.77	0.50
2:R:5:TYR:CD2	2:R:164:MET:HG2	2.47	0.50
2:V:19:CYS:CA	2:V:145:CYS:HB3	2.42	0.50
1:A:174:ASP:OD1	1:A:175:SER:N	2.43	0.50
1:A:495:LYS:HD3	8:A:1110:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:MET:HE2	1:C:67:LYS:HB2	1.93	0.50
1:C:300:PHE:HZ	1:C:376:MET:HE3	1.77	0.50
1:C:391:GLN:HG2	1:C:567:LEU:CD2	2.42	0.50
1:E:801:LEU:HD11	1:E:839:ILE:HD11	1.94	0.50
2:F:19:CYS:CB	2:F:46:MET:HG2	2.42	0.50
1:G:735:LEU:H	1:G:735:LEU:HD23	1.77	0.50
1:I:176:TRP:CD1	1:I:193:LEU:HB2	2.47	0.50
1:I:211:MET:HE2	1:I:246:VAL:CG2	2.42	0.50
1:K:426:MET:HE2	1:K:618:GLN:OE1	2.12	0.50
1:K:735:LEU:HD23	1:K:735:LEU:H	1.77	0.50
2:L:13:CYS:HB3	2:L:63:TYR:HB2	1.92	0.50
1:M:15:PRO:HD3	1:M:554:PHE:CE1	2.47	0.50
1:M:786:ASN:HD21	1:M:804:GLN:HA	1.76	0.50
1:O:782:ARG:HD3	1:O:864:ILE:O	2.12	0.50
2:R:114:MET:HE3	2:R:123:ALA:HB1	1.94	0.50
1:G:103:GLN:N	1:G:103:GLN:CD	2.70	0.49
2:H:13:CYS:HB3	2:H:63:TYR:HB2	1.93	0.49
2:H:176:ILE:HG22	2:H:177:LYS:HG3	1.94	0.49
2:J:177:LYS:N	2:J:178:PRO:HD3	2.27	0.49
2:N:19:CYS:HA	2:N:145:CYS:HA	1.93	0.49
2:N:210:PHE:HD2	2:N:213:ALA:HB2	1.77	0.49
1:Q:173:PRO:HA	1:Q:468:PHE:CE1	2.46	0.49
1:U:76:ILE:CG2	1:U:541:PRO:HG3	2.41	0.49
1:G:75:ARG:HH22	1:G:547:GLU:CD	2.19	0.49
1:G:141:PRO:CA	1:G:496:TYR:HB3	2.41	0.49
1:G:353:GLY:O	1:G:354:TRP:HB2	2.12	0.49
1:I:818:GLU:O	1:I:819:SER:HB2	2.12	0.49
2:J:106:LEU:HA	2:J:114:MET:HE2	1.94	0.49
2:J:210:PHE:CE2	2:J:251:ALA:HB1	2.46	0.49
1:M:15:PRO:HD3	1:M:554:PHE:CD1	2.47	0.49
1:M:322:GLU:HG3	1:M:327:VAL:O	2.11	0.49
2:N:20:PHE:CZ	2:N:24:MET:HE2	2.47	0.49
1:Q:176:TRP:CD1	1:Q:354:TRP:HE1	2.31	0.49
1:Q:195:ASN:HD21	1:Q:354:TRP:CD1	2.29	0.49
1:Q:800:ILE:HD12	1:Q:800:ILE:N	2.27	0.49
1:S:505:THR:O	1:S:506:ALA:C	2.56	0.49
1:U:433:PHE:CD1	1:U:433:PHE:N	2.80	0.49
1:A:45:GLU:HB3	8:A:1525:HOH:O	2.11	0.49
1:C:75:ARG:HH22	1:C:547:GLU:CD	2.20	0.49
1:C:387:TRP:CZ2	1:C:389:THR:HA	2.47	0.49
1:C:427:PHE:HB3	8:C:1029:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:ASN:HB2	8:C:1294:HOH:O	2.12	0.49
1:C:610:LYS:HB3	1:C:614:ALA:HB3	1.92	0.49
1:E:239:LYS:HE2	8:E:1602:HOH:O	2.12	0.49
1:E:250:PRO:HD3	5:E:904:MGD:C2	2.42	0.49
1:E:296:ASN:O	1:E:687:LYS:HB3	2.13	0.49
1:I:75:ARG:HH21	1:I:543:CYS:HA	1.76	0.49
1:K:153:ARG:O	1:K:157:TYR:HB3	2.12	0.49
1:K:602:ILE:HD13	8:K:1075:HOH:O	2.11	0.49
1:K:644:ASP:C	1:K:646:PRO:HD3	2.36	0.49
2:L:44:ARG:HB2	2:L:115:TYR:OH	2.11	0.49
1:M:617:GLU:HG3	1:M:631:TRP:CG	2.47	0.49
1:O:249:ASP:CG	5:O:904:MGD:H1'	2.37	0.49
1:O:476:GLN:HG2	8:O:1287:HOH:O	2.12	0.49
1:O:823:TYR:CE2	1:O:825:PRO:HG3	2.47	0.49
2:P:59:ASN:ND2	2:P:59:ASN:H	2.10	0.49
1:Q:176:TRP:CD2	1:Q:193:LEU:HD12	2.48	0.49
2:T:44:ARG:HG2	2:T:44:ARG:HH11	1.78	0.49
1:U:9:ASN:HA	1:U:576:GLN:HA	1.94	0.49
1:U:99:GLY:HA2	1:U:102:LYS:HE2	1.94	0.49
1:U:146:MET:HG2	5:U:903:MGD:N7	2.27	0.49
1:U:797:GLY:HA2	1:U:875:TYR:CE2	2.48	0.49
1:E:655:ARG:HB3	8:E:1401:HOH:O	2.11	0.49
1:I:476:GLN:OE1	1:I:708:ARG:NH2	2.44	0.49
1:M:56:LYS:HG2	1:M:57:THR:N	2.27	0.49
1:M:111:ARG:NH2	1:M:585:GLU:OE2	2.37	0.49
1:O:76:ILE:HG22	1:O:541:PRO:HG3	1.94	0.49
1:O:786:ASN:ND2	1:O:805:VAL:H	2.10	0.49
2:P:252:ASP:C	2:P:254:LYS:H	2.21	0.49
1:Q:458:GLY:HA3	8:Q:1540:HOH:O	2.12	0.49
1:S:116:GLU:O	1:S:120:ILE:HG13	2.11	0.49
1:W:489:LYS:HG3	8:W:1214:HOH:O	2.12	0.49
2:X:73:ASN:HD22	2:X:73:ASN:C	2.21	0.49
1:A:530:GLU:OE2	1:A:750:LYS:NZ	2.45	0.49
2:D:46:MET:HE3	2:D:46:MET:C	2.37	0.49
1:E:68:SER:HB3	1:E:753:TYR:CE2	2.47	0.49
1:E:452:ILE:N	1:E:453:PRO:CD	2.76	0.49
1:G:784:ILE:HD13	1:G:790:ILE:HG21	1.94	0.49
2:L:110:PRO:HB3	2:L:180:LEU:HD13	1.95	0.49
1:O:166:PHE:N	1:O:439:LEU:HD12	2.27	0.49
2:P:21:MET:CE	2:P:21:MET:CA	2.90	0.49
1:Q:451:LYS:HG3	1:Q:461:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:717:ALA:HB3	1:Q:720:SER:HB3	1.95	0.49
2:R:254:LYS:HD2	2:R:274:LEU:OXT	2.13	0.49
1:A:9:ASN:HA	1:A:576:GLN:HA	1.94	0.49
1:A:561:ILE:CG2	1:A:564:ASN:HB3	2.41	0.49
2:D:71:CYS:HB3	2:D:184:PRO:HA	1.95	0.49
1:E:173:PRO:HA	1:E:468:PHE:CE1	2.48	0.49
1:E:610:LYS:HB3	1:E:614:ALA:HB3	1.95	0.49
1:G:737:PRO:HG3	5:G:904:MGD:H2'	1.94	0.49
1:I:404:TYR:CD1	1:I:405:ALA:N	2.81	0.49
1:K:700:GLU:HG2	8:K:1568:HOH:O	2.12	0.49
2:N:105:LEU:HB3	2:N:114:MET:HE1	1.94	0.49
1:Q:103:GLN:CD	1:Q:103:GLN:N	2.70	0.49
2:V:205:VAL:HG13	2:V:254:LYS:NZ	2.28	0.49
1:W:197:GLU:OE2	1:W:665:THR:OG1	2.26	0.49
1:W:629:MET:HE2	1:W:634:PHE:CA	2.38	0.49
1:W:867:TRP:CD1	1:W:869:GLY:H	2.31	0.49
1:C:701:GLN:HG3	8:C:1665:HOH:O	2.12	0.49
1:E:565:TYR:C	1:E:567:LEU:H	2.21	0.49
1:G:176:TRP:O	1:G:177:GLU:C	2.55	0.49
2:H:106:LEU:HD23	2:H:114:MET:CE	2.43	0.49
2:H:142:MET:HE2	2:H:146:ALA:HB1	1.93	0.49
1:K:460:LYS:HE3	8:K:1234:HOH:O	2.13	0.49
1:K:847:TYR:CZ	1:K:853:CYS:HB3	2.48	0.49
1:M:855:MET:HB2	1:M:857:ASN:OD1	2.11	0.49
1:O:12:THR:HG23	8:O:1337:HOH:O	2.12	0.49
1:Q:753:TYR:HB3	2:R:24:MET:HE3	1.95	0.49
2:V:168:VAL:HG13	2:V:173:LEU:HB2	1.94	0.49
1:W:25:ILE:HG13	1:W:580:ILE:CG2	2.43	0.49
1:A:195:ASN:HD21	1:A:354:TRP:CD1	2.31	0.49
1:C:128:ILE:CD1	1:C:492:MET:HB2	2.43	0.49
1:I:96:ARG:HD2	1:I:514:TYR:O	2.12	0.49
1:K:100:LEU:CD1	1:K:105:PRO:HG3	2.42	0.49
1:K:218:ASP:OD2	1:K:253:ASN:HB2	2.12	0.49
1:K:610:LYS:HZ3	1:K:618:GLN:NE2	2.08	0.49
2:L:70:HIS:CD2	2:L:92:VAL:H	2.29	0.49
1:M:201:LEU:HD13	1:M:387:TRP:HB2	1.95	0.49
2:N:18:ASN:HB2	7:N:302:SF4:S1	2.53	0.49
2:P:125:LYS:HD2	2:P:126:CYS:O	2.11	0.49
1:Q:735:LEU:HD23	1:Q:735:LEU:H	1.77	0.49
1:A:141:PRO:CA	1:A:496:TYR:HB3	2.35	0.49
1:A:166:PHE:N	1:A:439:LEU:HD12	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:MET:CE	2:F:21:MET:HA	2.43	0.49
2:F:201:ALA:HB2	2:F:269:LEU:HB2	1.94	0.49
2:L:162:GLU:H	2:L:162:GLU:CD	2.20	0.49
1:Q:698:PHE:HA	1:Q:701:GLN:NE2	2.27	0.49
2:R:125:LYS:HD2	2:R:126:CYS:O	2.13	0.49
1:A:404:TYR:CD1	1:A:405:ALA:N	2.81	0.49
2:B:19:CYS:HB3	2:B:145:CYS:HB3	1.94	0.49
1:C:675:GLN:OE1	1:C:678:ARG:HA	2.13	0.49
1:E:104:ASP:N	1:E:105:PRO:HD3	2.27	0.49
1:G:257:ARG:HD3	2:H:61:ILE:HG21	1.95	0.49
1:I:202:LEU:HD23	1:I:394:PRO:HD3	1.95	0.49
1:I:755:ASN:OD1	1:I:761:ARG:HD2	2.13	0.49
2:J:40:GLN:HB3	2:J:43:HIS:CE1	2.47	0.49
1:K:138:LEU:HB2	1:K:490:ILE:CD1	2.43	0.49
1:M:17:PHE:CE2	1:M:31:MET:HE3	2.48	0.49
2:P:87:ARG:HB2	2:P:89:ASP:OD2	2.13	0.49
1:Q:99:GLY:N	1:Q:108:ASP:OD2	2.39	0.49
1:Q:176:TRP:NE1	1:Q:354:TRP:HE1	2.11	0.49
1:Q:630:THR:OG1	1:Q:633:GLU:HG3	2.13	0.49
1:S:277:ALA:HA	1:S:316:LYS:O	2.13	0.49
1:S:491:LYS:HD3	8:S:1563:HOH:O	2.12	0.49
1:U:107:SER:HB3	8:U:1627:HOH:O	2.12	0.49
1:U:823:TYR:CE2	1:U:825:PRO:HG3	2.48	0.49
1:W:159:ARG:HD2	1:W:409:ILE:O	2.12	0.49
1:W:211:MET:HE1	2:X:231:PHE:HZ	1.78	0.49
2:B:10:VAL:HG13	2:B:63:TYR:O	2.13	0.48
1:C:347:ALA:CB	1:C:388:SER:HA	2.43	0.48
1:C:395:LEU:HD12	1:C:566:GLN:HA	1.94	0.48
1:E:139:SER:OG	1:E:161:MET:HE2	2.13	0.48
1:E:181:TRP:HA	1:E:476:GLN:OE1	2.13	0.48
1:E:268:ILE:HG13	1:E:268:ILE:O	2.12	0.48
1:G:351:LEU:HG	1:G:391:GLN:NE2	2.28	0.48
1:I:187:TRP:CH2	1:I:196:PRO:HB3	2.48	0.48
1:K:644:ASP:OD1	1:K:646:PRO:HG3	2.13	0.48
2:L:59:ASN:ND2	2:L:59:ASN:N	2.56	0.48
1:M:197:GLU:OE2	1:M:665:THR:OG1	2.29	0.48
1:M:452:ILE:N	1:M:453:PRO:CD	2.76	0.48
1:O:548:ARG:HB2	8:O:1115:HOH:O	2.13	0.48
1:S:855:MET:HB2	1:S:857:ASN:OD1	2.13	0.48
2:T:252:ASP:C	2:T:254:LYS:H	2.19	0.48
1:W:333:ARG:HD3	1:W:337:ARG:NH2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:356:GLY:HA2	1:W:359:ARG:NH1	2.28	0.48
1:W:393:VAL:HG21	1:W:568:CYS:O	2.13	0.48
1:W:564:ASN:HD22	1:W:564:ASN:H	1.59	0.48
1:W:763:GLU:HA	1:W:768:LYS:HA	1.95	0.48
1:A:142:SER:CB	5:A:903:MGD:O1A	2.61	0.48
1:A:823:TYR:CE2	1:A:825:PRO:HG3	2.47	0.48
2:B:13:CYS:HB3	2:B:63:TYR:HB2	1.95	0.48
2:J:216:VAL:HG13	2:J:223:GLU:HG3	1.93	0.48
1:K:394:PRO:HG3	8:K:1322:HOH:O	2.12	0.48
1:K:402:PRO:HG2	1:K:422:PHE:CE1	2.48	0.48
2:L:176:ILE:HG22	2:L:177:LYS:HG3	1.94	0.48
1:M:68:SER:HB3	1:M:753:TYR:CE2	2.48	0.48
2:N:46:MET:HE1	2:N:65:PRO:C	2.38	0.48
2:N:198:TYR:HB3	2:N:238:ASP:HA	1.94	0.48
1:Q:166:PHE:H	1:Q:439:LEU:HD12	1.78	0.48
1:Q:296:ASN:O	1:Q:687:LYS:HB3	2.13	0.48
1:S:231:SER:HB2	1:S:235:ARG:HH12	1.78	0.48
1:S:561:ILE:N	1:S:562:PRO:HD3	2.27	0.48
1:W:644:ASP:OD1	1:W:646:PRO:HG3	2.12	0.48
1:A:114:TRP:CZ2	1:A:541:PRO:HD2	2.48	0.48
1:A:153:ARG:O	1:A:157:TYR:HB3	2.12	0.48
1:A:565:TYR:C	1:A:567:LEU:H	2.21	0.48
2:D:75:PRO:HD2	7:D:304:SF4:S4	2.54	0.48
2:D:256:TYR:HB2	2:D:274:LEU:HD21	1.95	0.48
1:I:282:TRP:HA	1:I:287:SER:OG	2.13	0.48
1:I:620:PHE:CZ	1:I:625:MET:HB3	2.48	0.48
2:P:247:VAL:O	2:P:257:SER:HA	2.13	0.48
1:U:708:ARG:HD3	8:U:1050:HOH:O	2.13	0.48
1:W:140:THR:HB	1:W:169:ALA:HB3	1.95	0.48
2:B:39:MET:HE2	2:B:45:TRP:CD2	2.48	0.48
1:C:1:MET:CE	1:C:22:ASP:HB3	2.43	0.48
1:C:253:ASN:O	1:C:257:ARG:HG3	2.13	0.48
1:C:748:ASP:O	1:C:750:LYS:HE2	2.14	0.48
1:E:85:PHE:CE2	1:E:87:PRO:HG3	2.48	0.48
1:I:501:LEU:HD13	1:I:823:TYR:CD2	2.48	0.48
2:L:105:LEU:HB3	2:L:114:MET:CE	2.42	0.48
1:M:165:GLY:CA	1:M:166:PHE:HB3	2.36	0.48
1:M:291:GLU:H	1:M:291:GLU:CD	2.21	0.48
1:O:563:ASP:HA	1:O:565:TYR:CE1	2.49	0.48
2:P:46:MET:HE2	2:P:48:ILE:HG12	1.95	0.48
1:Q:65:GLY:HA2	8:Q:1403:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:670:PRO:HG2	1:Q:675:GLN:CD	2.39	0.48
1:S:146:MET:HG2	5:S:903:MGD:N7	2.28	0.48
1:S:356:GLY:HA2	1:S:359:ARG:NH1	2.28	0.48
2:X:201:ALA:CB	2:X:269:LEU:HB2	2.35	0.48
1:A:17:PHE:CE2	1:A:31:MET:HE3	2.48	0.48
1:A:165:GLY:CA	1:A:166:PHE:HB3	2.42	0.48
1:C:561:ILE:CG2	1:C:564:ASN:HB3	2.38	0.48
2:D:4:TYR:CE2	2:D:158:LYS:HD2	2.48	0.48
2:D:40:GLN:HE21	2:D:117:ASN:HA	1.79	0.48
2:D:71:CYS:HB3	2:D:184:PRO:CA	2.43	0.48
1:G:645:ASN:HD21	1:G:648:ARG:HB3	1.74	0.48
2:H:87:ARG:HG3	2:H:91:ILE:O	2.13	0.48
1:I:610:LYS:HB3	1:I:614:ALA:HB3	1.95	0.48
1:I:716:PRO:HB2	8:I:1523:HOH:O	2.12	0.48
2:L:166:LYS:HG2	2:L:170:GLU:OE2	2.14	0.48
1:O:553:GLU:HB3	1:O:556:ASN:HB2	1.96	0.48
2:P:21:MET:CE	2:P:24:MET:HE3	2.43	0.48
1:S:644:ASP:O	1:S:646:PRO:HD3	2.14	0.48
1:S:656:TRP:CD2	1:S:663:LYS:HA	2.48	0.48
2:T:131:HIS:NE2	2:T:132:LEU:HG	2.28	0.48
1:W:138:LEU:HB2	1:W:490:ILE:CD1	2.39	0.48
2:X:20:PHE:CZ	2:X:24:MET:HE2	2.49	0.48
2:B:245:TYR:HB2	2:B:260:VAL:HG13	1.94	0.48
2:D:129:CYS:CB	2:D:132:LEU:HD12	2.44	0.48
1:G:74:LEU:HD12	1:G:750:LYS:CA	2.40	0.48
1:G:224:GLY:O	1:G:225:ILE:HB	2.14	0.48
2:L:203:ILE:N	2:L:203:ILE:HD12	2.29	0.48
1:M:21:LYS:CB	1:M:26:ILE:HD11	2.44	0.48
2:N:9:ASP:HA	2:N:189:LYS:HB3	1.95	0.48
1:O:39:ALA:HB1	8:O:1277:HOH:O	2.13	0.48
1:O:184:MET:HE2	1:O:190:SER:HA	1.95	0.48
3:O:901:ACT:H1	8:O:1043:HOH:O	2.13	0.48
1:Q:501:LEU:HD13	1:Q:823:TYR:CD2	2.49	0.48
1:S:587:MET:HE2	1:S:592:ILE:HA	1.95	0.48
1:S:701:GLN:HG3	8:S:1661:HOH:O	2.13	0.48
1:S:870:ASP:OD2	1:S:871:LYS:N	2.47	0.48
2:X:16:CYS:O	2:X:17:ASN:HB2	2.13	0.48
1:A:387:TRP:CZ2	1:A:389:THR:HA	2.48	0.48
1:A:610:LYS:HB3	1:A:614:ALA:HB3	1.95	0.48
1:E:257:ARG:HD3	2:F:61:ILE:HG21	1.94	0.48
2:F:21:MET:HE1	2:F:24:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:ARG:HD2	1:G:514:TYR:O	2.14	0.48
1:G:721:GLN:NE2	8:G:1285:HOH:O	2.47	0.48
2:H:165:ALA:HA	8:H:523:HOH:O	2.14	0.48
1:I:94:GLN:OE1	1:I:94:GLN:N	2.47	0.48
1:I:214:PHE:HA	1:I:347:ALA:HB3	1.95	0.48
1:M:730:TYR:CE1	1:M:794:ASN:HA	2.49	0.48
1:O:224:GLY:O	1:O:225:ILE:HB	2.14	0.48
1:Q:776:SER:HA	1:Q:805:VAL:CG1	2.44	0.48
1:U:427:PHE:HB3	8:U:1032:HOH:O	2.14	0.48
1:W:28:MET:HE2	8:W:1404:HOH:O	2.14	0.48
1:A:176:TRP:CD2	1:A:193:LEU:HD12	2.49	0.48
2:B:5:TYR:CD2	2:B:164:MET:HG2	2.49	0.48
1:C:395:LEU:HD13	1:C:571:ARG:HG2	1.96	0.48
1:E:37:VAL:HB	8:E:1156:HOH:O	2.13	0.48
1:E:165:GLY:HA3	1:E:166:PHE:CB	2.33	0.48
1:G:356:GLY:HA2	1:G:359:ARG:NH1	2.29	0.48
1:G:790:ILE:HD13	1:G:803:ALA:HB2	1.95	0.48
1:M:449:ARG:HD2	8:M:1038:HOH:O	2.12	0.48
2:N:114:MET:HG2	8:N:519:HOH:O	2.13	0.48
1:O:571:ARG:HB2	1:O:642:VAL:HB	1.96	0.48
1:Q:56:LYS:HG2	1:Q:57:THR:O	2.14	0.48
1:Q:111:ARG:NH2	1:Q:585:GLU:OE2	2.41	0.48
2:R:177:LYS:N	2:R:178:PRO:HD3	2.29	0.48
2:T:104:GLU:CD	2:T:104:GLU:H	2.22	0.48
2:V:106:LEU:HD22	2:V:114:MET:HG3	1.96	0.48
1:W:500:HIS:HA	1:W:503:THR:OG1	2.14	0.48
1:E:291:GLU:H	1:E:291:GLU:CD	2.22	0.48
2:F:216:VAL:HG13	2:F:223:GLU:HG3	1.96	0.48
1:I:528:TRP:CD2	1:I:750:LYS:HD3	2.49	0.48
1:I:602:ILE:HD13	8:I:1075:HOH:O	2.13	0.48
2:J:124:GLN:O	2:J:125:LYS:HB3	2.14	0.48
1:K:305:ASP:OD1	1:K:310:LYS:HD2	2.13	0.48
1:K:510:TYR:O	1:K:513:MET:HG2	2.14	0.48
2:L:103:LYS:O	2:L:106:LEU:HG	2.14	0.48
1:M:176:TRP:CD1	1:M:354:TRP:HE1	2.31	0.48
1:O:501:LEU:HD13	1:O:823:TYR:CD2	2.48	0.48
2:P:46:MET:HE1	2:P:65:PRO:C	2.39	0.48
1:S:74:LEU:HD12	1:S:750:LYS:HA	1.95	0.48
1:S:141:PRO:HA	1:S:496:TYR:HB3	1.96	0.48
1:S:249:ASP:CG	5:S:904:MGD:H1'	2.39	0.48
1:U:730:TYR:HB3	1:U:862:VAL:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:142:MET:HE2	2:V:147:HIS:CA	2.44	0.48
2:X:39:MET:HG2	2:X:40:GLN:N	2.27	0.48
1:A:426:MET:HE1	1:A:618:GLN:O	2.13	0.48
1:C:801:LEU:HD11	1:C:839:ILE:HD11	1.96	0.48
1:E:144:HIS:CE1	3:E:901:ACT:OXT	2.67	0.48
1:E:172:ASN:O	1:E:174:ASP:N	2.41	0.48
1:E:717:ALA:HB3	1:E:720:SER:HB3	1.94	0.48
1:E:776:SER:HA	1:E:805:VAL:HG13	1.96	0.48
1:G:197:GLU:HG3	1:G:199:TYR:CE1	2.49	0.48
1:M:649:LYS:HA	8:U:1001:HOH:O	2.14	0.48
2:N:5:TYR:CD2	2:N:164:MET:HG2	2.49	0.48
2:N:142:MET:HE1	8:N:430:HOH:O	2.14	0.48
2:P:92:VAL:HG11	7:P:304:SF4:S1	2.54	0.48
2:T:68:CYS:HA	2:T:113:VAL:HG11	1.95	0.48
2:T:87:ARG:HG3	2:T:91:ILE:O	2.13	0.48
2:T:260:VAL:HG13	2:T:260:VAL:O	2.14	0.48
1:U:21:LYS:CB	1:U:26:ILE:HD11	2.43	0.48
1:U:114:TRP:CZ2	1:U:587:MET:HG2	2.48	0.48
1:U:146:MET:HE2	1:U:544:THR:HB	1.96	0.48
1:W:142:SER:HB2	5:W:903:MGD:H5'2	1.96	0.48
2:X:142:MET:HE2	2:X:147:HIS:N	2.28	0.48
1:A:250:PRO:HD3	5:A:904:MGD:C2	2.44	0.47
1:A:457:MET:HA	1:A:516:HIS:CD2	2.49	0.47
1:C:744:HIS:HA	1:C:819:SER:HB3	1.95	0.47
2:D:26:GLU:HB2	2:D:144:ARG:NH1	2.29	0.47
1:E:4:VAL:HG22	1:E:21:LYS:HB2	1.95	0.47
1:G:533:VAL:HB	1:G:534:PRO:HD3	1.96	0.47
1:G:708:ARG:HD2	8:G:1045:HOH:O	2.14	0.47
2:H:142:MET:HE1	8:H:430:HOH:O	2.14	0.47
1:I:296:ASN:HB3	1:I:657:PHE:CZ	2.48	0.47
1:I:458:GLY:HA3	8:I:1543:HOH:O	2.15	0.47
2:J:5:TYR:HB2	2:J:157:LEU:HD12	1.96	0.47
2:L:50:ARG:HG2	2:L:63:TYR:CD2	2.49	0.47
2:L:142:MET:HE2	2:L:147:HIS:N	2.28	0.47
1:M:173:PRO:HA	1:M:468:PHE:CE1	2.49	0.47
1:O:15:PRO:HD3	1:O:554:PHE:CD1	2.49	0.47
1:O:75:ARG:NH2	1:O:543:CYS:HA	2.29	0.47
1:S:408:GLY:HA2	1:S:619:TYR:HE1	1.78	0.47
1:S:494:TRP:HE1	1:S:525:GLN:HE21	1.62	0.47
1:U:146:MET:CE	1:U:544:THR:HB	2.44	0.47
1:U:530:GLU:O	1:U:533:VAL:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:855:MET:HB2	1:W:857:ASN:OD1	2.13	0.47
1:A:42:TRP:CZ2	1:A:53:PRO:HD3	2.49	0.47
1:A:197:GLU:OE2	1:A:667:ASP:HB2	2.14	0.47
1:A:252:MET:HB3	1:A:808:CYS:HB3	1.96	0.47
2:B:46:MET:HE3	2:B:47:ASN:N	2.29	0.47
1:C:174:ASP:OD1	1:C:175:SER:N	2.44	0.47
1:C:716:PRO:HB3	1:C:723:HIS:CD2	2.49	0.47
1:E:346:LEU:HD23	1:E:386:MET:HE2	1.96	0.47
1:I:451:LYS:HG3	1:I:461:PHE:CE2	2.49	0.47
1:K:211:MET:HE1	1:K:338:GLN:CG	2.40	0.47
1:K:767:TYR:HB3	1:K:769:TYR:CE1	2.50	0.47
1:Q:13:GLY:O	1:Q:59:ILE:HA	2.13	0.47
1:S:257:ARG:HD3	2:T:61:ILE:HG21	1.96	0.47
2:T:106:LEU:CD2	2:T:114:MET:HG3	2.44	0.47
1:U:269:GLY:HA2	1:U:362:HIS:CE1	2.48	0.47
1:U:494:TRP:HE1	1:U:525:GLN:HE21	1.60	0.47
2:V:39:MET:HG2	2:V:40:GLN:N	2.29	0.47
1:W:139:SER:OG	1:W:161:MET:HE2	2.15	0.47
1:W:291:GLU:CD	1:W:291:GLU:H	2.22	0.47
1:W:772:MET:HB2	1:W:801:LEU:CD1	2.44	0.47
1:A:78:TYR:CE2	1:A:111:ARG:HD2	2.49	0.47
1:A:252:MET:HE3	1:A:263:TRP:CE3	2.50	0.47
1:A:391:GLN:HG2	1:A:567:LEU:HD23	1.95	0.47
1:A:648:ARG:NH1	8:A:1160:HOH:O	2.46	0.47
1:C:408:GLY:O	1:C:422:PHE:HE2	1.98	0.47
1:C:563:ASP:O	1:C:566:GLN:HG2	2.14	0.47
1:C:696:LYS:HD3	8:C:1682:HOH:O	2.14	0.47
1:K:561:ILE:N	1:K:562:PRO:HD3	2.30	0.47
1:M:563:ASP:O	1:M:566:GLN:HG2	2.14	0.47
2:N:94:ILE:O	2:N:96:PRO:HD3	2.14	0.47
1:O:14:GLY:HA2	1:O:554:PHE:CE1	2.48	0.47
1:S:560[A]:TYR:HD1	1:S:561:ILE:HG13	1.80	0.47
1:S:560[B]:TYR:HD1	1:S:561:ILE:HG13	1.80	0.47
1:U:501:LEU:HD13	1:U:823:TYR:CD2	2.49	0.47
2:X:21:MET:HE2	2:X:21:MET:N	2.29	0.47
2:X:52:GLU:HG2	2:X:61:ILE:HD12	1.95	0.47
1:A:558:SER:H	1:A:564:ASN:ND2	2.13	0.47
1:A:772:MET:HB2	1:A:801:LEU:HD13	1.95	0.47
2:B:245:TYR:HB2	2:B:260:VAL:CG1	2.44	0.47
1:C:211:MET:HE2	1:C:246:VAL:HG23	1.96	0.47
1:E:166:PHE:N	1:E:439:LEU:HD12	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:GLY:HA3	1:E:353:GLY:O	2.13	0.47
1:G:605:MET:N	1:G:605:MET:SD	2.86	0.47
2:H:56:TYR:HA	2:H:59:ASN:ND2	2.28	0.47
2:N:46:MET:HE3	2:N:47:ASN:N	2.30	0.47
1:O:162:ASN:CG	1:O:437:SER:HB2	2.40	0.47
2:P:142:MET:HE1	8:P:427:HOH:O	2.14	0.47
1:Q:394:PRO:HG3	8:Q:1324:HOH:O	2.13	0.47
1:S:9:ASN:HA	1:S:576:GLN:HA	1.97	0.47
1:S:176:TRP:NE1	1:S:354:TRP:HE1	2.12	0.47
1:S:744:HIS:CA	1:S:819:SER:HB3	2.44	0.47
1:U:75:ARG:HG2	8:U:1457:HOH:O	2.13	0.47
2:V:110:PRO:HB3	2:V:180:LEU:HD13	1.95	0.47
1:A:211:MET:HE2	1:A:246:VAL:CG2	2.44	0.47
1:E:292:TYR:CD2	1:E:378:GLY:HA2	2.50	0.47
2:F:104:GLU:H	2:F:104:GLU:CD	2.23	0.47
2:H:5:TYR:CD2	2:H:164:MET:HG2	2.49	0.47
1:K:512:LYS:HE3	1:K:830:GLY:O	2.14	0.47
1:M:176:TRP:O	1:M:177:GLU:C	2.57	0.47
1:M:184:MET:HE2	1:M:190:SER:HA	1.96	0.47
1:M:476:GLN:OE1	1:M:708:ARG:NH2	2.48	0.47
1:O:730:TYR:CE1	1:O:794:ASN:HA	2.50	0.47
1:S:521:PHE:CE2	1:S:523:VAL:CG2	2.97	0.47
1:S:717:ALA:HB3	1:S:720:SER:HB3	1.95	0.47
2:X:56:TYR:CD1	2:X:57:PRO:HA	2.49	0.47
2:X:69:MET:HB2	7:X:304:SF4:S2	2.55	0.47
1:A:505:THR:O	1:A:506:ALA:C	2.58	0.47
2:B:219:SER:C	2:B:221:GLY:H	2.21	0.47
2:D:94:ILE:O	2:D:96:PRO:HD3	2.14	0.47
2:D:167:LYS:HZ3	2:D:171:GLU:CD	2.23	0.47
1:E:645:ASN:HD22	1:E:648:ARG:HB3	1.73	0.47
1:E:786:ASN:ND2	1:E:804:GLN:HA	2.29	0.47
2:F:175:VAL:HG22	8:F:451:HOH:O	2.14	0.47
1:G:152:TYR:CD2	1:G:154:HIS:HD2	2.32	0.47
2:H:87:ARG:HB2	2:H:89:ASP:OD2	2.14	0.47
2:J:166:LYS:O	2:J:170:GLU:HG3	2.15	0.47
1:K:411:GLY:HA3	1:K:434:PRO:HB3	1.97	0.47
1:K:617:GLU:HG3	1:K:631:TRP:CG	2.49	0.47
1:K:695:LEU:HD22	1:K:708:ARG:HD3	1.97	0.47
1:O:400:TYR:CZ	1:O:421:LYS:HD2	2.50	0.47
1:O:847:TYR:CZ	1:O:853:CYS:HB3	2.49	0.47
1:Q:557:CYS:N	1:Q:564:ASN:HD21	1.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:452:ILE:N	1:S:453:PRO:CD	2.78	0.47
1:S:563:ASP:O	1:S:566:GLN:HG2	2.14	0.47
2:T:92:VAL:HG21	7:T:304:SF4:S1	2.55	0.47
1:U:737:PRO:HG3	5:U:904:MGD:H2'	1.95	0.47
1:A:734:MET:SD	1:A:839:ILE:HD12	2.55	0.47
1:C:171:HIS:O	1:C:467:GLY:HA2	2.14	0.47
1:C:628:TYR:CE2	1:C:643:PRO:HG2	2.49	0.47
1:E:27:ARG:NH2	2:F:132:LEU:HD21	2.30	0.47
2:F:95:ASP:HB3	2:F:98:LYS:HB2	1.96	0.47
2:F:247:VAL:O	2:F:257:SER:HA	2.15	0.47
1:G:452:ILE:HB	1:G:453:PRO:HD3	1.96	0.47
2:H:21:MET:HA	2:H:21:MET:CE	2.44	0.47
1:I:66:PHE:CD1	1:I:69:MET:HE3	2.50	0.47
2:J:114:MET:HE3	2:J:123:ALA:HB1	1.97	0.47
1:K:146:MET:HG2	5:K:903:MGD:N7	2.29	0.47
1:K:187:TRP:CH2	1:K:196:PRO:HB3	2.50	0.47
1:K:191:TRP:CD2	1:K:669:GLY:HA3	2.50	0.47
1:K:505:THR:O	1:K:506:ALA:C	2.57	0.47
1:M:547:GLU:OE1	1:M:582:PRO:HA	2.15	0.47
1:M:629:MET:HE2	1:M:634:PHE:CA	2.41	0.47
1:O:696:LYS:HG3	8:O:1041:HOH:O	2.14	0.47
1:Q:540:LEU:HA	1:Q:541:PRO:HD3	1.78	0.47
1:S:249:ASP:O	1:S:250:PRO:C	2.58	0.47
1:S:600:LEU:HB3	8:S:1078:HOH:O	2.15	0.47
2:V:70:HIS:CD2	2:V:92:VAL:H	2.23	0.47
2:V:204:LEU:HD23	2:V:209:CYS:HA	1.97	0.47
1:W:252:MET:HB3	1:W:808:CYS:HB3	1.97	0.47
1:W:394:PRO:HG3	8:W:1325:HOH:O	2.14	0.47
1:A:291:GLU:CD	1:A:291:GLU:N	2.72	0.47
2:B:87:ARG:HG3	2:B:91:ILE:O	2.15	0.47
1:C:223:SER:HB3	8:C:1340:HOH:O	2.14	0.47
2:F:106:LEU:HD23	2:F:114:MET:HE2	1.97	0.47
1:G:13:GLY:HA3	1:G:63:THR:OG1	2.15	0.47
1:G:258:LEU:HG	1:G:259:VAL:HG13	1.97	0.47
1:I:580:ILE:HA	8:I:1619:HOH:O	2.14	0.47
2:J:19:CYS:O	2:J:22:GLY:N	2.48	0.47
2:L:6:MET:HE3	2:L:156:PHE:CD1	2.50	0.47
2:L:162:GLU:CD	2:L:162:GLU:N	2.73	0.47
2:N:46:MET:HE1	2:N:65:PRO:CA	2.45	0.47
2:N:68:CYS:HB2	2:N:126:CYS:CB	2.43	0.47
1:O:28:MET:CE	1:O:67:LYS:N	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:561:ILE:CG2	1:O:564:ASN:HB3	2.40	0.47
2:P:87:ARG:NH2	2:P:91:ILE:HD12	2.29	0.47
1:S:55:ARG:HG3	8:S:1555:HOH:O	2.14	0.47
1:S:114:TRP:CZ2	1:S:541:PRO:HD2	2.50	0.47
1:S:387:TRP:CZ2	1:S:389:THR:HA	2.50	0.47
2:T:19:CYS:CB	2:T:145:CYS:HB3	2.26	0.47
1:U:361:SER:OG	1:U:717:ALA:HB1	2.15	0.47
1:U:452:ILE:N	1:U:453:PRO:CD	2.78	0.47
2:X:94:ILE:HG22	2:X:95:ASP:H	1.78	0.47
1:A:146:MET:HE2	1:A:544:THR:CB	2.43	0.47
2:D:128:MET:O	2:D:129:CYS:C	2.57	0.47
1:G:294:ALA:HA	8:G:1167:HOH:O	2.15	0.47
1:I:81:LYS:HE2	1:I:82:ARG:O	2.15	0.47
1:I:144:HIS:NE2	5:I:904:MGD:S13	2.87	0.47
2:J:142:MET:HE3	2:J:146:ALA:CB	2.43	0.47
1:K:571:ARG:HA	8:K:1027:HOH:O	2.13	0.47
1:K:737:PRO:CG	5:K:904:MGD:H2'	2.45	0.47
1:M:10:SER:HB3	1:M:147:TRP:HD1	1.80	0.47
1:M:174:ASP:O	1:M:177:GLU:HG2	2.15	0.47
1:O:262:LYS:HA	8:O:1449:HOH:O	2.14	0.47
1:Q:296:ASN:HB3	1:Q:657:PHE:CZ	2.50	0.47
1:S:186:MET:HE2	1:S:371:ILE:HG22	1.97	0.47
1:U:291:GLU:H	1:U:291:GLU:CD	2.23	0.47
1:U:530:GLU:OE2	1:U:750:LYS:NZ	2.48	0.47
1:W:378:GLY:O	1:W:381:LYS:HG2	2.15	0.47
1:W:454:GLU:H	1:W:454:GLU:CD	2.21	0.47
1:W:721:GLN:NE2	8:W:1287:HOH:O	2.48	0.47
1:W:794:ASN:HD21	1:W:842:LEU:HB3	1.79	0.47
1:C:756:TYR:CZ	2:D:41:ARG:HB3	2.50	0.47
2:D:19:CYS:CA	2:D:145:CYS:HB3	2.45	0.47
1:G:176:TRP:CD1	1:G:354:TRP:HE1	2.33	0.47
1:G:617:GLU:HG3	1:G:631:TRP:CG	2.50	0.47
1:I:480:TYR:HA	8:I:1177:HOH:O	2.15	0.47
2:J:125:LYS:HD2	2:J:126:CYS:O	2.15	0.47
2:L:52:GLU:CG	2:L:61:ILE:HD12	2.45	0.47
1:O:32:ASP:HB2	8:O:1663:HOH:O	2.14	0.47
1:O:784:ILE:HD13	1:O:790:ILE:HG21	1.97	0.47
2:P:114:MET:CB	2:P:125:LYS:HB3	2.44	0.47
1:Q:100:LEU:CD1	1:Q:105:PRO:HG3	2.43	0.47
1:Q:174:ASP:O	1:Q:177:GLU:HG2	2.14	0.47
1:S:744:HIS:C	1:S:819:SER:HB3	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:365:GLU:OE1	1:U:365:GLU:HA	2.14	0.47
2:V:19:CYS:HB3	2:V:145:CYS:CB	2.43	0.47
2:V:114:MET:HG2	8:V:516:HOH:O	2.15	0.47
2:X:164:MET:HE3	2:X:167:LYS:HB3	1.97	0.47
1:A:142:SER:HB3	5:A:903:MGD:O1A	2.14	0.46
1:A:433:PHE:N	1:A:433:PHE:CD1	2.83	0.46
1:A:711:MET:O	1:A:713:THR:HG23	2.15	0.46
1:C:322:GLU:HG3	1:C:327:VAL:O	2.15	0.46
1:C:744:HIS:HA	1:C:819:SER:CB	2.45	0.46
1:E:35:ASP:OD1	1:E:55:ARG:HD3	2.15	0.46
1:E:451:LYS:HG3	1:E:461:PHE:CE2	2.51	0.46
2:F:46:MET:CE	2:F:66:THR:H	2.24	0.46
1:I:162:ASN:CG	1:I:437:SER:HB2	2.39	0.46
1:I:175:SER:O	1:I:359:ARG:NH2	2.47	0.46
1:I:253:ASN:O	1:I:257:ARG:HG3	2.16	0.46
1:I:414:GLU:O	1:I:414:GLU:HG3	2.14	0.46
2:L:56:TYR:CD1	2:L:57:PRO:HA	2.50	0.46
1:M:139:SER:OG	1:M:161:MET:HE2	2.15	0.46
1:O:122:VAL:HG21	1:O:599:LYS:HG2	1.97	0.46
1:O:503:THR:O	1:O:504:MET:HE2	2.15	0.46
2:P:114:MET:HE3	2:P:123:ALA:HB1	1.95	0.46
1:Q:247:PHE:O	1:Q:263:TRP:HA	2.15	0.46
2:R:106:LEU:HD11	2:R:116:TRP:HB2	1.96	0.46
8:S:1335:HOH:O	2:T:29:LEU:HB2	2.15	0.46
2:T:8:ILE:HG23	2:T:153:VAL:HG12	1.97	0.46
1:U:21:LYS:HB2	1:U:26:ILE:HD11	1.96	0.46
1:U:68:SER:HB3	1:U:753:TYR:CD2	2.50	0.46
1:U:85:PHE:CE2	1:U:87:PRO:HG3	2.50	0.46
1:W:15:PRO:HD3	1:W:554:PHE:CD1	2.50	0.46
1:W:451:LYS:HG3	1:W:461:PHE:CE2	2.49	0.46
1:W:533:VAL:HB	1:W:534:PRO:HD3	1.96	0.46
1:W:794:ASN:HD22	1:W:862:VAL:HG12	1.80	0.46
1:A:461:PHE:HA	8:A:1503:HOH:O	2.15	0.46
1:E:95:LEU:HA	8:E:1538:HOH:O	2.13	0.46
1:G:165:GLY:HA3	1:G:166:PHE:CB	2.29	0.46
1:I:366:TRP:CD1	1:I:370:MET:HE3	2.51	0.46
1:I:580:ILE:HD12	8:I:1538:HOH:O	2.15	0.46
2:J:19:CYS:HB2	2:J:46:MET:HG2	1.96	0.46
2:L:247:VAL:O	2:L:257:SER:HA	2.15	0.46
1:M:408:GLY:HA2	1:M:619:TYR:HE1	1.80	0.46
1:Q:162:ASN:HD22	1:Q:166:PHE:HE2	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:21:MET:CE	2:R:21:MET:CA	2.93	0.46
2:T:73:ASN:C	2:T:73:ASN:HD22	2.23	0.46
2:V:71:CYS:CA	2:V:184:PRO:HA	2.44	0.46
2:X:185:ARG:NH1	2:X:185:ARG:CB	2.79	0.46
2:B:5:TYR:HB2	2:B:157:LEU:HD13	1.96	0.46
1:C:540:LEU:HA	1:C:541:PRO:HD3	1.79	0.46
2:F:168:VAL:HA	2:F:173:LEU:HD12	1.98	0.46
1:G:433:PHE:N	1:G:433:PHE:CD1	2.83	0.46
1:G:451:LYS:HG3	1:G:461:PHE:CE2	2.50	0.46
1:I:162:ASN:ND2	1:I:437:SER:HB2	2.30	0.46
2:J:21:MET:HE3	2:J:21:MET:CA	2.43	0.46
2:L:185:ARG:HB3	2:L:185:ARG:CZ	2.45	0.46
1:M:505:THR:O	1:M:506:ALA:C	2.58	0.46
1:M:670:PRO:HG2	1:M:675:GLN:CD	2.40	0.46
1:M:737:PRO:CG	5:M:904:MGD:H2'	2.46	0.46
2:N:4:TYR:O	2:N:185:ARG:HD3	2.15	0.46
1:O:533:VAL:HB	1:O:534:PRO:HD3	1.97	0.46
1:O:557:CYS:H	1:O:564:ASN:ND2	2.02	0.46
2:P:96:PRO:O	2:P:100:LYS:HG3	2.15	0.46
2:T:114:MET:CA	2:T:125:LYS:HB3	2.46	0.46
2:V:64:ARG:NH1	8:V:416:HOH:O	2.48	0.46
2:X:5:TYR:HB2	2:X:157:LEU:HD11	1.96	0.46
1:A:452:ILE:HB	1:A:453:PRO:HD3	1.96	0.46
1:A:627:LYS:NZ	8:A:1223:HOH:O	2.49	0.46
2:D:56:TYR:CA	2:D:59:ASN:HD22	2.24	0.46
2:F:9:ASP:HA	2:F:189:LYS:HB3	1.98	0.46
2:F:21:MET:HA	2:F:21:MET:HE3	1.98	0.46
1:G:76:ILE:CG2	1:G:541:PRO:HG3	2.45	0.46
2:H:71:CYS:HB2	2:H:182:THR:O	2.15	0.46
1:I:302:GLU:OE1	1:I:302:GLU:N	2.40	0.46
2:J:18:ASN:HB2	7:J:302:SF4:S1	2.56	0.46
1:K:494:TRP:HE1	1:K:525:GLN:HE21	1.63	0.46
1:M:587:MET:HG3	1:M:592:ILE:HG13	1.97	0.46
1:O:195:ASN:OD1	1:O:353:GLY:HA3	2.15	0.46
2:P:3:GLN:O	2:P:158:LYS:HA	2.15	0.46
1:Q:119:ASP:OD1	1:Q:599:LYS:HE3	2.15	0.46
1:U:737:PRO:CG	5:U:904:MGD:H2'	2.44	0.46
2:V:175:VAL:HG23	2:V:178:PRO:HG3	1.97	0.46
1:W:27:ARG:HB2	2:X:25:ASP:OD1	2.15	0.46
2:X:124:GLN:HB2	8:X:403:HOH:O	2.16	0.46
1:C:75:ARG:NH2	1:C:543:CYS:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:21:LYS:HB3	1:G:26:ILE:HD11	1.97	0.46
1:I:153:ARG:O	1:I:157:TYR:HB3	2.15	0.46
1:I:565:TYR:C	1:I:567:LEU:H	2.24	0.46
2:J:87:ARG:HB2	2:J:89:ASP:OD2	2.15	0.46
1:K:501:LEU:O	1:K:507:THR:HG21	2.16	0.46
8:L:568:HOH:O	2:T:85:TYR:HB2	2.15	0.46
1:M:478:HIS:HD2	8:M:1206:HOH:O	1.98	0.46
1:O:218:ASP:OD2	1:O:253:ASN:HB2	2.16	0.46
1:O:561:ILE:N	1:O:562:PRO:HD3	2.31	0.46
2:P:75:PRO:HD2	7:P:304:SF4:S4	2.56	0.46
2:P:198:TYR:HB3	2:P:238:ASP:HA	1.98	0.46
1:U:81:LYS:HG2	1:U:82:ARG:N	2.31	0.46
1:U:783:GLY:O	1:U:866:LYS:HD2	2.15	0.46
1:W:114:TRP:CZ2	1:W:541:PRO:HD2	2.50	0.46
1:W:176:TRP:O	1:W:177:GLU:C	2.59	0.46
1:W:564:ASN:C	1:W:566:GLN:N	2.72	0.46
1:A:211:MET:CE	2:B:231:PHE:CZ	2.96	0.46
1:A:753:TYR:OH	2:B:28:GLU:HB3	2.16	0.46
1:C:528:TRP:CE2	1:C:750:LYS:HD3	2.51	0.46
1:G:282:TRP:HA	1:G:287:SER:OG	2.15	0.46
1:I:175:SER:C	1:I:359:ARG:HH21	2.24	0.46
1:K:784:ILE:HD13	1:K:790:ILE:HG21	1.96	0.46
1:M:200:ASP:HB3	8:M:1059:HOH:O	2.15	0.46
1:O:155:SER:OG	1:O:409:ILE:HG12	2.15	0.46
1:Q:114:TRP:CZ2	1:Q:541:PRO:HD2	2.50	0.46
1:U:142:SER:HB3	5:U:903:MGD:O1A	2.15	0.46
1:W:495:LYS:HD3	8:W:1109:HOH:O	2.15	0.46
1:A:501:LEU:HD13	1:A:823:TYR:CD2	2.51	0.46
1:E:796:ARG:NH2	1:E:844:PRO:HB3	2.31	0.46
1:G:508:ASN:O	1:G:512:LYS:HG3	2.15	0.46
1:G:554:PHE:HB3	8:G:1026:HOH:O	2.16	0.46
1:G:730:TYR:CZ	1:G:794:ASN:HA	2.51	0.46
1:K:67:LYS:NZ	2:L:25:ASP:O	2.41	0.46
2:L:198:TYR:HB3	2:L:238:ASP:HA	1.98	0.46
2:L:273:LYS:O	2:L:274:LEU:HD23	2.15	0.46
1:O:143:SER:HB3	3:O:901:ACT:H3	1.97	0.46
1:O:163:MET:HE1	1:O:606:PHE:HA	1.98	0.46
1:O:753:TYR:HB3	2:P:24:MET:CE	2.41	0.46
1:S:253:ASN:O	1:S:257:ARG:HG3	2.14	0.46
1:U:239:LYS:HE3	8:U:1097:HOH:O	2.15	0.46
1:U:417:ALA:CB	1:U:559:GLY:HA2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:78:TYR:HA	1:W:541:PRO:HG2	1.97	0.46
1:W:337:ARG:O	1:W:341:LYS:HG2	2.15	0.46
1:W:452:ILE:N	1:W:453:PRO:CD	2.78	0.46
2:X:252:ASP:HB3	2:X:254:LYS:HE2	1.96	0.46
1:A:81:LYS:HB2	1:A:112:ILE:HD13	1.98	0.46
1:C:629:MET:HE2	1:C:634:PHE:N	2.31	0.46
2:F:4:TYR:CE2	2:F:158:LYS:HD2	2.50	0.46
2:F:122:VAL:HG22	2:F:123:ALA:N	2.31	0.46
2:H:52:GLU:HG3	2:H:61:ILE:HD12	1.98	0.46
1:I:138:LEU:HB2	1:I:490:ILE:HD12	1.98	0.46
1:I:426:MET:HE2	1:I:618:GLN:HG2	1.96	0.46
1:I:558:SER:H	1:I:564:ASN:ND2	2.14	0.46
2:L:168:VAL:HG13	2:L:173:LEU:HB2	1.98	0.46
1:M:187:TRP:CH2	1:M:196:PRO:HB3	2.51	0.46
1:O:620:PHE:CZ	1:O:625:MET:HB3	2.51	0.46
1:O:696:LYS:HD3	8:O:1679:HOH:O	2.15	0.46
1:Q:17:PHE:CE2	1:Q:31:MET:HE3	2.51	0.46
1:Q:427:PHE:HB3	8:Q:1028:HOH:O	2.14	0.46
1:S:753:TYR:CB	2:T:21:MET:HE2	2.41	0.46
1:U:387:TRP:CE2	1:U:389:THR:HA	2.50	0.46
1:U:527:ILE:HG23	1:U:542:ALA:O	2.16	0.46
2:V:110:PRO:CB	2:V:180:LEU:HD13	2.46	0.46
1:W:268:ILE:O	1:W:270:THR:HG23	2.16	0.46
2:X:71:CYS:HB3	2:X:184:PRO:N	2.31	0.46
1:A:176:TRP:CE2	1:A:193:LEU:HD12	2.51	0.46
2:B:142:MET:HE3	2:B:146:ALA:HB1	1.97	0.46
2:B:175:VAL:HG23	2:B:178:PRO:HG3	1.98	0.46
1:C:504:MET:HE2	1:C:504:MET:HA	1.98	0.46
1:C:533:VAL:HB	1:C:534:PRO:HD3	1.97	0.46
2:D:254:LYS:HD2	2:D:274:LEU:OXT	2.16	0.46
1:E:400:TYR:HA	8:E:1457:HOH:O	2.16	0.46
1:I:364:ILE:HD13	1:I:708:ARG:HG3	1.98	0.46
1:I:395:LEU:HD12	1:I:566:GLN:HA	1.98	0.46
1:I:452:ILE:HB	1:I:453:PRO:HD3	1.98	0.46
1:I:744:HIS:HA	1:I:819:SER:HB3	1.98	0.46
1:M:138:LEU:HB2	1:M:490:ILE:CD1	2.42	0.46
1:M:726:LEU:HD23	8:M:1374:HOH:O	2.15	0.46
2:P:5:TYR:CE2	2:P:164:MET:HG2	2.51	0.46
1:S:121:VAL:O	1:S:125:ILE:HG13	2.15	0.46
1:U:124:GLU:HG3	1:U:521:PHE:CD2	2.51	0.46
1:U:284:LYS:HE2	1:U:308:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:168:VAL:HG21	8:X:525:HOH:O	2.15	0.46
1:A:528:TRP:CD2	1:A:750:LYS:HD3	2.51	0.46
1:C:274:LEU:O	1:C:278:ILE:HG13	2.16	0.46
1:E:162:ASN:CG	1:E:437:SER:HB2	2.41	0.46
1:E:166:PHE:H	1:E:439:LEU:HD12	1.80	0.46
1:E:630:THR:OG1	1:E:633:GLU:HG3	2.15	0.46
2:F:157:LEU:HD12	2:F:157:LEU:H	1.81	0.46
1:G:505:THR:O	1:G:506:ALA:C	2.59	0.46
1:I:28:MET:HE2	1:I:67:LYS:HB2	1.98	0.46
2:J:211:GLU:HG3	2:J:230:ASN:C	2.41	0.46
1:M:296:ASN:HB3	1:M:657:PHE:CZ	2.51	0.46
2:P:126:CYS:HB2	8:P:462:HOH:O	2.16	0.46
1:Q:152:TYR:CD2	1:Q:154:HIS:HD2	2.34	0.46
1:U:1:MET:HB2	1:U:22:ASP:OD1	2.16	0.46
2:V:15:ASP:HB2	2:V:63:TYR:CD2	2.51	0.46
1:W:495:LYS:HE3	1:W:497:GLY:O	2.16	0.46
1:C:426:MET:HE2	1:C:618:GLN:HG2	1.93	0.45
1:C:784:ILE:HD13	1:C:790:ILE:HG21	1.97	0.45
1:I:610:LYS:HZ3	1:I:618:GLN:HE22	1.61	0.45
1:K:378:GLY:O	1:K:381:LYS:HG2	2.16	0.45
1:O:737:PRO:CG	5:O:904:MGD:H2'	2.46	0.45
1:Q:75:ARG:HH21	1:Q:543:CYS:HA	1.79	0.45
2:T:83:ALA:HB1	2:T:105:LEU:HD11	1.98	0.45
1:W:173:PRO:HG3	1:W:180:HIS:CG	2.51	0.45
1:W:222:ASN:HA	5:W:904:MGD:H22	1.81	0.45
1:W:498:GLY:N	1:W:499:PRO:HD3	2.31	0.45
2:X:69:MET:N	7:X:304:SF4:S2	2.89	0.45
1:C:28:MET:HE1	1:C:67:LYS:N	2.31	0.45
1:C:737:PRO:CG	5:C:904:MGD:H2'	2.46	0.45
1:E:775:ASN:HA	1:E:806:THR:O	2.17	0.45
1:G:152:TYR:HD2	1:G:154:HIS:HD2	1.62	0.45
1:G:162:ASN:CG	1:G:437:SER:HB2	2.42	0.45
1:I:111:ARG:HB3	8:I:1473:HOH:O	2.16	0.45
2:J:87:ARG:HG3	2:J:91:ILE:O	2.16	0.45
1:K:267:LYS:HG3	1:K:325:SER:O	2.16	0.45
1:K:656:TRP:CD2	1:K:663:LYS:HA	2.51	0.45
2:L:18:ASN:HB2	7:L:302:SF4:S1	2.56	0.45
1:M:75:ARG:HH21	1:M:543:CYS:HA	1.80	0.45
1:M:162:ASN:HD22	1:M:166:PHE:HE2	1.65	0.45
1:M:426:MET:HA	1:M:426:MET:CE	2.42	0.45
1:M:630:THR:OG1	1:M:633:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:28:MET:CE	1:O:67:LYS:H	2.28	0.45
1:Q:451:LYS:HA	1:Q:454:GLU:OE1	2.16	0.45
1:S:15:PRO:HB2	1:S:31:MET:SD	2.56	0.45
1:S:250:PRO:HD3	5:S:904:MGD:C2	2.46	0.45
1:U:11:SER:C	1:U:13:GLY:N	2.74	0.45
1:U:620:PHE:CZ	1:U:625:MET:HB3	2.51	0.45
1:U:744:HIS:HA	1:U:819:SER:HB3	1.98	0.45
2:X:3:GLN:HB3	2:X:89:ASP:O	2.17	0.45
1:A:187:TRP:CH2	1:A:196:PRO:HB3	2.52	0.45
1:A:366:TRP:O	1:A:370:MET:HG2	2.16	0.45
2:D:81:ASN:OD1	2:D:81:ASN:O	2.34	0.45
1:E:176:TRP:O	1:E:177:GLU:C	2.59	0.45
1:G:530:GLU:CD	1:G:750:LYS:HZ2	2.25	0.45
1:G:753:TYR:HB3	2:H:24:MET:HE3	1.98	0.45
1:K:165:GLY:CA	1:K:166:PHE:HB3	2.40	0.45
2:L:44:ARG:HA	8:L:509:HOH:O	2.16	0.45
2:L:50:ARG:HG2	2:L:63:TYR:HD2	1.82	0.45
1:M:239:LYS:HE2	8:M:1601:HOH:O	2.16	0.45
1:O:734:MET:HB2	1:O:814:VAL:HG23	1.99	0.45
2:P:39:MET:HG2	2:P:40:GLN:N	2.30	0.45
1:Q:501:LEU:HD13	1:Q:823:TYR:CG	2.51	0.45
1:S:66:PHE:HA	1:S:69:MET:HE3	1.97	0.45
1:S:268:ILE:HG13	1:S:268:ILE:O	2.14	0.45
2:T:247:VAL:O	2:T:257:SER:HA	2.16	0.45
1:U:17:PHE:CE2	1:U:31:MET:HE3	2.51	0.45
1:U:162:ASN:ND2	1:U:437:SER:HB2	2.31	0.45
1:U:482:TYR:CD1	1:U:483:PRO:HA	2.52	0.45
1:U:721:GLN:HG3	8:U:1309:HOH:O	2.15	0.45
1:W:608:GLU:HB3	1:W:610:LYS:HE3	1.97	0.45
2:X:68:CYS:CB	2:X:113:VAL:HG21	2.46	0.45
1:A:166:PHE:H	1:A:439:LEU:HD12	1.82	0.45
1:A:452:ILE:N	1:A:453:PRO:CD	2.79	0.45
1:A:460:LYS:HA	1:A:482:TYR:O	2.16	0.45
2:B:21:MET:HA	2:B:21:MET:CE	2.47	0.45
2:D:85:TYR:HA	8:D:557:HOH:O	2.17	0.45
1:G:644:ASP:C	1:G:646:PRO:HD3	2.41	0.45
2:H:23:CYS:O	2:H:26:GLU:N	2.48	0.45
2:H:46:MET:HE1	2:H:65:PRO:C	2.42	0.45
1:K:316:LYS:HD2	1:K:320:TRP:CH2	2.51	0.45
1:M:745:THR:HB	1:M:821:ALA:HB2	1.98	0.45
2:N:122:VAL:HG22	2:N:123:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:262:LYS:HG2	2:P:232:PHE:CE1	2.51	0.45
1:Q:670:PRO:HB3	1:Q:682:GLN:HB2	1.99	0.45
1:Q:721:GLN:NE2	8:Q:1286:HOH:O	2.50	0.45
1:S:13:GLY:HA3	1:S:63:THR:OG1	2.16	0.45
1:S:29:THR:HG22	2:T:144:ARG:HH21	1.81	0.45
1:S:478:HIS:HD2	8:S:1211:HOH:O	1.99	0.45
1:U:75:ARG:NH2	1:U:543:CYS:HA	2.31	0.45
1:U:454:GLU:CD	1:U:454:GLU:N	2.74	0.45
2:V:73:ASN:HD22	2:V:73:ASN:HA	1.64	0.45
1:W:66:PHE:HA	1:W:69:MET:HE3	1.98	0.45
2:X:64:ARG:HD2	2:X:176:ILE:HD11	1.97	0.45
1:A:249:ASP:OD2	5:A:904:MGD:H1'	2.16	0.45
1:C:498:GLY:N	1:C:499:PRO:HD3	2.31	0.45
1:C:505:THR:O	1:C:506:ALA:C	2.59	0.45
2:D:185:ARG:HB3	2:D:185:ARG:CZ	2.47	0.45
1:E:239:LYS:HG3	8:E:1513:HOH:O	2.15	0.45
2:F:92:VAL:HG11	7:F:304:SF4:S1	2.57	0.45
2:F:199:VAL:HG12	2:F:237:PHE:HB2	1.98	0.45
1:I:268:ILE:HG13	1:I:268:ILE:O	2.16	0.45
1:I:678:ARG:HD2	8:I:1590:HOH:O	2.16	0.45
1:K:701:GLN:HG3	8:K:1665:HOH:O	2.16	0.45
1:K:797:GLY:HA2	1:K:875:TYR:CE2	2.52	0.45
1:M:165:GLY:HA3	1:M:166:PHE:CB	2.30	0.45
1:M:557:CYS:H	1:M:564:ASN:ND2	1.96	0.45
1:M:717:ALA:HB3	1:M:720:SER:HB3	1.98	0.45
1:O:44:ILE:HG21	1:O:206:LEU:HD12	1.98	0.45
1:O:269:GLY:HA2	1:O:362:HIS:CG	2.51	0.45
1:Q:265:SER:O	1:Q:810:GLN:NE2	2.50	0.45
1:S:55:ARG:HD2	8:S:1644:HOH:O	2.17	0.45
1:S:100:LEU:CD1	1:S:105:PRO:HG3	2.46	0.45
1:U:421:LYS:HA	1:U:424:TRP:HD1	1.82	0.45
1:U:426:MET:HE1	1:U:618:GLN:O	2.16	0.45
1:U:561:ILE:CG2	1:U:564:ASN:HB3	2.45	0.45
1:W:701:GLN:HG3	8:W:1660:HOH:O	2.17	0.45
1:W:725:PRO:HD2	8:W:1197:HOH:O	2.17	0.45
2:X:120:GLU:O	2:X:121:ASN:C	2.58	0.45
1:A:816:SER:HB3	1:A:839:ILE:HG13	1.98	0.45
2:B:56:TYR:HA	2:B:59:ASN:HD22	1.79	0.45
2:B:69:MET:HB3	2:B:184:PRO:HB3	1.98	0.45
1:C:452:ILE:N	1:C:453:PRO:CD	2.79	0.45
1:E:738:HIS:HE2	5:E:903:MGD:H15	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:MET:CE	2:F:146:ALA:HB1	2.46	0.45
2:H:58:ARG:HD2	2:H:268:ASP:OD1	2.17	0.45
1:I:482:TYR:HA	1:I:483:PRO:C	2.40	0.45
1:K:400:TYR:CE1	1:K:421:LYS:HD2	2.52	0.45
1:K:708:ARG:HD2	8:K:1046:HOH:O	2.16	0.45
1:K:730:TYR:CE1	1:K:794:ASN:HA	2.51	0.45
1:M:265:SER:O	1:M:810:GLN:NE2	2.48	0.45
1:O:15:PRO:HD2	8:O:1003:HOH:O	2.16	0.45
2:R:69:MET:HB3	2:R:184:PRO:HB3	1.99	0.45
1:S:79:PRO:HB2	1:S:112:ILE:O	2.15	0.45
1:S:434:PRO:O	1:S:436:PRO:HD3	2.16	0.45
1:U:454:GLU:CD	1:U:454:GLU:H	2.25	0.45
1:W:56:LYS:HG2	1:W:57:THR:N	2.32	0.45
1:W:62:TYR:HB3	1:W:742:SER:HA	1.99	0.45
1:W:214:PHE:HA	1:W:347:ALA:HB3	1.99	0.45
1:W:773:ARG:HH11	1:W:773:ARG:HG3	1.81	0.45
1:A:117:ALA:O	1:A:121:VAL:HG23	2.16	0.45
1:E:563:ASP:HA	1:E:565:TYR:CE1	2.52	0.45
2:F:46:MET:HE1	2:F:65:PRO:CA	2.46	0.45
2:F:142:MET:HE2	2:F:146:ALA:HB1	1.98	0.45
1:G:139:SER:CB	1:G:161:MET:HE2	2.47	0.45
2:H:114:MET:CE	2:H:123:ALA:HB1	2.40	0.45
1:I:100:LEU:CD1	1:I:105:PRO:HG3	2.46	0.45
1:I:247:PHE:CZ	1:I:255:THR:HG22	2.52	0.45
1:K:176:TRP:NE1	1:K:354:TRP:HE1	2.15	0.45
1:K:291:GLU:H	1:K:291:GLU:CD	2.25	0.45
1:M:498:GLY:N	1:M:499:PRO:HD3	2.32	0.45
1:M:839:ILE:HD13	1:M:839:ILE:HA	1.86	0.45
1:O:139:SER:OG	1:O:161:MET:HE2	2.17	0.45
1:O:359:ARG:HG3	1:O:359:ARG:O	2.17	0.45
1:O:425:ARG:HD3	1:O:622:ALA:O	2.16	0.45
2:P:4:TYR:CZ	2:P:158:LYS:HD2	2.52	0.45
2:P:21:MET:CA	2:P:21:MET:HE3	2.47	0.45
1:Q:617:GLU:HG3	1:Q:631:TRP:CG	2.52	0.45
1:W:780:GLU:CD	1:W:780:GLU:C	2.84	0.45
2:X:141:LYS:HA	8:X:502:HOH:O	2.15	0.45
1:A:220:GLU:CD	1:A:235:ARG:HH21	2.24	0.45
2:B:1:MET:HE2	2:B:88:GLU:OE2	2.17	0.45
1:I:786:ASN:ND2	1:I:804:GLN:HA	2.32	0.45
2:N:70:HIS:HD2	2:N:92:VAL:N	2.03	0.45
2:N:106:LEU:HD23	2:N:114:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:247:VAL:O	2:N:257:SER:HA	2.17	0.45
1:S:99:GLY:HA2	1:S:102:LYS:HG2	1.98	0.45
1:S:176:TRP:CD1	1:S:354:TRP:HE1	2.35	0.45
1:S:772:MET:HB2	1:S:801:LEU:HD13	1.98	0.45
1:U:144:HIS:HB2	5:U:903:MGD:O1B	2.17	0.45
1:U:642:VAL:HA	1:U:643:PRO:HD3	1.84	0.45
1:U:756:TYR:HD1	2:V:24:MET:HE1	1.80	0.45
1:W:253:ASN:O	1:W:257:ARG:HG3	2.17	0.45
1:W:426:MET:CE	1:W:618:GLN:HG2	2.47	0.45
1:W:730:TYR:CE1	1:W:794:ASN:HA	2.52	0.45
1:A:75:ARG:HH22	1:A:547:GLU:CD	2.25	0.45
1:A:282:TRP:HA	1:A:287:SER:OG	2.17	0.45
2:B:106:LEU:HD11	2:B:116:TRP:HB2	1.99	0.45
1:E:15:PRO:HD3	1:E:554:PHE:CD1	2.52	0.45
1:E:501:LEU:HD13	1:E:823:TYR:CG	2.52	0.45
2:F:245:TYR:HB2	2:F:260:VAL:CG1	2.47	0.45
1:G:140:THR:O	1:G:140:THR:HG23	2.17	0.45
1:G:404:TYR:CD1	1:G:405:ALA:N	2.85	0.45
1:G:741:PHE:CD2	1:G:757:ILE:HD13	2.52	0.45
2:H:211:GLU:HB2	2:H:231:PHE:HA	1.98	0.45
1:I:563:ASP:HA	8:I:1045:HOH:O	2.17	0.45
1:K:395:LEU:HD12	1:K:566:GLN:HA	1.99	0.45
1:K:725:PRO:HD2	8:K:1196:HOH:O	2.15	0.45
1:M:163:MET:HE1	1:M:605:MET:O	2.17	0.45
1:M:249:ASP:CG	5:M:904:MGD:H1'	2.42	0.45
2:N:59:ASN:ND2	2:N:59:ASN:H	2.15	0.45
1:O:683:THR:HB	1:O:689:GLU:OE1	2.17	0.45
2:P:210:PHE:O	2:P:233:GLY:HA2	2.17	0.45
1:Q:152:TYR:HD2	1:Q:154:HIS:HD2	1.64	0.45
2:R:105:LEU:HB3	2:R:114:MET:HE1	1.99	0.45
1:U:224:GLY:O	1:U:225:ILE:HB	2.17	0.45
2:V:8:ILE:HG23	2:V:153:VAL:CG1	2.47	0.45
1:W:75:ARG:HH21	1:W:543:CYS:HA	1.82	0.45
1:W:95:LEU:HD21	8:W:1493:HOH:O	2.17	0.45
1:W:271:ASP:CG	5:W:904:MGD:HN1	2.24	0.45
1:W:730:TYR:CZ	1:W:794:ASN:HA	2.52	0.45
1:A:253:ASN:O	1:A:257:ARG:HG3	2.17	0.45
2:B:73:ASN:HB3	2:B:182:THR:HA	1.99	0.45
1:C:142:SER:HB3	5:C:903:MGD:O1A	2.17	0.45
1:C:201:LEU:HD13	1:C:387:TRP:HB2	1.99	0.45
1:E:610:LYS:HZ1	1:E:618:GLN:NE2	2.07	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:339:TRP:CH2	1:G:346:LEU:HD13	2.52	0.45
1:G:394:PRO:HG3	8:G:1323:HOH:O	2.16	0.45
1:G:647:ASN:O	1:G:648:ARG:C	2.60	0.45
2:H:72:GLU:OE1	2:H:183:LYS:HD2	2.17	0.45
2:H:104:GLU:H	2:H:104:GLU:CD	2.25	0.45
1:I:128:ILE:HD13	1:I:492:MET:HB2	1.99	0.45
1:I:227:ALA:O	1:I:228:GLY:C	2.60	0.45
1:K:224:GLY:O	1:K:225:ILE:HB	2.16	0.45
1:M:433:PHE:CD1	1:M:433:PHE:N	2.85	0.45
2:N:164:MET:O	2:N:168:VAL:HG23	2.18	0.45
2:P:21:MET:HE3	2:P:21:MET:N	2.31	0.45
1:Q:253:ASN:O	1:Q:257:ARG:HG3	2.16	0.45
1:Q:257:ARG:HD3	2:R:61:ILE:HG21	1.98	0.45
1:S:387:TRP:CE2	1:S:389:THR:HA	2.52	0.45
2:T:87:ARG:HB2	2:T:89:ASP:OD2	2.16	0.45
2:T:141:LYS:HA	8:T:497:HOH:O	2.17	0.45
2:T:217:LEU:HB2	2:T:237:PHE:CE1	2.52	0.45
1:U:454:GLU:HA	8:U:1002:HOH:O	2.16	0.45
1:U:857:ASN:HB3	5:U:903:MGD:N19	2.31	0.45
1:W:806:THR:OG1	1:W:807:GLU:N	2.49	0.45
1:W:857:ASN:HB3	5:W:903:MGD:N19	2.32	0.45
1:A:353:GLY:O	1:A:354:TRP:HB2	2.17	0.44
1:A:786:ASN:ND2	1:A:804:GLN:HA	2.32	0.44
1:C:214:PHE:HA	1:C:347:ALA:HB3	1.99	0.44
1:C:393:VAL:HA	1:C:394:PRO:HD3	1.77	0.44
2:F:19:CYS:O	2:F:22:GLY:N	2.47	0.44
2:H:69:MET:HE2	2:H:69:MET:HA	1.99	0.44
1:I:164:MET:SD	1:I:164:MET:C	3.00	0.44
1:I:719:GLU:O	1:I:859:THR:HB	2.17	0.44
1:K:21:LYS:HB3	1:K:26:ILE:HD11	1.98	0.44
1:K:720:SER:O	1:K:724:SER:HB3	2.17	0.44
1:K:823:TYR:CE2	1:K:825:PRO:HG3	2.51	0.44
2:L:1:MET:HE2	2:L:88:GLU:OE2	2.18	0.44
1:M:452:ILE:HB	1:M:453:PRO:HD3	1.99	0.44
1:O:166:PHE:H	1:O:439:LEU:HD12	1.82	0.44
1:O:426:MET:HA	1:O:426:MET:CE	2.45	0.44
2:P:69:MET:O	2:P:70:HIS:C	2.60	0.44
1:Q:656:TRP:CD2	1:Q:663:LYS:HA	2.51	0.44
2:R:27:HIS:HB2	2:R:39:MET:HE3	1.99	0.44
1:U:505:THR:O	1:U:506:ALA:C	2.60	0.44
1:W:704:ILE:HG23	8:W:1649:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:764:VAL:O	1:W:765:ASP:HB2	2.16	0.44
1:W:816:SER:OG	1:W:839:ILE:HG13	2.18	0.44
2:X:84:VAL:CG2	2:X:94:ILE:HG12	2.40	0.44
1:C:138:LEU:HB2	1:C:490:ILE:HD12	1.98	0.44
1:C:610:LYS:HZ3	1:C:618:GLN:HE22	1.61	0.44
1:C:797:GLY:HA2	1:C:875:TYR:CE2	2.52	0.44
1:C:806:THR:OG1	1:C:807:GLU:N	2.50	0.44
2:D:235:PHE:C	2:D:235:PHE:CD1	2.94	0.44
1:E:251:HIS:O	1:E:253:ASN:N	2.50	0.44
1:E:362:HIS:HB3	1:E:717:ALA:HB2	1.99	0.44
1:E:493:PHE:HB2	1:E:519:LEU:HD21	1.98	0.44
2:F:68:CYS:HB3	2:F:126:CYS:HB3	1.94	0.44
2:F:69:MET:HE2	2:F:69:MET:HA	1.99	0.44
2:F:176:ILE:HG22	2:F:177:LYS:HG3	1.98	0.44
2:H:59:ASN:ND2	2:H:59:ASN:H	2.15	0.44
1:I:296:ASN:O	1:I:687:LYS:HB3	2.17	0.44
1:I:505:THR:O	1:I:506:ALA:C	2.60	0.44
1:K:263:TRP:CZ2	1:K:265:SER:HB2	2.52	0.44
2:L:92:VAL:HG11	7:L:304:SF4:S1	2.56	0.44
1:Q:857:ASN:HB3	5:Q:903:MGD:N19	2.32	0.44
1:S:677:CYS:C	1:S:678:ARG:HG2	2.41	0.44
1:S:797:GLY:HA2	1:S:875:TYR:CE2	2.52	0.44
1:U:847:TYR:CZ	1:U:853:CYS:HB3	2.52	0.44
1:W:212:ILE:CD1	1:W:238:LEU:HD13	2.47	0.44
1:W:224:GLY:O	1:W:225:ILE:HB	2.17	0.44
1:W:393:VAL:HG23	1:W:566:GLN:O	2.17	0.44
1:W:770:TRP:HB3	1:W:801:LEU:CD2	2.47	0.44
2:X:51:ARG:O	2:X:61:ILE:HG13	2.16	0.44
1:A:144:HIS:HB2	5:A:903:MGD:O1B	2.17	0.44
2:B:68:CYS:CB	2:B:126:CYS:CB	2.91	0.44
1:E:400:TYR:CE1	1:E:421:LYS:HD2	2.52	0.44
1:E:533:VAL:HB	1:E:534:PRO:HD3	1.99	0.44
2:H:68:CYS:HB2	2:H:126:CYS:HB3	1.98	0.44
2:H:204:LEU:HD23	2:H:209:CYS:HA	1.99	0.44
1:I:249:ASP:OD2	5:I:904:MGD:H1'	2.17	0.44
1:I:736:SER:OG	5:I:903:MGD:N19	2.44	0.44
1:M:391:GLN:HG2	1:M:567:LEU:CD2	2.47	0.44
1:O:277:ALA:HA	1:O:316:LYS:O	2.16	0.44
2:P:55:THR:O	2:P:56:TYR:C	2.60	0.44
2:P:77:VAL:HG22	2:P:84:VAL:HG12	1.97	0.44
1:W:300:PHE:HZ	1:W:376:MET:HE3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:445:GLN:HB2	1:W:484:ALA:HB3	1.99	0.44
1:W:576:GLN:HB3	8:W:1108:HOH:O	2.17	0.44
1:W:790:ILE:HD13	1:W:803:ALA:HB2	1.99	0.44
1:E:215:TRP:CE3	1:E:370:MET:HE1	2.52	0.44
1:E:322:GLU:HG3	1:E:327:VAL:O	2.18	0.44
1:G:303:TRP:HA	1:G:711:MET:HE2	1.99	0.44
1:I:139:SER:OG	1:I:161:MET:HE2	2.18	0.44
1:I:211:MET:HE2	1:I:246:VAL:HG21	1.99	0.44
1:K:855:MET:HE2	1:K:857:ASN:OD1	2.17	0.44
1:M:9:ASN:HA	1:M:576:GLN:HA	1.99	0.44
1:M:730:TYR:HB3	1:M:862:VAL:CA	2.48	0.44
1:M:730:TYR:HB3	1:M:862:VAL:C	2.43	0.44
1:Q:164:MET:HE2	1:Q:494:TRP:CZ3	2.53	0.44
1:Q:776:SER:HA	1:Q:805:VAL:HG13	1.99	0.44
1:S:103:GLN:CD	1:S:103:GLN:N	2.75	0.44
1:S:426:MET:HE1	1:S:618:GLN:O	2.16	0.44
1:S:736:SER:HG	5:S:903:MGD:H191	1.66	0.44
2:T:70:HIS:CD2	2:T:92:VAL:H	2.33	0.44
1:U:201:LEU:HD13	1:U:387:TRP:HB2	2.00	0.44
1:U:393:VAL:CG1	1:U:395:LEU:HG	2.47	0.44
2:B:247:VAL:O	2:B:257:SER:HA	2.18	0.44
1:C:165:GLY:CA	1:C:166:PHE:HB3	2.45	0.44
1:G:56:LYS:HG2	1:G:57:THR:O	2.17	0.44
2:H:106:LEU:HD11	2:H:116:TRP:HB2	1.99	0.44
1:K:269:GLY:HA2	1:K:362:HIS:CE1	2.53	0.44
1:K:452:ILE:N	1:K:453:PRO:CD	2.80	0.44
1:M:564:ASN:H	1:M:564:ASN:HD22	1.65	0.44
2:N:17:ASN:HB2	8:N:563:HOH:O	2.16	0.44
1:O:15:PRO:HD3	1:O:554:PHE:CE1	2.51	0.44
1:O:471:GLY:HA3	1:O:475:HIS:CE1	2.53	0.44
2:R:23:CYS:O	2:R:26:GLU:N	2.48	0.44
2:T:60:ASP:C	2:T:60:ASP:OD1	2.61	0.44
2:T:185:ARG:HB3	2:T:185:ARG:CZ	2.48	0.44
1:U:302:GLU:OE1	1:U:302:GLU:N	2.46	0.44
1:U:414:GLU:O	1:U:414:GLU:CG	2.65	0.44
1:W:9:ASN:HA	1:W:576:GLN:HA	1.98	0.44
1:W:553:GLU:CD	1:W:556:ASN:HD22	2.26	0.44
2:X:3:GLN:NE2	2:X:161:PRO:HG3	2.32	0.44
2:X:157:LEU:HD12	2:X:157:LEU:O	2.18	0.44
2:X:162:GLU:CD	2:X:162:GLU:H	2.25	0.44
2:X:203:ILE:HD12	2:X:203:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:HG2	1:A:57:THR:O	2.18	0.44
1:A:142:SER:OG	5:A:903:MGD:O1A	2.26	0.44
1:C:400:TYR:CE1	1:C:421:LYS:HD2	2.53	0.44
2:D:19:CYS:CB	2:D:46:MET:HG2	2.45	0.44
1:E:75:ARG:HH21	1:E:543:CYS:HA	1.83	0.44
2:F:40:GLN:NE2	2:F:118:GLU:H	2.16	0.44
1:G:504:MET:HE3	8:G:1038:HOH:O	2.16	0.44
1:I:12:THR:O	1:I:226:TYR:HA	2.17	0.44
1:K:501:LEU:HD13	1:K:823:TYR:CD2	2.53	0.44
1:M:571:ARG:HA	8:M:1026:HOH:O	2.18	0.44
1:Q:757:ILE:HD11	8:R:566:HOH:O	2.16	0.44
1:S:27:ARG:NH2	2:T:132:LEU:HD21	2.31	0.44
1:S:656:TRP:CG	1:S:663:LYS:HA	2.53	0.44
1:U:753:TYR:CE1	2:V:28:GLU:HG3	2.53	0.44
2:V:142:MET:HE2	2:V:147:HIS:HA	1.98	0.44
2:X:126:CYS:HB2	8:X:468:HOH:O	2.18	0.44
2:X:247:VAL:O	2:X:257:SER:HA	2.18	0.44
1:A:489:LYS:HG3	8:A:1214:HOH:O	2.17	0.44
1:A:708:ARG:HD2	8:A:1046:HOH:O	2.18	0.44
1:E:670:PRO:HG2	1:E:675:GLN:CD	2.42	0.44
1:E:734:MET:HE1	1:E:839:ILE:HG23	1.99	0.44
1:E:857:ASN:HB3	5:E:903:MGD:N19	2.33	0.44
2:F:87:ARG:HG3	2:F:91:ILE:O	2.18	0.44
1:G:141:PRO:HD3	1:G:157:TYR:CZ	2.53	0.44
1:I:85:PHE:CE2	1:I:87:PRO:HG3	2.52	0.44
1:I:252:MET:HE3	1:I:263:TRP:CE3	2.53	0.44
1:O:588:SER:HA	8:O:1370:HOH:O	2.18	0.44
1:O:610:LYS:HB3	1:O:614:ALA:HB3	1.98	0.44
1:Q:716:PRO:HB3	1:Q:723:HIS:CD2	2.53	0.44
1:Q:770:TRP:HB3	1:Q:801:LEU:HD23	2.00	0.44
2:R:142:MET:CE	2:R:146:ALA:HB1	2.48	0.44
2:T:49:GLU:HG3	2:T:64:ARG:HH21	1.80	0.44
1:U:144:HIS:CE1	1:U:225:ILE:HD11	2.53	0.44
1:U:452:ILE:HB	1:U:453:PRO:HD3	2.00	0.44
1:U:676:VAL:HG13	8:U:1058:HOH:O	2.18	0.44
1:W:118:THR:O	1:W:122:VAL:HG23	2.18	0.44
2:B:157:LEU:HD12	2:B:157:LEU:N	2.33	0.44
2:B:198:TYR:CD1	2:B:198:TYR:C	2.96	0.44
1:C:433:PHE:N	1:C:433:PHE:CD1	2.86	0.44
1:E:292:TYR:HE1	1:E:658:ALA:HA	1.81	0.44
1:G:105:PRO:HD2	8:G:1427:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:ASP:HB3	8:G:1059:HOH:O	2.18	0.44
2:H:198:TYR:CD1	2:H:198:TYR:C	2.95	0.44
1:I:159:ARG:O	1:I:163:MET:HG3	2.18	0.44
1:I:271:ASP:CG	5:I:904:MGD:HN1	2.25	0.44
1:K:184:MET:HE2	1:K:190:SER:HA	2.00	0.44
1:K:498:GLY:N	1:K:499:PRO:HD3	2.32	0.44
2:L:71:CYS:CA	2:L:184:PRO:HA	2.44	0.44
2:N:128:MET:O	2:N:129:CYS:C	2.61	0.44
1:O:68:SER:HB3	1:O:753:TYR:CD2	2.52	0.44
1:Q:47:ARG:HD2	1:Q:241:LEU:HD22	2.00	0.44
2:R:70:HIS:HD2	2:R:92:VAL:N	2.03	0.44
2:T:129:CYS:HB3	2:T:131:HIS:HE1	1.79	0.44
1:U:76:ILE:HA	1:U:77:PRO:HD3	1.82	0.44
2:V:20:PHE:CE2	2:V:24:MET:HE2	2.53	0.44
1:W:75:ARG:NH2	1:W:547:GLU:OE1	2.43	0.44
1:W:244:ASP:C	1:W:245:PHE:HD2	2.26	0.44
1:W:362:HIS:HB3	1:W:717:ALA:HB2	1.99	0.44
1:W:737:PRO:CG	5:W:904:MGD:H2'	2.48	0.44
1:W:748:ASP:O	1:W:750:LYS:HG3	2.17	0.44
1:A:155:SER:OG	1:A:409:ILE:HG12	2.18	0.44
1:C:790:ILE:HD13	1:C:803:ALA:HB2	2.00	0.44
2:D:121:ASN:CG	1:S:608:GLU:O	2.61	0.44
2:F:21:MET:HE2	2:F:24:MET:HE3	1.99	0.44
1:I:81:LYS:HB2	1:I:112:ILE:HD13	1.99	0.44
1:I:540:LEU:HA	1:I:541:PRO:HD3	1.76	0.44
1:I:625:MET:N	1:I:626:PRO:CD	2.81	0.44
1:I:847:TYR:CZ	1:I:853:CYS:HB3	2.52	0.44
1:K:311:THR:HG21	8:K:1500:HOH:O	2.17	0.44
1:K:730:TYR:CZ	1:K:794:ASN:HA	2.52	0.44
2:N:176:ILE:HG22	2:N:177:LYS:HG3	1.99	0.44
2:N:211:GLU:HB2	2:N:231:PHE:HA	1.99	0.44
2:P:59:ASN:H	2:P:59:ASN:HD22	1.64	0.44
1:Q:454:GLU:H	1:Q:454:GLU:CD	2.26	0.44
2:R:142:MET:HE2	2:R:147:HIS:N	2.33	0.44
1:S:427:PHE:CG	1:S:434:PRO:HG3	2.53	0.44
1:U:28:MET:CE	1:U:67:LYS:N	2.81	0.44
2:V:129:CYS:HB3	2:V:131:HIS:CE1	2.53	0.44
2:X:152:PHE:N	2:X:152:PHE:CD1	2.86	0.44
2:B:53:ARG:HB2	2:B:60:ASP:OD1	2.17	0.43
1:C:15:PRO:HD3	1:C:554:PHE:CD1	2.53	0.43
1:C:139:SER:OG	1:C:161:MET:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:HIS:NE2	5:C:904:MGD:S13	2.91	0.43
1:G:381:LYS:NZ	8:G:1249:HOH:O	2.51	0.43
2:H:27:HIS:HE1	8:H:472:HOH:O	2.00	0.43
2:H:46:MET:HE1	2:H:65:PRO:CA	2.48	0.43
1:I:265:SER:O	1:I:810:GLN:NE2	2.51	0.43
1:I:499:PRO:HG3	5:I:903:MGD:O5'	2.18	0.43
1:K:39:ALA:HA	1:K:40:PRO:HD3	1.89	0.43
2:L:2:GLU:HG2	2:L:158:LYS:HG2	1.99	0.43
1:Q:39:ALA:HA	1:Q:40:PRO:HD3	1.88	0.43
1:Q:339:TRP:CH2	1:Q:346:LEU:HD13	2.54	0.43
1:S:1:MET:H3	1:S:22:ASP:CG	2.26	0.43
1:S:277:ALA:HB2	1:S:321:ALA:HB2	2.00	0.43
1:S:629:MET:HE2	1:S:634:PHE:CA	2.48	0.43
2:T:177:LYS:HA	2:T:179:GLU:OE1	2.18	0.43
1:U:353:GLY:O	1:U:354:TRP:HB2	2.18	0.43
1:U:571:ARG:HA	8:U:1030:HOH:O	2.18	0.43
1:W:156:THR:HB	8:W:1302:HOH:O	2.18	0.43
2:X:1:MET:SD	2:X:88:GLU:HB3	2.58	0.43
2:X:179:GLU:HG2	2:X:180:LEU:H	1.81	0.43
1:A:602:ILE:CG2	8:A:1075:HOH:O	2.64	0.43
2:F:58:ARG:HD2	2:F:268:ASP:OD1	2.18	0.43
2:F:128:MET:O	2:F:129:CYS:C	2.61	0.43
2:H:21:MET:HB2	8:H:562:HOH:O	2.18	0.43
2:H:95:ASP:HB3	2:H:98:LYS:HB2	1.99	0.43
2:H:210:PHE:CE2	2:H:251:ALA:HB1	2.53	0.43
1:K:277:ALA:HB2	1:K:321:ALA:HB2	2.00	0.43
1:K:676:VAL:HG13	8:K:1054:HOH:O	2.18	0.43
1:K:705:ASP:OD2	1:K:849:SER:OG	2.35	0.43
1:Q:452:ILE:N	1:Q:453:PRO:CD	2.81	0.43
1:S:138:LEU:HB2	1:S:490:ILE:HD12	2.00	0.43
1:S:422:PHE:O	1:S:423:ALA:C	2.59	0.43
1:U:69:MET:HE2	1:U:754:MET:HE3	2.00	0.43
1:U:182:GLY:HA3	1:U:364:ILE:HG23	2.00	0.43
1:U:187:TRP:CH2	1:U:196:PRO:HB3	2.53	0.43
1:U:197:GLU:OE2	1:U:667:ASP:HB2	2.19	0.43
2:V:90:GLY:HA3	2:V:185:ARG:CZ	2.48	0.43
1:W:452:ILE:HB	1:W:453:PRO:HD3	2.00	0.43
1:A:676:VAL:HG13	8:A:1054:HOH:O	2.16	0.43
1:C:495:LYS:HD2	1:C:514:TYR:OH	2.19	0.43
1:C:649:LYS:HE2	8:C:1465:HOH:O	2.17	0.43
1:E:111:ARG:NH2	1:E:585:GLU:OE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:ARG:O	1:G:157:TYR:HB3	2.19	0.43
2:H:18:ASN:HB2	7:H:302:SF4:S1	2.58	0.43
2:H:75:PRO:HD2	7:H:304:SF4:S4	2.58	0.43
1:I:387:TRP:CZ2	1:I:389:THR:HA	2.54	0.43
1:K:13:GLY:HA3	1:K:63:THR:OG1	2.19	0.43
2:L:40:GLN:HE22	2:L:117:ASN:HA	1.82	0.43
1:M:404:TYR:CD1	1:M:405:ALA:N	2.86	0.43
1:Q:11:SER:HA	1:Q:147:TRP:HB2	2.00	0.43
1:Q:176:TRP:CE2	1:Q:193:LEU:HD12	2.54	0.43
2:R:159:THR:OG1	2:R:160:THR:N	2.52	0.43
2:R:213:ALA:HB1	2:R:251:ALA:HB2	2.00	0.43
1:S:263:TRP:HZ3	2:T:59:ASN:HD21	1.67	0.43
2:T:201:ALA:HB2	2:T:269:LEU:HB2	2.00	0.43
2:X:56:TYR:HA	2:X:59:ASN:ND2	2.33	0.43
1:A:776:SER:HA	1:A:805:VAL:HG13	2.01	0.43
1:C:726:LEU:HB2	8:C:1197:HOH:O	2.17	0.43
2:D:210:PHE:CE2	2:D:251:ALA:HB1	2.54	0.43
1:E:200:ASP:HB3	8:E:1061:HOH:O	2.18	0.43
1:E:482:TYR:HA	1:E:483:PRO:C	2.44	0.43
2:H:112:GLY:HA2	8:H:518:HOH:O	2.17	0.43
1:I:478:HIS:HD2	8:I:1207:HOH:O	2.00	0.43
1:K:21:LYS:HG2	1:K:22:ASP:OD2	2.18	0.43
1:M:647:ASN:O	1:M:648:ARG:C	2.59	0.43
1:O:211:MET:HE2	1:O:246:VAL:CG2	2.49	0.43
1:Q:96:ARG:HH12	1:Q:519:LEU:HB3	1.81	0.43
1:Q:597:ALA:HB1	1:Q:603:GLU:HA	2.00	0.43
1:S:855:MET:HE2	1:S:857:ASN:OD1	2.19	0.43
1:U:223:SER:HB2	8:U:1036:HOH:O	2.17	0.43
1:U:630:THR:OG1	1:U:633:GLU:HG3	2.18	0.43
2:V:5:TYR:CE2	2:V:164:MET:HG2	2.53	0.43
2:X:4:TYR:CZ	2:X:158:LYS:HD2	2.53	0.43
2:X:210:PHE:CE2	2:X:251:ALA:HB1	2.52	0.43
1:A:39:ALA:HA	1:A:40:PRO:HD3	1.87	0.43
1:A:211:MET:O	1:A:344:THR:HA	2.18	0.43
1:C:144:HIS:HB2	5:C:903:MGD:O1B	2.19	0.43
1:C:406:GLU:O	1:C:418:ALA:HB2	2.18	0.43
1:C:446:HIS:CD2	1:C:466:LYS:HG3	2.54	0.43
1:C:625:MET:N	1:C:626:PRO:CD	2.82	0.43
1:E:288:TYR:HB2	1:E:376:MET:O	2.17	0.43
1:G:797:GLY:HA2	1:G:875:TYR:CZ	2.54	0.43
2:J:58:ARG:HD2	2:J:268:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:204:LEU:O	2:J:274:LEU:N	2.51	0.43
2:L:64:ARG:NH1	8:L:419:HOH:O	2.43	0.43
2:N:21:MET:HE3	2:N:21:MET:CA	2.47	0.43
2:N:69:MET:HE2	2:N:69:MET:HA	1.99	0.43
1:O:656:TRP:CD2	1:O:663:LYS:HA	2.54	0.43
1:O:797:GLY:HA2	1:O:875:TYR:CE2	2.54	0.43
1:Q:478:HIS:HD2	8:Q:1208:HOH:O	2.00	0.43
2:R:210:PHE:HD2	2:R:213:ALA:HB2	1.84	0.43
1:S:610:LYS:HB3	1:S:614:ALA:HB3	1.99	0.43
1:U:269:GLY:HA2	1:U:362:HIS:CG	2.52	0.43
1:U:349:GLY:HA3	1:U:353:GLY:O	2.18	0.43
1:U:744:HIS:HA	1:U:819:SER:CB	2.49	0.43
1:W:25:ILE:HG13	1:W:580:ILE:HG21	1.99	0.43
1:W:104:ASP:N	1:W:105:PRO:HD3	2.34	0.43
1:C:691:ILE:HD11	1:C:711:MET:HE3	2.01	0.43
2:D:204:LEU:HD23	2:D:209:CYS:HA	2.01	0.43
1:E:866:LYS:HE2	1:E:866:LYS:HB3	1.84	0.43
2:F:2:GLU:HG2	2:F:158:LYS:HG2	2.01	0.43
2:F:46:MET:HE3	2:F:47:ASN:N	2.34	0.43
1:G:187:TRP:CE3	1:G:379:MET:HE1	2.54	0.43
1:G:393:VAL:HA	1:G:394:PRO:HD3	1.79	0.43
1:I:218:ASP:OD2	1:I:253:ASN:HB2	2.18	0.43
1:M:117:ALA:O	1:M:121:VAL:HG23	2.19	0.43
1:M:152:TYR:CD2	1:M:154:HIS:HD2	2.36	0.43
2:P:56:TYR:CD1	2:P:57:PRO:HA	2.54	0.43
1:Q:408:GLY:HA2	1:Q:619:TYR:HE1	1.83	0.43
1:Q:454:GLU:CD	1:Q:454:GLU:N	2.77	0.43
1:Q:505:THR:O	1:Q:506:ALA:C	2.61	0.43
1:Q:558:SER:H	1:Q:564:ASN:ND2	2.16	0.43
1:Q:657:PHE:CE1	1:Q:681:LEU:HG	2.54	0.43
2:R:46:MET:HE3	2:R:47:ASN:N	2.34	0.43
1:S:550:ASP:HA	1:S:616:CYS:SG	2.58	0.43
1:S:738:HIS:HE2	5:S:903:MGD:H15	1.66	0.43
1:S:850:LYS:NZ	8:S:1283:HOH:O	2.51	0.43
1:U:78:TYR:C	1:U:541:PRO:HG2	2.44	0.43
1:U:498:GLY:N	1:U:499:PRO:HD3	2.33	0.43
1:U:571:ARG:HB2	1:U:642:VAL:HB	2.01	0.43
2:V:210:PHE:CE2	2:V:251:ALA:HB1	2.54	0.43
2:X:26:GLU:HB2	2:X:144:ARG:NH1	2.34	0.43
2:X:106:LEU:HD22	2:X:114:MET:O	2.18	0.43
1:A:76:ILE:HG22	1:A:541:PRO:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:TYR:HA	2:B:59:ASN:ND2	2.34	0.43
1:C:182:GLY:HA3	1:C:364:ILE:HG23	2.00	0.43
1:C:436:PRO:HG3	8:C:1462:HOH:O	2.18	0.43
2:D:17:ASN:HB2	8:D:567:HOH:O	2.17	0.43
2:D:19:CYS:HA	2:D:145:CYS:HB3	1.99	0.43
1:E:103:GLN:CD	1:E:103:GLN:N	2.76	0.43
1:G:68:SER:HB3	1:G:753:TYR:CZ	2.54	0.43
1:G:81:LYS:HB2	1:G:112:ILE:HD13	2.00	0.43
1:G:482:TYR:HA	1:G:483:PRO:C	2.44	0.43
2:H:105:LEU:CB	2:H:114:MET:HE1	2.49	0.43
1:I:776:SER:HA	1:I:805:VAL:HG13	2.00	0.43
1:K:867:TRP:CE2	1:K:869:GLY:HA2	2.54	0.43
1:M:347:ALA:HB1	1:M:388:SER:HA	2.01	0.43
1:O:816:SER:OG	1:O:839:ILE:HG13	2.18	0.43
2:P:106:LEU:HD23	2:P:114:MET:HE2	2.00	0.43
1:S:542:ALA:HA	1:S:587:MET:O	2.19	0.43
2:T:76:CYS:HA	2:T:108:THR:HB	2.01	0.43
1:W:219:PRO:HD2	1:W:255:THR:HG21	1.99	0.43
1:W:696:LYS:O	1:W:700:GLU:HG3	2.19	0.43
1:A:252:MET:HE1	8:B:470:HOH:O	2.17	0.43
1:C:78:TYR:C	1:C:541:PRO:HG2	2.44	0.43
1:C:140:THR:HG22	1:C:493:PHE:HE2	1.84	0.43
1:C:598:LYS:HG3	8:C:1262:HOH:O	2.18	0.43
2:D:21:MET:HE3	8:D:567:HOH:O	2.19	0.43
1:E:521:PHE:CE2	1:E:523:VAL:CG2	3.02	0.43
1:G:114:TRP:CZ2	1:G:541:PRO:HD2	2.54	0.43
1:G:482:TYR:CD1	1:G:483:PRO:HA	2.54	0.43
1:G:501:LEU:HD13	1:G:823:TYR:CD2	2.53	0.43
1:I:141:PRO:CA	1:I:496:TYR:HB3	2.46	0.43
1:K:553:GLU:HG2	1:K:556:ASN:HB2	1.99	0.43
1:M:10:SER:HA	1:M:15:PRO:HA	2.00	0.43
1:M:66:PHE:CD1	1:M:69:MET:CE	3.02	0.43
1:M:825:PRO:HD2	8:M:1338:HOH:O	2.18	0.43
1:S:361:SER:OG	1:S:717:ALA:HB1	2.19	0.43
1:S:696:LYS:O	1:S:700:GLU:HG3	2.19	0.43
1:S:730:TYR:CE1	1:S:794:ASN:HA	2.53	0.43
1:U:152:TYR:CD2	1:U:154:HIS:HD2	2.36	0.43
2:V:139:ALA:HB3	2:V:140:PRO:HD3	2.00	0.43
1:W:724:SER:HA	1:W:725:PRO:HD3	1.86	0.43
2:X:27:HIS:HB2	2:X:39:MET:HE3	2.00	0.43
1:A:425:ARG:HD3	1:A:622:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LYS:O	1:A:700:GLU:HG3	2.19	0.43
2:B:92:VAL:O	2:B:125:LYS:NZ	2.46	0.43
2:B:228:GLU:OE2	2:H:214:LYS:NZ	2.41	0.43
1:C:155:SER:HB2	1:C:408:GLY:HA3	2.00	0.43
1:C:454:GLU:CD	1:C:454:GLU:N	2.77	0.43
2:D:109:CYS:HA	2:D:110:PRO:HD3	1.83	0.43
1:E:825:PRO:HD2	8:E:1340:HOH:O	2.19	0.43
1:I:165:GLY:CA	1:I:166:PHE:HB3	2.45	0.43
2:J:39:MET:HE2	2:J:45:TRP:CD2	2.53	0.43
1:K:93:PRO:HG2	8:K:1156:HOH:O	2.18	0.43
1:K:142:SER:HB3	5:K:903:MGD:O1A	2.19	0.43
1:K:187:TRP:HB2	1:K:681:LEU:HD13	2.01	0.43
1:K:455:CYS:O	1:K:459:GLY:HA2	2.19	0.43
1:M:224:GLY:O	1:M:225:ILE:HB	2.17	0.43
1:O:262:LYS:HD2	8:O:1449:HOH:O	2.19	0.43
1:O:677:CYS:C	1:O:678:ARG:HG2	2.44	0.43
1:O:831:LYS:O	1:O:873:GLU:HA	2.18	0.43
1:Q:291:GLU:CD	1:Q:291:GLU:N	2.76	0.43
1:Q:378:GLY:O	1:Q:381:LYS:HG2	2.18	0.43
1:Q:395:LEU:HD13	1:Q:571:ARG:CG	2.49	0.43
2:R:58:ARG:NH1	2:R:270:GLY:HA2	2.34	0.43
1:S:377:GLN:O	1:S:381:LYS:HE2	2.19	0.43
2:T:26:GLU:HB2	2:T:144:ARG:HH11	1.84	0.43
1:U:753:TYR:HB3	2:V:24:MET:CE	2.29	0.43
1:W:222:ASN:HA	5:W:904:MGD:N22	2.34	0.43
2:X:176:ILE:HG22	2:X:177:LYS:HG3	2.01	0.43
1:A:272:HIS:ND1	1:A:272:HIS:N	2.67	0.43
1:C:211:MET:HE2	1:C:246:VAL:CG2	2.49	0.43
1:C:530:GLU:CD	1:C:750:LYS:HZ3	2.26	0.43
1:E:540:LEU:HA	1:E:541:PRO:HD3	1.80	0.43
1:E:670:PRO:HB3	1:E:682:GLN:HB2	2.01	0.43
1:G:75:ARG:HH21	1:G:543:CYS:HA	1.84	0.43
1:G:390:THR:O	1:G:567:LEU:HA	2.19	0.43
2:H:166:LYS:O	2:H:170:GLU:HG3	2.18	0.43
1:I:499:PRO:CB	1:I:745:THR:HG21	2.48	0.43
2:J:5:TYR:CD2	2:J:164:MET:HG2	2.54	0.43
1:K:76:ILE:CG2	1:K:541:PRO:HG3	2.48	0.43
2:L:183:LYS:N	2:L:184:PRO:HD3	2.34	0.43
1:M:56:LYS:HG2	1:M:57:THR:O	2.19	0.43
1:M:176:TRP:CE2	1:M:193:LEU:HD12	2.54	0.43
1:O:227:ALA:O	1:O:228:GLY:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:499:PRO:HG3	5:O:903:MGD:O5'	2.19	0.43
1:O:617:GLU:HG3	1:O:631:TRP:CG	2.54	0.43
2:P:185:ARG:CZ	2:P:185:ARG:CB	2.96	0.43
1:Q:401:PHE:HA	1:Q:402:PRO:HD3	1.84	0.43
1:Q:588:SER:O	1:Q:592:ILE:HG13	2.19	0.43
2:T:20:PHE:CE2	2:T:24:MET:HE2	2.53	0.43
1:U:401:PHE:HA	1:U:402:PRO:HD3	1.80	0.43
1:U:549:TRP:CG	1:U:613:LEU:HD13	2.54	0.43
1:W:56:LYS:HG2	1:W:57:THR:O	2.18	0.43
1:W:753:TYR:HB3	2:X:24:MET:CE	2.49	0.43
1:W:773:ARG:HG3	1:W:773:ARG:NH1	2.34	0.43
1:A:124:GLU:HG2	8:A:1501:HOH:O	2.17	0.42
1:A:395:LEU:HD13	1:A:571:ARG:HG3	2.01	0.42
1:C:141:PRO:HD3	1:C:157:TYR:CZ	2.53	0.42
1:C:855:MET:HE2	1:C:857:ASN:OD1	2.18	0.42
2:D:5:TYR:CD2	2:D:164:MET:HG2	2.54	0.42
1:G:251:HIS:HA	1:G:809:LEU:HD23	2.00	0.42
1:I:76:ILE:HA	1:I:77:PRO:HD3	1.85	0.42
1:I:197:GLU:OE2	1:I:667:ASP:HB2	2.18	0.42
1:I:521:PHE:CE2	1:I:523:VAL:CG2	3.02	0.42
1:K:31:MET:HE1	1:K:639:TYR:CG	2.54	0.42
1:K:665:THR:HB	1:K:666:PRO:CD	2.49	0.42
1:M:786:ASN:HD22	1:M:786:ASN:HA	1.58	0.42
1:O:104:ASP:OD2	1:O:107:SER:HB3	2.18	0.42
1:O:696:LYS:O	1:O:700:GLU:HG3	2.19	0.42
1:O:732:LEU:CD1	1:O:864:ILE:HG12	2.49	0.42
2:P:87:ARG:HG3	2:P:91:ILE:O	2.18	0.42
1:Q:96:ARG:HD2	1:Q:514:TYR:O	2.19	0.42
1:Q:162:ASN:CG	1:Q:437:SER:HB2	2.43	0.42
1:Q:691:ILE:CD1	1:Q:711:MET:HE3	2.43	0.42
2:R:164:MET:O	2:R:168:VAL:HG23	2.18	0.42
2:T:201:ALA:O	2:T:234:GLU:HA	2.19	0.42
1:U:501:LEU:HB2	8:U:1368:HOH:O	2.18	0.42
1:U:549:TRP:CZ3	1:U:577:ALA:HA	2.54	0.42
2:V:5:TYR:HB2	2:V:157:LEU:HD12	2.01	0.42
2:V:114:MET:CB	2:V:125:LYS:HB3	2.49	0.42
2:V:122:VAL:HG22	2:V:123:ALA:N	2.34	0.42
2:V:126:CYS:HB2	8:V:465:HOH:O	2.18	0.42
1:W:44:ILE:HG21	1:W:206:LEU:HD12	2.01	0.42
1:W:478:HIS:CD2	8:W:1208:HOH:O	2.71	0.42
1:W:602:ILE:CG2	8:W:1074:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:109:CYS:HB2	2:X:114:MET:SD	2.59	0.42
1:C:265:SER:O	1:C:810:GLN:NE2	2.51	0.42
1:C:600:LEU:HB3	8:C:1076:HOH:O	2.19	0.42
1:C:720:SER:O	1:C:724:SER:HB3	2.19	0.42
1:E:197:GLU:OE2	1:E:667:ASP:HB2	2.18	0.42
1:G:44:ILE:HD11	1:G:394:PRO:CG	2.49	0.42
1:G:452:ILE:N	1:G:453:PRO:CD	2.82	0.42
1:G:571:ARG:HB2	1:G:642:VAL:HB	2.01	0.42
1:I:144:HIS:CE1	3:I:901:ACT:OXT	2.73	0.42
1:I:355:GLY:HA2	5:I:904:MGD:O1B	2.19	0.42
1:I:408:GLY:HA2	1:I:619:TYR:HE1	1.84	0.42
2:J:189:LYS:O	2:J:190:ASN:HB2	2.19	0.42
2:J:245:TYR:HB2	2:J:260:VAL:CG1	2.49	0.42
1:K:521:PHE:CE2	1:K:523:VAL:CG2	3.02	0.42
1:K:770:TRP:HB3	1:K:801:LEU:CD2	2.49	0.42
1:O:870:ASP:HB3	1:O:872:TYR:CE1	2.53	0.42
1:U:267:LYS:HB3	1:U:721:GLN:NE2	2.33	0.42
1:U:629:MET:HE2	1:U:633:GLU:C	2.44	0.42
1:W:65:GLY:HA3	2:X:21:MET:HG3	2.01	0.42
1:W:505:THR:O	1:W:506:ALA:C	2.61	0.42
1:A:730:TYR:CZ	1:A:794:ASN:HA	2.55	0.42
1:C:530:GLU:O	1:C:533:VAL:HG23	2.18	0.42
1:C:767:TYR:HB3	1:C:769:TYR:CE1	2.54	0.42
1:E:13:GLY:HA3	1:E:63:THR:OG1	2.19	0.42
1:G:29:THR:HG22	2:H:144:ARG:NH2	2.35	0.42
1:G:269:GLY:HA2	1:G:362:HIS:CE1	2.54	0.42
1:K:227:ALA:O	1:K:228:GLY:C	2.60	0.42
1:K:433:PHE:CD1	1:K:433:PHE:N	2.88	0.42
1:K:721:GLN:HE21	1:K:721:GLN:HB2	1.73	0.42
2:L:87:ARG:NH2	2:L:91:ILE:HD12	2.35	0.42
1:M:166:PHE:N	1:M:439:LEU:HD12	2.34	0.42
2:N:250:ASP:HB2	8:N:537:HOH:O	2.19	0.42
1:O:540:LEU:HA	1:O:541:PRO:HD3	1.78	0.42
1:O:730:TYR:HB3	1:O:862:VAL:CA	2.49	0.42
1:S:20:VAL:HG12	8:S:1605:HOH:O	2.19	0.42
1:W:2:GLY:O	1:W:21:LYS:HE3	2.18	0.42
1:W:478:HIS:HD2	8:W:1208:HOH:O	2.02	0.42
2:X:6:MET:CE	2:X:143:PRO:HG2	2.49	0.42
2:X:78:ALA:C	2:X:80:GLY:H	2.27	0.42
2:X:175:VAL:CG2	2:X:178:PRO:HG3	2.43	0.42
1:A:128:ILE:HD13	1:A:492:MET:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HB2	1:C:22:ASP:OD1	2.19	0.42
1:C:76:ILE:HA	1:C:77:PRO:HD3	1.79	0.42
1:C:561:ILE:N	1:C:562:PRO:HD3	2.35	0.42
1:C:783:GLY:O	1:C:866:LYS:HD2	2.19	0.42
2:D:185:ARG:CB	2:D:185:ARG:NH1	2.82	0.42
1:E:501:LEU:HD13	1:E:823:TYR:CD2	2.55	0.42
1:G:602:ILE:HG23	8:G:1074:HOH:O	2.19	0.42
2:H:5:TYR:HB2	2:H:157:LEU:CD1	2.49	0.42
2:H:105:LEU:HB3	2:H:114:MET:HE1	2.02	0.42
1:I:280:TYR:OH	1:I:284:LYS:HE3	2.20	0.42
2:J:26:GLU:HB2	2:J:144:ARG:HH11	1.84	0.42
1:K:358:CYS:O	1:K:363:GLY:HA3	2.19	0.42
1:M:402:PRO:HG2	1:M:422:PHE:CE1	2.54	0.42
2:P:191:LEU:HD12	2:P:191:LEU:O	2.20	0.42
2:P:203:ILE:HD12	2:P:203:ILE:N	2.35	0.42
1:Q:354:TRP:HB3	1:Q:355:GLY:H	1.64	0.42
1:Q:602:ILE:HG23	8:Q:1075:HOH:O	2.20	0.42
1:S:165:GLY:CA	1:S:166:PHE:HB3	2.49	0.42
1:S:360:ALA:HB1	1:S:859:THR:CG2	2.40	0.42
1:S:708:ARG:CD	8:S:1049:HOH:O	2.67	0.42
1:U:78:TYR:O	1:U:80:MET:HG3	2.20	0.42
1:U:263:TRP:CZ2	1:U:265:SER:HB2	2.53	0.42
2:V:21:MET:CE	2:V:21:MET:CA	2.97	0.42
1:W:644:ASP:C	1:W:646:PRO:HD3	2.44	0.42
2:X:159:THR:OG1	2:X:160:THR:N	2.51	0.42
3:A:901:ACT:H1	8:A:1043:HOH:O	2.19	0.42
1:C:249:ASP:CG	5:C:904:MGD:H1'	2.44	0.42
1:C:597:ALA:HB1	1:C:603:GLU:HA	2.00	0.42
2:D:7:VAL:HB	2:D:155:GLU:HB3	2.01	0.42
2:D:69:MET:HB2	7:D:304:SF4:S2	2.60	0.42
1:E:116:GLU:O	1:E:120:ILE:HG13	2.20	0.42
1:E:224:GLY:O	1:E:225:ILE:HB	2.19	0.42
2:F:260:VAL:O	2:F:260:VAL:HG13	2.19	0.42
1:G:461:PHE:HA	8:G:1503:HOH:O	2.19	0.42
2:H:203:ILE:HD11	2:H:249:ILE:HD13	2.01	0.42
1:I:742:SER:O	5:I:904:MGD:N18	2.48	0.42
1:I:866:LYS:HE2	1:I:866:LYS:HB3	1.88	0.42
1:K:69:MET:HE2	1:K:754:MET:HE3	2.01	0.42
1:K:696:LYS:HA	1:K:699:GLU:CG	2.50	0.42
1:M:80:MET:HB2	1:M:539:ILE:HB	2.01	0.42
1:O:75:ARG:HH21	1:O:543:CYS:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:494:TRP:HE1	1:O:525:GLN:HE21	1.67	0.42
2:P:52:GLU:HG3	2:P:61:ILE:HD12	2.02	0.42
1:Q:209:ALA:HB2	1:Q:345:TYR:CE1	2.54	0.42
1:Q:425:ARG:HD3	1:Q:622:ALA:O	2.20	0.42
1:S:508:ASN:HB2	8:S:1299:HOH:O	2.19	0.42
2:T:69:MET:HB2	7:T:304:SF4:S2	2.59	0.42
2:V:44:ARG:HG2	2:V:44:ARG:HH11	1.85	0.42
1:W:557:CYS:H	1:W:564:ASN:ND2	2.08	0.42
1:W:563:ASP:O	1:W:566:GLN:HG2	2.19	0.42
1:W:625:MET:N	1:W:626:PRO:CD	2.82	0.42
2:X:44:ARG:HG2	2:X:44:ARG:HH11	1.84	0.42
2:X:60:ASP:OD1	2:X:60:ASP:C	2.62	0.42
1:A:68:SER:HB3	1:A:753:TYR:CE2	2.55	0.42
1:A:173:PRO:HA	1:A:468:PHE:CE1	2.54	0.42
2:B:3:GLN:O	2:B:158:LYS:HA	2.19	0.42
1:C:146:MET:HE2	1:C:544:THR:CB	2.47	0.42
1:C:498:GLY:HA3	1:C:532:GLU:HB2	2.00	0.42
1:C:598:LYS:HA	1:C:603:GLU:HB2	2.01	0.42
2:D:9:ASP:O	2:D:153:VAL:HG13	2.19	0.42
1:E:174:ASP:O	1:E:177:GLU:HG2	2.19	0.42
1:E:607:SER:O	1:E:608:GLU:HB2	2.18	0.42
1:G:233:ILE:O	1:G:236:GLN:HB3	2.20	0.42
1:G:256:ALA:HA	1:G:260:ALA:HB2	2.01	0.42
1:G:269:GLY:HA2	1:G:362:HIS:ND1	2.35	0.42
1:G:776:SER:HA	1:G:805:VAL:HG13	2.02	0.42
1:I:174:ASP:OD1	1:I:175:SER:N	2.48	0.42
1:I:269:GLY:HA2	1:I:362:HIS:CG	2.55	0.42
2:J:129:CYS:HB3	2:J:131:HIS:CE1	2.54	0.42
2:L:159:THR:OG1	2:L:160:THR:N	2.52	0.42
2:L:175:VAL:HG23	2:L:178:PRO:HG3	2.02	0.42
2:N:177:LYS:N	2:N:178:PRO:HD3	2.34	0.42
1:O:587:MET:HE2	1:O:592:ILE:HA	2.02	0.42
1:O:597:ALA:HB1	1:O:603:GLU:HA	2.02	0.42
1:Q:319:GLU:CG	1:U:726:LEU:HD13	2.43	0.42
1:U:31:MET:HE1	1:U:639:TYR:CG	2.55	0.42
1:U:78:TYR:CD1	1:U:111:ARG:HG3	2.54	0.42
1:U:144:HIS:NE2	5:U:904:MGD:S13	2.92	0.42
1:U:251:HIS:HA	1:U:809:LEU:HD23	2.00	0.42
1:W:745:THR:HG22	1:W:819:SER:O	2.19	0.42
2:X:62:ASN:CG	2:X:193:ARG:HB3	2.45	0.42
1:A:81:LYS:HE3	1:A:82:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:VAL:HB	1:A:534:PRO:HD3	2.02	0.42
1:A:553:GLU:OE1	1:A:556:ASN:ND2	2.49	0.42
1:A:730:TYR:CE1	1:A:794:ASN:HA	2.55	0.42
2:B:46:MET:CE	2:B:66:THR:N	2.81	0.42
2:B:112:GLY:HA2	8:B:518:HOH:O	2.19	0.42
1:G:351:LEU:HG	1:G:391:GLN:HE21	1.84	0.42
1:G:563:ASP:O	1:G:566:GLN:HG2	2.19	0.42
1:G:565:TYR:C	1:G:567:LEU:N	2.78	0.42
2:H:21:MET:HE2	2:H:24:MET:HE3	2.01	0.42
2:H:40:GLN:HG3	8:H:443:HOH:O	2.19	0.42
1:I:119:ASP:OD1	1:I:599:LYS:NZ	2.52	0.42
1:I:165:GLY:HA3	1:I:166:PHE:CB	2.38	0.42
1:I:651:THR:HG21	1:I:664:ASP:O	2.20	0.42
2:L:127:THR:HG22	8:L:527:HOH:O	2.19	0.42
1:M:69:MET:HE2	1:M:754:MET:HE3	2.00	0.42
1:O:74:LEU:HD12	1:O:750:LYS:CA	2.43	0.42
1:Q:197:GLU:OE2	1:Q:667:ASP:HB2	2.20	0.42
2:R:207:GLY:CA	1:U:728:VAL:HG12	2.31	0.42
1:S:80:MET:HE1	1:S:529:PHE:CE1	2.55	0.42
2:X:229:THR:HB	2:X:233:GLY:HA2	2.00	0.42
1:A:402:PRO:CD	1:A:623:THR:HG22	2.49	0.42
1:A:433:PHE:HA	1:A:434:PRO:HD3	1.81	0.42
1:A:697:ASN:ND2	8:A:1203:HOH:O	2.52	0.42
1:C:65:GLY:CA	2:D:21:MET:HG3	2.49	0.42
1:C:277:ALA:HA	1:C:316:LYS:O	2.19	0.42
2:D:31:GLU:O	2:D:33:PRO:HD3	2.19	0.42
1:G:39:ALA:O	1:G:55:ARG:NH2	2.41	0.42
1:I:770:TRP:HB3	1:I:801:LEU:HD23	2.01	0.42
1:K:269:GLY:HA2	1:K:362:HIS:CG	2.55	0.42
1:K:560[B]:TYR:C	1:K:562:PRO:HD3	2.45	0.42
1:K:831:LYS:O	1:K:873:GLU:HA	2.20	0.42
1:K:855:MET:HB2	1:K:857:ASN:OD1	2.20	0.42
2:L:126:CYS:HB2	8:L:470:HOH:O	2.18	0.42
1:M:249:ASP:OD2	5:M:904:MGD:H1'	2.19	0.42
1:M:349:GLY:HA3	1:M:353:GLY:O	2.19	0.42
1:M:782:ARG:HH11	1:M:782:ARG:HG3	1.84	0.42
1:M:826:LEU:HD12	1:M:833:ALA:HB3	2.02	0.42
1:M:848:ILE:HG13	1:M:854:GLY:O	2.19	0.42
1:O:1:MET:H3	1:O:22:ASP:CG	2.28	0.42
1:S:177:GLU:HA	1:S:177:GLU:OE2	2.20	0.42
1:S:857:ASN:HB3	5:S:903:MGD:N19	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:114:MET:HE3	2:T:123:ALA:HB1	2.02	0.42
2:T:159:THR:OG1	2:T:160:THR:N	2.51	0.42
1:U:77:PRO:HB2	1:U:78:TYR:CD2	2.54	0.42
1:U:625:MET:N	1:U:626:PRO:CD	2.82	0.42
1:U:806:THR:OG1	1:U:807:GLU:N	2.53	0.42
1:W:96:ARG:HD2	1:W:514:TYR:O	2.20	0.42
1:W:263:TRP:CZ2	1:W:265:SER:HB2	2.55	0.42
2:X:111:TYR:N	2:X:111:TYR:CD1	2.87	0.42
1:A:31:MET:HE1	1:A:639:TYR:CG	2.54	0.42
1:A:498:GLY:N	1:A:499:PRO:HD3	2.35	0.42
1:C:269:GLY:HA2	1:C:362:HIS:CE1	2.55	0.42
1:C:732:LEU:CD1	1:C:864:ILE:HG12	2.50	0.42
1:E:518:SER:HB2	8:E:1557:HOH:O	2.20	0.42
1:G:28:MET:HE1	1:G:66:PHE:CB	2.42	0.42
1:G:149:ASN:HB2	1:G:551:ILE:O	2.19	0.42
1:G:288:TYR:HA	8:G:1506:HOH:O	2.19	0.42
1:I:140:THR:CB	1:I:169:ALA:HB3	2.48	0.42
2:J:247:VAL:O	2:J:257:SER:HA	2.20	0.42
2:N:10:VAL:HG13	2:N:63:TYR:O	2.20	0.42
1:O:21:LYS:CB	1:O:26:ILE:HD11	2.49	0.42
1:O:288:TYR:HB2	1:O:376:MET:O	2.20	0.42
2:P:9:ASP:HA	2:P:189:LYS:HB3	2.02	0.42
1:Q:292:TYR:CD2	1:Q:378:GLY:HA2	2.55	0.42
1:Q:361:SER:OG	1:Q:717:ALA:HB1	2.19	0.42
1:Q:433:PHE:CD1	1:Q:433:PHE:N	2.88	0.42
1:S:53:PRO:HA	1:S:54:PRO:HD3	1.87	0.42
2:V:198:TYR:CD1	2:V:198:TYR:C	2.98	0.42
1:A:724:SER:OG	1:A:726:LEU:HB2	2.20	0.42
2:D:17:ASN:N	2:D:17:ASN:ND2	2.67	0.42
2:D:40:GLN:HE22	2:D:118:GLU:H	1.67	0.42
1:E:114:TRP:CH2	1:E:541:PRO:HD2	2.55	0.42
1:E:211:MET:HE1	1:E:338:GLN:HG2	2.02	0.42
1:E:503:THR:C	1:E:504:MET:HE2	2.45	0.42
2:H:53:ARG:HB2	2:H:60:ASP:OD1	2.20	0.42
2:H:142:MET:HE2	2:H:146:ALA:C	2.45	0.42
1:I:426:MET:HE3	1:I:426:MET:CA	2.45	0.42
2:J:231:PHE:HD1	8:J:484:HOH:O	2.02	0.42
2:L:52:GLU:HB2	8:L:437:HOH:O	2.19	0.42
1:O:56:LYS:HG2	1:O:57:THR:O	2.20	0.42
1:O:587:MET:HG3	1:O:592:ILE:CG1	2.49	0.42
2:P:210:PHE:HD2	2:P:213:ALA:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:269:GLY:HA2	1:Q:362:HIS:ND1	2.35	0.42
1:Q:404:TYR:CD1	1:Q:405:ALA:N	2.88	0.42
2:R:40:GLN:HB3	2:R:43:HIS:CE1	2.55	0.42
2:R:166:LYS:HE2	2:R:170:GLU:OE2	2.20	0.42
1:S:146:MET:HE2	1:S:544:THR:HA	2.01	0.42
1:S:227:ALA:O	1:S:228:GLY:C	2.63	0.42
1:U:471:GLY:HA3	1:U:475:HIS:CE1	2.54	0.42
1:W:521:PHE:CE2	1:W:523:VAL:CG2	3.03	0.42
1:W:739:PRO:HG2	1:W:742:SER:O	2.20	0.42
2:X:104:GLU:H	2:X:104:GLU:CD	2.28	0.42
1:A:391:GLN:HG2	1:A:567:LEU:CD2	2.50	0.41
2:B:9:ASP:HA	2:B:189:LYS:HB3	2.01	0.41
2:B:210:PHE:HD2	2:B:213:ALA:HB2	1.85	0.41
1:C:73:ASP:C	1:C:73:ASP:OD1	2.62	0.41
1:C:356:GLY:H	5:C:904:MGD:H5'1	1.82	0.41
1:C:656:TRP:CD2	1:C:663:LYS:HA	2.54	0.41
1:C:857:ASN:HB3	5:C:903:MGD:N19	2.35	0.41
1:E:390:THR:O	1:E:567:LEU:HA	2.20	0.41
2:F:94:ILE:CD1	2:F:125:LYS:HG3	2.50	0.41
2:F:164:MET:HE3	2:F:167:LYS:HB3	2.02	0.41
1:G:15:PRO:HD3	1:G:554:PHE:CD1	2.54	0.41
1:G:144:HIS:HE2	3:G:901:ACT:C	2.33	0.41
1:I:192:ARG:CZ	1:I:562:PRO:HD2	2.50	0.41
1:K:69:MET:HE2	1:K:754:MET:HE1	2.01	0.41
1:K:563:ASP:HA	1:K:565:TYR:CE1	2.55	0.41
2:L:114:MET:CA	2:L:125:LYS:HB3	2.49	0.41
1:M:76:ILE:HA	1:M:77:PRO:HD3	1.82	0.41
1:M:103:GLN:CD	1:M:103:GLN:N	2.78	0.41
1:M:272:HIS:ND1	1:M:272:HIS:N	2.67	0.41
1:O:11:SER:C	1:O:13:GLY:H	2.26	0.41
1:O:140:THR:HB	1:O:169:ALA:HB3	2.02	0.41
1:O:482:TYR:HA	1:O:483:PRO:C	2.44	0.41
1:O:564:ASN:H	1:O:564:ASN:HD22	1.66	0.41
2:P:16:CYS:O	2:P:17:ASN:HB2	2.20	0.41
1:S:730:TYR:CZ	1:S:794:ASN:HA	2.55	0.41
2:T:5:TYR:HB2	2:T:157:LEU:HD12	1.99	0.41
2:T:76:CYS:HB3	2:T:108:THR:CB	2.49	0.41
2:T:106:LEU:HD23	2:T:114:MET:CE	2.48	0.41
1:U:146:MET:HE2	1:U:544:THR:CB	2.49	0.41
1:U:162:ASN:ND2	1:U:166:PHE:HE2	2.17	0.41
1:U:277:ALA:HA	1:U:316:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:499:PRO:CB	1:U:745:THR:HG21	2.49	0.41
2:V:203:ILE:HD12	2:V:203:ILE:N	2.35	0.41
1:W:44:ILE:HD11	1:W:394:PRO:CG	2.49	0.41
1:W:224:GLY:HA2	8:W:1331:HOH:O	2.20	0.41
1:W:561:ILE:N	1:W:562:PRO:HD3	2.34	0.41
2:X:168:VAL:O	2:X:168:VAL:HG12	2.20	0.41
1:C:280:TYR:CE2	1:C:317:THR:HG22	2.55	0.41
1:C:700:GLU:HG2	8:C:1572:HOH:O	2.20	0.41
1:G:225:ILE:HG12	1:G:226:TYR:CD1	2.55	0.41
2:J:106:LEU:N	2:J:114:MET:HE2	2.35	0.41
1:K:144:HIS:NE2	3:K:901:ACT:OXT	2.53	0.41
1:O:144:HIS:NE2	5:O:904:MGD:S13	2.93	0.41
1:O:498:GLY:N	1:O:499:PRO:HD3	2.35	0.41
2:P:217:LEU:O	2:P:224:VAL:N	2.42	0.41
1:S:139:SER:OG	1:S:161:MET:HE2	2.20	0.41
1:S:489:LYS:HD3	8:S:1024:HOH:O	2.20	0.41
1:S:610:LYS:HZ3	1:S:618:GLN:NE2	2.14	0.41
1:U:855:MET:HB2	1:U:857:ASN:OD1	2.20	0.41
2:V:142:MET:HE1	8:V:429:HOH:O	2.19	0.41
1:W:11:SER:C	1:W:13:GLY:N	2.78	0.41
1:W:74:LEU:HD12	1:W:750:LYS:CA	2.45	0.41
1:W:143:SER:CB	3:W:901:ACT:H3	2.49	0.41
1:W:171:HIS:O	1:W:467:GLY:HA2	2.20	0.41
1:W:826:LEU:HD21	1:W:835:ARG:HD3	2.01	0.41
2:X:198:TYR:CD1	2:X:236:LYS:HE3	2.55	0.41
1:A:354:TRP:HB3	1:A:355:GLY:H	1.66	0.41
1:C:662:GLU:OE1	1:C:662:GLU:N	2.50	0.41
1:E:142:SER:OG	5:E:903:MGD:O1A	2.36	0.41
1:E:227:ALA:O	1:E:228:GLY:C	2.63	0.41
1:E:291:GLU:CD	1:E:291:GLU:N	2.78	0.41
1:E:526:SER:HB3	8:E:1116:HOH:O	2.19	0.41
1:G:176:TRP:CD1	1:G:193:LEU:HB2	2.56	0.41
1:G:411:GLY:HA3	1:G:434:PRO:HB3	2.02	0.41
1:G:857:ASN:HB3	5:G:903:MGD:N19	2.35	0.41
2:H:142:MET:CE	2:H:146:ALA:HB1	2.49	0.41
1:I:192:ARG:NH2	1:I:562:PRO:HB2	2.35	0.41
1:I:655:ARG:HB3	8:I:1400:HOH:O	2.19	0.41
1:K:144:HIS:NE2	3:K:901:ACT:C	2.83	0.41
1:K:214:PHE:HA	1:K:347:ALA:HB3	2.02	0.41
2:L:104:GLU:CD	2:L:104:GLU:H	2.28	0.41
1:M:39:ALA:HA	1:M:40:PRO:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:171:HIS:HD2	8:O:1464:HOH:O	2.03	0.41
2:P:81:ASN:OD1	2:P:81:ASN:O	2.39	0.41
1:Q:521:PHE:CE2	1:Q:523:VAL:HG22	2.55	0.41
1:Q:548:ARG:NH1	1:Q:550:ASP:OD2	2.47	0.41
2:R:1:MET:HE2	2:R:88:GLU:OE2	2.21	0.41
1:S:354:TRP:CZ2	1:S:561:ILE:HD11	2.55	0.41
1:U:361:SER:N	1:U:856:ALA:HB1	2.36	0.41
1:U:691:ILE:CD1	1:U:711:MET:HE3	2.45	0.41
1:U:730:TYR:CE1	1:U:794:ASN:HA	2.56	0.41
1:U:734:MET:HB2	1:U:814:VAL:HG23	2.01	0.41
1:U:757:ILE:HD11	8:V:563:HOH:O	2.20	0.41
1:W:215:TRP:CZ3	1:W:370:MET:HE1	2.56	0.41
1:W:564:ASN:C	1:W:566:GLN:H	2.27	0.41
1:A:501:LEU:HA	1:A:507:THR:HB	2.03	0.41
2:B:21:MET:HE2	2:B:24:MET:HE3	2.01	0.41
1:C:1:MET:HE2	1:C:22:ASP:HB3	2.03	0.41
1:C:521:PHE:CE2	1:C:523:VAL:CG2	3.03	0.41
1:E:146:MET:HE2	1:E:544:THR:CB	2.48	0.41
2:F:159:THR:OG1	2:F:160:THR:N	2.53	0.41
1:G:166:PHE:CE1	1:G:168:TYR:HB2	2.55	0.41
1:G:220:GLU:HB3	2:H:14:GLN:OE1	2.20	0.41
1:G:738:HIS:ND1	5:G:904:MGD:N15	2.65	0.41
2:H:164:MET:O	2:H:168:VAL:HG23	2.20	0.41
1:I:460:LYS:HE3	8:I:1233:HOH:O	2.19	0.41
2:J:128:MET:O	2:J:129:CYS:C	2.63	0.41
2:J:198:TYR:HB3	2:J:238:ASP:HA	2.02	0.41
1:K:277:ALA:HA	1:K:316:LYS:O	2.20	0.41
1:K:581:GLU:O	1:K:582:PRO:C	2.63	0.41
1:O:316:LYS:HD2	1:O:320:TRP:CH2	2.55	0.41
1:O:364:ILE:HB	8:O:1350:HOH:O	2.20	0.41
1:O:744:HIS:HA	1:O:819:SER:CB	2.50	0.41
1:O:744:HIS:HA	1:O:819:SER:HB3	2.02	0.41
2:P:154:TYR:CE1	7:P:302:SF4:S4	3.14	0.41
2:P:205:VAL:HG13	2:P:254:LYS:HZ1	1.82	0.41
2:P:238:ASP:O	2:P:239:ALA:HB3	2.20	0.41
1:Q:117:ALA:O	1:Q:121:VAL:HG23	2.20	0.41
1:Q:794:ASN:ND2	1:Q:842:LEU:HB3	2.34	0.41
1:U:28:MET:CE	1:U:67:LYS:H	2.32	0.41
1:U:390:THR:HB	1:U:567:LEU:CD2	2.50	0.41
1:U:548:ARG:NH1	8:U:1204:HOH:O	2.44	0.41
2:V:106:LEU:HD23	2:V:114:MET:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:87:ARG:HB2	2:X:89:ASP:OD2	2.20	0.41
1:A:197:GLU:HG2	1:A:199:TYR:HD1	1.86	0.41
2:D:90:GLY:HA3	2:D:185:ARG:CZ	2.51	0.41
2:D:106:LEU:HD11	2:D:116:TRP:HB2	2.02	0.41
2:D:213:ALA:O	2:D:228:GLU:HA	2.19	0.41
1:E:125:ILE:HD11	1:E:494:TRP:HZ3	1.86	0.41
2:H:69:MET:HB2	7:H:304:SF4:S2	2.61	0.41
2:H:106:LEU:HD23	2:H:114:MET:HG3	2.03	0.41
1:I:730:TYR:CE1	1:I:794:ASN:HA	2.55	0.41
1:K:249:ASP:CG	5:K:904:MGD:H1'	2.45	0.41
2:L:91:ILE:HG22	2:L:93:LEU:HG	2.03	0.41
2:L:142:MET:CE	2:L:146:ALA:HB1	2.50	0.41
2:L:142:MET:HE3	2:L:146:ALA:HB1	2.03	0.41
1:M:138:LEU:HA	1:M:167:THR:O	2.20	0.41
2:N:73:ASN:HB3	2:N:182:THR:HA	2.02	0.41
1:O:426:MET:HE2	1:O:618:GLN:HG2	2.03	0.41
2:P:230:ASN:OD1	2:P:232:PHE:HB2	2.21	0.41
2:R:122:VAL:HG22	2:R:123:ALA:N	2.35	0.41
1:S:272:HIS:ND1	1:S:272:HIS:N	2.69	0.41
2:T:3:GLN:NE2	2:T:161:PRO:HG3	2.36	0.41
2:T:203:ILE:N	2:T:203:ILE:HD12	2.35	0.41
1:U:96:ARG:HD2	1:U:514:TYR:O	2.21	0.41
1:U:364:ILE:HD13	1:U:708:ARG:HG3	2.03	0.41
1:U:433:PHE:HA	1:U:434:PRO:HD3	1.91	0.41
1:W:454:GLU:CD	1:W:454:GLU:N	2.79	0.41
1:W:744:HIS:HA	1:W:819:SER:CB	2.51	0.41
2:X:94:ILE:CG2	2:X:95:ASP:N	2.82	0.41
2:X:185:ARG:HB3	2:X:185:ARG:NH1	2.34	0.41
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.72	0.41
1:C:510:TYR:O	1:C:513:MET:HG2	2.20	0.41
1:E:756:TYR:HB2	2:F:24:MET:HE1	2.03	0.41
1:G:501:LEU:HA	1:G:507:THR:HB	2.03	0.41
1:G:540:LEU:HA	1:G:541:PRO:HD3	1.85	0.41
1:I:152:TYR:HD2	1:I:154:HIS:HD2	1.68	0.41
1:I:175:SER:HA	1:I:359:ARG:NH2	2.35	0.41
1:I:402:PRO:HD3	1:I:623:THR:HG22	2.01	0.41
1:K:68:SER:HB3	1:K:753:TYR:CD2	2.55	0.41
1:K:211:MET:CE	2:L:231:PHE:CZ	3.03	0.41
1:K:356:GLY:HA2	1:K:359:ARG:NH1	2.36	0.41
1:K:393:VAL:HA	1:K:394:PRO:HD3	1.79	0.41
2:L:129:CYS:HB3	2:L:131:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:291:GLU:CD	1:M:291:GLU:N	2.78	0.41
1:M:400:TYR:CE1	1:M:421:LYS:HD2	2.56	0.41
1:O:512:LYS:HE3	1:O:830:GLY:O	2.21	0.41
1:Q:138:LEU:HD12	1:Q:167:THR:O	2.21	0.41
1:Q:839:ILE:C	1:Q:841:ILE:H	2.27	0.41
1:S:174:ASP:OD1	1:S:175:SER:N	2.52	0.41
1:S:526:SER:HB3	8:S:1119:HOH:O	2.19	0.41
1:W:744:HIS:HA	1:W:819:SER:HB3	2.03	0.41
2:X:154:TYR:HE1	7:X:302:SF4:S4	2.43	0.41
1:C:191:TRP:CE2	1:C:669:GLY:HA3	2.55	0.41
1:C:226:TYR:HE2	1:C:743:MET:HE2	1.86	0.41
1:C:650:LYS:N	1:C:650:LYS:HD3	2.35	0.41
2:D:2:GLU:HG3	2:D:159:THR:C	2.45	0.41
1:E:302:GLU:OE1	1:E:302:GLU:N	2.45	0.41
1:E:412:ASP:OD1	1:E:415:ASN:N	2.49	0.41
1:E:797:GLY:HA2	1:E:875:TYR:CZ	2.56	0.41
1:E:839:ILE:C	1:E:841:ILE:H	2.29	0.41
1:G:162:ASN:HD22	1:G:166:PHE:HE2	1.69	0.41
1:G:291:GLU:CD	1:G:291:GLU:N	2.79	0.41
1:I:220:GLU:HB3	2:J:14:GLN:OE1	2.19	0.41
1:I:257:ARG:HD3	2:J:61:ILE:HG21	2.03	0.41
2:J:13:CYS:HB3	2:J:63:TYR:HB2	2.03	0.41
2:J:245:TYR:HB2	2:J:260:VAL:HG13	2.02	0.41
1:M:451:LYS:HG3	1:M:461:PHE:CE2	2.55	0.41
1:O:388:SER:C	1:O:389:THR:HG23	2.46	0.41
1:O:452:ILE:N	1:O:453:PRO:CD	2.83	0.41
1:O:476:GLN:OE1	1:O:708:ARG:NH2	2.53	0.41
1:O:707:HIS:HA	1:O:715:VAL:HG11	2.01	0.41
2:P:122:VAL:HG22	2:P:123:ALA:N	2.35	0.41
1:U:69:MET:SD	1:U:747:GLY:HA2	2.60	0.41
1:U:268:ILE:O	1:U:268:ILE:HG13	2.20	0.41
2:V:192:TYR:HA	2:V:196:LYS:HG2	2.02	0.41
2:X:46:MET:HE3	2:X:47:ASN:N	2.36	0.41
2:X:164:MET:HE3	2:X:164:MET:HA	2.03	0.41
1:A:262:LYS:NZ	1:A:331:GLU:OE2	2.52	0.41
1:A:402:PRO:HD3	1:A:623:THR:HG22	2.02	0.41
1:C:35:ASP:OD1	1:C:55:ARG:HD3	2.21	0.41
1:C:677:CYS:C	1:C:678:ARG:HG2	2.44	0.41
1:E:55:ARG:HD2	8:E:1642:HOH:O	2.19	0.41
2:F:106:LEU:HD11	2:F:116:TRP:HB2	2.02	0.41
1:G:146:MET:HE2	1:G:544:THR:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:786:ASN:ND2	1:G:804:GLN:HA	2.36	0.41
1:K:141:PRO:CA	1:K:496:TYR:HB3	2.48	0.41
1:K:548:ARG:HB2	8:K:1113:HOH:O	2.21	0.41
1:M:393:VAL:HA	1:M:394:PRO:HD3	1.76	0.41
1:O:280:TYR:CE2	1:O:317:THR:HG22	2.56	0.41
2:P:1:MET:HG2	2:P:88:GLU:O	2.21	0.41
2:P:164:MET:O	2:P:164:MET:HE3	2.20	0.41
1:S:146:MET:HE2	1:S:544:THR:CA	2.50	0.41
1:S:301:GLU:CD	1:S:301:GLU:N	2.79	0.41
2:T:175:VAL:CG2	2:T:178:PRO:HG3	2.44	0.41
1:U:355:GLY:N	5:U:904:MGD:O2A	2.50	0.41
2:X:68:CYS:HB2	2:X:113:VAL:HG21	2.03	0.41
1:A:162:ASN:ND2	1:A:437:SER:HB2	2.36	0.41
1:A:162:ASN:CG	1:A:437:SER:HB2	2.45	0.41
1:A:211:MET:HE2	1:A:246:VAL:HG21	2.02	0.41
1:A:249:ASP:CG	5:A:904:MGD:H1'	2.46	0.41
1:A:292:TYR:CD2	1:A:378:GLY:HA2	2.56	0.41
1:A:737:PRO:CG	5:A:904:MGD:H2'	2.50	0.41
1:C:34:ASP:HB3	1:C:37:VAL:HG22	2.03	0.41
1:C:706:GLU:HB2	8:C:1601:HOH:O	2.21	0.41
1:C:847:TYR:CD2	1:C:853:CYS:HA	2.56	0.41
2:D:94:ILE:CD1	2:D:125:LYS:HG2	2.51	0.41
1:E:127:ARG:HA	8:E:1253:HOH:O	2.20	0.41
1:E:296:ASN:HB3	1:E:657:PHE:CZ	2.55	0.41
1:E:675:GLN:NE2	1:E:680:GLY:O	2.42	0.41
1:G:66:PHE:CD1	1:G:69:MET:HE3	2.56	0.41
1:G:387:TRP:CZ2	1:G:389:THR:HA	2.56	0.41
1:G:610:LYS:HB3	1:G:614:ALA:CB	2.48	0.41
1:G:644:ASP:OD2	1:G:645:ASN:N	2.54	0.41
1:G:717:ALA:HB3	1:G:720:SER:HB3	2.02	0.41
1:G:734:MET:HB2	1:G:814:VAL:HG23	2.03	0.41
1:G:734:MET:HB2	1:G:814:VAL:CG2	2.51	0.41
1:G:780:GLU:C	1:G:780:GLU:OE1	2.64	0.41
2:H:23:CYS:O	2:H:24:MET:C	2.64	0.41
2:H:129:CYS:HB3	2:H:132:LEU:HD12	2.03	0.41
1:I:300:PHE:HZ	1:I:376:MET:HE3	1.85	0.41
1:I:433:PHE:CD1	1:I:433:PHE:N	2.89	0.41
1:K:21:LYS:CB	1:K:26:ILE:HD11	2.51	0.41
1:K:53:PRO:HA	1:K:54:PRO:HD3	1.89	0.41
2:L:20:PHE:CZ	2:L:24:MET:HE2	2.56	0.41
1:M:35:ASP:OD1	1:M:55:ARG:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:165:GLY:HA3	1:O:166:PHE:CB	2.35	0.41
1:O:387:TRP:CE2	1:O:389:THR:HA	2.56	0.41
1:O:454:GLU:CD	1:O:454:GLU:N	2.79	0.41
2:P:51:ARG:O	2:P:61:ILE:HG13	2.21	0.41
1:Q:144:HIS:NE2	5:Q:904:MGD:S13	2.93	0.41
1:Q:625:MET:N	1:Q:626:PRO:CD	2.84	0.41
2:R:99:ALA:C	2:R:122:VAL:HG23	2.46	0.41
2:R:106:LEU:HA	2:R:114:MET:HG3	2.03	0.41
1:S:66:PHE:HD1	1:S:69:MET:HE3	1.79	0.41
1:S:95:LEU:HD21	8:S:1500:HOH:O	2.20	0.41
1:S:338:GLN:HG2	2:T:231:PHE:CZ	2.56	0.41
1:S:498:GLY:N	1:S:499:PRO:HD3	2.35	0.41
2:T:117:ASN:HB2	2:T:124:GLN:OE1	2.20	0.41
1:U:269:GLY:HA2	1:U:362:HIS:ND1	2.36	0.41
1:U:296:ASN:HB3	1:U:657:PHE:CZ	2.55	0.41
1:U:565:TYR:C	1:U:567:LEU:H	2.28	0.41
2:V:229:THR:HB	2:V:233:GLY:CA	2.47	0.41
1:W:433:PHE:HA	1:W:434:PRO:HD3	1.89	0.41
1:W:495:LYS:CD	1:W:514:TYR:OH	2.69	0.41
1:W:499:PRO:HB2	1:W:745:THR:HG21	2.02	0.41
2:X:15:ASP:HB2	2:X:63:TYR:CG	2.56	0.41
2:X:210:PHE:O	2:X:233:GLY:HA2	2.20	0.41
1:A:476:GLN:OE1	1:A:708:ARG:NH2	2.54	0.41
1:C:195:ASN:HD21	1:C:354:TRP:CD1	2.39	0.41
1:E:65:GLY:HA3	2:F:21:MET:HG3	2.03	0.41
1:E:721:GLN:NE2	8:E:1287:HOH:O	2.53	0.41
1:G:56:LYS:HG2	1:G:57:THR:N	2.35	0.41
1:G:144:HIS:CE1	3:G:901:ACT:OXT	2.74	0.41
1:G:164:MET:HE2	1:G:494:TRP:CZ3	2.56	0.41
1:G:350:GLY:O	1:G:390:THR:HG21	2.21	0.41
1:G:823:TYR:CE2	1:G:825:PRO:HG3	2.56	0.41
1:I:730:TYR:HB3	1:I:862:VAL:CA	2.51	0.41
1:I:744:HIS:HA	1:I:819:SER:CB	2.51	0.41
1:K:499:PRO:HG3	5:K:903:MGD:O5'	2.21	0.41
1:K:610:LYS:HB3	1:K:614:ALA:HB3	2.02	0.41
2:L:23:CYS:O	2:L:27:HIS:N	2.44	0.41
2:L:46:MET:HE1	2:L:65:PRO:C	2.46	0.41
2:L:103:LYS:HG2	2:L:116:TRP:CD2	2.56	0.41
1:M:800:ILE:C	1:M:801:LEU:HG	2.46	0.41
2:N:4:TYR:CE2	2:N:158:LYS:HD2	2.56	0.41
1:O:176:TRP:O	1:O:179:TRP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:408:GLY:HA2	1:O:619:TYR:HE1	1.86	0.41
1:Q:436:PRO:HG3	8:Q:1461:HOH:O	2.21	0.41
1:Q:691:ILE:HG12	1:Q:711:MET:HB2	2.03	0.41
1:Q:722:LYS:HD3	8:Q:1563:HOH:O	2.20	0.41
1:Q:753:TYR:CE1	2:R:28:GLU:HG3	2.56	0.41
1:S:139:SER:CB	1:S:161:MET:HE2	2.51	0.41
1:S:558:SER:H	1:S:564:ASN:HD22	1.66	0.41
2:T:44:ARG:HG2	2:T:44:ARG:NH1	2.36	0.41
1:U:428:ASP:HB2	8:U:1235:HOH:O	2.21	0.41
1:U:451:LYS:HG3	1:U:461:PHE:CE2	2.56	0.41
1:U:550:ASP:HA	1:U:616:CYS:SG	2.61	0.41
1:W:128:ILE:CG2	1:W:136:ALA:HB3	2.51	0.41
1:W:755:ASN:OD1	1:W:761:ARG:HD2	2.21	0.41
1:A:565:TYR:CE2	1:A:571:ARG:HD2	2.56	0.40
2:B:124:GLN:O	2:B:125:LYS:HB3	2.22	0.40
2:B:142:MET:HE3	2:B:146:ALA:CB	2.51	0.40
1:C:114:TRP:CZ2	1:C:587:MET:HG2	2.57	0.40
1:C:134:PRO:HD2	8:C:1363:HOH:O	2.21	0.40
1:C:173:PRO:HG3	1:C:180:HIS:CG	2.56	0.40
2:D:69:MET:O	2:D:70:HIS:C	2.63	0.40
2:D:177:LYS:HD3	2:D:180:LEU:HD11	2.02	0.40
2:F:20:PHE:CE2	2:F:24:MET:HE2	2.55	0.40
2:H:201:ALA:HB3	2:H:235:PHE:CE2	2.55	0.40
2:H:210:PHE:CD2	2:H:213:ALA:HB2	2.54	0.40
1:I:74:LEU:HD23	1:I:74:LEU:HA	1.82	0.40
2:J:68:CYS:HB2	2:J:126:CYS:HB2	2.04	0.40
2:J:166:LYS:HG2	2:J:170:GLU:OE2	2.22	0.40
1:K:116:GLU:O	1:K:120:ILE:HG13	2.21	0.40
1:M:656:TRP:CD2	1:M:663:LYS:HA	2.56	0.40
2:N:16:CYS:O	2:N:17:ASN:HB2	2.21	0.40
2:N:75:PRO:HD2	7:N:304:SF4:S4	2.61	0.40
1:O:806:THR:OG1	1:O:807:GLU:N	2.54	0.40
1:S:783:GLY:O	1:S:866:LYS:HD2	2.22	0.40
1:S:845:ASP:OD2	1:S:845:ASP:N	2.48	0.40
1:U:25:ILE:HG13	1:U:580:ILE:HG21	2.02	0.40
1:U:78:TYR:O	1:U:79:PRO:C	2.64	0.40
1:U:771:ILE:HG22	1:U:772:MET:N	2.35	0.40
1:U:791:ARG:NH2	8:U:1584:HOH:O	2.36	0.40
1:U:867:TRP:CD1	1:U:869:GLY:H	2.38	0.40
1:W:468:PHE:N	1:W:468:PHE:CD1	2.89	0.40
1:W:571:ARG:HB2	1:W:642:VAL:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:734:MET:HB2	1:W:814:VAL:HG23	2.03	0.40
2:X:7:VAL:HG13	2:X:173:LEU:HD22	2.02	0.40
2:B:177:LYS:HD3	2:B:180:LEU:HD11	2.04	0.40
1:C:528:TRP:CG	1:C:750:LYS:HD3	2.56	0.40
1:C:848:ILE:HG13	1:C:854:GLY:O	2.21	0.40
1:E:66:PHE:CD1	1:E:69:MET:CE	3.05	0.40
1:E:770:TRP:HB3	1:E:801:LEU:HD23	2.02	0.40
2:F:39:MET:HE2	2:F:45:TRP:CD2	2.57	0.40
1:G:454:GLU:H	1:G:454:GLU:CD	2.29	0.40
1:G:499:PRO:HG3	5:G:903:MGD:O5'	2.21	0.40
1:G:722:LYS:HG2	8:G:1568:HOH:O	2.21	0.40
1:G:736:SER:OG	5:G:903:MGD:N19	2.51	0.40
2:H:196:LYS:HD3	2:H:196:LYS:HA	1.87	0.40
1:I:138:LEU:HD12	1:I:167:THR:O	2.21	0.40
1:I:189:PHE:HZ	1:I:654:LEU:HD21	1.87	0.40
1:I:774:VAL:O	1:I:805:VAL:HA	2.20	0.40
1:K:142:SER:CB	5:K:903:MGD:O1A	2.69	0.40
2:L:69:MET:HB2	7:L:304:SF4:S2	2.61	0.40
1:O:104:ASP:N	1:O:105:PRO:HD3	2.36	0.40
1:O:153:ARG:O	1:O:157:TYR:HB3	2.21	0.40
1:O:192:ARG:NH2	1:O:562:PRO:HB2	2.37	0.40
2:P:139:ALA:N	2:P:140:PRO:CD	2.85	0.40
1:Q:12:THR:HG23	8:Q:1331:HOH:O	2.21	0.40
1:Q:15:PRO:HD3	1:Q:554:PHE:CE1	2.57	0.40
1:S:699:GLU:HG2	1:S:699:GLU:H	1.63	0.40
2:T:106:LEU:HD23	2:T:114:MET:HG3	2.03	0.40
1:U:73:ASP:HB3	8:U:1622:HOH:O	2.20	0.40
1:U:730:TYR:HB3	1:U:862:VAL:CA	2.51	0.40
2:V:164:MET:O	2:V:168:VAL:HG23	2.22	0.40
1:W:361:SER:N	1:W:856:ALA:HB1	2.35	0.40
1:W:401:PHE:HA	1:W:402:PRO:HD3	1.94	0.40
1:W:402:PRO:HB2	1:W:619:TYR:OH	2.22	0.40
1:W:422:PHE:O	1:W:423:ALA:C	2.64	0.40
1:W:426:MET:HE1	1:W:618:GLN:C	2.46	0.40
1:W:729:LYS:HD2	8:W:1134:HOH:O	2.19	0.40
2:X:35:TYR:O	2:X:36:THR:HB	2.21	0.40
1:A:296:ASN:HB3	1:A:657:PHE:CZ	2.56	0.40
1:A:726:LEU:HD12	1:A:726:LEU:HA	1.96	0.40
1:C:11:SER:C	1:C:13:GLY:N	2.79	0.40
1:C:501:LEU:HA	1:C:507:THR:HB	2.04	0.40
2:D:124:GLN:O	2:D:125:LYS:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ILE:HA	1:E:77:PRO:HD3	1.79	0.40
1:E:220:GLU:CD	1:E:235:ARG:HH21	2.30	0.40
1:G:118:THR:O	1:G:122:VAL:HG23	2.21	0.40
1:G:217:SER:C	1:G:219:PRO:HD3	2.46	0.40
1:G:253:ASN:O	1:G:257:ARG:HG3	2.20	0.40
1:G:476:GLN:OE1	1:G:708:ARG:NH2	2.54	0.40
1:G:501:LEU:HD13	1:G:823:TYR:CG	2.56	0.40
1:G:855:MET:HE2	1:G:857:ASN:OD1	2.21	0.40
1:I:512:LYS:HA	8:I:1367:HOH:O	2.21	0.40
1:I:855:MET:HB2	1:I:857:ASN:OD1	2.21	0.40
2:J:201:ALA:HB3	2:J:235:PHE:CE2	2.56	0.40
1:K:748:ASP:O	1:K:750:LYS:HG3	2.20	0.40
2:L:213:ALA:CB	2:L:251:ALA:HB2	2.51	0.40
1:M:162:ASN:ND2	1:M:437:SER:HB2	2.36	0.40
1:M:227:ALA:O	1:M:230:GLU:HG2	2.20	0.40
1:M:280:TYR:OH	1:M:284:LYS:HE3	2.21	0.40
1:M:695:LEU:O	1:M:699:GLU:HG2	2.22	0.40
1:M:724:SER:HA	1:M:725:PRO:HD3	1.99	0.40
2:N:189:LYS:O	2:N:190:ASN:HB2	2.22	0.40
1:O:521:PHE:CE2	1:O:523:VAL:CG2	3.04	0.40
1:O:767:TYR:HB3	1:O:769:TYR:CE1	2.56	0.40
1:Q:187:TRP:CH2	1:Q:196:PRO:HB3	2.56	0.40
1:Q:650:LYS:HG2	8:S:1004:HOH:O	2.21	0.40
1:Q:855:MET:HE2	1:Q:857:ASN:ND2	2.36	0.40
2:R:164:MET:HE3	2:R:167:LYS:HB3	2.03	0.40
1:S:99:GLY:N	1:S:108:ASP:OD2	2.44	0.40
1:S:328:PRO:O	1:S:332:ILE:HG13	2.21	0.40
1:S:503:THR:HA	1:S:840:ASN:ND2	2.35	0.40
1:S:510:TYR:O	1:S:513:MET:HG2	2.21	0.40
1:S:540:LEU:HA	1:S:541:PRO:HD3	1.79	0.40
1:S:541:PRO:HB2	1:S:586:SER:HA	2.03	0.40
1:S:620:PHE:CZ	1:S:625:MET:HB3	2.56	0.40
2:T:199:VAL:HG13	2:T:199:VAL:O	2.21	0.40
1:W:21:LYS:HB2	1:W:26:ILE:HD11	2.04	0.40
1:W:153:ARG:O	1:W:157:TYR:HB3	2.21	0.40
1:W:155:SER:O	1:W:410:SER:HB3	2.20	0.40
1:W:395:LEU:HD13	1:W:571:ARG:HG2	2.03	0.40
2:X:26:GLU:HB2	2:X:144:ARG:HH11	1.84	0.40
2:X:206:GLN:N	8:X:425:HOH:O	2.55	0.40
2:X:218:LYS:HG2	2:X:222:LYS:C	2.45	0.40
1:A:721:GLN:NE2	8:A:1286:HOH:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:MET:CE	2:B:146:ALA:HB1	2.50	0.40
1:C:433:PHE:HA	1:C:434:PRO:HD3	1.81	0.40
1:C:724:SER:HA	1:C:725:PRO:HD3	1.95	0.40
2:D:46:MET:CE	2:D:66:THR:H	2.34	0.40
2:D:87:ARG:HG3	2:D:91:ILE:O	2.22	0.40
1:E:311:THR:HG21	8:E:1501:HOH:O	2.22	0.40
1:E:642:VAL:HA	1:E:643:PRO:HD3	1.90	0.40
1:E:782:ARG:HG3	1:E:782:ARG:HH11	1.87	0.40
1:E:831:LYS:O	1:E:873:GLU:HA	2.21	0.40
1:G:739:PRO:HG2	1:G:742:SER:O	2.22	0.40
1:I:767:TYR:HB3	1:I:769:TYR:CE1	2.57	0.40
1:I:825:PRO:HD2	8:I:1339:HOH:O	2.21	0.40
1:K:433:PHE:HA	1:K:434:PRO:HD3	1.84	0.40
1:K:482:TYR:HA	1:K:483:PRO:C	2.46	0.40
1:K:560[A]:TYR:C	1:K:562:PRO:HD3	2.45	0.40
1:K:587:MET:HG3	1:K:592:ILE:HG13	2.03	0.40
1:M:540:LEU:HA	1:M:541:PRO:HD3	1.74	0.40
2:N:23:CYS:O	2:N:26:GLU:N	2.55	0.40
1:O:553:GLU:HB3	1:O:556:ASN:HB3	2.04	0.40
1:Q:162:ASN:ND2	1:Q:437:SER:HB2	2.36	0.40
2:R:167:LYS:HG3	2:R:171:GLU:OE2	2.20	0.40
1:S:152:TYR:CD2	1:S:154:HIS:HD2	2.40	0.40
1:S:651:THR:HB	1:S:665:THR:HG22	2.04	0.40
2:T:7:VAL:HB	2:T:155:GLU:HB3	2.03	0.40
2:T:166:LYS:HG2	2:T:170:GLU:OE2	2.22	0.40
2:T:211:GLU:HG3	2:T:230:ASN:C	2.46	0.40
1:U:426:MET:HE3	1:U:622:ALA:HB2	2.02	0.40
1:U:656:TRP:CD2	1:U:663:LYS:HA	2.56	0.40
1:W:427:PHE:HA	1:W:432:THR:HG23	2.04	0.40
1:W:775:ASN:HA	1:W:806:THR:O	2.21	0.40
1:A:55:ARG:HD2	8:A:1645:HOH:O	2.20	0.40
1:A:119:ASP:OD1	1:A:599:LYS:HE2	2.22	0.40
1:A:505:THR:HG22	1:A:857:ASN:HD21	1.86	0.40
1:E:625:MET:N	1:E:626:PRO:CD	2.84	0.40
1:E:693:THR:HG22	8:E:1626:HOH:O	2.20	0.40
1:G:30:PRO:HG3	1:G:59:ILE:HG12	2.03	0.40
1:G:354:TRP:HB3	1:G:355:GLY:H	1.67	0.40
1:G:753:TYR:CE1	2:H:28:GLU:HG3	2.56	0.40
2:H:46:MET:HE1	2:H:65:PRO:HA	2.04	0.40
1:I:262:LYS:HG2	2:J:232:PHE:CE1	2.56	0.40
1:I:292:TYR:CD2	1:I:378:GLY:HA2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:724:SER:OG	1:I:726:LEU:HB2	2.21	0.40
1:K:11:SER:HA	1:K:147:TRP:HB2	2.03	0.40
1:M:737:PRO:HG3	5:M:904:MGD:H2'	2.03	0.40
1:O:602:ILE:CG2	8:O:1075:HOH:O	2.68	0.40
1:O:649:LYS:HE3	1:O:651:THR:HG22	2.04	0.40
2:P:73:ASN:O	2:P:75:PRO:HD3	2.21	0.40
2:P:142:MET:HE3	2:P:146:ALA:HB1	2.04	0.40
1:Q:250:PRO:HD3	5:Q:904:MGD:C2	2.51	0.40
1:Q:553:GLU:HB3	1:Q:556:ASN:HB2	2.03	0.40
1:S:78:TYR:CD1	1:S:111:ARG:HG3	2.57	0.40
1:S:132:TYR:CD2	1:S:491:LYS:HG3	2.57	0.40
1:S:274:LEU:O	1:S:278:ILE:HG13	2.22	0.40
2:T:58:ARG:NE	2:T:234:GLU:OE2	2.51	0.40
1:U:171:HIS:O	1:U:467:GLY:HA2	2.21	0.40
1:U:252:MET:HB3	1:U:808:CYS:HB3	2.03	0.40
2:V:69:MET:O	2:V:70:HIS:C	2.65	0.40
1:W:102:LYS:HE2	8:W:1489:HOH:O	2.21	0.40
2:X:73:ASN:C	2:X:73:ASN:ND2	2.78	0.40
2:X:115:TYR:CD1	2:X:115:TYR:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	875/875 (100%)	821 (94%)	49 (6%)	5 (1%)	21	24
1	C	875/875 (100%)	804 (92%)	65 (7%)	6 (1%)	18	20
1	E	875/875 (100%)	807 (92%)	61 (7%)	7 (1%)	16	17
1	G	875/875 (100%)	820 (94%)	50 (6%)	5 (1%)	21	24
1	I	875/875 (100%)	816 (93%)	54 (6%)	5 (1%)	21	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	875/875 (100%)	813 (93%)	57 (6%)	5 (1%)	21	24
1	M	875/875 (100%)	814 (93%)	57 (6%)	4 (0%)	24	27
1	O	875/875 (100%)	819 (94%)	51 (6%)	5 (1%)	21	24
1	Q	875/875 (100%)	815 (93%)	52 (6%)	8 (1%)	14	14
1	S	875/875 (100%)	815 (93%)	52 (6%)	8 (1%)	14	14
1	U	875/875 (100%)	808 (92%)	63 (7%)	4 (0%)	24	27
1	W	875/875 (100%)	803 (92%)	65 (7%)	7 (1%)	16	17
2	B	272/274 (99%)	256 (94%)	15 (6%)	1 (0%)	30	34
2	D	272/274 (99%)	254 (93%)	17 (6%)	1 (0%)	30	34
2	F	272/274 (99%)	249 (92%)	22 (8%)	1 (0%)	30	34
2	H	272/274 (99%)	255 (94%)	16 (6%)	1 (0%)	30	34
2	J	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	34
2	L	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	34
2	N	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	30	34
2	P	272/274 (99%)	254 (93%)	17 (6%)	1 (0%)	30	34
2	R	272/274 (99%)	259 (95%)	12 (4%)	1 (0%)	30	34
2	T	272/274 (99%)	251 (92%)	20 (7%)	1 (0%)	30	34
2	V	272/274 (99%)	257 (94%)	13 (5%)	2 (1%)	18	20
2	X	272/274 (99%)	239 (88%)	30 (11%)	3 (1%)	11	11
All	All	13764/13788 (100%)	12807 (93%)	873 (6%)	84 (1%)	21	24

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	C	177	GLU
1	E	177	GLU
1	G	177	GLU
1	G	225	ILE
1	I	177	GLU
1	I	225	ILE
1	K	177	GLU
1	K	225	ILE
1	O	141	PRO
1	O	177	GLU

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Mol	Chain	Res	Type
1	Q	177	GLU
1	S	177	GLU
1	U	177	GLU
1	W	177	GLU
1	A	141	PRO
1	C	141	PRO
1	E	225	ILE
1	K	141	PRO
1	M	177	GLU
1	O	225	ILE
1	Q	225	ILE
1	S	141	PRO
1	U	225	ILE
1	W	141	PRO
1	C	531	GLY
1	E	35	ASP
1	E	141	PRO
1	G	141	PRO
1	I	141	PRO
1	K	858	ASN
1	M	141	PRO
2	P	67	PRO
1	Q	141	PRO
1	Q	228	GLY
1	S	35	ASP
1	U	141	PRO
1	U	858	ASN
1	W	225	ILE
1	A	648	ARG
2	D	67	PRO
2	F	67	PRO
1	K	507	THR
1	M	225	ILE
1	M	858	ASN
2	N	67	PRO
1	S	507	THR
1	S	555	ALA
1	S	858	ASN
1	W	35	ASP
2	X	81	ASN
2	X	221	GLY
1	A	225	ILE

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Mol	Chain	Res	Type
1	C	225	ILE
1	C	421	LYS
1	E	252	MET
1	E	421	LYS
1	E	808	CYS
2	J	67	PRO
1	O	858	ASN
1	Q	253	ASN
1	Q	421	LYS
2	R	67	PRO
1	S	225	ILE
2	V	19	CYS
1	W	786	ASN
1	W	808	CYS
1	I	421	LYS
1	S	228	GLY
2	V	221	GLY
2	X	129	CYS
2	H	67	PRO
2	B	67	PRO
1	G	534	PRO
1	Q	182	GLY
1	Q	531	GLY
1	W	228	GLY
1	C	394	PRO
2	L	221	GLY
1	G	737	PRO
1	I	394	PRO
1	O	394	PRO
2	T	67	PRO
1	A	394	PRO

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	731/729 (100%)	716 (98%)	15 (2%)	47	61
1	C	731/729 (100%)	722 (99%)	9 (1%)	63	77
1	E	731/729 (100%)	723 (99%)	8 (1%)	65	79
1	G	731/729 (100%)	719 (98%)	12 (2%)	55	70
1	I	731/729 (100%)	721 (99%)	10 (1%)	59	73
1	K	731/729 (100%)	721 (99%)	10 (1%)	59	73
1	M	731/729 (100%)	720 (98%)	11 (2%)	57	72
1	O	731/729 (100%)	718 (98%)	13 (2%)	51	66
1	Q	731/729 (100%)	718 (98%)	13 (2%)	51	66
1	S	731/729 (100%)	722 (99%)	9 (1%)	63	77
1	U	731/729 (100%)	723 (99%)	8 (1%)	65	79
1	W	731/729 (100%)	724 (99%)	7 (1%)	68	81
2	B	235/235 (100%)	225 (96%)	10 (4%)	26	34
2	D	235/235 (100%)	222 (94%)	13 (6%)	19	24
2	F	235/235 (100%)	223 (95%)	12 (5%)	21	26
2	H	235/235 (100%)	222 (94%)	13 (6%)	19	24
2	J	235/235 (100%)	225 (96%)	10 (4%)	26	34
2	L	235/235 (100%)	224 (95%)	11 (5%)	23	30
2	N	235/235 (100%)	223 (95%)	12 (5%)	21	26
2	P	235/235 (100%)	226 (96%)	9 (4%)	29	39
2	R	235/235 (100%)	225 (96%)	10 (4%)	26	34
2	T	235/235 (100%)	223 (95%)	12 (5%)	21	26
2	V	235/235 (100%)	224 (95%)	11 (5%)	23	30
2	X	235/235 (100%)	225 (96%)	10 (4%)	26	34
All	All	11592/11568 (100%)	11334 (98%)	258 (2%)	47	59

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	A	142	SER
1	A	373	LEU

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Mol	Chain	Res	Type
1	A	379	MET
1	A	426	MET
1	A	499	PRO
1	A	560[A]	TYR
1	A	560[B]	TYR
1	A	564	ASN
1	A	599	LYS
1	A	605	MET
1	A	726	LEU
1	A	743	MET
1	A	800	ILE
1	A	839	ILE
2	B	19	CYS
2	B	21	MET
2	B	24	MET
2	B	71	CYS
2	B	104	GLU
2	B	109	CYS
2	B	129	CYS
2	B	145	CYS
2	B	149	CYS
2	B	157	LEU
1	C	108	ASP
1	C	142	SER
1	C	373	LEU
1	C	499	PRO
1	C	560[A]	TYR
1	C	560[B]	TYR
1	C	605	MET
1	C	743	MET
1	C	780	GLU
2	D	13	CYS
2	D	17	ASN
2	D	19	CYS
2	D	21	MET
2	D	71	CYS
2	D	73	ASN
2	D	104	GLU
2	D	109	CYS
2	D	129	CYS
2	D	145	CYS
2	D	149	CYS

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Mol	Chain	Res	Type
2	D	157	LEU
2	D	252	ASP
1	E	142	SER
1	E	499	PRO
1	E	560[A]	TYR
1	E	560[B]	TYR
1	E	564	ASN
1	E	678	ARG
1	E	726	LEU
1	E	800	ILE
2	F	13	CYS
2	F	19	CYS
2	F	21	MET
2	F	24	MET
2	F	67	PRO
2	F	71	CYS
2	F	109	CYS
2	F	129	CYS
2	F	145	CYS
2	F	149	CYS
2	F	157	LEU
2	F	252	ASP
1	G	100	LEU
1	G	142	SER
1	G	274	LEU
1	G	373	LEU
1	G	414	GLU
1	G	426	MET
1	G	499	PRO
1	G	564	ASN
1	G	605	MET
1	G	726	LEU
1	G	743	MET
1	G	800	ILE
2	H	13	CYS
2	H	19	CYS
2	H	21	MET
2	H	24	MET
2	H	29	LEU
2	H	71	CYS
2	H	76	CYS
2	H	109	CYS

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Mol	Chain	Res	Type
2	H	129	CYS
2	H	145	CYS
2	H	148	ASN
2	H	149	CYS
2	H	157	LEU
1	I	142	SER
1	I	373	LEU
1	I	499	PRO
1	I	560[A]	TYR
1	I	560[B]	TYR
1	I	564	ASN
1	I	726	LEU
1	I	743	MET
1	I	800	ILE
1	I	839	ILE
2	J	13	CYS
2	J	19	CYS
2	J	21	MET
2	J	71	CYS
2	J	76	CYS
2	J	109	CYS
2	J	114	MET
2	J	129	CYS
2	J	145	CYS
2	J	149	CYS
1	K	142	SER
1	K	414	GLU
1	K	499	PRO
1	K	560[A]	TYR
1	K	560[B]	TYR
1	K	564	ASN
1	K	582	PRO
1	K	605	MET
1	K	708	ARG
1	K	726	LEU
2	L	13	CYS
2	L	19	CYS
2	L	21	MET
2	L	24	MET
2	L	59	ASN
2	L	71	CYS
2	L	109	CYS

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Mol	Chain	Res	Type
2	L	129	CYS
2	L	145	CYS
2	L	149	CYS
2	L	157	LEU
1	M	142	SER
1	M	272	HIS
1	M	373	LEU
1	M	426	MET
1	M	560[A]	TYR
1	M	560[B]	TYR
1	M	564	ASN
1	M	743	MET
1	M	786	ASN
1	M	818	GLU
1	M	839	ILE
2	N	13	CYS
2	N	19	CYS
2	N	21	MET
2	N	24	MET
2	N	29	LEU
2	N	57	PRO
2	N	71	CYS
2	N	109	CYS
2	N	129	CYS
2	N	145	CYS
2	N	149	CYS
2	N	157	LEU
1	O	142	SER
1	O	373	LEU
1	O	426	MET
1	O	499	PRO
1	O	560[A]	TYR
1	O	560[B]	TYR
1	O	564	ASN
1	O	582	PRO
1	O	605	MET
1	O	726	LEU
1	O	743	MET
1	O	786	ASN
1	O	841	ILE
2	P	13	CYS
2	P	19	CYS

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Mol	Chain	Res	Type
2	P	21	MET
2	P	24	MET
2	P	71	CYS
2	P	109	CYS
2	P	129	CYS
2	P	145	CYS
2	P	149	CYS
1	Q	100	LEU
1	Q	142	SER
1	Q	373	LEU
1	Q	499	PRO
1	Q	560[A]	TYR
1	Q	560[B]	TYR
1	Q	564	ASN
1	Q	599	LYS
1	Q	678	ARG
1	Q	726	LEU
1	Q	743	MET
1	Q	801	LEU
1	Q	839	ILE
2	R	13	CYS
2	R	19	CYS
2	R	21	MET
2	R	71	CYS
2	R	76	CYS
2	R	109	CYS
2	R	129	CYS
2	R	145	CYS
2	R	149	CYS
2	R	157	LEU
1	S	17	PHE
1	S	142	SER
1	S	373	LEU
1	S	499	PRO
1	S	605	MET
1	S	678	ARG
1	S	726	LEU
1	S	743	MET
1	S	786	ASN
2	T	13	CYS
2	T	19	CYS
2	T	21	MET

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Mol	Chain	Res	Type
2	T	24	MET
2	T	57	PRO
2	T	71	CYS
2	T	104	GLU
2	T	109	CYS
2	T	129	CYS
2	T	145	CYS
2	T	149	CYS
2	T	157	LEU
1	U	426	MET
1	U	499	PRO
1	U	560[A]	TYR
1	U	560[B]	TYR
1	U	564	ASN
1	U	726	LEU
1	U	743	MET
1	U	786	ASN
2	V	13	CYS
2	V	19	CYS
2	V	21	MET
2	V	24	MET
2	V	59	ASN
2	V	71	CYS
2	V	73	ASN
2	V	109	CYS
2	V	129	CYS
2	V	145	CYS
2	V	149	CYS
1	W	272	HIS
1	W	499	PRO
1	W	560[A]	TYR
1	W	560[B]	TYR
1	W	564	ASN
1	W	608	GLU
1	W	743	MET
2	X	13	CYS
2	X	17	ASN
2	X	19	CYS
2	X	21	MET
2	X	29	LEU
2	X	71	CYS
2	X	129	CYS

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Mol	Chain	Res	Type
2	X	145	CYS
2	X	149	CYS
2	X	252	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (278) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	130	HIS
1	A	154	HIS
1	A	162	ASN
1	A	222	ASN
1	A	232	ASN
1	A	298	HIS
1	A	440	ASN
1	A	478	HIS
1	A	525	GLN
1	A	564	ASN
1	A	618	GLN
1	A	621	ASN
1	A	673	ASN
1	A	674	ASN
1	A	697	ASN
1	A	701	GLN
1	A	723	HIS
1	A	786	ASN
2	B	40	GLN
2	B	59	ASN
2	B	70	HIS
2	B	73	ASN
2	B	81	ASN
1	C	130	HIS
1	C	154	HIS
1	C	162	ASN
1	C	171	HIS
1	C	222	ASN
1	C	440	ASN
1	C	462	GLN
1	C	478	HIS
1	C	525	GLN
1	C	564	ASN
1	C	576	GLN

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Mol	Chain	Res	Type
1	C	618	GLN
1	C	674	ASN
1	C	697	ASN
1	C	701	GLN
1	C	721	GLN
1	C	786	ASN
2	D	17	ASN
2	D	18	ASN
2	D	27	HIS
2	D	40	GLN
2	D	59	ASN
2	D	73	ASN
2	D	81	ASN
2	D	121	ASN
1	E	162	ASN
1	E	222	ASN
1	E	391	GLN
1	E	440	ASN
1	E	462	GLN
1	E	478	HIS
1	E	525	GLN
1	E	564	ASN
1	E	618	GLN
1	E	647	ASN
1	E	674	ASN
1	E	697	ASN
1	E	701	GLN
1	E	786	ASN
1	E	810	GLN
2	F	27	HIS
2	F	30	ASN
2	F	40	GLN
2	F	59	ASN
2	F	70	HIS
2	F	73	ASN
2	F	81	ASN
1	G	154	HIS
1	G	162	ASN
1	G	171	HIS
1	G	391	GLN
1	G	415	ASN
1	G	440	ASN

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Mol	Chain	Res	Type
1	G	478	HIS
1	G	525	GLN
1	G	564	ASN
1	G	576	GLN
1	G	618	GLN
1	G	674	ASN
1	G	697	ASN
1	G	701	GLN
1	G	721	GLN
1	G	786	ASN
1	G	810	GLN
2	H	27	HIS
2	H	40	GLN
2	H	59	ASN
2	H	70	HIS
2	H	73	ASN
2	H	81	ASN
1	I	154	HIS
1	I	162	ASN
1	I	391	GLN
1	I	415	ASN
1	I	440	ASN
1	I	462	GLN
1	I	478	HIS
1	I	525	GLN
1	I	564	ASN
1	I	576	GLN
1	I	618	GLN
1	I	673	ASN
1	I	674	ASN
1	I	697	ASN
1	I	701	GLN
1	I	721	GLN
1	I	786	ASN
1	I	804	GLN
2	J	17	ASN
2	J	18	ASN
2	J	40	GLN
2	J	59	ASN
2	J	70	HIS
2	J	73	ASN
1	K	154	HIS

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Mol	Chain	Res	Type
1	K	162	ASN
1	K	222	ASN
1	K	391	GLN
1	K	462	GLN
1	K	478	HIS
1	K	525	GLN
1	K	564	ASN
1	K	576	GLN
1	K	618	GLN
1	K	647	ASN
1	K	673	ASN
1	K	674	ASN
1	K	697	ASN
1	K	701	GLN
1	K	721	GLN
1	K	786	ASN
2	L	40	GLN
2	L	59	ASN
2	L	70	HIS
2	L	73	ASN
2	L	81	ASN
2	L	86	GLN
1	M	88	ASN
1	M	154	HIS
1	M	162	ASN
1	M	232	ASN
1	M	298	HIS
1	M	391	GLN
1	M	415	ASN
1	M	440	ASN
1	M	462	GLN
1	M	478	HIS
1	M	525	GLN
1	M	564	ASN
1	M	576	GLN
1	M	618	GLN
1	M	673	ASN
1	M	697	ASN
1	M	701	GLN
1	M	721	GLN
1	M	786	ASN
2	N	18	ASN

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Mol	Chain	Res	Type
2	N	59	ASN
2	N	70	HIS
2	N	73	ASN
2	N	190	ASN
1	O	154	HIS
1	O	162	ASN
1	O	171	HIS
1	O	222	ASN
1	O	415	ASN
1	O	440	ASN
1	O	462	GLN
1	O	478	HIS
1	O	525	GLN
1	O	564	ASN
1	O	618	GLN
1	O	673	ASN
1	O	674	ASN
1	O	697	ASN
1	O	701	GLN
1	O	721	GLN
1	O	786	ASN
2	P	18	ASN
2	P	30	ASN
2	P	40	GLN
2	P	59	ASN
2	P	70	HIS
2	P	81	ASN
2	P	121	ASN
1	Q	154	HIS
1	Q	162	ASN
1	Q	171	HIS
1	Q	391	GLN
1	Q	462	GLN
1	Q	478	HIS
1	Q	525	GLN
1	Q	564	ASN
1	Q	576	GLN
1	Q	618	GLN
1	Q	621	ASN
1	Q	697	ASN
1	Q	701	GLN
1	Q	721	GLN

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Mol	Chain	Res	Type
1	Q	786	ASN
2	R	27	HIS
2	R	40	GLN
2	R	59	ASN
2	R	70	HIS
2	R	73	ASN
2	R	81	ASN
1	S	88	ASN
1	S	154	HIS
1	S	162	ASN
1	S	208	HIS
1	S	222	ASN
1	S	478	HIS
1	S	525	GLN
1	S	564	ASN
1	S	576	GLN
1	S	618	GLN
1	S	674	ASN
1	S	697	ASN
1	S	701	GLN
1	S	707	HIS
1	S	786	ASN
2	T	3	GLN
2	T	18	ASN
2	T	40	GLN
2	T	59	ASN
2	T	73	ASN
1	U	154	HIS
1	U	162	ASN
1	U	171	HIS
1	U	222	ASN
1	U	232	ASN
1	U	415	ASN
1	U	440	ASN
1	U	478	HIS
1	U	525	GLN
1	U	564	ASN
1	U	618	GLN
1	U	673	ASN
1	U	674	ASN
1	U	697	ASN
1	U	701	GLN

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Mol	Chain	Res	Type
1	U	786	ASN
2	V	17	ASN
2	V	40	GLN
2	V	59	ASN
2	V	70	HIS
2	V	73	ASN
2	V	81	ASN
2	V	131	HIS
1	W	88	ASN
1	W	154	HIS
1	W	162	ASN
1	W	171	HIS
1	W	222	ASN
1	W	415	ASN
1	W	462	GLN
1	W	478	HIS
1	W	525	GLN
1	W	564	ASN
1	W	576	GLN
1	W	618	GLN
1	W	645	ASN
1	W	674	ASN
1	W	697	ASN
1	W	701	GLN
1	W	721	GLN
1	W	786	ASN
2	X	3	GLN
2	X	17	ASN
2	X	40	GLN
2	X	59	ASN
2	X	73	ASN
2	X	121	ASN
2	X	148	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 108 ligands modelled in this entry, 36 are monoatomic - leaving 72 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	S	901	6	3,3,3	1.27	0	3,3,3	1.02	0
7	SF4	R	304	2	0,12,12	-	-	-		
3	ACT	I	901	6	3,3,3	1.18	0	3,3,3	0.97	0
5	MGD	E	904	6	47,52,52	2.40	14 (29%)	58,81,81	1.10	2 (3%)
5	MGD	Q	904	6	47,52,52	2.21	14 (29%)	58,81,81	1.23	3 (5%)
3	ACT	E	901	6	3,3,3	1.17	0	3,3,3	1.17	0
5	MGD	W	904	6	47,52,52	2.25	14 (29%)	58,81,81	1.12	3 (5%)
5	MGD	M	904	6	47,52,52	2.30	14 (29%)	58,81,81	1.27	2 (3%)
7	SF4	X	303	2	0,12,12	-	-	-		
3	ACT	U	901	6	3,3,3	1.31	0	3,3,3	0.95	0
7	SF4	R	302	2	0,12,12	-	-	-		
5	MGD	C	904	6	47,52,52	2.34	14 (29%)	58,81,81	1.09	3 (5%)
5	MGD	G	903	6	47,52,52	2.18	14 (29%)	58,81,81	2.14	9 (15%)
5	MGD	I	904	6	47,52,52	2.19	13 (27%)	58,81,81	1.66	5 (8%)
3	ACT	W	901	6	3,3,3	1.31	0	3,3,3	0.82	0
7	SF4	F	304	2	0,12,12	-	-	-		
7	SF4	V	303	2	0,12,12	-	-	-		
7	SF4	H	304	2	0,12,12	-	-	-		
7	SF4	N	304	2	0,12,12	-	-	-		
7	SF4	V	304	2	0,12,12	-	-	-		
7	SF4	N	302	2	0,12,12	-	-	-		
7	SF4	B	304	2	0,12,12	-	-	-		
7	SF4	J	304	2	0,12,12	-	-	-		
7	SF4	L	303	2	0,12,12	-	-	-		
7	SF4	T	304	2	0,12,12	-	-	-		
7	SF4	X	304	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	A	901	6	3,3,3	1.28	0	3,3,3	0.85	0
7	SF4	L	304	2	0,12,12	-	-	-		
5	MGD	O	903	6	47,52,52	2.13	16 (34%)	58,81,81	2.14	7 (12%)
7	SF4	D	302	2	0,12,12	-	-	-		
5	MGD	E	903	6	47,52,52	2.20	15 (31%)	58,81,81	2.07	8 (13%)
5	MGD	G	904	6	47,52,52	2.15	14 (29%)	58,81,81	1.14	4 (6%)
7	SF4	B	302	2	0,12,12	-	-	-		
5	MGD	K	903	6	47,52,52	1.82	12 (25%)	58,81,81	2.06	7 (12%)
5	MGD	U	903	6	47,52,52	2.19	13 (27%)	58,81,81	2.14	9 (15%)
3	ACT	M	901	6	3,3,3	1.17	0	3,3,3	1.18	0
7	SF4	F	302	2	0,12,12	-	-	-		
3	ACT	C	901	6	3,3,3	1.11	0	3,3,3	1.07	0
7	SF4	H	302	2	0,12,12	-	-	-		
7	SF4	T	303	2	0,12,12	-	-	-		
7	SF4	D	304	2	0,12,12	-	-	-		
5	MGD	A	904	6	47,52,52	2.37	12 (25%)	58,81,81	1.21	4 (6%)
7	SF4	J	302	2	0,12,12	-	-	-		
5	MGD	S	903	6	47,52,52	1.95	13 (27%)	58,81,81	2.23	9 (15%)
7	SF4	P	303	2	0,12,12	-	-	-		
3	ACT	K	901	6	3,3,3	1.24	0	3,3,3	1.07	0
7	SF4	T	302	2	0,12,12	-	-	-		
7	SF4	X	302	2	0,12,12	-	-	-		
5	MGD	O	904	6	47,52,52	2.30	14 (29%)	58,81,81	1.19	3 (5%)
3	ACT	O	901	6	3,3,3	1.22	0	3,3,3	1.03	0
5	MGD	Q	903	6	47,52,52	2.14	15 (31%)	58,81,81	2.19	8 (13%)
5	MGD	I	903	6	47,52,52	2.30	11 (23%)	58,81,81	2.14	8 (13%)
5	MGD	U	904	6	47,52,52	2.34	14 (29%)	58,81,81	1.09	3 (5%)
7	SF4	F	303	2	0,12,12	-	-	-		
5	MGD	K	904	6	47,52,52	2.28	15 (31%)	58,81,81	1.16	3 (5%)
5	MGD	M	903	6	47,52,52	2.11	13 (27%)	58,81,81	2.17	9 (15%)
5	MGD	W	903	6	47,52,52	2.35	13 (27%)	58,81,81	1.98	7 (12%)
7	SF4	J	303	2	0,12,12	-	-	-		
3	ACT	G	901	6	3,3,3	1.20	0	3,3,3	1.05	0
7	SF4	V	302	2	0,12,12	-	-	-		
5	MGD	C	903	6	47,52,52	2.14	15 (31%)	58,81,81	2.09	7 (12%)
7	SF4	B	303	2	0,12,12	-	-	-		
7	SF4	L	302	2	0,12,12	-	-	-		
7	SF4	P	302	2	0,12,12	-	-	-		
7	SF4	P	304	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SF4	D	303	2	0,12,12	-	-	-		
5	MGD	S	904	6	47,52,52	2.31	14 (29%)	58,81,81	1.12	4 (6%)
7	SF4	H	303	2	0,12,12	-	-	-		
7	SF4	N	303	2	0,12,12	-	-	-		
7	SF4	R	303	2	0,12,12	-	-	-		
5	MGD	A	903	6	47,52,52	1.88	11 (23%)	58,81,81	2.09	7 (12%)
3	ACT	Q	901	6	3,3,3	1.23	0	3,3,3	0.93	0

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
7	SF4	R	304	2	-	-	0/6/5/5
5	MGD	E	904	6	-	5/22/66/66	0/6/6/6
5	MGD	Q	904	6	-	5/22/66/66	0/6/6/6
5	MGD	W	904	6	-	5/22/66/66	0/6/6/6
7	SF4	X	303	2	-	-	0/6/5/5
5	MGD	M	904	6	-	5/22/66/66	0/6/6/6
7	SF4	R	302	2	-	-	0/6/5/5
5	MGD	C	904	6	-	4/22/66/66	0/6/6/6
5	MGD	G	903	6	-	10/22/66/66	0/6/6/6
5	MGD	I	904	6	-	3/22/66/66	0/6/6/6
7	SF4	F	304	2	-	-	0/6/5/5
7	SF4	V	303	2	-	-	0/6/5/5
7	SF4	H	304	2	-	-	0/6/5/5
7	SF4	N	304	2	-	-	0/6/5/5
7	SF4	V	304	2	-	-	0/6/5/5
7	SF4	N	302	2	-	-	0/6/5/5
7	SF4	B	304	2	-	-	0/6/5/5
7	SF4	J	304	2	-	-	0/6/5/5
7	SF4	L	303	2	-	-	0/6/5/5
7	SF4	T	304	2	-	-	0/6/5/5
7	SF4	X	304	2	-	-	0/6/5/5
7	SF4	L	304	2	-	-	0/6/5/5
5	MGD	O	903	6	-	9/22/66/66	0/6/6/6
7	SF4	D	302	2	-	-	0/6/5/5
5	MGD	E	903	6	-	9/22/66/66	0/6/6/6
5	MGD	G	904	6	-	5/22/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	B	302	2	-	-	0/6/5/5
5	MGD	K	903	6	-	7/22/66/66	0/6/6/6
5	MGD	U	903	6	-	9/22/66/66	0/6/6/6
7	SF4	F	302	2	-	-	0/6/5/5
7	SF4	H	302	2	-	-	0/6/5/5
7	SF4	T	303	2	-	-	0/6/5/5
7	SF4	D	304	2	-	-	0/6/5/5
5	MGD	A	904	6	-	5/22/66/66	0/6/6/6
7	SF4	J	302	2	-	-	0/6/5/5
5	MGD	S	903	6	-	11/22/66/66	0/6/6/6
7	SF4	P	303	2	-	-	0/6/5/5
7	SF4	T	302	2	-	-	0/6/5/5
7	SF4	X	302	2	-	-	0/6/5/5
5	MGD	O	904	6	-	4/22/66/66	0/6/6/6
5	MGD	Q	903	6	-	7/22/66/66	0/6/6/6
5	MGD	U	904	6	-	4/22/66/66	0/6/6/6
5	MGD	I	903	6	-	7/22/66/66	0/6/6/6
7	SF4	F	303	2	-	-	0/6/5/5
5	MGD	K	904	6	-	4/22/66/66	0/6/6/6
5	MGD	M	903	6	-	8/22/66/66	0/6/6/6
5	MGD	W	903	6	-	10/22/66/66	0/6/6/6
7	SF4	J	303	2	-	-	0/6/5/5
7	SF4	V	302	2	-	-	0/6/5/5
5	MGD	C	903	6	-	7/22/66/66	0/6/6/6
7	SF4	B	303	2	-	-	0/6/5/5
7	SF4	L	302	2	-	-	0/6/5/5
7	SF4	P	302	2	-	-	0/6/5/5
7	SF4	P	304	2	-	-	0/6/5/5
7	SF4	D	303	2	-	-	0/6/5/5
5	MGD	S	904	6	-	4/22/66/66	0/6/6/6
7	SF4	H	303	2	-	-	0/6/5/5
7	SF4	N	303	2	-	-	0/6/5/5
7	SF4	R	303	2	-	-	0/6/5/5
5	MGD	A	903	6	-	7/22/66/66	0/6/6/6

All (327) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	904	MGD	C23-C14	7.21	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	904	MGD	C14-N15	7.16	1.54	1.46
5	S	904	MGD	C14-N15	7.06	1.54	1.46
5	K	904	MGD	C14-N15	7.04	1.54	1.46
5	I	903	MGD	C14-N15	6.97	1.54	1.46
5	Q	904	MGD	C14-N15	6.95	1.54	1.46
5	U	904	MGD	C23-C14	6.77	1.59	1.53
5	A	904	MGD	C14-N15	6.76	1.54	1.46
5	I	904	MGD	C23-C14	6.63	1.58	1.53
5	M	904	MGD	C14-N15	6.56	1.53	1.46
5	O	904	MGD	C14-N15	6.56	1.53	1.46
5	E	904	MGD	C14-N15	6.51	1.53	1.46
5	W	903	MGD	C21-N22	6.45	1.42	1.35
5	G	904	MGD	C14-N15	6.41	1.53	1.46
5	W	903	MGD	C14-N15	6.36	1.53	1.46
5	C	904	MGD	C14-N15	6.29	1.53	1.46
5	C	903	MGD	C14-N15	6.13	1.53	1.46
5	W	904	MGD	C14-N15	6.05	1.53	1.46
5	M	904	MGD	PA-O3B	6.05	1.66	1.59
5	E	903	MGD	C14-N15	6.05	1.53	1.46
5	Q	903	MGD	C14-N15	5.94	1.53	1.46
5	G	903	MGD	C14-N15	5.90	1.53	1.46
5	C	904	MGD	C21-N22	5.88	1.41	1.35
5	A	904	MGD	PA-O3B	5.88	1.65	1.59
5	O	904	MGD	C23-C14	5.80	1.58	1.53
5	O	903	MGD	C14-N15	5.80	1.53	1.46
5	I	903	MGD	C23-C14	5.69	1.58	1.53
5	K	903	MGD	C14-N15	5.58	1.52	1.46
5	U	904	MGD	C21-N22	5.58	1.41	1.35
5	U	903	MGD	C14-N15	5.55	1.52	1.46
5	E	904	MGD	C21-N22	5.53	1.41	1.35
5	W	904	MGD	C21-N22	5.51	1.41	1.35
5	W	904	MGD	C23-C14	5.48	1.58	1.53
5	O	904	MGD	C21-N22	5.45	1.41	1.35
5	C	904	MGD	C23-C14	5.44	1.58	1.53
5	A	903	MGD	C14-N15	5.44	1.52	1.46
5	S	904	MGD	C21-N22	5.36	1.41	1.35
5	A	904	MGD	C21-N22	5.33	1.41	1.35
5	M	903	MGD	PA-O3B	5.22	1.65	1.59
5	I	904	MGD	C14-N15	5.21	1.52	1.46
5	O	903	MGD	C21-N22	5.20	1.41	1.35
5	G	903	MGD	C21-N22	5.16	1.40	1.35
5	I	903	MGD	C21-N22	5.14	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	903	MGD	C21-N22	5.13	1.40	1.35
5	K	904	MGD	C23-C14	5.08	1.57	1.53
5	U	903	MGD	PA-O3B	5.06	1.65	1.59
5	A	904	MGD	C23-C14	5.03	1.57	1.53
5	E	903	MGD	C21-N22	5.01	1.40	1.35
5	C	903	MGD	C23-C14	4.94	1.57	1.53
5	E	903	MGD	PA-O3B	4.94	1.64	1.59
5	C	903	MGD	C21-N22	4.92	1.40	1.35
5	G	904	MGD	C21-N22	4.90	1.40	1.35
5	S	904	MGD	C23-C14	4.89	1.57	1.53
5	M	903	MGD	C14-N15	4.89	1.52	1.46
5	G	904	MGD	C23-C14	4.89	1.57	1.53
5	M	903	MGD	C21-N22	4.88	1.40	1.35
5	I	904	MGD	C21-N22	4.86	1.40	1.35
5	Q	903	MGD	C21-N22	4.84	1.40	1.35
5	S	903	MGD	C14-N15	4.81	1.51	1.46
5	W	903	MGD	PA-O3B	4.81	1.64	1.59
5	W	904	MGD	O11-C11	4.76	1.52	1.43
5	Q	904	MGD	C21-N22	4.75	1.40	1.35
5	I	903	MGD	C16-N15	4.74	1.49	1.37
5	Q	903	MGD	C16-N15	4.72	1.48	1.37
5	M	904	MGD	C16-N15	4.70	1.48	1.37
5	K	904	MGD	C16-N15	4.67	1.48	1.37
5	C	904	MGD	PA-O3B	4.66	1.64	1.59
5	Q	904	MGD	C16-N15	4.66	1.48	1.37
5	M	904	MGD	C21-N22	4.64	1.40	1.35
5	K	904	MGD	PA-O3B	4.63	1.64	1.59
5	Q	904	MGD	C23-C14	4.56	1.57	1.53
5	K	904	MGD	C21-N22	4.55	1.40	1.35
5	G	903	MGD	C16-N15	4.54	1.48	1.37
5	A	903	MGD	C16-N15	4.54	1.48	1.37
5	E	903	MGD	C16-N15	4.54	1.48	1.37
5	C	903	MGD	C16-N15	4.50	1.48	1.37
5	O	903	MGD	O11-C11	4.49	1.52	1.43
5	O	904	MGD	C16-N15	4.48	1.48	1.37
5	S	903	MGD	C16-N15	4.46	1.48	1.37
5	E	904	MGD	PA-O3B	4.45	1.64	1.59
5	E	904	MGD	C16-N15	4.45	1.48	1.37
5	I	904	MGD	C16-N15	4.38	1.48	1.37
5	A	903	MGD	C21-N22	4.32	1.40	1.35
5	U	903	MGD	C16-N15	4.30	1.47	1.37
5	W	903	MGD	C23-C14	4.29	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	903	MGD	C16-N15	4.29	1.47	1.37
5	S	904	MGD	PA-O3B	4.26	1.64	1.59
5	Q	903	MGD	C23-C14	4.25	1.57	1.53
5	C	903	MGD	O11-C11	4.22	1.51	1.43
5	M	903	MGD	C16-N15	4.20	1.47	1.37
5	W	903	MGD	C16-N15	4.20	1.47	1.37
5	W	903	MGD	O11-C11	4.20	1.51	1.43
5	C	904	MGD	C16-N15	4.19	1.47	1.37
5	G	903	MGD	O11-C11	4.18	1.51	1.43
5	S	904	MGD	C16-N15	4.18	1.47	1.37
5	C	904	MGD	O11-C11	4.18	1.51	1.43
5	S	903	MGD	C21-N22	4.17	1.39	1.35
5	U	903	MGD	O11-C11	4.17	1.51	1.43
5	O	903	MGD	C16-N15	4.17	1.47	1.37
5	S	903	MGD	O11-C11	4.15	1.51	1.43
5	G	904	MGD	C16-N15	4.14	1.47	1.37
5	W	904	MGD	O11-C23	4.14	1.49	1.43
5	E	903	MGD	O11-C11	4.13	1.51	1.43
5	O	904	MGD	O11-C11	4.12	1.51	1.43
5	I	903	MGD	PA-O3B	4.12	1.63	1.59
5	A	904	MGD	C16-N15	4.11	1.47	1.37
5	M	904	MGD	C23-C14	4.07	1.56	1.53
5	W	904	MGD	C16-N15	4.03	1.47	1.37
5	A	904	MGD	O11-C23	4.01	1.49	1.43
5	Q	903	MGD	O11-C11	3.99	1.51	1.43
5	G	903	MGD	PA-O3B	3.98	1.63	1.59
5	I	903	MGD	O11-C11	3.98	1.51	1.43
5	U	904	MGD	C16-N15	3.97	1.47	1.37
5	S	904	MGD	O11-C23	3.87	1.49	1.43
5	O	904	MGD	O11-C23	3.84	1.49	1.43
5	Q	904	MGD	O11-C11	3.79	1.50	1.43
5	C	904	MGD	C21-N20	3.77	1.42	1.36
5	K	904	MGD	O11-C23	3.76	1.49	1.43
5	G	904	MGD	O11-C23	3.74	1.49	1.43
5	A	904	MGD	O11-C11	3.73	1.50	1.43
5	E	904	MGD	O11-C11	3.66	1.50	1.43
5	S	904	MGD	O11-C11	3.66	1.50	1.43
5	U	904	MGD	O11-C11	3.65	1.50	1.43
5	M	904	MGD	O11-C11	3.60	1.50	1.43
5	Q	903	MGD	PA-O3B	3.60	1.63	1.59
5	E	904	MGD	C21-N20	3.60	1.41	1.36
5	K	903	MGD	C21-N22	3.59	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	903	MGD	O11-C11	3.59	1.50	1.43
5	O	904	MGD	PA-O3B	3.59	1.63	1.59
5	M	903	MGD	O11-C11	3.59	1.50	1.43
5	S	904	MGD	C21-N20	3.56	1.41	1.36
5	G	904	MGD	O11-C11	3.55	1.50	1.43
5	U	904	MGD	O11-C23	3.54	1.48	1.43
5	I	904	MGD	O11-C11	3.52	1.50	1.43
5	O	903	MGD	C23-C14	3.51	1.56	1.53
5	E	903	MGD	C17-N18	3.51	1.45	1.38
5	G	903	MGD	C23-C14	3.49	1.56	1.53
5	U	903	MGD	C21-N20	3.48	1.41	1.36
5	A	904	MGD	C17-N18	3.48	1.45	1.38
5	M	904	MGD	C17-N18	3.47	1.45	1.38
5	W	903	MGD	C21-N20	3.46	1.41	1.36
5	I	903	MGD	C21-N20	3.45	1.41	1.36
5	K	904	MGD	O11-C11	3.43	1.50	1.43
5	M	904	MGD	C21-N20	3.41	1.41	1.36
5	E	903	MGD	C23-C14	3.40	1.56	1.53
5	S	903	MGD	C23-C14	3.39	1.56	1.53
5	E	904	MGD	C17-N18	3.39	1.45	1.38
5	Q	904	MGD	O11-C23	3.39	1.48	1.43
5	K	903	MGD	C21-N20	3.39	1.41	1.36
5	M	903	MGD	C17-N18	3.38	1.45	1.38
5	I	904	MGD	C17-N18	3.37	1.45	1.38
5	G	904	MGD	C17-N18	3.35	1.45	1.38
5	A	903	MGD	C21-N20	3.33	1.41	1.36
5	I	904	MGD	C16-C21	3.31	1.44	1.38
5	O	903	MGD	PA-O3B	3.30	1.63	1.59
5	U	904	MGD	PA-O3B	3.25	1.63	1.59
5	A	904	MGD	C21-N20	3.25	1.41	1.36
5	Q	904	MGD	C17-N18	3.21	1.44	1.38
5	Q	903	MGD	C17-N18	3.20	1.44	1.38
5	Q	904	MGD	C21-N20	3.20	1.41	1.36
5	Q	904	MGD	PA-O3B	3.19	1.62	1.59
5	C	903	MGD	C17-N18	3.17	1.44	1.38
5	U	903	MGD	C17-N18	3.17	1.44	1.38
5	M	903	MGD	C23-N22	3.16	1.50	1.45
5	M	904	MGD	O11-C23	3.16	1.48	1.43
5	C	904	MGD	C17-N18	3.16	1.44	1.38
5	G	903	MGD	C23-N22	3.16	1.50	1.45
5	G	903	MGD	C17-N18	3.15	1.44	1.38
5	A	903	MGD	C17-N18	3.14	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	904	MGD	C23-N22	3.13	1.50	1.45
5	M	904	MGD	C16-C21	3.13	1.44	1.38
5	K	903	MGD	O11-C11	3.12	1.49	1.43
5	G	903	MGD	C21-N20	3.09	1.40	1.36
5	I	903	MGD	C23-N22	3.08	1.50	1.45
5	C	904	MGD	C16-C21	3.08	1.43	1.38
5	C	903	MGD	C21-N20	3.07	1.40	1.36
5	K	904	MGD	C21-N20	3.05	1.40	1.36
5	S	904	MGD	C17-N18	3.05	1.44	1.38
5	W	903	MGD	C17-N18	3.03	1.44	1.38
5	I	904	MGD	C21-N20	3.03	1.40	1.36
5	O	903	MGD	C17-N18	3.02	1.44	1.38
5	U	904	MGD	C17-N18	3.02	1.44	1.38
5	M	903	MGD	C23-C14	3.02	1.56	1.53
5	U	903	MGD	C23-C14	3.02	1.56	1.53
5	E	903	MGD	C21-N20	3.01	1.40	1.36
5	M	903	MGD	C21-N20	3.00	1.40	1.36
5	K	904	MGD	C17-N18	2.99	1.44	1.38
5	W	904	MGD	PA-O3B	2.99	1.62	1.59
5	Q	904	MGD	C16-C21	2.98	1.43	1.38
5	G	904	MGD	C21-N20	2.98	1.40	1.36
5	O	904	MGD	C16-C21	2.98	1.43	1.38
5	S	903	MGD	C21-N20	2.97	1.40	1.36
5	S	904	MGD	C16-C21	2.97	1.43	1.38
5	S	903	MGD	C17-N18	2.96	1.44	1.38
5	E	904	MGD	C16-C21	2.96	1.43	1.38
5	E	903	MGD	C23-N22	2.96	1.50	1.45
5	K	904	MGD	C16-C21	2.95	1.43	1.38
5	O	903	MGD	C21-N20	2.93	1.40	1.36
5	I	903	MGD	C17-N18	2.93	1.44	1.38
5	U	904	MGD	C21-N20	2.88	1.40	1.36
5	K	903	MGD	C17-N18	2.88	1.44	1.38
5	C	904	MGD	O11-C23	2.87	1.47	1.43
5	O	904	MGD	C21-N20	2.86	1.40	1.36
5	W	903	MGD	C23-N22	2.84	1.49	1.45
5	S	903	MGD	C23-N22	2.84	1.49	1.45
5	O	904	MGD	C17-N18	2.83	1.44	1.38
5	W	904	MGD	C16-C21	2.82	1.43	1.38
5	S	904	MGD	C23-N22	2.81	1.49	1.45
5	E	904	MGD	O11-C23	2.80	1.47	1.43
5	U	904	MGD	C16-C21	2.80	1.43	1.38
5	Q	903	MGD	C21-N20	2.78	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	903	MGD	O11-C23	2.75	1.47	1.43
5	Q	903	MGD	C23-N22	2.75	1.49	1.45
5	U	903	MGD	C23-N22	2.74	1.49	1.45
5	G	904	MGD	PA-O3B	2.74	1.62	1.59
5	K	903	MGD	O4'-C1'	2.69	1.48	1.42
5	G	904	MGD	C16-C21	2.68	1.43	1.38
5	M	903	MGD	C6-N1	2.66	1.43	1.38
5	S	904	MGD	C6-N1	2.65	1.43	1.38
5	I	904	MGD	PA-O3B	2.64	1.62	1.59
5	I	903	MGD	C16-C21	2.63	1.43	1.38
5	A	904	MGD	C16-C21	2.63	1.43	1.38
5	O	904	MGD	C6-N1	2.63	1.43	1.38
5	E	903	MGD	C16-C21	2.62	1.43	1.38
5	S	903	MGD	PA-O3B	2.60	1.62	1.59
5	O	903	MGD	C23-N22	2.59	1.49	1.45
5	W	904	MGD	C21-N20	2.59	1.40	1.36
5	C	903	MGD	C16-C21	2.59	1.43	1.38
5	U	904	MGD	C6-N1	2.58	1.43	1.38
5	C	904	MGD	O17-C17	2.56	1.28	1.23
5	C	903	MGD	O11-C23	2.55	1.47	1.43
5	C	903	MGD	C23-N22	2.54	1.49	1.45
5	E	903	MGD	PB-O3B	2.53	1.62	1.59
5	U	904	MGD	O17-C17	2.53	1.28	1.23
5	O	903	MGD	C6-N1	2.52	1.43	1.38
5	W	903	MGD	C16-C21	2.50	1.42	1.38
5	A	903	MGD	C23-N22	2.50	1.49	1.45
5	W	904	MGD	C17-N18	2.50	1.43	1.38
5	U	903	MGD	O17-C17	2.48	1.28	1.23
5	G	903	MGD	O11-C23	2.48	1.47	1.43
5	I	904	MGD	C23-N22	2.46	1.49	1.45
5	W	904	MGD	C23-N22	2.46	1.49	1.45
5	O	904	MGD	C23-N22	2.46	1.49	1.45
5	S	903	MGD	C16-C21	2.45	1.42	1.38
5	G	903	MGD	C16-C21	2.45	1.42	1.38
5	M	903	MGD	O17-C17	2.45	1.28	1.23
5	U	904	MGD	C23-N22	2.45	1.49	1.45
5	K	904	MGD	C6-N1	2.45	1.43	1.38
5	Q	904	MGD	C23-N22	2.43	1.49	1.45
5	W	903	MGD	O17-C17	2.43	1.28	1.23
5	O	903	MGD	O17-C17	2.42	1.28	1.23
5	E	904	MGD	O17-C17	2.40	1.28	1.23
5	A	903	MGD	O4'-C1'	2.40	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	903	MGD	C16-C21	2.39	1.42	1.38
5	Q	903	MGD	C16-C21	2.39	1.42	1.38
5	W	904	MGD	O17-C17	2.39	1.28	1.23
5	Q	904	MGD	O17-C17	2.39	1.28	1.23
5	M	904	MGD	C23-N22	2.37	1.49	1.45
5	E	904	MGD	C23-N22	2.36	1.49	1.45
5	I	904	MGD	O11-C23	2.33	1.47	1.43
5	G	903	MGD	C6-N1	2.33	1.43	1.38
5	S	903	MGD	O17-C17	2.32	1.28	1.23
5	C	904	MGD	C6-N1	2.32	1.43	1.38
5	A	904	MGD	O17-C17	2.32	1.28	1.23
5	G	903	MGD	O17-C17	2.32	1.28	1.23
5	G	904	MGD	C23-N22	2.31	1.49	1.45
5	O	903	MGD	O11-C23	2.31	1.47	1.43
5	S	904	MGD	O17-C17	2.30	1.27	1.23
5	K	904	MGD	O6-C6	2.29	1.27	1.23
5	C	903	MGD	C6-N1	2.29	1.43	1.38
5	Q	903	MGD	C6-N1	2.29	1.43	1.38
5	A	903	MGD	C8-N9	2.29	1.42	1.37
5	O	904	MGD	O6-C6	2.28	1.27	1.23
5	Q	904	MGD	C6-N1	2.28	1.43	1.38
5	M	904	MGD	O17-C17	2.28	1.27	1.23
5	C	903	MGD	C8-N9	2.26	1.42	1.37
5	I	904	MGD	O17-C17	2.26	1.27	1.23
5	W	904	MGD	C6-N1	2.24	1.43	1.38
5	G	903	MGD	O6-C6	2.24	1.27	1.23
5	G	904	MGD	O6-C6	2.24	1.27	1.23
5	E	904	MGD	C6-N1	2.24	1.43	1.38
5	K	903	MGD	C23-N22	2.24	1.48	1.45
5	C	903	MGD	O4'-C1'	2.24	1.47	1.42
5	G	904	MGD	C6-N1	2.23	1.43	1.38
5	E	903	MGD	O17-C17	2.23	1.27	1.23
5	U	903	MGD	O6-C6	2.22	1.27	1.23
5	K	904	MGD	C23-N22	2.22	1.48	1.45
5	W	904	MGD	C10-C11	2.22	1.54	1.51
5	Q	903	MGD	C8-N9	2.21	1.42	1.37
5	M	904	MGD	C4-N3	2.21	1.39	1.34
5	G	904	MGD	O17-C17	2.18	1.27	1.23
5	K	904	MGD	O17-C17	2.18	1.27	1.23
5	O	904	MGD	C10-C11	2.18	1.54	1.51
5	Q	904	MGD	O6-C6	2.18	1.27	1.23
5	U	903	MGD	C6-N1	2.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	903	MGD	O6-C6	2.17	1.27	1.23
5	K	903	MGD	O6-C6	2.17	1.27	1.23
5	M	903	MGD	C16-C21	2.17	1.42	1.38
5	A	903	MGD	C6-N1	2.17	1.42	1.38
5	W	903	MGD	O6-C6	2.16	1.27	1.23
5	O	903	MGD	O6-C6	2.16	1.27	1.23
5	A	904	MGD	C10-C11	2.15	1.54	1.51
5	I	904	MGD	C6-N1	2.14	1.42	1.38
5	S	904	MGD	O6-C6	2.14	1.27	1.23
5	O	903	MGD	C16-C21	2.14	1.42	1.38
5	Q	903	MGD	O17-C17	2.12	1.27	1.23
5	C	903	MGD	PA-O3B	2.11	1.61	1.59
5	K	903	MGD	C6-N1	2.11	1.42	1.38
5	S	903	MGD	O6-C6	2.11	1.27	1.23
5	C	903	MGD	O17-C17	2.10	1.27	1.23
5	M	904	MGD	C6-N1	2.10	1.42	1.38
5	S	903	MGD	C6-N1	2.10	1.42	1.38
5	A	903	MGD	C16-C21	2.09	1.42	1.38
5	I	903	MGD	C6-N1	2.08	1.42	1.38
5	E	904	MGD	C10-C11	2.06	1.54	1.51
5	K	903	MGD	C8-N9	2.06	1.42	1.37
5	K	904	MGD	C8-N9	2.05	1.42	1.37
5	E	903	MGD	C6-N1	2.05	1.42	1.38
5	U	904	MGD	C10-C11	2.03	1.54	1.51
5	K	903	MGD	O17-C17	2.03	1.27	1.23
5	E	903	MGD	C2-N2	2.03	1.38	1.34
5	C	904	MGD	C4-N3	2.02	1.38	1.34
5	Q	903	MGD	PB-O3B	2.02	1.61	1.59
5	O	903	MGD	C2-N1	2.02	1.42	1.37
5	E	903	MGD	O6-C6	2.01	1.27	1.23
5	M	903	MGD	O6-C6	2.00	1.27	1.23
5	O	903	MGD	C4-N3	2.00	1.38	1.34

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	903	MGD	O2A-PA-O3B	-10.89	77.85	107.27
5	O	903	MGD	O2A-PA-O3B	-10.77	78.16	107.27
5	S	903	MGD	O2A-PA-O3B	-10.57	78.71	107.27
5	M	903	MGD	O2A-PA-O3B	-10.53	78.82	107.27
5	G	903	MGD	O2A-PA-O3B	-10.42	79.12	107.27
5	K	903	MGD	O2A-PA-O3B	-10.24	79.60	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	903	MGD	O2A-PA-O3B	-10.13	79.89	107.27
5	U	903	MGD	O2A-PA-O3B	-10.09	79.99	107.27
5	E	903	MGD	O2A-PA-O3B	-10.09	79.99	107.27
5	C	903	MGD	O2A-PA-O3B	-9.88	80.57	107.27
5	W	903	MGD	O2A-PA-O3B	-9.70	81.04	107.27
5	A	903	MGD	O2A-PA-O3B	-9.67	81.14	107.27
5	I	904	MGD	O11-C23-C14	-7.86	103.72	108.96
5	S	903	MGD	C23-C14-N15	5.71	113.48	107.87
5	E	903	MGD	O2A-PA-O3A	-5.66	81.91	107.57
5	W	903	MGD	O2A-PA-O3A	-5.65	81.94	107.57
5	M	903	MGD	O2A-PA-O3A	-5.64	82.01	107.57
5	I	904	MGD	O4'-C4'-C5'	-5.56	91.52	109.33
5	O	903	MGD	O2A-PA-O3A	-5.55	82.40	107.57
5	I	903	MGD	O2A-PA-O3A	-5.53	82.49	107.57
5	U	903	MGD	O2A-PA-O3A	-5.51	82.59	107.57
5	C	903	MGD	O2A-PA-O3A	-5.43	82.95	107.57
5	M	903	MGD	C23-C14-N15	5.38	113.15	107.87
5	Q	903	MGD	O2A-PA-O3A	-5.30	83.52	107.57
5	A	903	MGD	C23-C14-N15	5.20	112.97	107.87
5	K	903	MGD	O2A-PA-O3A	-5.14	84.25	107.57
5	O	903	MGD	C23-C14-N15	5.12	112.90	107.87
5	A	903	MGD	O2A-PA-O3A	-5.08	84.56	107.57
5	G	903	MGD	C23-C14-N15	5.05	112.83	107.87
5	S	903	MGD	O2A-PA-O1A	-5.04	89.01	112.44
5	G	903	MGD	O2A-PA-O3A	-5.03	84.79	107.57
5	G	903	MGD	O2A-PA-O1A	-5.01	89.16	112.44
5	M	904	MGD	O11-C23-C14	-4.96	105.66	108.96
5	Q	903	MGD	C23-C14-N15	4.94	112.72	107.87
5	S	903	MGD	O2A-PA-O3A	-4.88	85.44	107.57
5	C	903	MGD	C23-C14-N15	4.88	112.66	107.87
5	U	903	MGD	C23-C14-N15	4.85	112.63	107.87
5	S	903	MGD	O11-C23-C14	4.83	112.19	108.96
5	E	903	MGD	C23-C14-N15	4.80	112.58	107.87
5	W	903	MGD	O2A-PA-O1A	-4.78	90.19	112.44
5	A	903	MGD	O2A-PA-O1A	-4.78	90.21	112.44
5	I	903	MGD	O2A-PA-O1A	-4.78	90.21	112.44
5	U	903	MGD	O2A-PA-O1A	-4.77	90.27	112.44
5	K	903	MGD	O2A-PA-O1A	-4.69	90.61	112.44
5	Q	903	MGD	O2A-PA-O1A	-4.62	90.95	112.44
5	E	903	MGD	O2A-PA-O1A	-4.55	91.26	112.44
5	M	903	MGD	O2A-PA-O1A	-4.54	91.33	112.44
5	K	903	MGD	C23-C14-N15	4.50	112.29	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	904	MGD	O11-C23-C14	-4.50	105.96	108.96
5	A	904	MGD	O4'-C4'-C5'	-4.44	95.12	109.33
5	I	903	MGD	C23-C14-N15	4.38	112.17	107.87
5	M	904	MGD	O4'-C4'-C5'	-4.38	95.32	109.33
5	I	903	MGD	O11-C23-C14	4.36	111.87	108.96
5	W	903	MGD	C23-C14-N15	4.33	112.12	107.87
5	Q	904	MGD	O11-C23-C14	-4.32	106.08	108.96
5	G	904	MGD	O4'-C4'-C5'	-4.29	95.60	109.33
5	O	903	MGD	O2A-PA-O1A	-4.28	92.52	112.44
5	S	903	MGD	O3B-PA-O1A	4.19	123.31	110.70
5	C	903	MGD	O2A-PA-O1A	-4.19	92.95	112.44
5	K	904	MGD	O4'-C4'-C5'	-4.16	96.02	109.33
5	Q	904	MGD	O4'-C4'-C5'	-4.15	96.03	109.33
5	U	904	MGD	O4'-C4'-C5'	-4.10	96.20	109.33
5	G	903	MGD	O11-C23-C14	4.10	111.70	108.96
5	G	903	MGD	O3B-PA-O1A	4.01	122.77	110.70
5	U	903	MGD	O3B-PA-O1A	3.98	122.67	110.70
5	O	904	MGD	O4'-C4'-C5'	-3.86	96.97	109.33
5	S	904	MGD	O4'-C4'-C5'	-3.82	97.11	109.33
5	Q	903	MGD	O3B-PA-O1A	3.79	122.12	110.70
5	Q	903	MGD	O11-C23-C14	3.79	111.49	108.96
5	M	903	MGD	O3B-PA-O1A	3.78	122.07	110.70
5	A	903	MGD	O3A-C10-C11	-3.72	99.39	108.58
5	M	903	MGD	O11-C23-C14	3.70	111.43	108.96
5	I	903	MGD	O3B-PA-O1A	3.68	121.78	110.70
5	I	904	MGD	O11-C23-N22	-3.64	105.30	108.61
5	E	903	MGD	O3B-PA-O1A	3.60	121.54	110.70
5	C	904	MGD	O11-C23-C14	-3.57	106.58	108.96
5	O	903	MGD	O11-C23-C14	3.55	111.33	108.96
5	C	903	MGD	O3A-C10-C11	-3.54	99.84	108.58
5	U	903	MGD	O11-C23-C14	3.51	111.30	108.96
5	O	903	MGD	O3B-PA-O1A	3.50	121.22	110.70
5	A	903	MGD	O11-C23-C14	3.46	111.28	108.96
5	K	903	MGD	O3A-C10-C11	-3.43	100.10	108.58
5	C	903	MGD	O11-C23-C14	3.41	111.24	108.96
5	W	904	MGD	O4'-C4'-C5'	-3.40	98.45	109.33
5	A	904	MGD	O11-C23-C14	-3.39	106.70	108.96
5	W	903	MGD	O3B-PA-O1A	3.30	120.65	110.70
5	C	904	MGD	O4'-C4'-C5'	-3.27	98.87	109.33
5	U	903	MGD	O3A-C10-C11	-3.26	100.54	108.58
5	K	903	MGD	O3B-PA-O1A	3.23	120.43	110.70
5	E	904	MGD	O4'-C4'-C5'	-3.22	99.01	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	903	MGD	O3B-PA-O1A	3.15	120.17	110.70
5	I	903	MGD	O4'-C4'-C5'	-3.11	99.36	109.33
5	I	903	MGD	O3A-C10-C11	-3.09	100.95	108.58
5	C	903	MGD	O3B-PA-O1A	3.03	119.82	110.70
5	A	904	MGD	O3A-C10-C11	2.96	115.90	108.58
5	S	904	MGD	O11-C23-C14	-2.88	107.05	108.96
5	K	904	MGD	O11-C23-C14	-2.80	107.09	108.96
5	U	903	MGD	O4'-C4'-C5'	-2.78	100.42	109.33
5	Q	903	MGD	O4'-C4'-C5'	-2.77	100.45	109.33
5	W	904	MGD	O11-C23-C14	-2.75	107.13	108.96
5	S	903	MGD	O11-C23-N22	2.72	111.07	108.61
5	W	904	MGD	C23-C14-N15	2.71	110.53	107.87
5	E	904	MGD	C23-C14-N15	2.68	110.50	107.87
5	G	904	MGD	O11-C23-C14	-2.66	107.19	108.96
5	U	904	MGD	C23-C14-N15	2.65	110.47	107.87
5	Q	903	MGD	O3A-C10-C11	-2.63	102.08	108.58
5	M	903	MGD	O4'-C4'-C5'	-2.63	100.92	109.33
5	M	903	MGD	O3A-C10-C11	-2.53	102.33	108.58
5	E	903	MGD	O3A-C10-C11	-2.50	102.41	108.58
5	E	903	MGD	O4'-C4'-C5'	-2.50	101.34	109.33
5	O	903	MGD	O11-C23-N22	2.47	110.85	108.61
5	G	903	MGD	O4'-C4'-C5'	-2.45	101.48	109.33
5	A	904	MGD	C23-C14-N15	2.45	110.27	107.87
5	S	903	MGD	O4'-C4'-C5'	-2.45	101.50	109.33
5	U	903	MGD	O11-C23-N22	2.43	110.81	108.61
5	E	903	MGD	O11-C23-C14	2.40	110.56	108.96
5	U	904	MGD	O11-C23-C14	-2.35	107.40	108.96
5	S	904	MGD	O3A-C10-C11	2.30	114.25	108.58
5	S	903	MGD	O3A-C10-C11	-2.29	102.91	108.58
5	G	903	MGD	O11-C23-N22	2.29	110.68	108.61
5	W	903	MGD	O4'-C4'-C5'	-2.28	102.02	109.33
5	K	903	MGD	O11-C23-C14	2.28	110.48	108.96
5	G	904	MGD	O3A-C10-C11	2.21	114.03	108.58
5	S	904	MGD	C23-C14-N15	2.21	110.04	107.87
5	M	903	MGD	O11-C23-N22	2.20	110.60	108.61
5	I	904	MGD	PB-O5'-C5'	-2.19	108.79	121.35
5	G	904	MGD	C23-C14-N15	2.15	109.98	107.87
5	K	904	MGD	C17-C16-N15	2.14	122.09	116.27
5	Q	904	MGD	O3A-C10-C11	2.11	113.80	108.58
5	G	903	MGD	O3A-C10-C11	-2.08	103.45	108.58
5	O	904	MGD	O3A-C10-C11	2.04	113.62	108.58
5	C	904	MGD	O2A-PA-O1A	2.01	121.81	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	904	MGD	C3'-C2'-C1'	2.01	105.26	101.46
5	W	903	MGD	O3A-PA-O1A	2.00	116.87	108.94

There are no chirality outliers.

All (154) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	903	MGD	C5'-O5'-PB-O1B
5	A	903	MGD	C5'-O5'-PB-O2B
5	A	903	MGD	C5'-O5'-PB-O3B
5	A	903	MGD	C10-O3A-PA-O2A
5	A	903	MGD	O3A-C10-C11-O11
5	A	903	MGD	O3A-C10-C11-C12
5	A	904	MGD	PA-O3B-PB-O5'
5	A	904	MGD	C5'-O5'-PB-O1B
5	A	904	MGD	C5'-O5'-PB-O3B
5	C	903	MGD	C5'-O5'-PB-O1B
5	C	903	MGD	C5'-O5'-PB-O2B
5	C	903	MGD	C5'-O5'-PB-O3B
5	C	903	MGD	C10-O3A-PA-O2A
5	C	903	MGD	O3A-C10-C11-O11
5	C	903	MGD	O3A-C10-C11-C12
5	C	904	MGD	C5'-O5'-PB-O1B
5	C	904	MGD	C5'-O5'-PB-O3B
5	E	903	MGD	C5'-O5'-PB-O1B
5	E	903	MGD	C5'-O5'-PB-O3B
5	E	903	MGD	C10-O3A-PA-O2A
5	E	904	MGD	C5'-O5'-PB-O1B
5	E	904	MGD	C5'-O5'-PB-O3B
5	G	903	MGD	C5'-O5'-PB-O1B
5	G	903	MGD	C5'-O5'-PB-O3B
5	G	903	MGD	C10-O3A-PA-O2A
5	G	904	MGD	C5'-O5'-PB-O1B
5	G	904	MGD	C5'-O5'-PB-O3B
5	I	903	MGD	PA-O3B-PB-O5'
5	I	903	MGD	C5'-O5'-PB-O1B
5	I	903	MGD	C5'-O5'-PB-O3B
5	I	903	MGD	C10-O3A-PA-O2A
5	I	904	MGD	C5'-O5'-PB-O1B
5	I	904	MGD	C5'-O5'-PB-O2B
5	I	904	MGD	C5'-O5'-PB-O3B
5	K	903	MGD	C5'-O5'-PB-O1B

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Mol	Chain	Res	Type	Atoms
5	K	903	MGD	C5'-O5'-PB-O2B
5	K	903	MGD	C5'-O5'-PB-O3B
5	K	903	MGD	C10-O3A-PA-O2A
5	K	903	MGD	O3A-C10-C11-O11
5	K	903	MGD	O3A-C10-C11-C12
5	K	904	MGD	PA-O3B-PB-O5'
5	K	904	MGD	C5'-O5'-PB-O1B
5	K	904	MGD	C5'-O5'-PB-O3B
5	M	903	MGD	C5'-O5'-PB-O1B
5	M	903	MGD	C5'-O5'-PB-O3B
5	M	903	MGD	C10-O3A-PA-O2A
5	M	904	MGD	C5'-O5'-PB-O1B
5	M	904	MGD	C5'-O5'-PB-O3B
5	O	903	MGD	C5'-O5'-PB-O1B
5	O	903	MGD	C5'-O5'-PB-O3B
5	O	903	MGD	C10-O3A-PA-O2A
5	O	904	MGD	C5'-O5'-PB-O1B
5	O	904	MGD	C5'-O5'-PB-O3B
5	Q	903	MGD	C5'-O5'-PB-O1B
5	Q	903	MGD	C5'-O5'-PB-O3B
5	Q	903	MGD	C10-O3A-PA-O2A
5	Q	904	MGD	PA-O3B-PB-O5'
5	Q	904	MGD	C5'-O5'-PB-O1B
5	Q	904	MGD	C5'-O5'-PB-O3B
5	S	903	MGD	PA-O3B-PB-O5'
5	S	903	MGD	C5'-O5'-PB-O1B
5	S	903	MGD	C5'-O5'-PB-O3B
5	S	903	MGD	C10-O3A-PA-O2A
5	S	903	MGD	O3A-C10-C11-O11
5	S	903	MGD	O3A-C10-C11-C12
5	S	904	MGD	C5'-O5'-PB-O1B
5	S	904	MGD	C5'-O5'-PB-O3B
5	U	903	MGD	C5'-O5'-PB-O1B
5	U	903	MGD	C5'-O5'-PB-O3B
5	U	903	MGD	C10-O3A-PA-O2A
5	U	904	MGD	PA-O3B-PB-O5'
5	U	904	MGD	C5'-O5'-PB-O1B
5	U	904	MGD	C5'-O5'-PB-O3B
5	W	903	MGD	C5'-O5'-PB-O1B
5	W	903	MGD	C5'-O5'-PB-O3B
5	W	903	MGD	C10-O3A-PA-O2A
5	W	904	MGD	C5'-O5'-PB-O1B

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Mol	Chain	Res	Type	Atoms
5	W	904	MGD	C5'-O5'-PB-O3B
5	U	903	MGD	O3A-C10-C11-O11
5	W	903	MGD	O3A-C10-C11-O11
5	C	904	MGD	PA-O3B-PB-O5'
5	E	903	MGD	PA-O3B-PB-O5'
5	E	904	MGD	PA-O3B-PB-O5'
5	G	904	MGD	PA-O3B-PB-O5'
5	M	903	MGD	PA-O3B-PB-O5'
5	M	904	MGD	PA-O3B-PB-O5'
5	O	903	MGD	PA-O3B-PB-O5'
5	O	904	MGD	PA-O3B-PB-O5'
5	Q	903	MGD	PA-O3B-PB-O5'
5	S	904	MGD	PA-O3B-PB-O5'
5	U	903	MGD	PA-O3B-PB-O5'
5	W	904	MGD	PA-O3B-PB-O5'
5	G	903	MGD	PA-O3B-PB-O1B
5	U	903	MGD	O3A-C10-C11-C12
5	W	903	MGD	O3A-C10-C11-C12
5	A	903	MGD	C10-O3A-PA-O3B
5	A	904	MGD	C5'-O5'-PB-O2B
5	C	903	MGD	C10-O3A-PA-O3B
5	C	904	MGD	C5'-O5'-PB-O2B
5	E	903	MGD	C5'-O5'-PB-O2B
5	E	903	MGD	C10-O3A-PA-O3B
5	E	904	MGD	C5'-O5'-PB-O2B
5	G	903	MGD	C5'-O5'-PB-O2B
5	G	903	MGD	C10-O3A-PA-O3B
5	G	904	MGD	C5'-O5'-PB-O2B
5	I	903	MGD	C5'-O5'-PB-O2B
5	I	903	MGD	C10-O3A-PA-O3B
5	K	903	MGD	C10-O3A-PA-O3B
5	K	904	MGD	C5'-O5'-PB-O2B
5	M	903	MGD	C5'-O5'-PB-O2B
5	M	903	MGD	C10-O3A-PA-O3B
5	M	904	MGD	C5'-O5'-PB-O2B
5	O	903	MGD	C5'-O5'-PB-O2B
5	O	903	MGD	C10-O3A-PA-O3B
5	O	904	MGD	C5'-O5'-PB-O2B
5	Q	903	MGD	C5'-O5'-PB-O2B
5	Q	903	MGD	C10-O3A-PA-O3B
5	Q	904	MGD	C5'-O5'-PB-O2B
5	S	903	MGD	C5'-O5'-PB-O2B

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Mol	Chain	Res	Type	Atoms
5	S	903	MGD	C10-O3A-PA-O3B
5	S	904	MGD	C5'-O5'-PB-O2B
5	U	903	MGD	C5'-O5'-PB-O2B
5	U	903	MGD	C10-O3A-PA-O3B
5	U	904	MGD	C5'-O5'-PB-O2B
5	W	903	MGD	C5'-O5'-PB-O2B
5	W	903	MGD	C10-O3A-PA-O3B
5	W	904	MGD	C5'-O5'-PB-O2B
5	W	903	MGD	PA-O3B-PB-O1B
5	E	903	MGD	O3A-C10-C11-O11
5	G	903	MGD	O3A-C10-C11-O11
5	M	903	MGD	O3A-C10-C11-O11
5	O	903	MGD	O3A-C10-C11-O11
5	O	903	MGD	PA-O3B-PB-O1B
5	S	903	MGD	PB-O3B-PA-O1A
5	G	903	MGD	PA-O3B-PB-O5'
5	W	903	MGD	PA-O3B-PB-O5'
5	A	904	MGD	O4'-C4'-C5'-O5'
5	E	903	MGD	O4'-C4'-C5'-O5'
5	M	904	MGD	O4'-C4'-C5'-O5'
5	U	903	MGD	O4'-C4'-C5'-O5'
5	S	903	MGD	PA-O3B-PB-O2B
5	E	904	MGD	O4'-C4'-C5'-O5'
5	I	903	MGD	O4'-C4'-C5'-O5'
5	M	903	MGD	O4'-C4'-C5'-O5'
5	O	903	MGD	O4'-C4'-C5'-O5'
5	Q	903	MGD	O4'-C4'-C5'-O5'
5	W	903	MGD	O4'-C4'-C5'-O5'
5	E	903	MGD	O3A-C10-C11-C12
5	G	903	MGD	O3A-C10-C11-C12
5	S	903	MGD	PA-O3B-PB-O1B
5	G	903	MGD	O4'-C4'-C5'-O5'
5	G	904	MGD	O4'-C4'-C5'-O5'
5	Q	904	MGD	O4'-C4'-C5'-O5'
5	W	904	MGD	O4'-C4'-C5'-O5'

There are no ring outliers.

69 monomers are involved in 212 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	S	901	ACT	1	0
7	R	304	SF4	2	0

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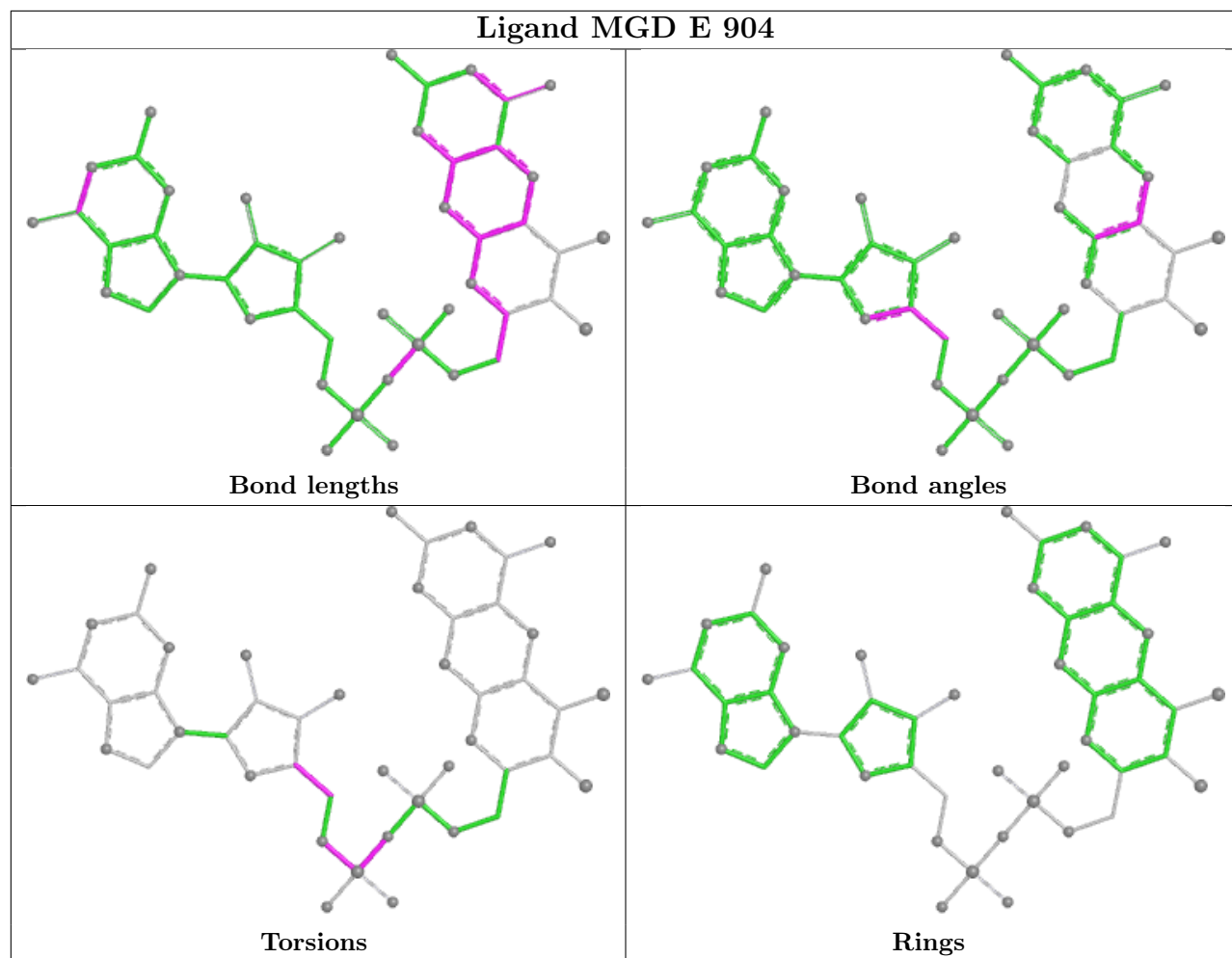
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	901	ACT	3	0
5	E	904	MGD	3	0
5	Q	904	MGD	4	0
3	E	901	ACT	2	0
5	W	904	MGD	7	0
5	M	904	MGD	7	0
7	X	303	SF4	2	0
3	U	901	ACT	1	0
7	R	302	SF4	1	0
5	C	904	MGD	6	0
5	G	903	MGD	6	0
5	I	904	MGD	7	0
3	W	901	ACT	2	0
7	F	304	SF4	1	0
7	V	303	SF4	2	0
7	H	304	SF4	2	0
7	N	304	SF4	1	0
7	V	304	SF4	1	0
7	N	302	SF4	1	0
7	B	304	SF4	1	0
7	L	303	SF4	2	0
7	T	304	SF4	4	0
7	X	304	SF4	3	0
3	A	901	ACT	1	0
7	L	304	SF4	3	0
5	O	903	MGD	5	0
7	D	302	SF4	1	0
5	E	903	MGD	5	0
5	G	904	MGD	4	0
5	K	903	MGD	6	0
5	U	903	MGD	7	0
3	M	901	ACT	1	0
3	C	901	ACT	3	0
7	H	302	SF4	1	0
7	T	303	SF4	2	0
7	D	304	SF4	2	0
5	A	904	MGD	6	0
7	J	302	SF4	1	0
5	S	903	MGD	6	0
7	P	303	SF4	2	0
3	K	901	ACT	3	0
7	T	302	SF4	1	0

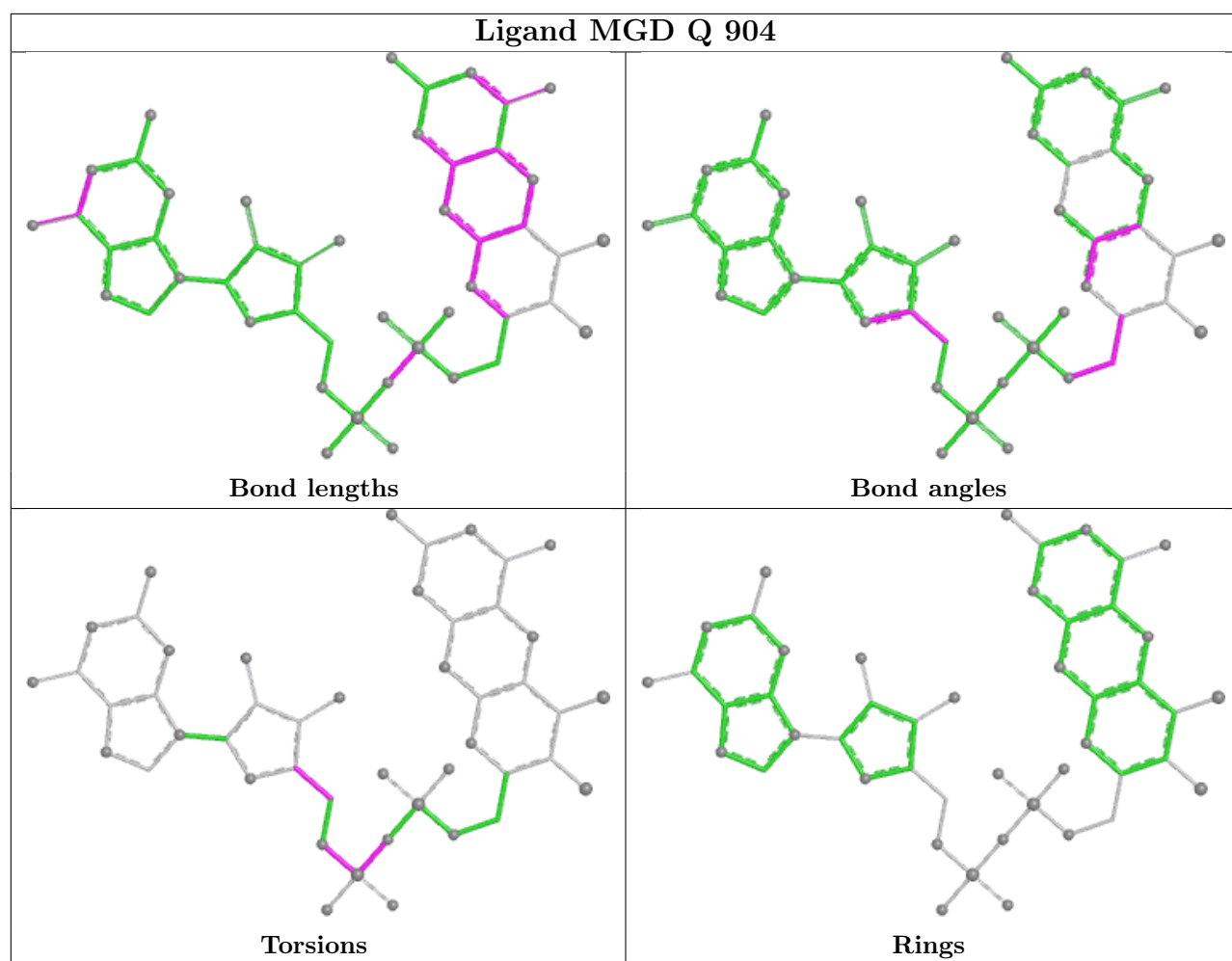
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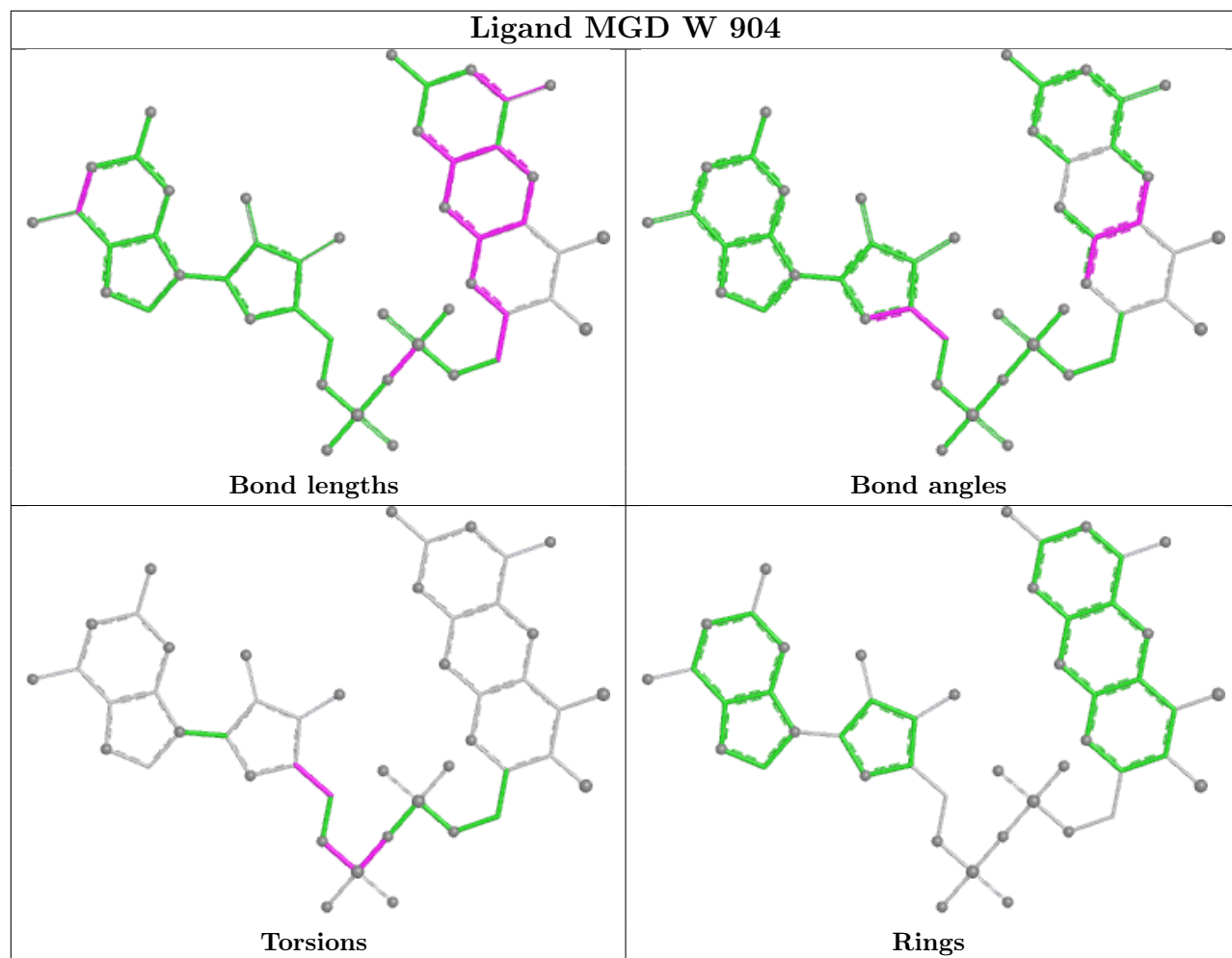
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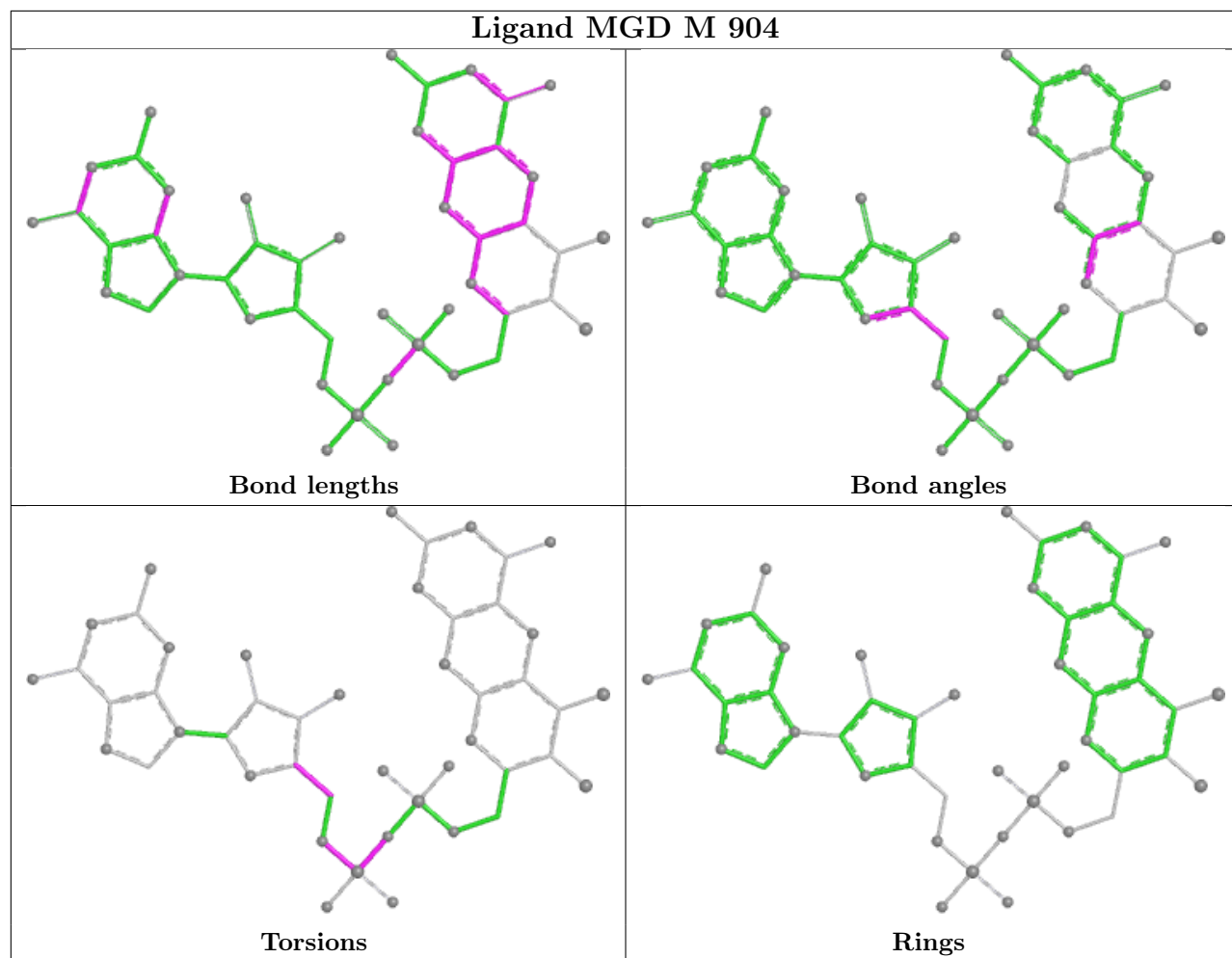
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	X	302	SF4	2	0
5	O	904	MGD	5	0
3	O	901	ACT	2	0
5	Q	903	MGD	5	0
5	I	903	MGD	5	0
5	U	904	MGD	7	0
7	F	303	SF4	2	0
5	K	904	MGD	4	0
5	M	903	MGD	4	0
5	W	903	MGD	6	0
7	J	303	SF4	2	0
3	G	901	ACT	3	0
7	V	302	SF4	1	0
5	C	903	MGD	5	0
7	B	303	SF4	2	0
7	L	302	SF4	1	0
7	P	302	SF4	2	0
7	P	304	SF4	2	0
7	D	303	SF4	2	0
5	S	904	MGD	5	0
7	H	303	SF4	2	0
7	N	303	SF4	2	0
7	R	303	SF4	2	0
5	A	903	MGD	6	0
3	Q	901	ACT	1	0

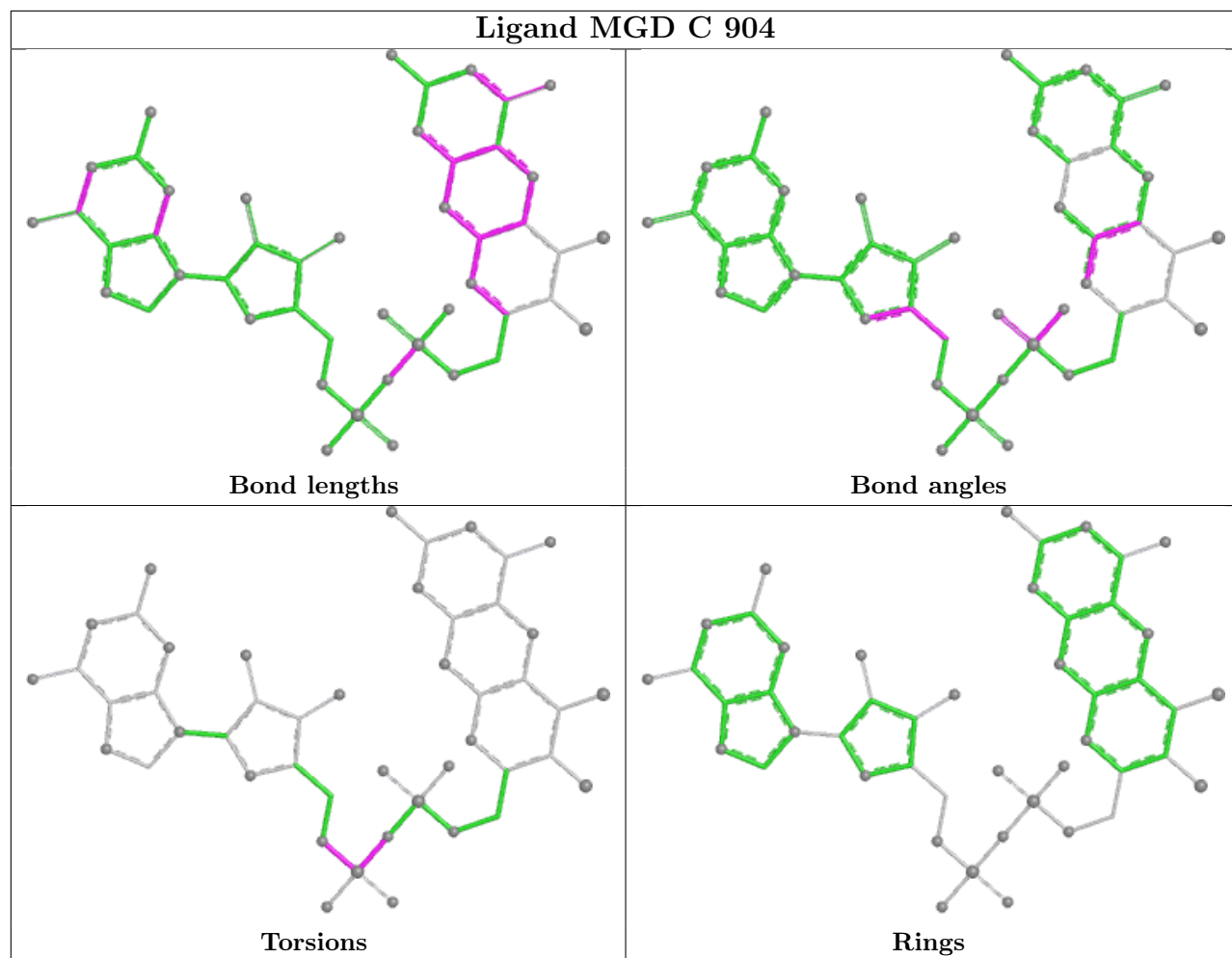
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

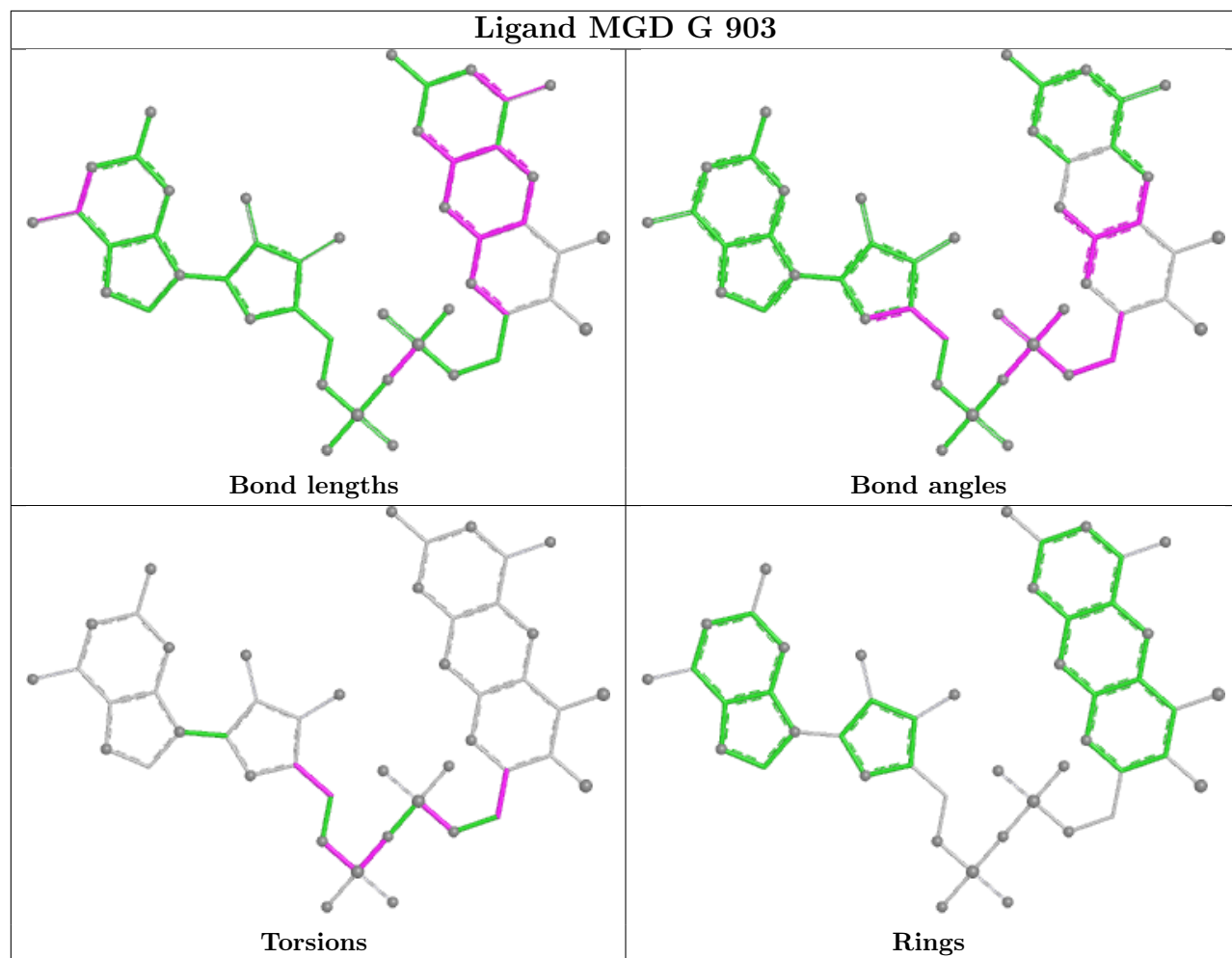


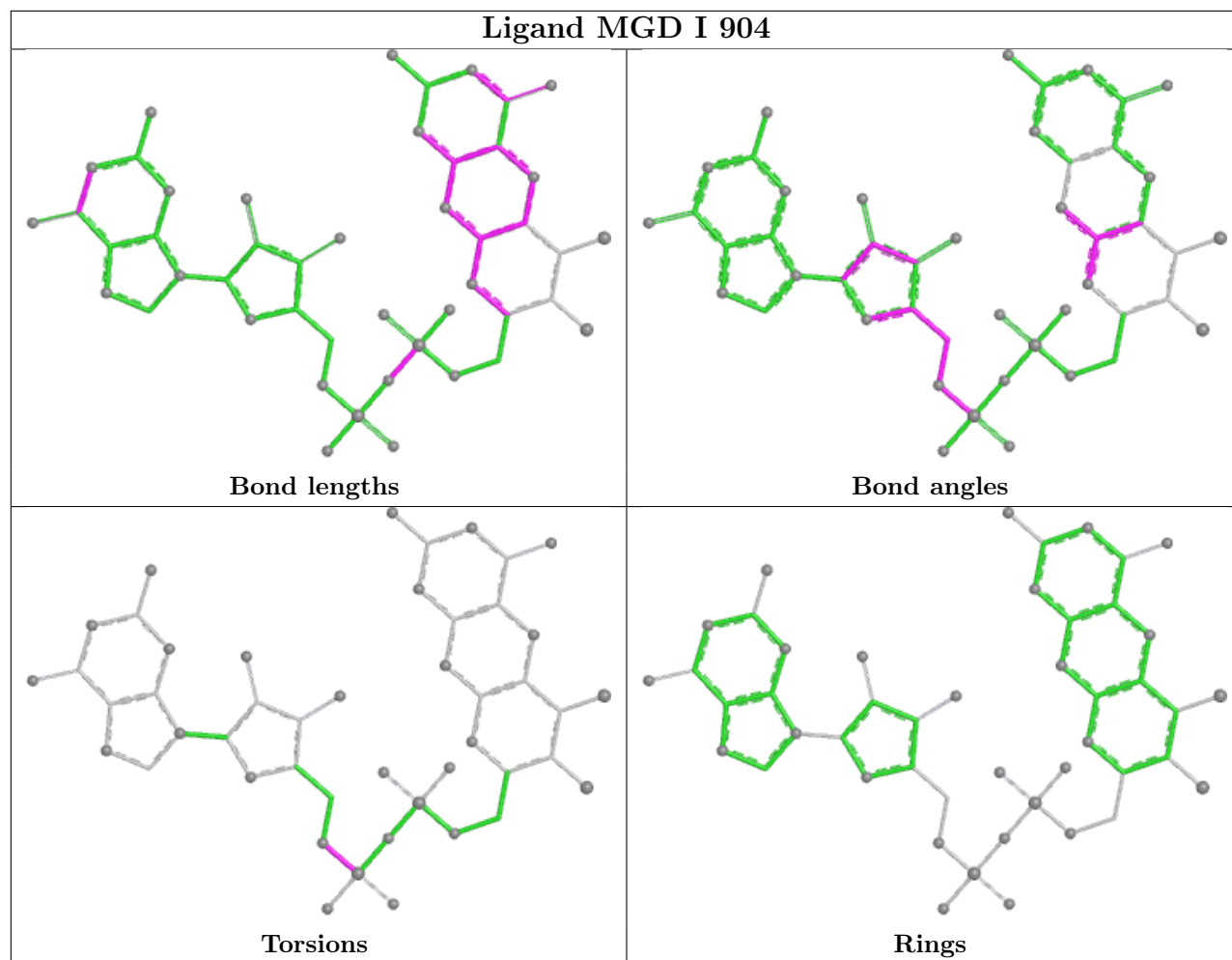


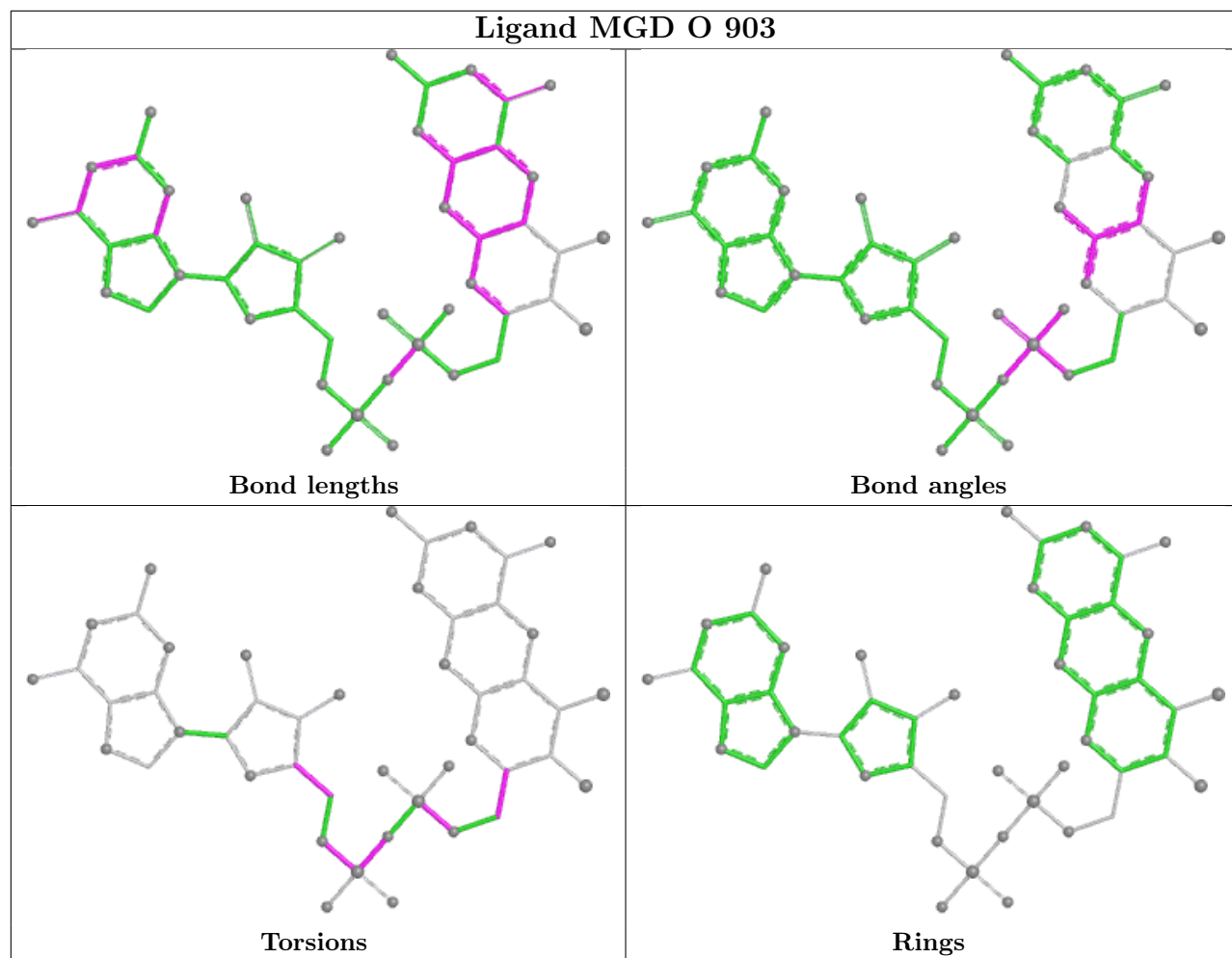


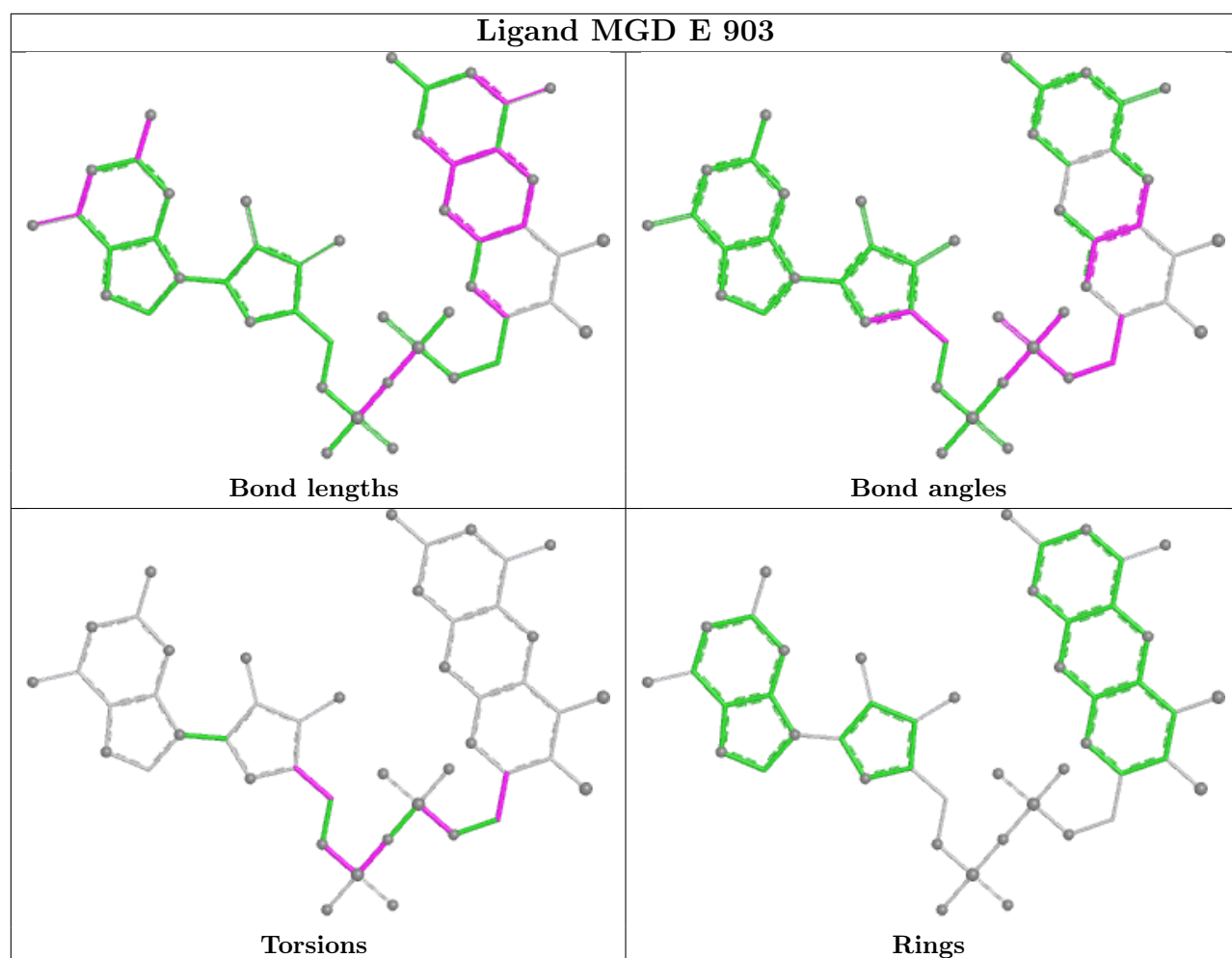


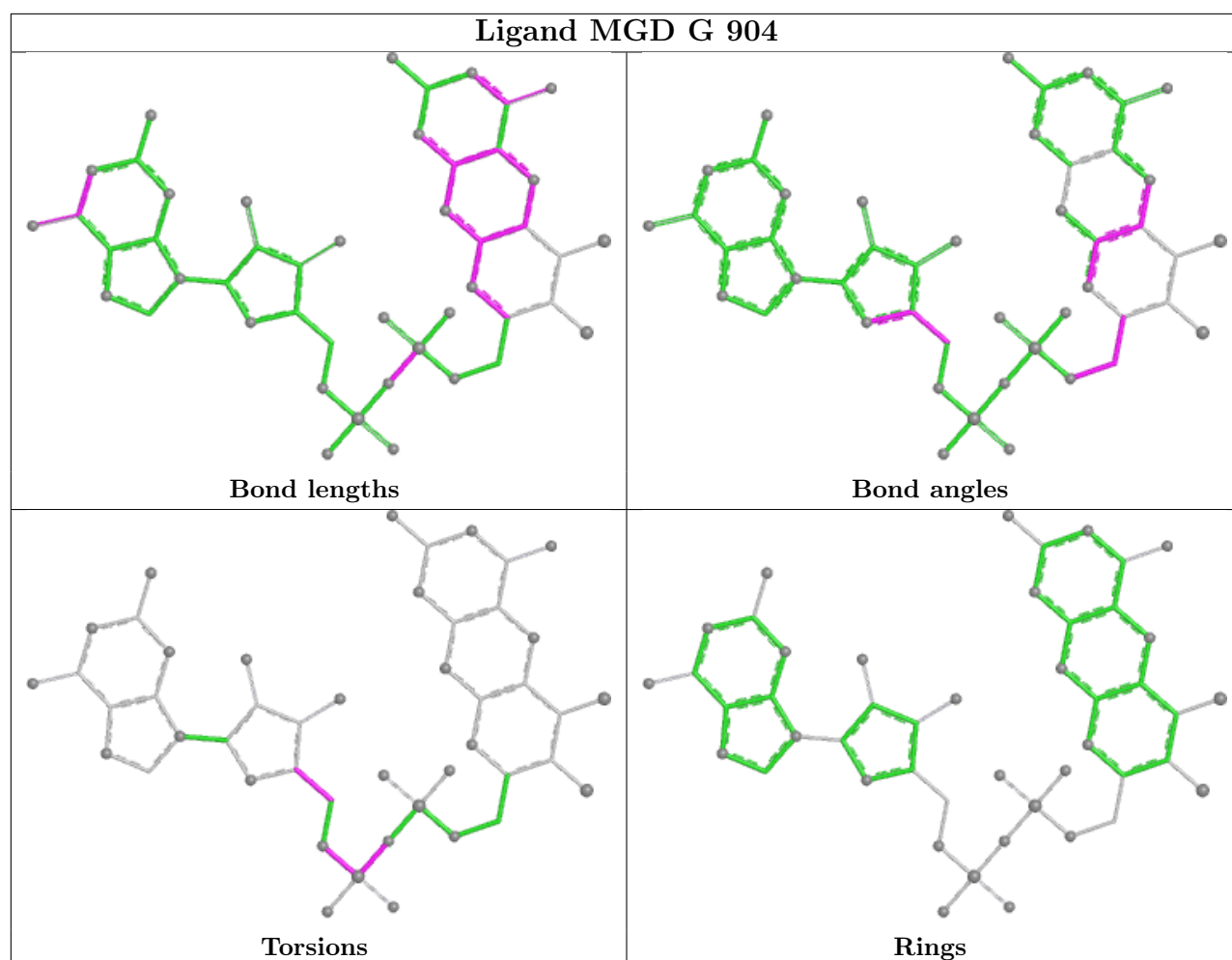


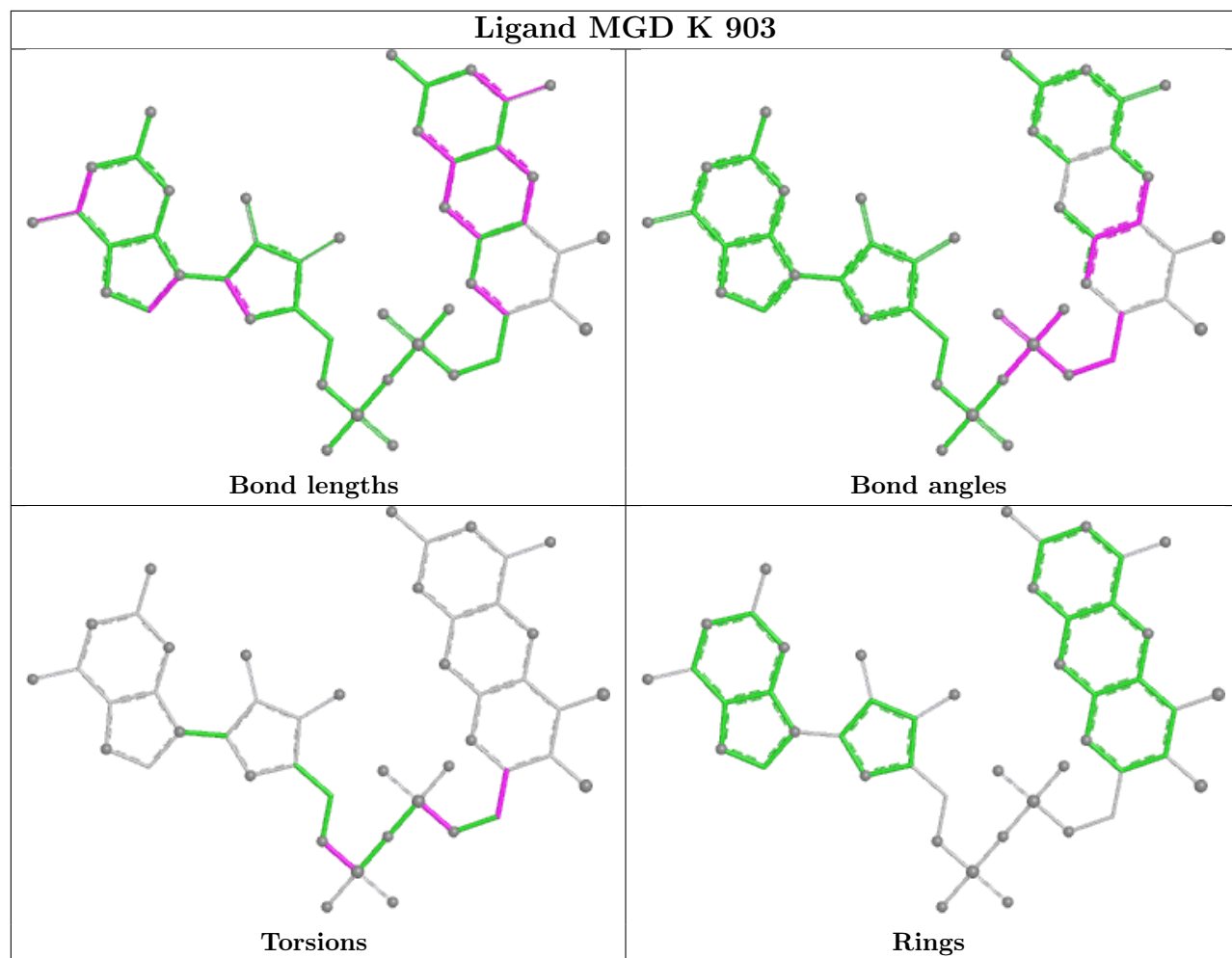


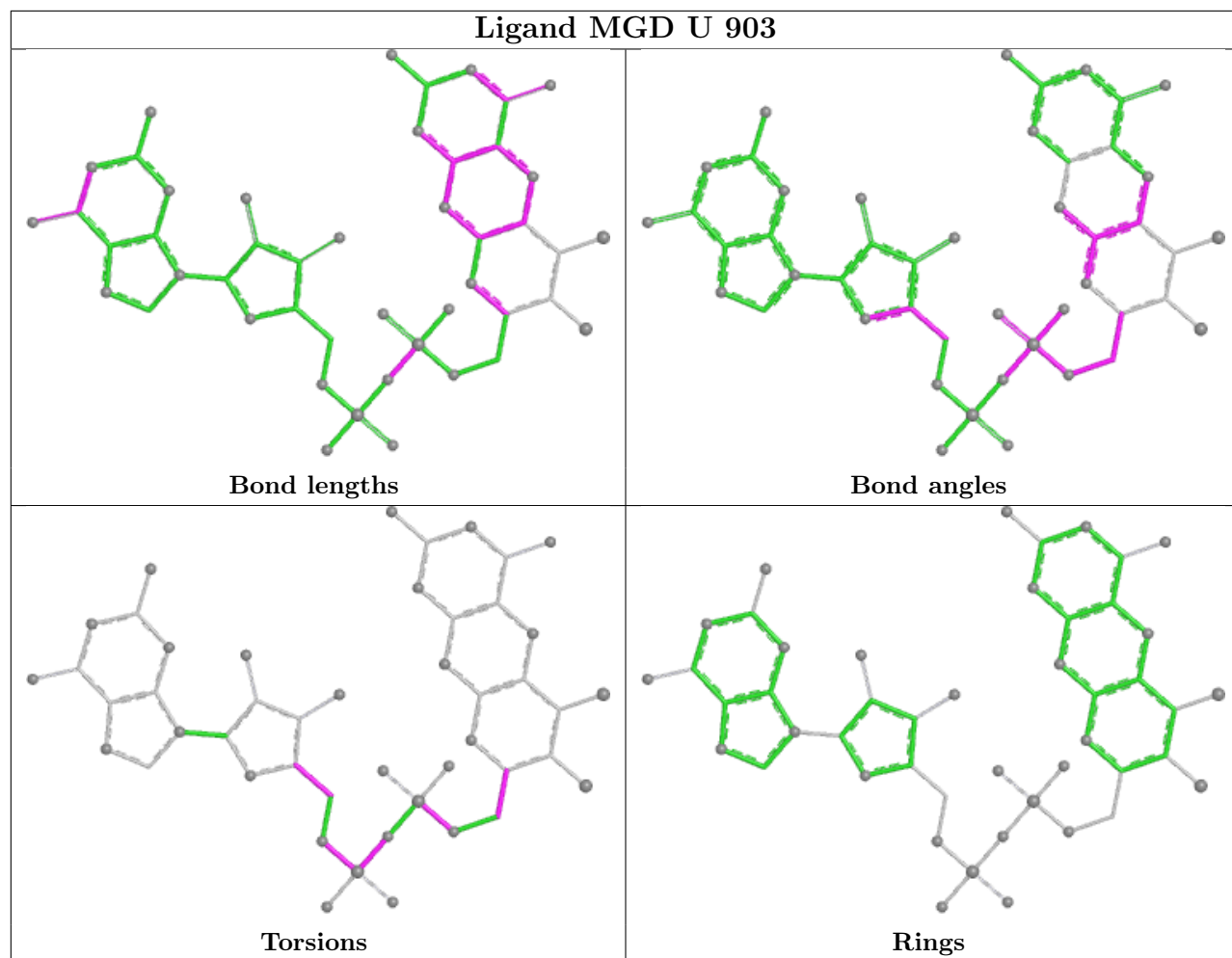


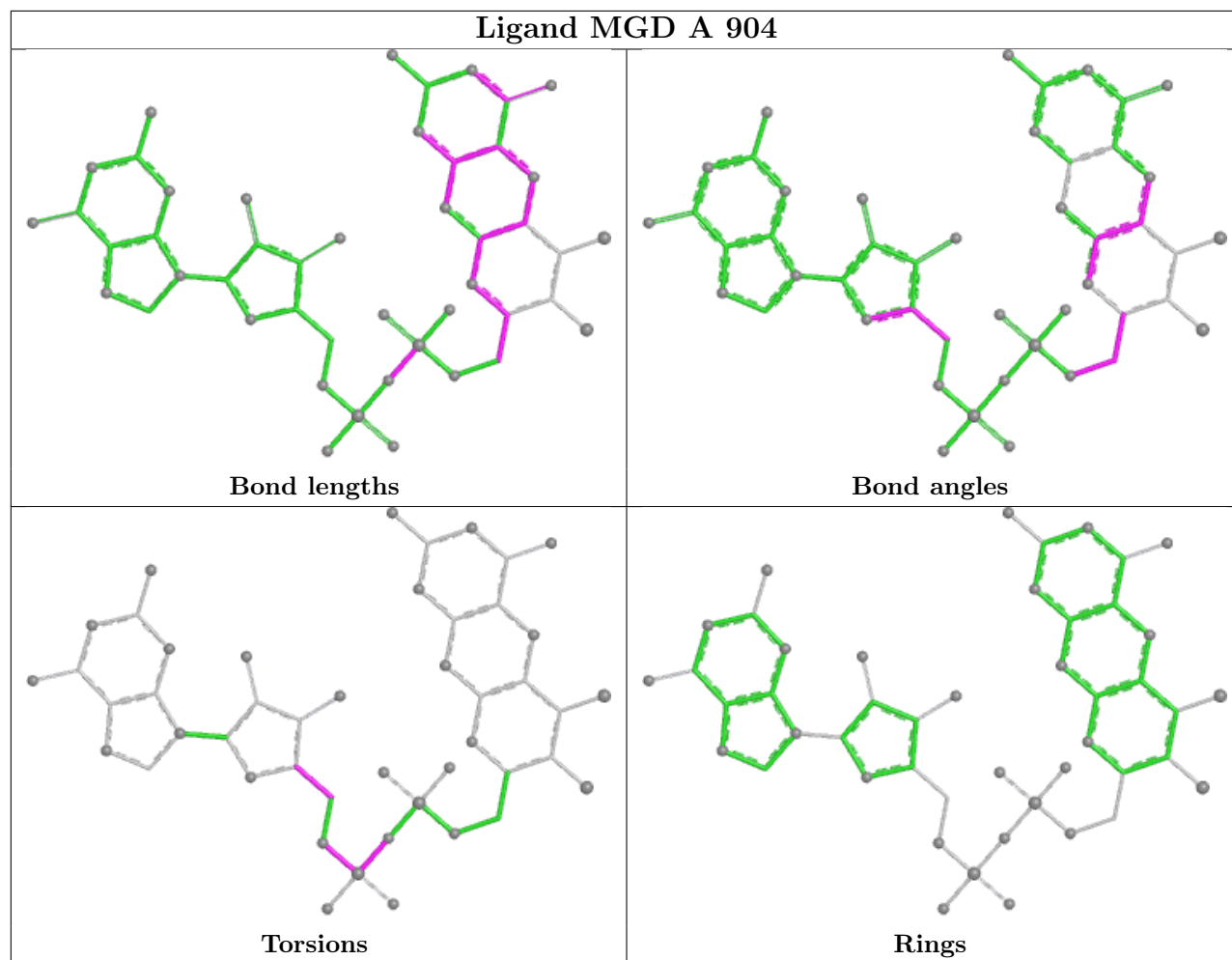


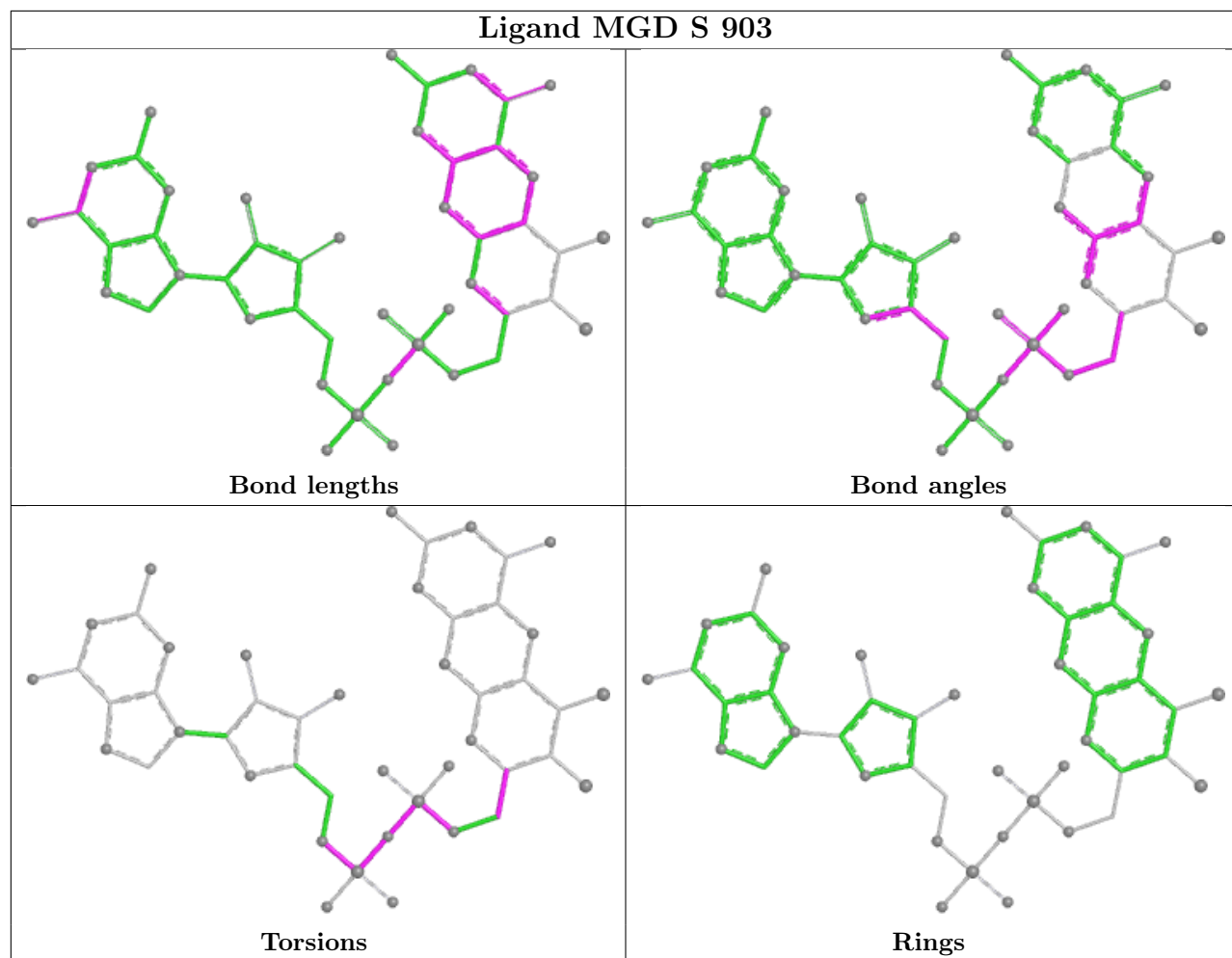


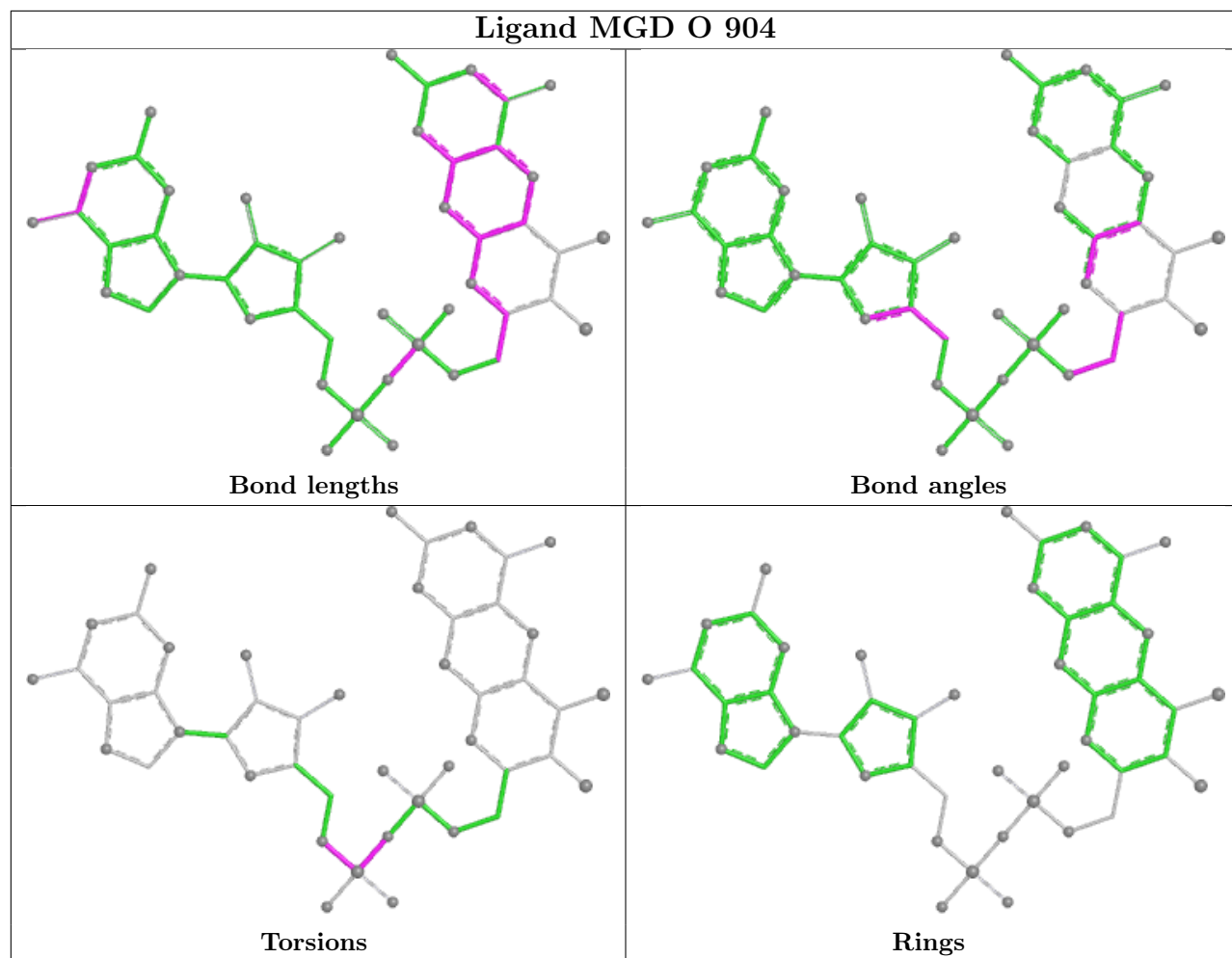


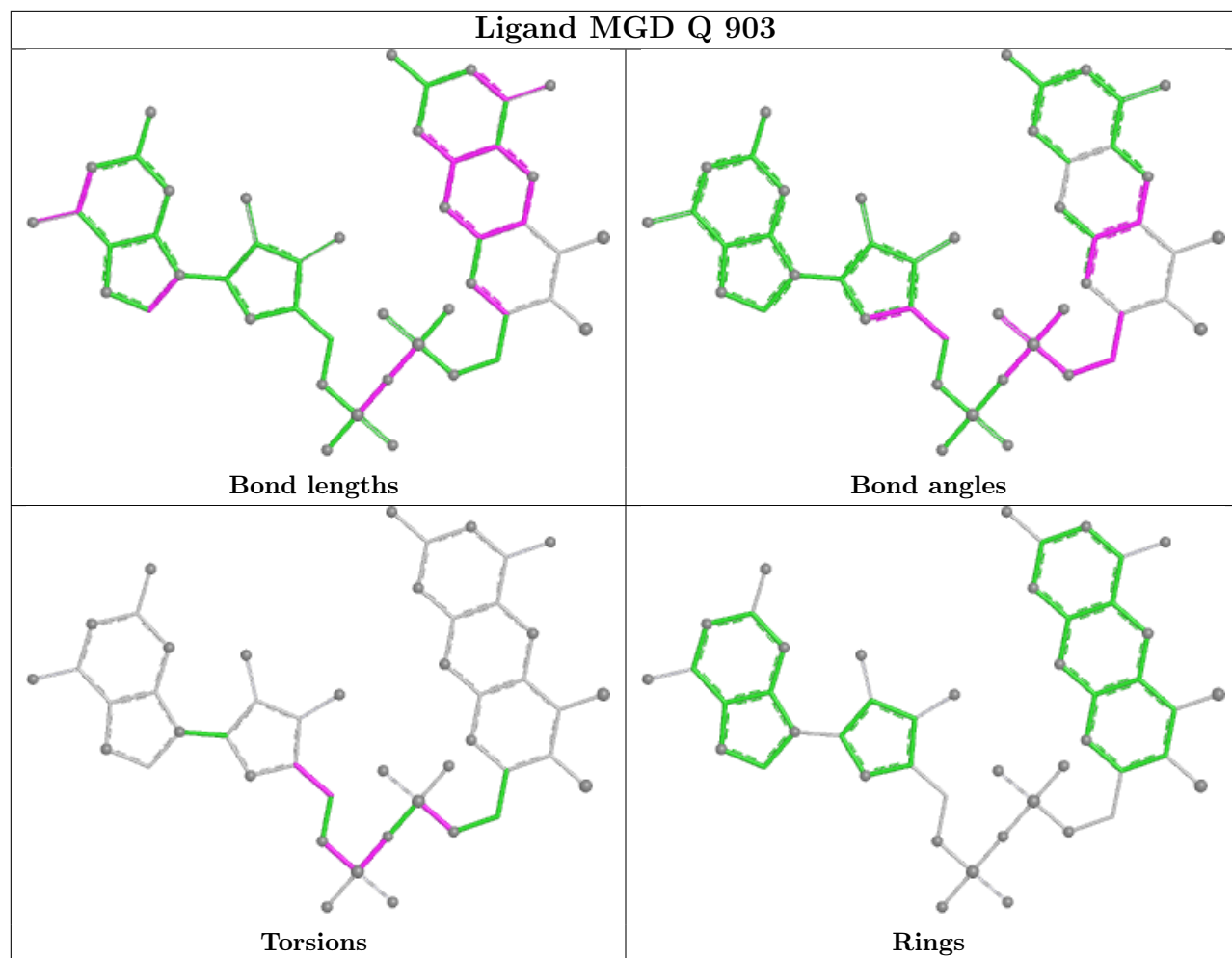


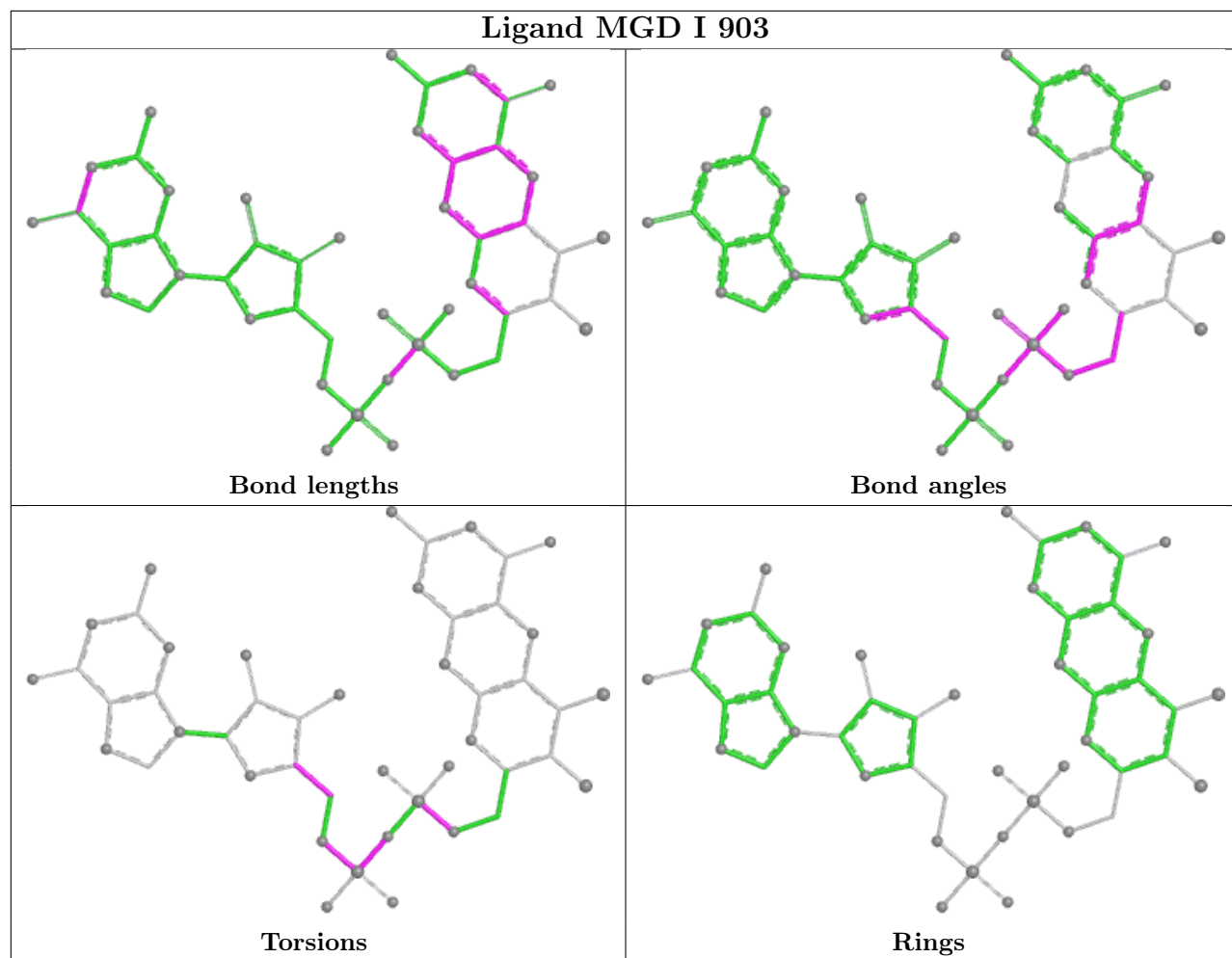


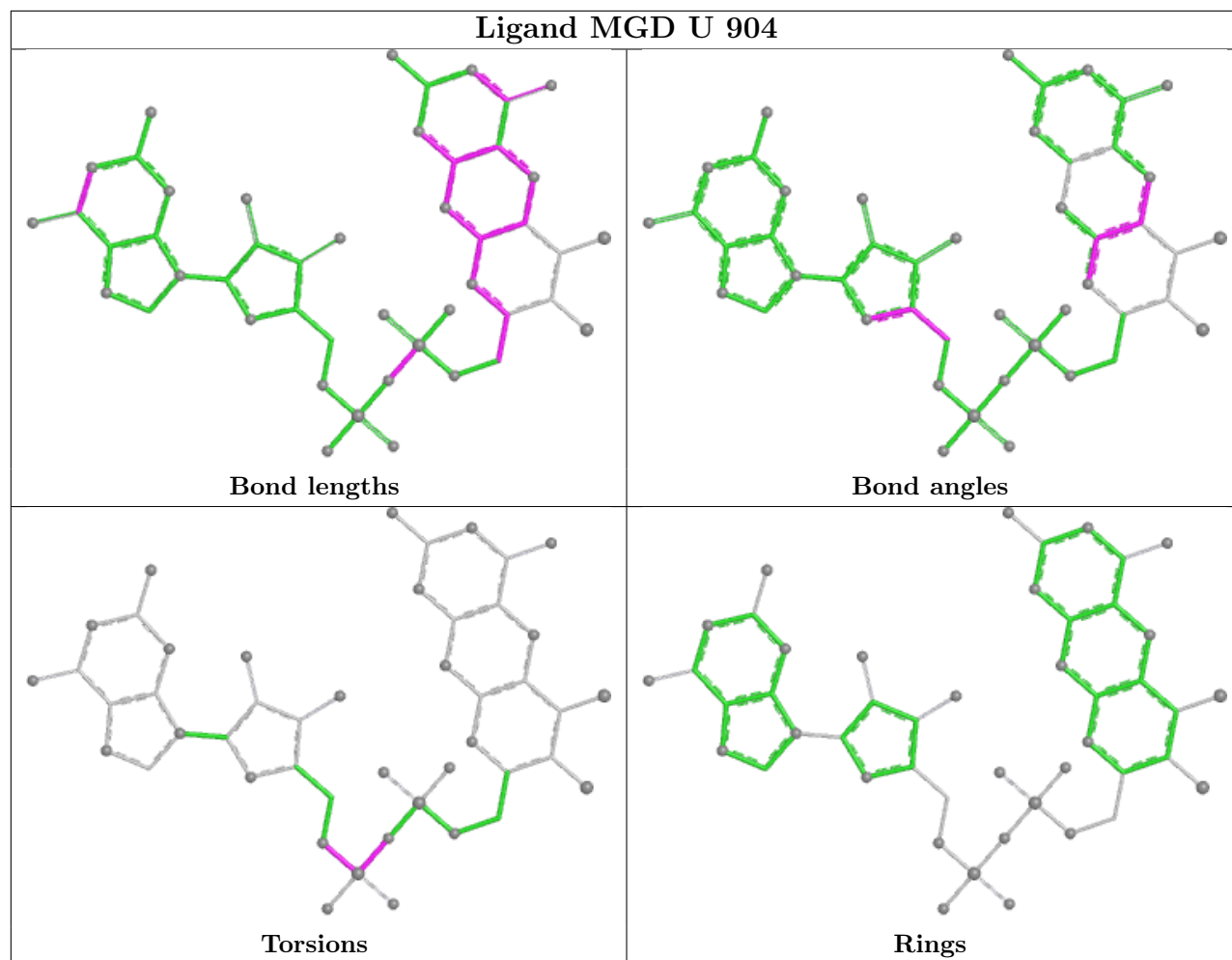


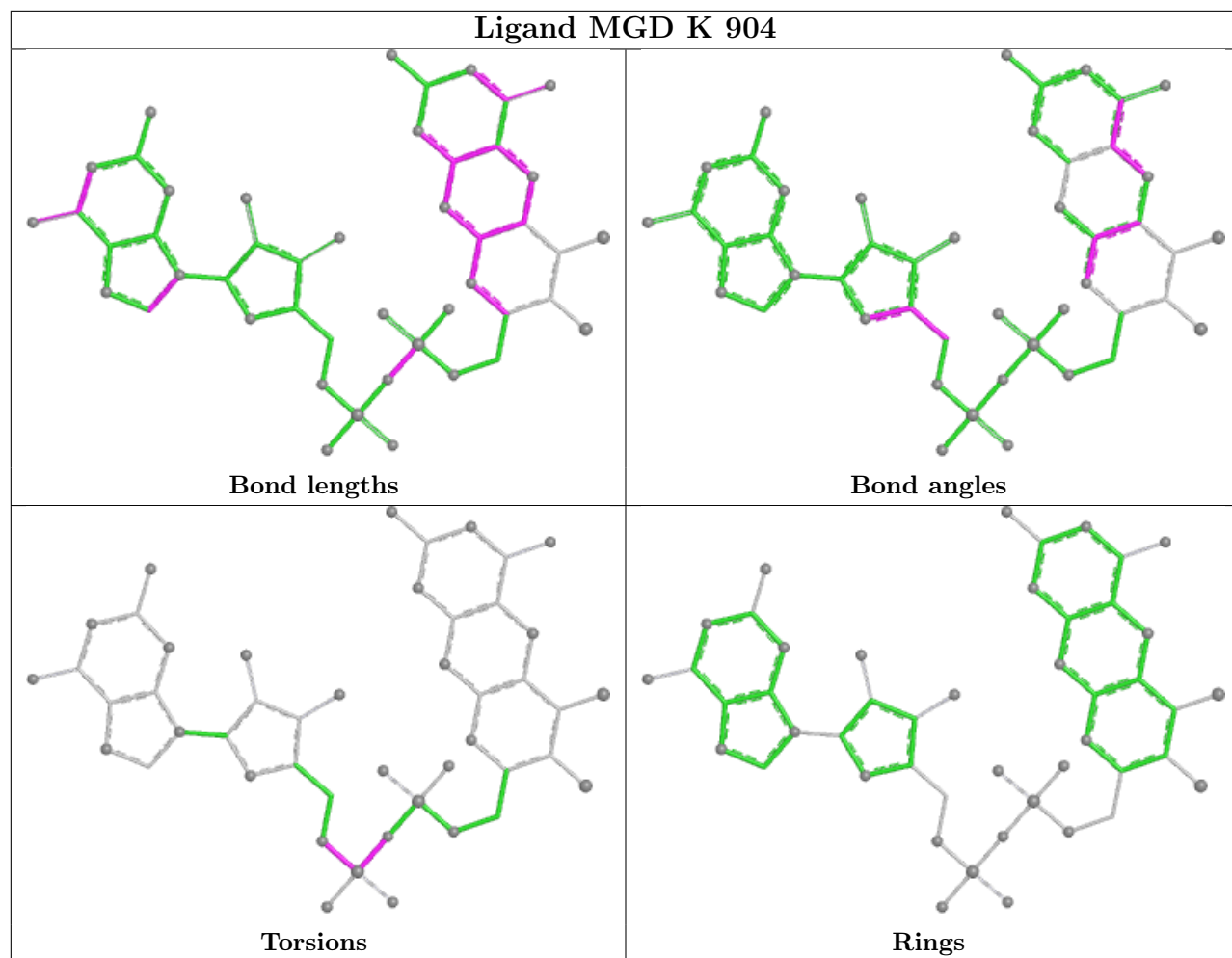


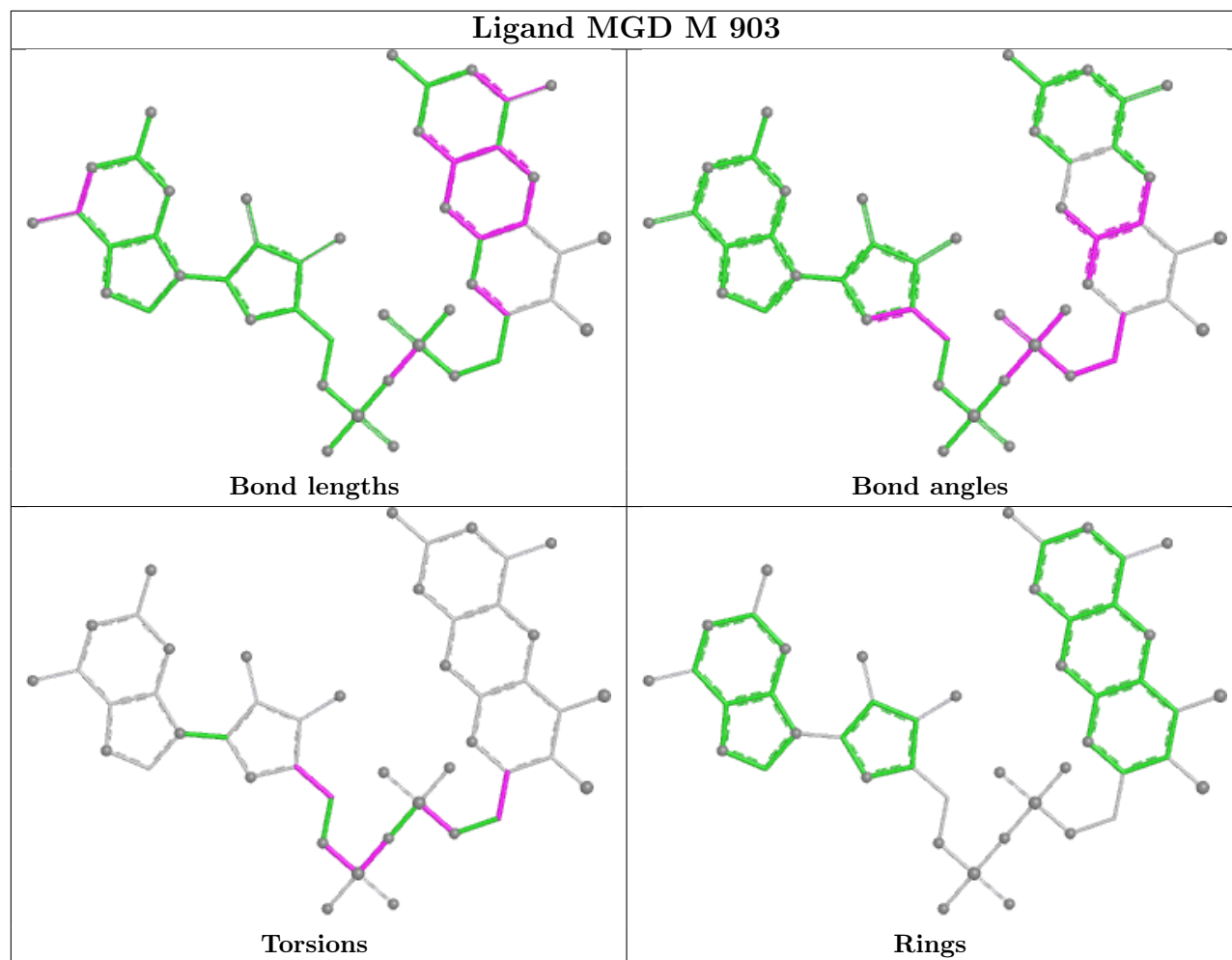


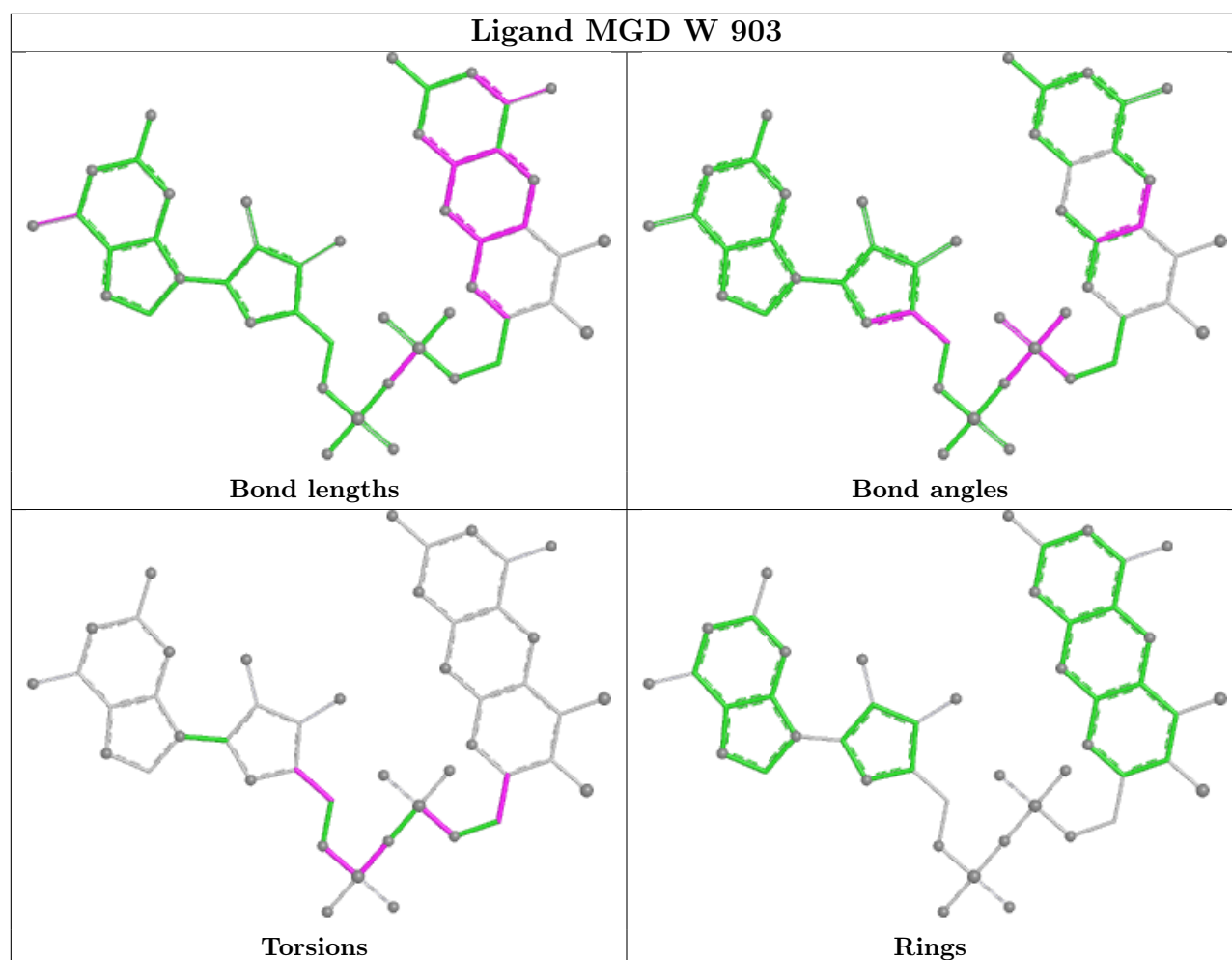


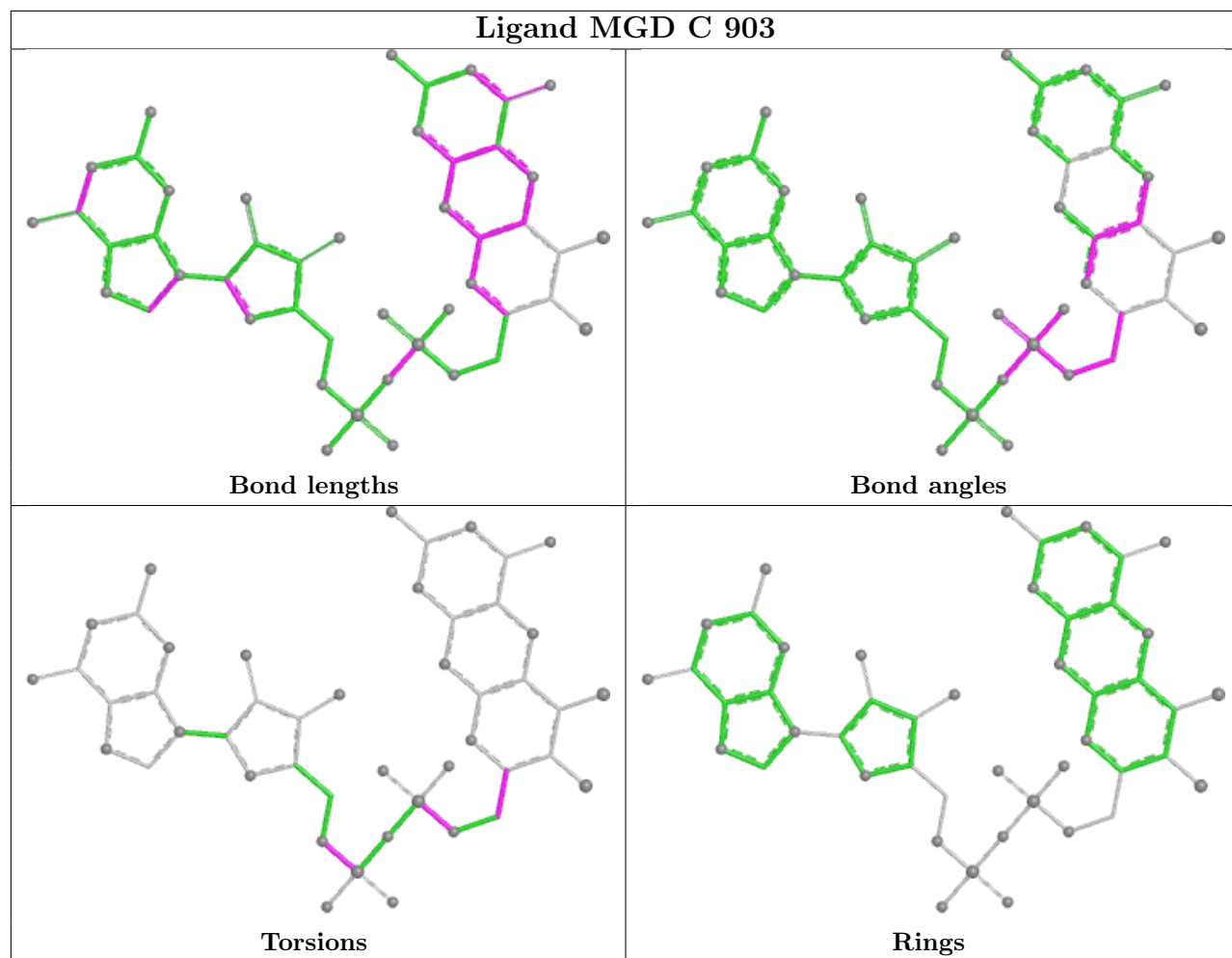


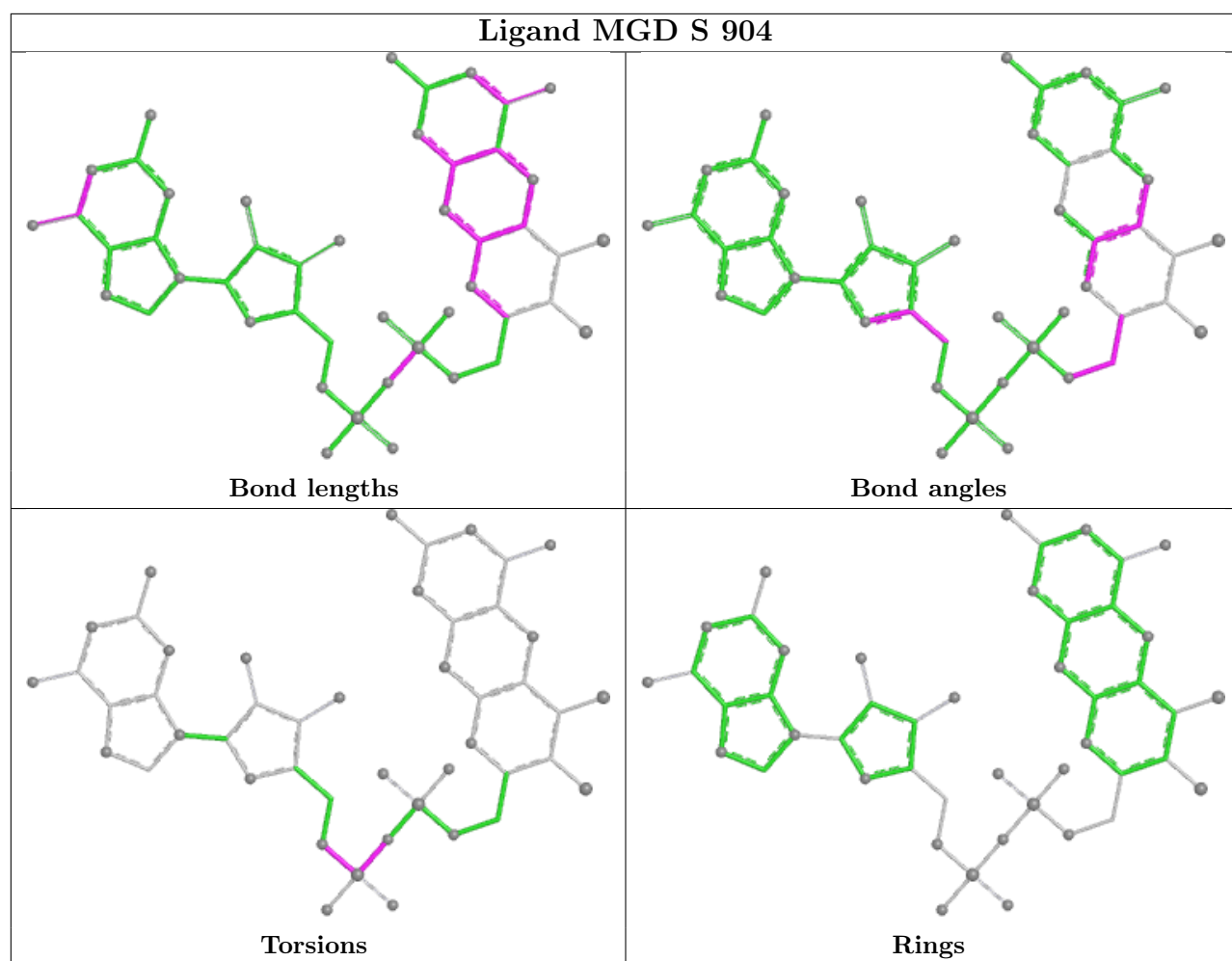


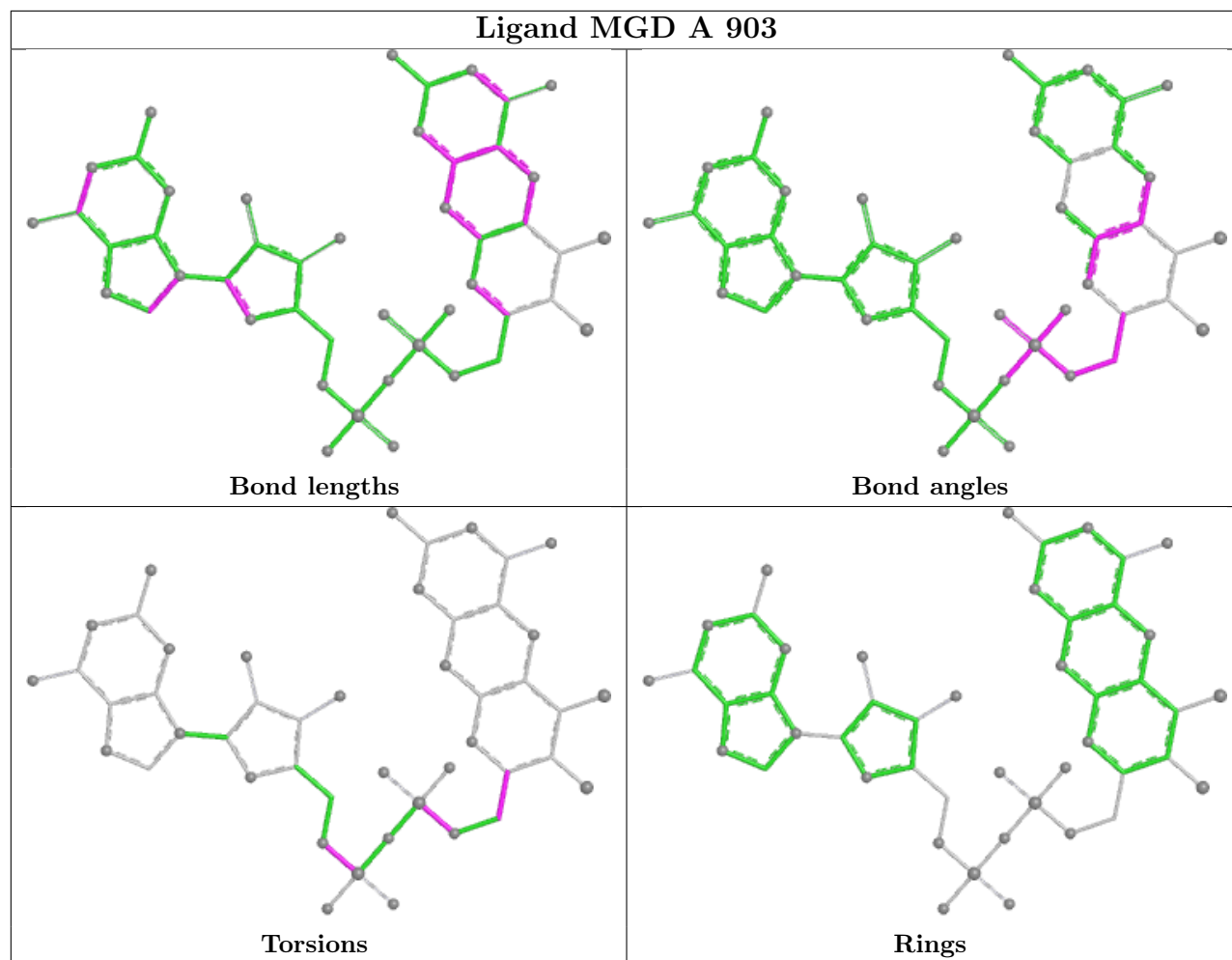












5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.