



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:47 AM EDT

PDB ID : 4V4E / pdb_00004v4e
Title : Crystal Structure of Pyrogallol-Phloroglucinol Transhydroxylase from *Pelobacter acidigallici* complexed with inhibitor 1,2,4,5-tetrahydroxy-benzene
Authors : Messerschmidt, A.; Niessen, H.; Abt, D.; Einsle, O.; Schink, B.; Kroneck, P.M.H.
Deposited on : 2004-06-02
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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)	:	2.50

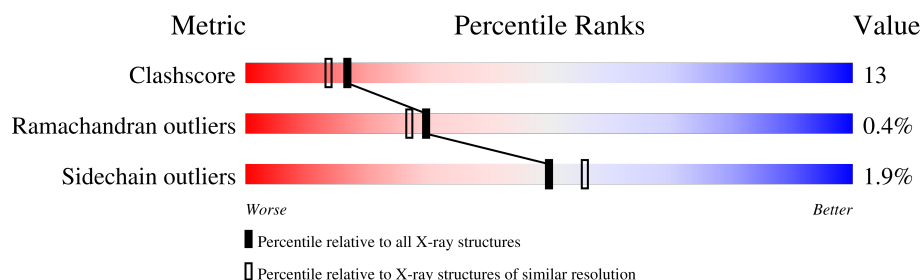
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

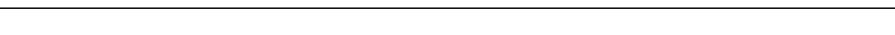
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	875	75% 23% .
1	C	875	74% 24% .
1	E	875	78% 21% .
1	G	875	77% 22% .
1	I	875	75% 24% .
1	K	875	77% 21% .
1	M	875	76% 23% .
1	O	875	77% 21% .

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Mol	Chain	Length	Quality of chain
1	Q	875	 74% 24% .
1	S	875	 74% 24% .
1	U	875	 75% 23% .
1	W	875	 76% 22% .
2	B	274	 74% 23% ..
2	D	274	 65% 31% .
2	F	274	 68% 29% .
2	H	274	 70% 26% ..
2	J	274	 69% 27% ..
2	L	274	 69% 27% .
2	N	274	 69% 27% .
2	P	274	 72% 24% .
2	R	274	 70% 26% .
2	T	274	 69% 28% .
2	V	274	 71% 26% .
2	X	274	 66% 31% ..

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
7	SF4	B	303	-	-	X	-
7	SF4	D	303	-	-	X	-
7	SF4	F	303	-	-	X	-
7	SF4	H	303	-	-	X	-
7	SF4	J	303	-	-	X	-
7	SF4	L	303	-	-	X	-
7	SF4	N	303	-	-	X	-
7	SF4	P	303	-	-	X	-
7	SF4	R	303	-	-	X	-
7	SF4	T	303	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	V	303	-	-	X	-
7	SF4	X	303	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 121823 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	0	0
			6998	4464	1189	1297	48			
1	C	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	E	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	G	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	I	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	K	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	M	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	O	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	Q	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	S	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	U	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	W	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	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 CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

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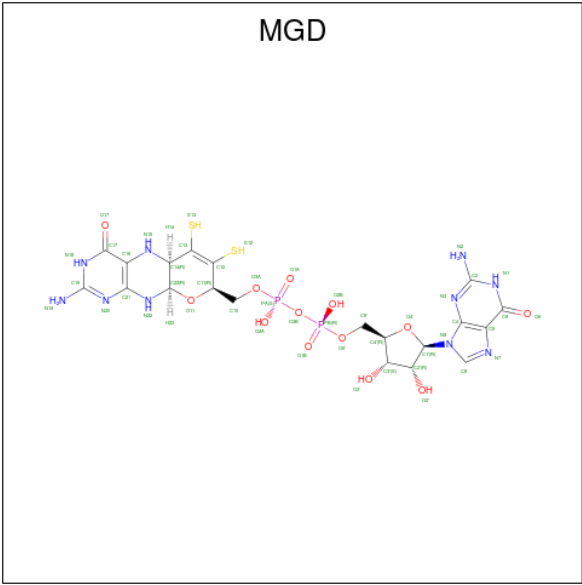
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Ca 1	0	0
3	D	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0
3	G	1	Total 1	Ca 1	0	0
3	H	1	Total 1	Ca 1	0	0
3	I	1	Total 1	Ca 1	0	0
3	J	1	Total 1	Ca 1	0	0
3	K	1	Total 1	Ca 1	0	0
3	L	1	Total 1	Ca 1	0	0
3	M	1	Total 1	Ca 1	0	0
3	N	1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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	1	Total	Ca	0	0
			1	1		

- Molecule 4 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
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
4	I	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
4	I	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	M	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	M	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	O	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	O	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	S	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	S	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	U	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	U	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
4	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 5 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo).

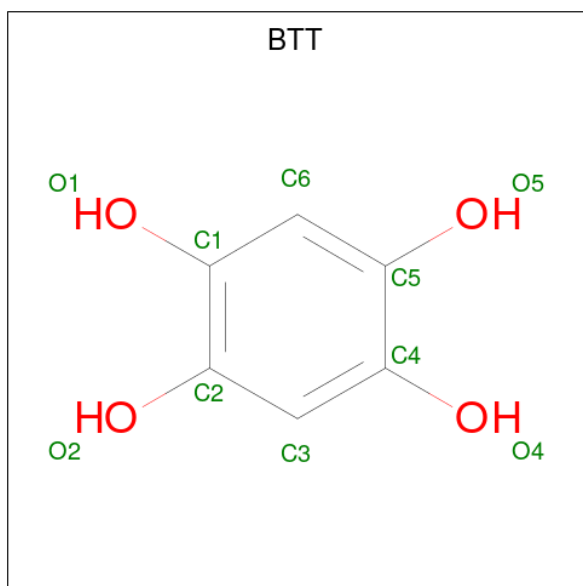
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mo 1	0	0
5	C	1	Total 1	Mo 1	0	0
5	E	1	Total 1	Mo 1	0	0
5	G	1	Total 1	Mo 1	0	0

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

- Molecule 6 is BENZENE-1,2,4,5-TETROL (CCD ID: BTT) (formula: C₆H₆O₄).



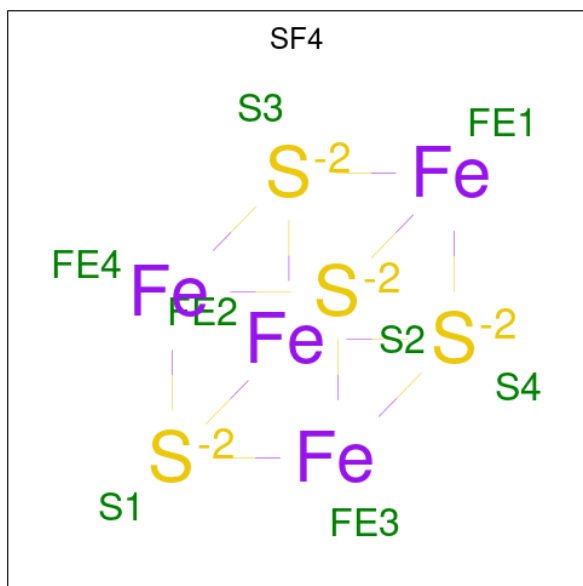
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	E	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			10	6	4		
6	I	1	Total	C	O	0	0
			10	6	4		
6	K	1	Total	C	O	0	0
			10	6	4		
6	M	1	Total	C	O	0	0
			10	6	4		
6	O	1	Total	C	O	0	0
			10	6	4		
6	Q	1	Total	C	O	0	0
			10	6	4		
6	S	1	Total	C	O	0	0
			10	6	4		
6	U	1	Total	C	O	0	0
			10	6	4		
6	W	1	Total	C	O	0	0
			10	6	4		

- 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	681	Total 681	O 681	0	0
8	B	169	Total 169	O 169	0	0
8	C	684	Total 684	O 684	0	0
8	D	162	Total 162	O 162	0	0
8	E	688	Total 688	O 688	0	0
8	F	160	Total 160	O 160	0	0

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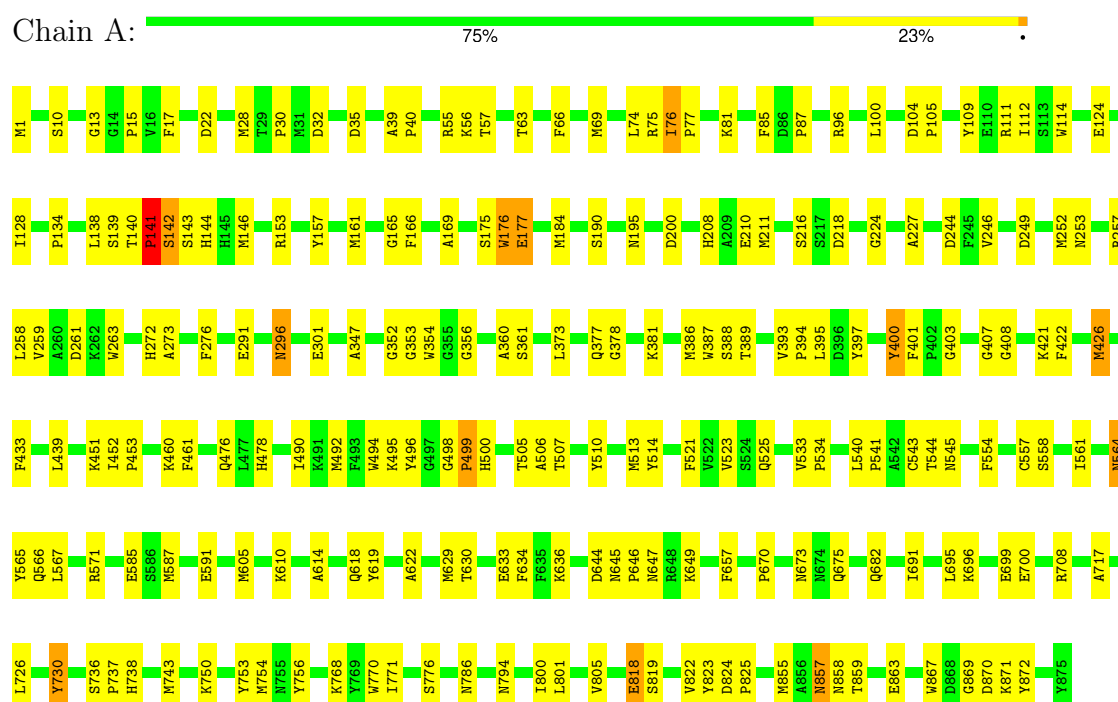
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	682	Total 682	O 682	0	0
8	H	161	Total 161	O 161	0	0
8	I	671	Total 671	O 671	0	0
8	J	168	Total 168	O 168	0	0
8	K	681	Total 681	O 681	0	0
8	L	165	Total 165	O 165	0	0
8	M	682	Total 682	O 682	0	0
8	N	160	Total 160	O 160	0	0
8	O	675	Total 675	O 675	0	0
8	P	160	Total 160	O 160	0	0
8	Q	693	Total 693	O 693	0	0
8	R	158	Total 158	O 158	0	0
8	S	665	Total 665	O 665	0	0
8	T	162	Total 162	O 162	0	0
8	U	670	Total 670	O 670	0	0
8	V	154	Total 154	O 154	0	0
8	W	675	Total 675	O 675	0	0
8	X	165	Total 165	O 165	0	0

3 Residue-property plots

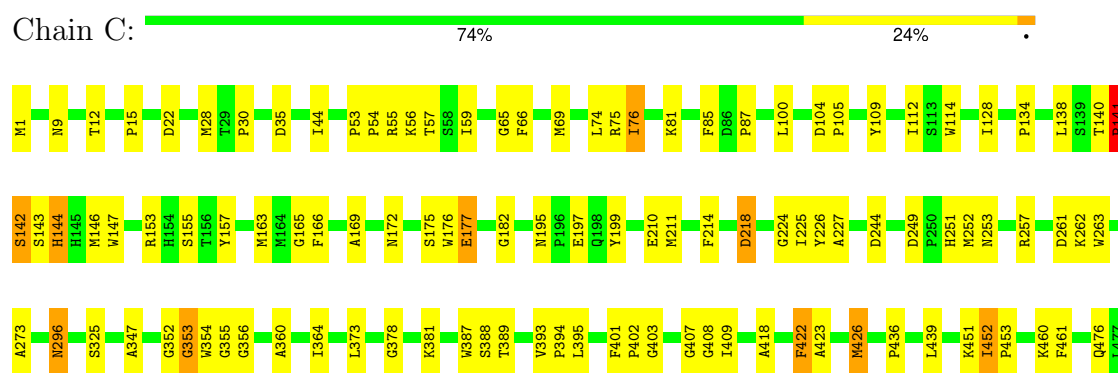
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



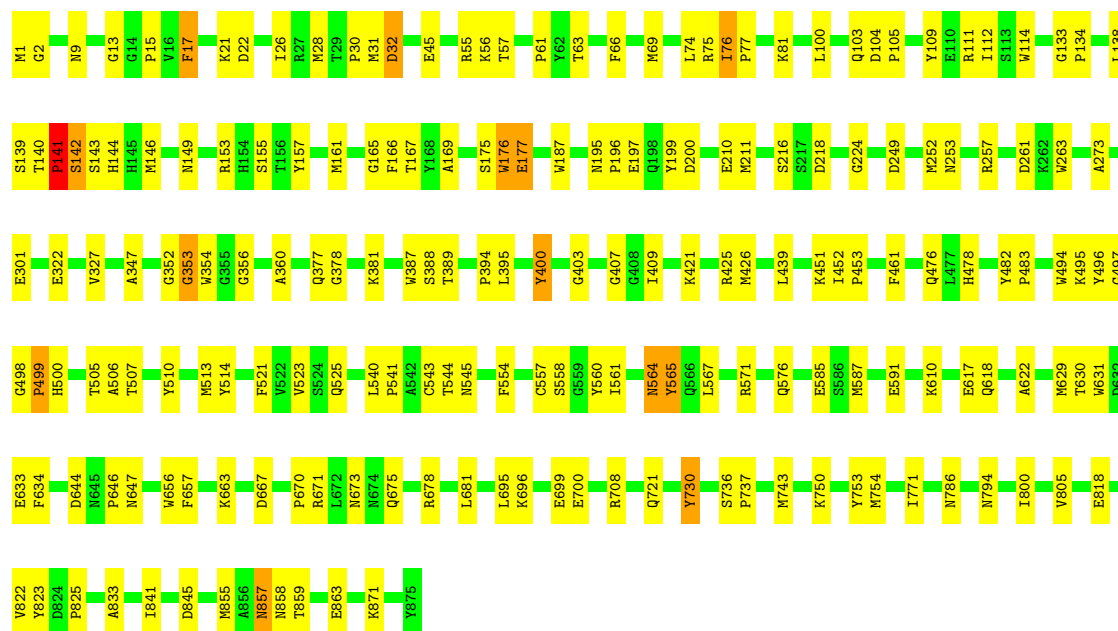
- Molecule 1: Pyrogallol hydroxytransferase large subunit





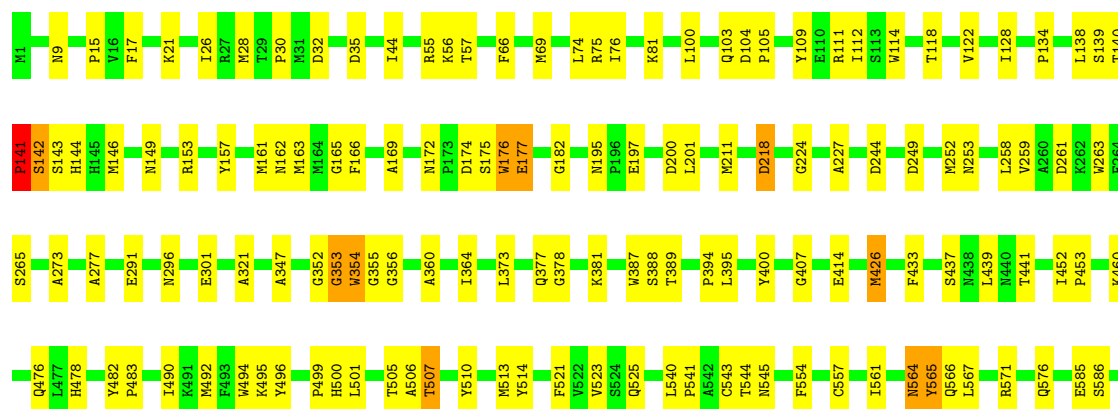
● Molecule 1: Pyrogallol hydroxytransferase large subunit

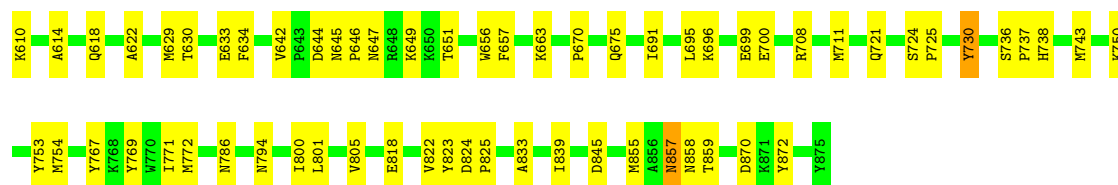
Chain E: 78% 21%



● Molecule 1: Pyrogallol hydroxytransferase large subunit

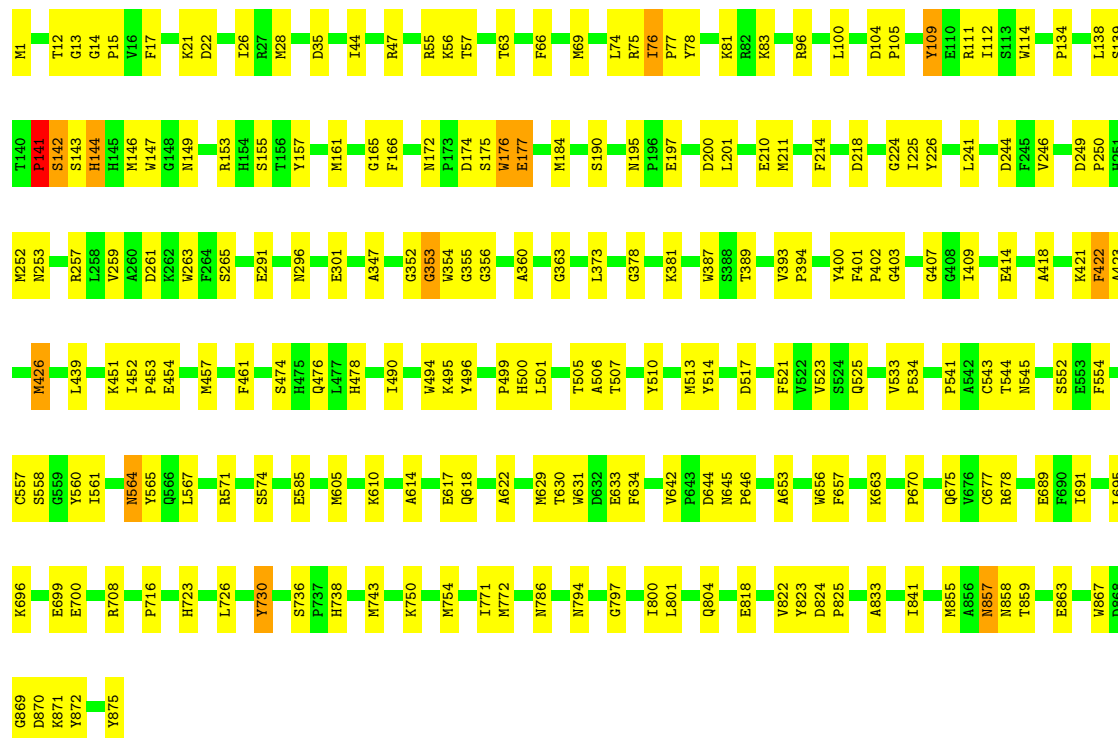
Chain G: 77% 22%





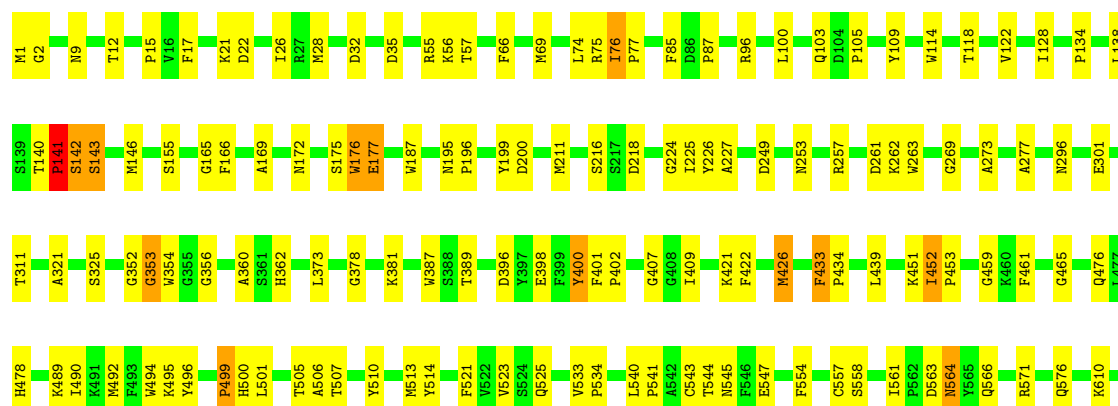
• Molecule 1: Pyrogallol hydroxytransferase large subunit

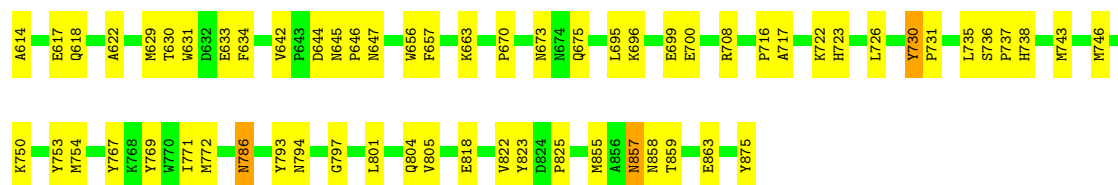
Chain I: 75% 24% •



• Molecule 1: Pyrogallol hydroxytransferase large subunit

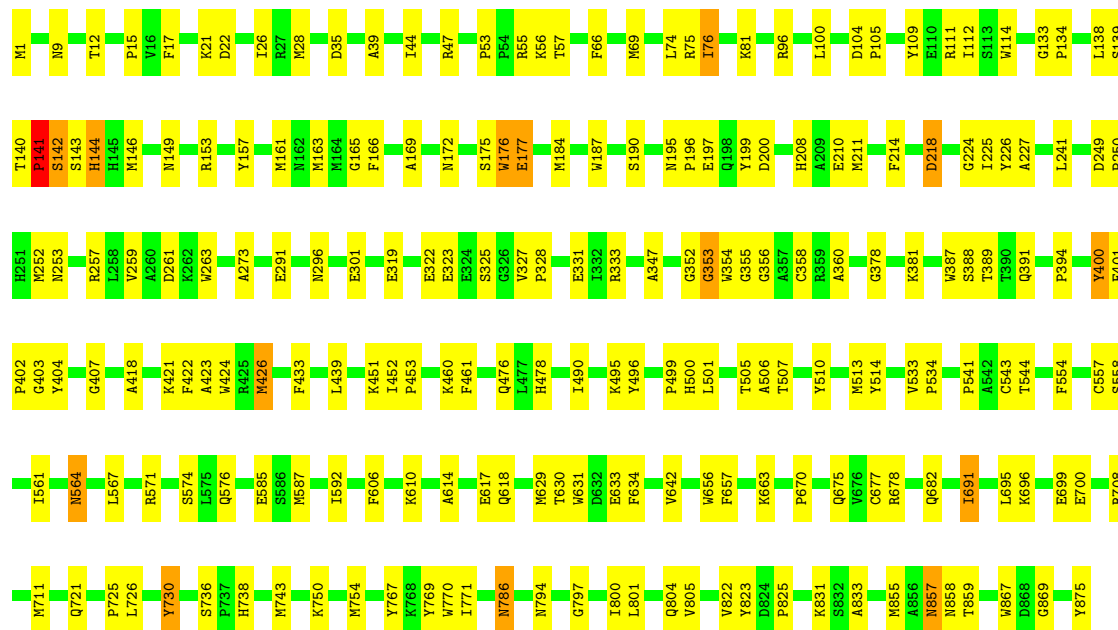
Chain K: 77% 21% •





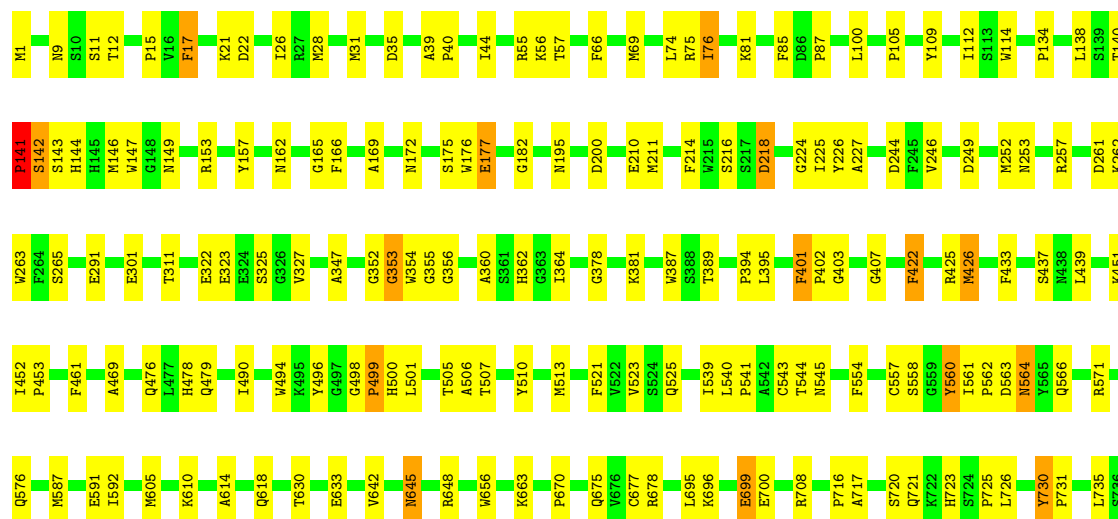
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain M: 76% 23% •



• Molecule 1: Pyrogallol hydroxytransferase large subunit

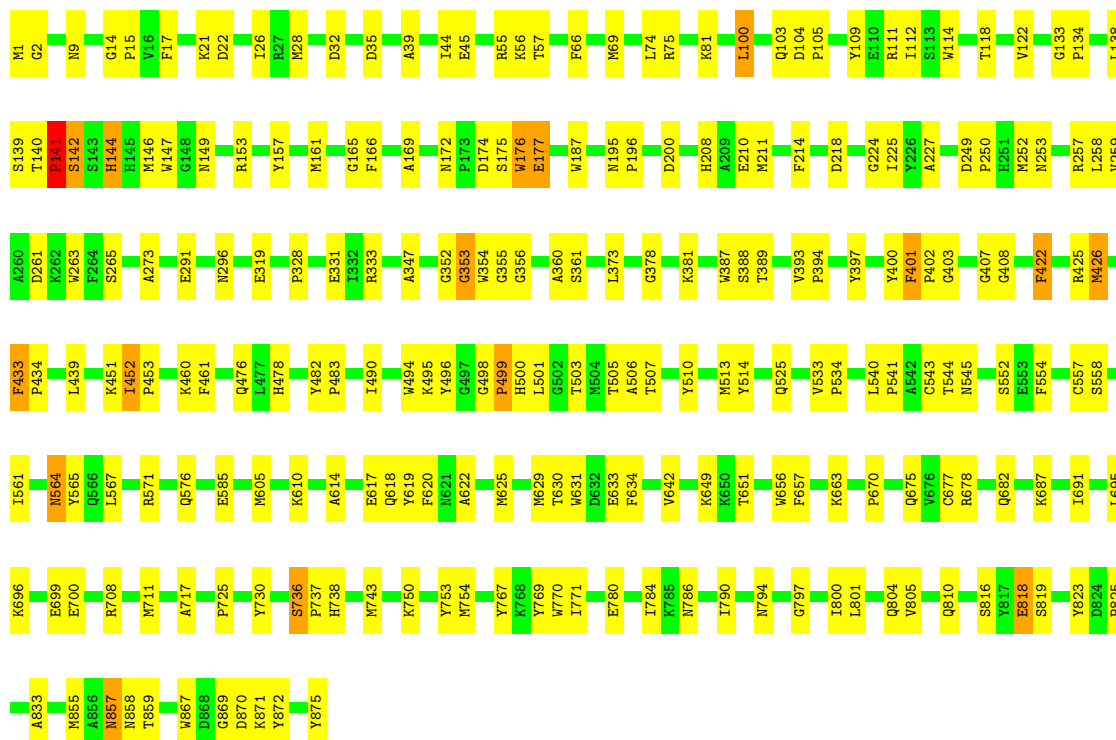
Chain O: 77% 21% •





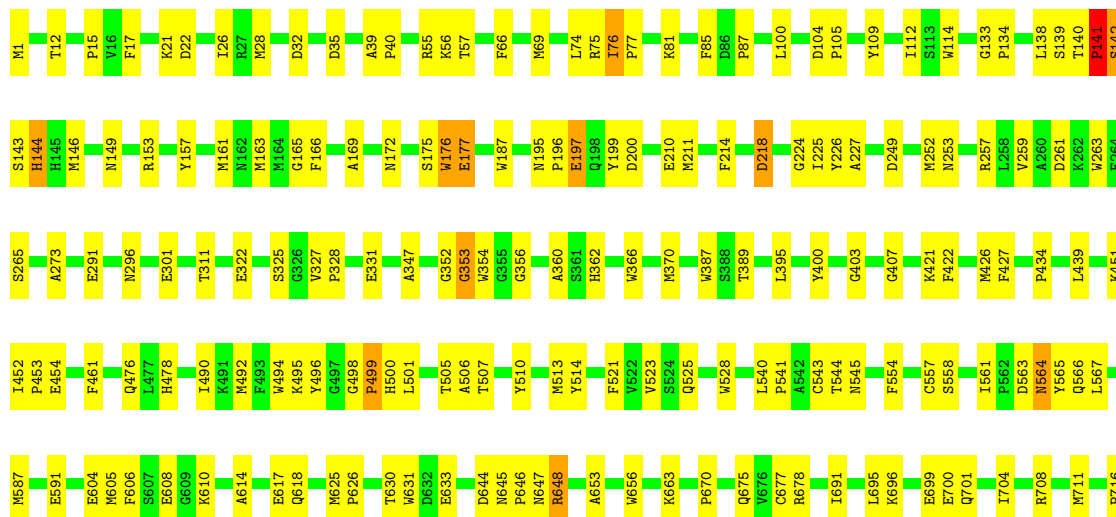
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain Q: 74% 24%



• Molecule 1: Pyrogallol hydroxytransferase large subunit

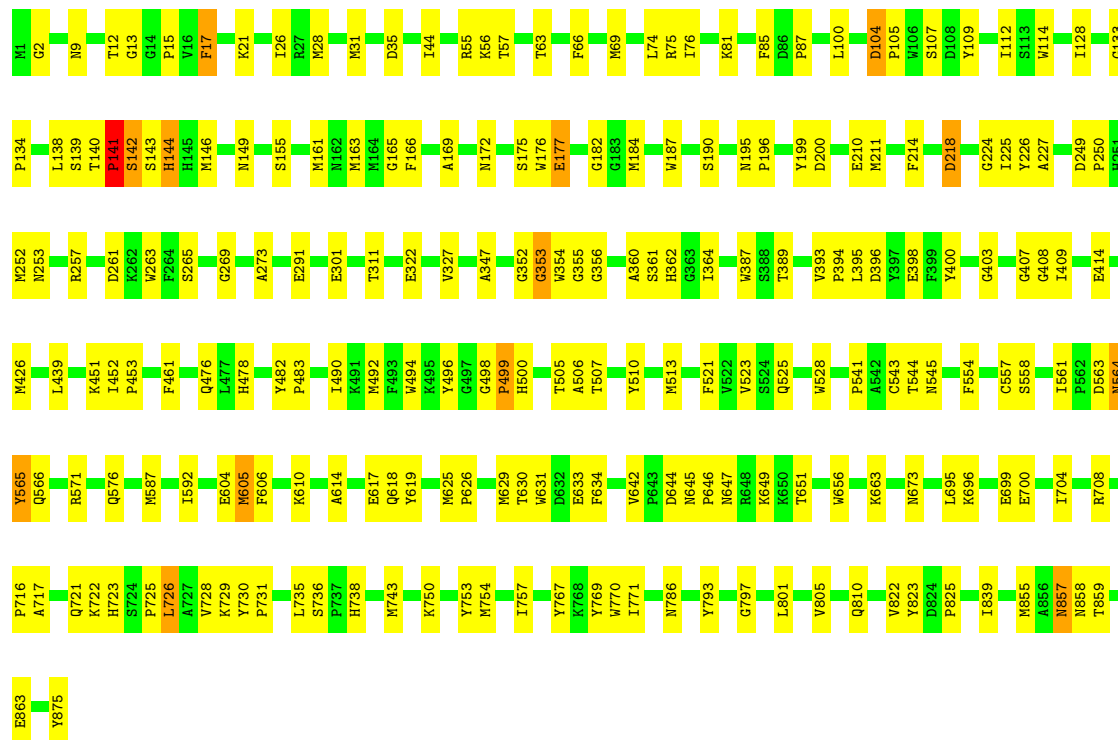
Chain S: 74% 24%





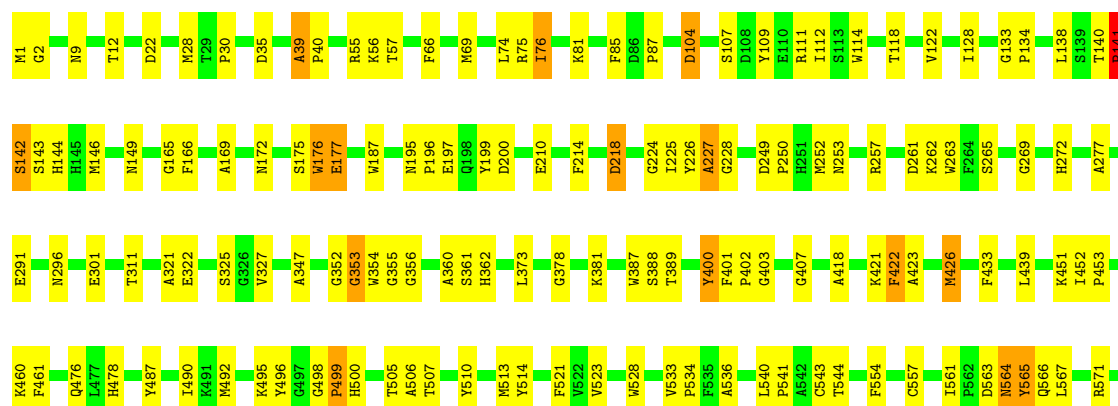
- Molecule 1: Pyrogallol hydroxytransferase large subunit

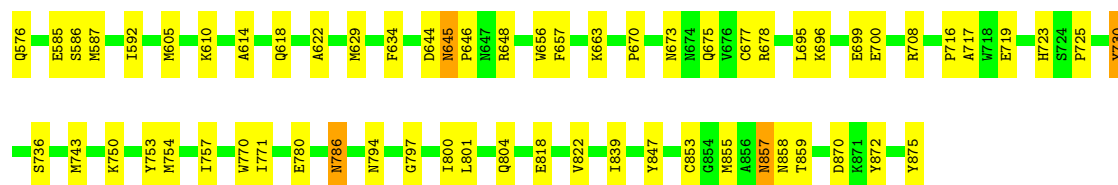
Chain U: 75% 23% .



- Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain W: 76% 22% .





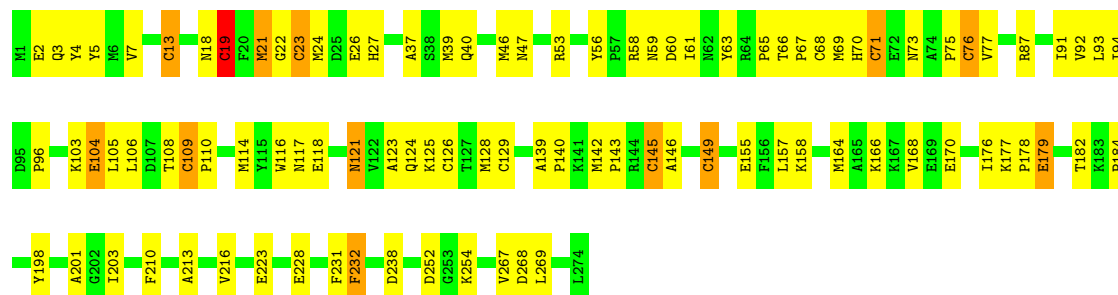
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain B: 74% 23%



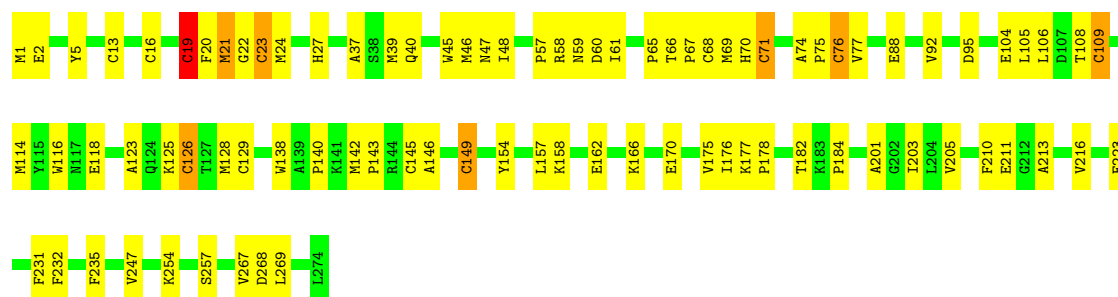
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain D: 65% 31%



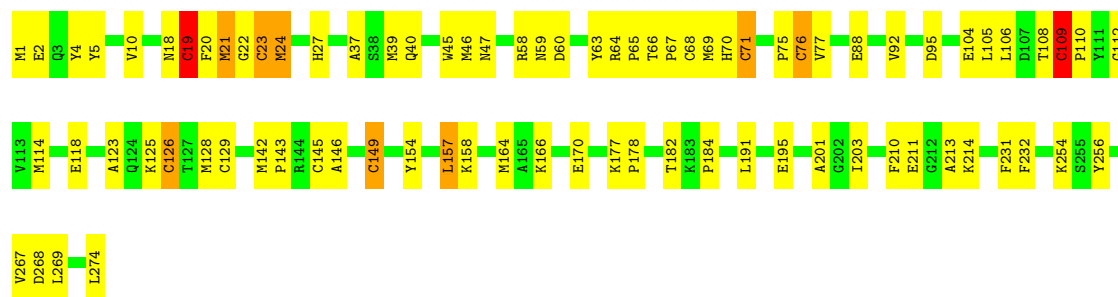
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain F: 68% 29%



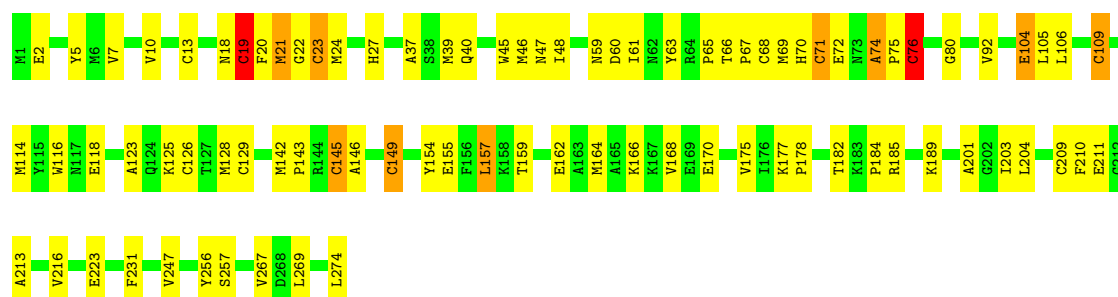
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain H: 70% 26%



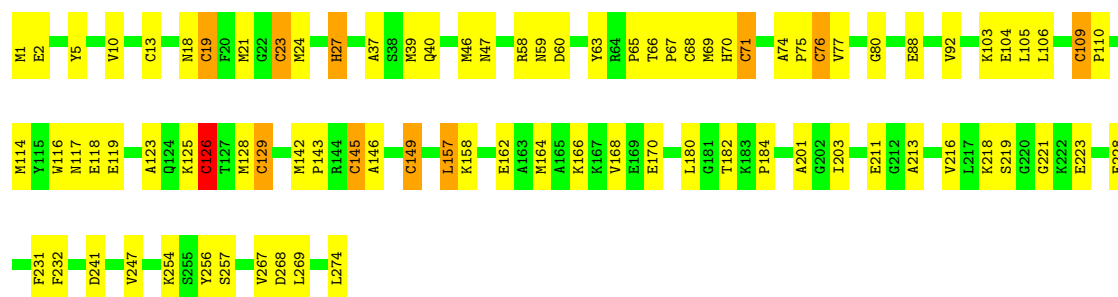
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain J: 69% 27%



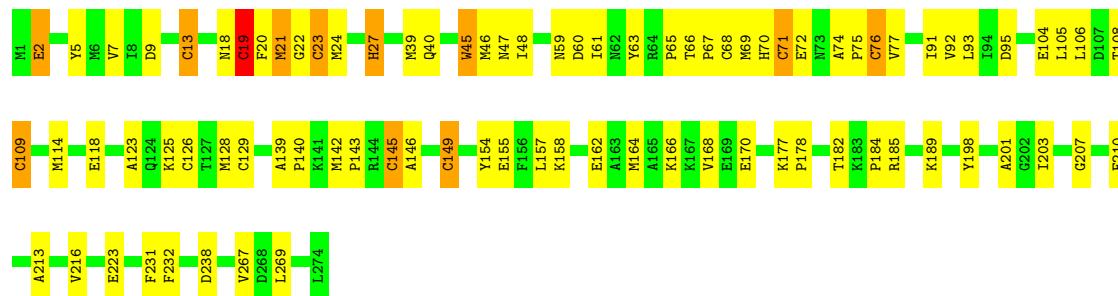
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain L: 69% 27%



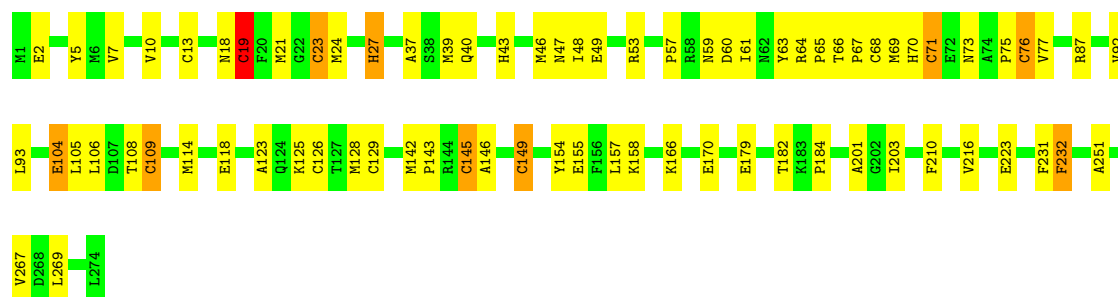
- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain N: 69% 27%



- Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain P:  72% 24% .



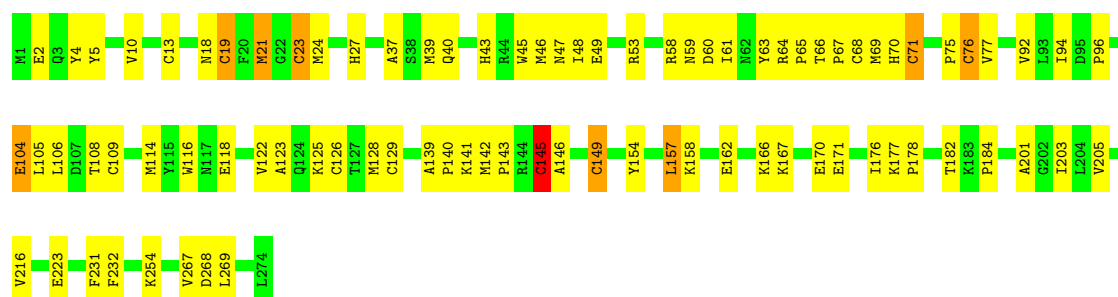
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain R:  70% 26% .



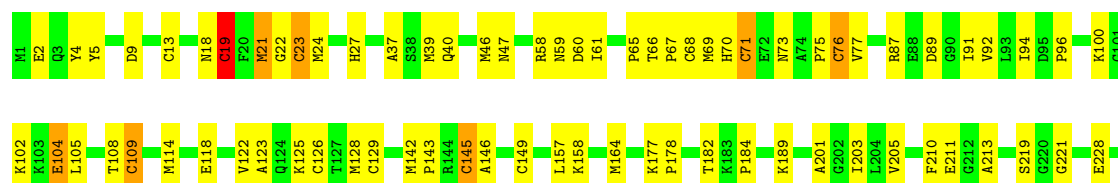
• Molecule 2: Pyrogallol hydroxytransferase small subunit

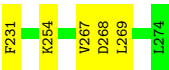
Chain T:  69% 28% .



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain V:  71% 26% .





● 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	172.57Å 178.44Å 179.66Å 63.83° 64.40° 65.04°	Depositor
Resolution (Å)	24.99 – 2.00	Depositor
% Data completeness (in resolution range)	96.5 (24.99-2.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.172 , 0.203	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	121823	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: SF4, CA, MGD, 4MO, BTT

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	0.37	0/7219	0.96	46/9786 (0.5%)
1	C	0.36	0/7219	0.96	41/9786 (0.4%)
1	E	0.38	0/7219	0.97	39/9786 (0.4%)
1	G	0.37	0/7219	0.97	41/9786 (0.4%)
1	I	0.36	0/7219	0.96	46/9786 (0.5%)
1	K	0.38	0/7219	0.97	41/9786 (0.4%)
1	M	0.37	0/7219	0.96	47/9786 (0.5%)
1	O	0.37	0/7219	0.96	39/9786 (0.4%)
1	Q	0.37	0/7219	0.97	42/9786 (0.4%)
1	S	0.37	0/7219	0.97	47/9786 (0.5%)
1	U	0.37	0/7219	0.96	43/9786 (0.4%)
1	W	0.36	0/7219	0.96	47/9786 (0.5%)
2	B	0.49	0/2231	1.00	13/3009 (0.4%)
2	D	0.40	0/2231	0.93	7/3009 (0.2%)
2	F	0.46	0/2231	1.01	17/3009 (0.6%)
2	H	0.48	0/2231	1.02	16/3009 (0.5%)
2	J	0.46	0/2231	0.97	12/3009 (0.4%)
2	L	0.45	0/2231	1.00	14/3009 (0.5%)
2	N	0.47	0/2231	0.99	15/3009 (0.5%)
2	P	0.44	0/2231	0.96	11/3009 (0.4%)
2	R	0.47	1/2231 (0.0%)	1.00	13/3009 (0.4%)
2	T	0.42	0/2231	0.96	9/3009 (0.3%)
2	V	0.41	0/2231	0.94	6/3009 (0.2%)
2	X	0.39	0/2231	0.91	6/3009 (0.2%)
All	All	0.39	1/113400 (0.0%)	0.97	658/153540 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	23	CYS	CA-C	-5.10	1.46	1.52

All (658) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	353	GLY	N-CA-C	-9.80	100.09	111.85
1	S	353	GLY	N-CA-C	-9.63	100.30	111.85
1	M	352	GLY	N-CA-C	-9.60	90.42	113.18
1	W	507	THR	N-CA-C	9.54	124.31	112.87
2	B	23	CYS	CB-CA-C	-9.51	95.95	110.88
1	Q	507	THR	N-CA-C	9.45	124.21	112.87
1	W	353	GLY	N-CA-C	-9.33	100.65	111.85
1	A	507	THR	N-CA-C	9.25	123.97	112.87
1	E	353	GLY	N-CA-C	-9.21	100.80	111.85
1	I	352	GLY	N-CA-C	-9.13	91.55	113.18
1	G	353	GLY	N-CA-C	-9.11	100.92	111.85
1	Q	352	GLY	N-CA-C	-9.10	91.61	113.18
2	N	23	CYS	CB-CA-C	-9.06	97.00	110.96
1	A	352	GLY	N-CA-C	-9.05	91.74	113.18
1	M	507	THR	N-CA-C	9.03	123.70	112.87
1	S	507	THR	N-CA-C	9.02	123.69	112.87
1	E	352	GLY	N-CA-C	-8.98	91.90	113.18
1	W	352	GLY	N-CA-C	-8.95	91.96	113.18
1	C	507	THR	N-CA-C	8.94	123.60	112.87
1	K	352	GLY	N-CA-C	-8.91	92.06	113.18
1	E	507	THR	N-CA-C	8.87	123.52	112.87
1	O	507	THR	N-CA-C	8.86	123.50	112.87
1	C	352	GLY	N-CA-C	-8.85	92.19	113.18
2	J	23	CYS	CB-CA-C	-8.83	97.01	110.88
1	G	352	GLY	N-CA-C	-8.82	92.28	113.18
1	Q	353	GLY	N-CA-C	-8.82	100.41	111.70
1	S	352	GLY	N-CA-C	-8.80	92.32	113.18
2	R	23	CYS	CB-CA-C	-8.80	97.41	110.96
2	H	145	CYS	CB-CA-C	-8.76	97.47	110.96
2	P	23	CYS	CB-CA-C	-8.72	97.18	110.88
1	O	352	GLY	N-CA-C	-8.67	92.63	113.18
1	K	353	GLY	N-CA-C	-8.65	100.63	111.70
2	L	23	CYS	CB-CA-C	-8.54	97.47	110.88
1	W	857	ASN	N-CA-C	8.51	121.32	111.11
1	G	507	THR	N-CA-C	8.48	123.04	112.87
1	U	352	GLY	N-CA-C	-8.44	93.19	113.18
2	F	23	CYS	CB-CA-C	-8.42	97.66	110.88
1	I	507	THR	N-CA-C	8.40	122.96	112.87
2	D	77	VAL	N-CA-C	-8.33	101.92	111.00
1	U	857	ASN	N-CA-C	8.32	121.09	111.11
1	O	353	GLY	N-CA-C	-8.14	101.28	111.70
1	M	407	GLY	N-CA-C	8.04	124.65	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	23	CYS	CB-CA-C	-8.04	98.26	110.88
1	Q	500	HIS	N-CA-C	8.04	120.95	111.71
1	G	76	ILE	CA-C-N	7.99	127.56	118.85
1	G	76	ILE	C-N-CA	7.99	127.56	118.85
1	K	76	ILE	CA-C-N	7.97	127.54	118.85
1	K	76	ILE	C-N-CA	7.97	127.54	118.85
1	A	857	ASN	N-CA-C	7.96	120.66	111.11
1	S	857	ASN	N-CA-C	7.94	120.64	111.11
1	I	353	GLY	N-CA-C	-7.93	101.55	111.70
1	G	500	HIS	N-CA-C	7.91	121.87	111.75
2	T	77	VAL	N-CA-C	-7.83	103.23	110.82
1	M	353	GLY	N-CA-C	-7.82	101.69	111.70
1	C	857	ASN	N-CA-C	7.80	120.48	111.11
2	N	77	VAL	N-CA-C	-7.80	103.25	110.82
1	O	857	ASN	N-CA-C	7.79	120.46	111.11
2	D	19	CYS	CB-CA-C	-7.79	98.97	110.96
1	G	141	PRO	N-CA-C	-7.69	96.63	112.47
1	A	353	GLY	N-CA-C	-7.67	101.48	111.52
1	C	353	GLY	N-CA-C	-7.66	100.81	111.76
1	Q	857	ASN	N-CA-C	7.62	120.26	111.11
1	M	857	ASN	N-CA-C	7.62	120.25	111.11
1	K	857	ASN	N-CA-C	7.57	120.19	111.11
2	F	77	VAL	N-CA-C	-7.51	102.81	111.00
1	G	857	ASN	N-CA-C	7.50	120.40	111.33
2	L	149	CYS	CB-CA-C	-7.49	98.22	109.90
1	S	500	HIS	N-CA-C	7.47	121.32	111.75
1	W	730	TYR	CA-C-N	7.43	127.07	119.56
1	W	730	TYR	C-N-CA	7.43	127.07	119.56
1	U	407	GLY	N-CA-C	7.42	123.91	115.08
1	A	407	GLY	N-CA-C	7.42	123.91	115.08
1	A	141	PRO	N-CA-C	-7.38	97.28	112.47
1	A	500	HIS	N-CA-C	7.37	121.18	111.75
1	I	500	HIS	N-CA-C	7.33	121.13	111.75
2	T	23	CYS	CB-CA-C	-7.32	99.39	110.88
1	I	76	ILE	CA-C-N	7.30	126.81	118.85
1	I	76	ILE	C-N-CA	7.30	126.81	118.85
2	F	19	CYS	CB-CA-C	-7.30	95.89	110.42
1	Q	141	PRO	N-CA-C	-7.29	97.45	112.47
2	B	76	CYS	CB-CA-C	-7.29	99.44	110.88
2	H	19	CYS	CB-CA-C	-7.28	95.93	110.42
2	H	77	VAL	N-CA-C	-7.26	103.09	111.00
1	S	261	ASP	N-CA-C	-7.25	104.57	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	149	CYS	CB-CA-C	-7.24	98.04	109.70
1	U	730	TYR	CA-C-N	7.19	126.83	119.56
1	U	730	TYR	C-N-CA	7.19	126.83	119.56
1	M	500	HIS	N-CA-C	7.13	120.87	111.75
1	K	730	TYR	CA-C-N	7.12	126.75	119.56
1	K	730	TYR	C-N-CA	7.12	126.75	119.56
2	L	19	CYS	CB-CA-C	-7.11	96.27	110.42
1	K	141	PRO	N-CA-C	-7.09	97.86	112.47
1	O	407	GLY	N-CA-C	7.08	123.51	115.08
1	C	730	TYR	CA-C-N	7.08	126.71	119.56
1	C	730	TYR	C-N-CA	7.08	126.71	119.56
2	R	19	CYS	CB-CA-C	-7.08	96.33	110.42
2	H	109	CYS	CB-CA-C	-7.07	101.79	109.85
1	I	224	GLY	N-CA-C	-7.06	96.46	113.18
1	S	736	SER	CA-C-N	7.05	128.65	119.84
1	S	736	SER	C-N-CA	7.05	128.65	119.84
1	Q	224	GLY	N-CA-C	-7.04	96.50	113.18
2	B	19	CYS	CB-CA-C	-7.02	96.45	110.42
2	X	77	VAL	N-CA-C	-7.01	102.46	112.35
1	S	141	PRO	N-CA-C	-7.01	98.03	112.47
1	I	141	PRO	N-CA-C	-6.98	98.09	112.47
2	V	23	CYS	CB-CA-C	-6.97	99.94	110.88
2	B	149	CYS	CB-CA-C	-6.95	98.19	109.72
1	E	500	HIS	N-CA-C	6.95	120.64	111.75
1	C	76	ILE	CA-C-N	6.95	126.76	119.05
1	C	76	ILE	C-N-CA	6.95	126.76	119.05
1	K	500	HIS	N-CA-C	6.94	119.70	111.71
1	E	76	ILE	CA-C-N	6.92	126.40	118.85
1	E	76	ILE	C-N-CA	6.92	126.40	118.85
2	L	267	VAL	N-CA-C	6.92	117.80	108.11
1	S	76	ILE	CA-C-N	6.92	126.39	118.85
1	S	76	ILE	C-N-CA	6.92	126.39	118.85
1	M	261	ASP	N-CA-C	-6.91	105.00	113.50
1	U	261	ASP	N-CA-C	-6.91	105.00	113.50
1	K	507	THR	N-CA-C	6.90	125.50	110.80
2	V	77	VAL	N-CA-C	-6.90	103.48	111.00
1	W	433	PHE	CA-C-N	6.90	126.83	120.21
1	W	433	PHE	C-N-CA	6.90	126.83	120.21
1	A	224	GLY	N-CA-C	-6.86	96.92	113.18
1	O	261	ASP	N-CA-C	-6.85	105.08	113.50
1	O	224	GLY	N-CA-C	-6.85	96.95	113.18
1	G	730	TYR	CA-C-N	6.82	126.44	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	730	TYR	C-N-CA	6.82	126.44	119.56
1	O	422	PHE	N-CA-C	6.81	118.36	111.07
2	F	27	HIS	N-CA-C	6.80	122.25	113.88
1	K	422	PHE	N-CA-C	6.80	118.35	111.07
1	U	141	PRO	N-CA-C	-6.80	98.45	112.47
1	C	500	HIS	N-CA-C	6.79	120.44	111.75
2	T	19	CYS	CB-CA-C	-6.78	96.93	110.42
2	N	19	CYS	CB-CA-C	-6.78	96.94	110.42
2	J	19	CYS	CB-CA-C	-6.76	96.96	110.42
1	S	407	GLY	N-CA-C	6.76	124.00	115.42
1	W	141	PRO	N-CA-C	-6.76	98.55	112.47
2	P	77	VAL	N-CA-C	-6.74	103.65	111.00
1	C	645	ASN	CA-C-N	6.73	126.99	119.32
1	C	645	ASN	C-N-CA	6.73	126.99	119.32
1	M	76	ILE	CA-C-N	6.71	126.17	118.85
1	M	76	ILE	C-N-CA	6.71	126.17	118.85
1	S	645	ASN	CA-C-N	6.71	128.22	119.84
1	S	645	ASN	C-N-CA	6.71	128.22	119.84
1	O	645	ASN	CA-C-N	6.70	126.96	119.32
1	O	645	ASN	C-N-CA	6.70	126.96	119.32
1	O	141	PRO	N-CA-C	-6.70	98.67	112.47
2	D	23	CYS	CB-CA-C	-6.69	100.65	110.96
1	Q	401	PHE	CA-C-N	6.69	126.65	119.76
1	Q	401	PHE	C-N-CA	6.69	126.65	119.76
1	Q	407	GLY	N-CA-C	6.69	123.04	115.08
1	M	141	PRO	N-CA-C	-6.67	98.72	112.47
1	W	407	GLY	N-CA-C	6.64	122.98	115.08
1	C	407	GLY	N-CA-C	6.64	122.98	115.08
1	G	224	GLY	N-CA-C	-6.63	97.46	113.18
2	P	19	CYS	CB-CA-C	-6.63	97.22	110.42
2	H	149	CYS	CB-CA-C	-6.61	99.05	109.70
1	C	141	PRO	N-CA-C	-6.61	98.85	112.47
2	L	77	VAL	N-CA-C	-6.59	104.34	110.53
2	N	145	CYS	CB-CA-C	-6.59	97.31	110.42
1	S	730	TYR	CA-C-N	6.59	126.21	119.56
1	S	730	TYR	C-N-CA	6.59	126.21	119.56
1	E	224	GLY	N-CA-C	-6.58	97.58	113.18
1	K	224	GLY	N-CA-C	-6.57	97.60	113.18
1	A	261	ASP	N-CA-C	-6.55	105.44	113.50
1	O	500	HIS	N-CA-C	6.53	120.10	111.75
1	W	76	ILE	CA-C-N	6.50	126.08	119.19
1	W	76	ILE	C-N-CA	6.50	126.08	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	109	CYS	CB-CA-C	-6.50	103.73	110.17
1	W	224	GLY	N-CA-C	-6.48	97.81	113.18
2	H	27	HIS	N-CA-C	6.48	122.27	113.97
2	R	149	CYS	CB-CA-C	-6.48	98.96	109.72
1	A	730	TYR	CA-C-N	6.48	126.10	119.56
1	A	730	TYR	C-N-CA	6.48	126.10	119.56
2	F	145	CYS	CB-CA-C	-6.47	97.54	110.42
1	U	224	GLY	N-CA-C	-6.47	97.86	113.18
1	K	261	ASP	N-CA-C	-6.46	105.56	113.50
1	G	104	ASP	CA-C-N	6.45	125.95	119.24
1	G	104	ASP	C-N-CA	6.45	125.95	119.24
2	B	145	CYS	CB-CA-C	-6.45	97.59	110.42
1	G	407	GLY	N-CA-C	6.44	122.75	115.08
2	R	145	CYS	CB-CA-C	-6.42	97.64	110.42
1	A	210	GLU	N-CA-C	-6.42	106.08	114.04
1	G	109	TYR	N-CA-C	6.42	119.99	109.85
2	N	149	CYS	CB-CA-C	-6.42	99.07	109.72
1	O	730	TYR	CA-C-N	6.41	126.03	119.56
1	O	730	TYR	C-N-CA	6.41	126.03	119.56
2	L	145	CYS	CB-CA-C	-6.39	97.70	110.42
1	Q	858	ASN	N-CA-C	6.39	122.19	113.37
2	V	267	VAL	N-CA-C	6.38	117.79	108.53
1	C	296	ASN	N-CA-C	6.38	121.11	112.88
1	I	730	TYR	CA-C-N	6.38	126.00	119.56
1	I	730	TYR	C-N-CA	6.38	126.00	119.56
2	L	109	CYS	CB-CA-C	-6.37	103.86	110.17
1	I	407	GLY	N-CA-C	6.37	123.64	114.67
1	W	422	PHE	N-CA-C	6.36	117.88	111.07
1	A	422	PHE	N-CA-C	6.36	117.87	111.07
1	Q	149	ASN	N-CA-C	6.35	117.86	111.07
1	M	273	ALA	N-CA-C	-6.34	104.45	111.36
1	E	141	PRO	N-CA-C	-6.34	99.41	112.47
1	G	261	ASP	N-CA-C	-6.33	105.72	113.50
1	E	407	GLY	N-CA-C	6.32	123.58	114.67
1	E	109	TYR	N-CA-C	6.32	119.83	109.72
1	K	407	GLY	N-CA-C	6.31	122.59	115.08
1	M	149	ASN	N-CA-C	6.30	117.81	111.07
2	N	109	CYS	CB-CA-C	-6.29	102.67	109.85
1	K	433	PHE	CA-C-N	6.29	126.26	120.03
1	K	433	PHE	C-N-CA	6.29	126.26	120.03
1	S	218	ASP	CA-C-N	6.29	125.78	119.24
1	S	218	ASP	C-N-CA	6.29	125.78	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	224	GLY	N-CA-C	-6.29	98.28	113.18
2	X	19	CYS	CB-CA-C	-6.29	97.91	110.42
1	A	109	TYR	N-CA-C	6.26	119.73	109.85
1	I	857	ASN	N-CA-C	6.25	121.69	111.37
2	V	19	CYS	CB-CA-C	-6.25	97.98	110.42
2	P	149	CYS	CB-CA-C	-6.25	99.35	109.72
2	B	267	VAL	N-CA-C	6.24	117.47	108.48
1	S	224	GLY	N-CA-C	-6.23	98.41	113.18
1	K	645	ASN	CA-C-N	6.23	126.42	119.32
1	K	645	ASN	C-N-CA	6.23	126.42	119.32
1	C	401	PHE	CA-C-N	6.21	126.16	119.76
1	C	401	PHE	C-N-CA	6.21	126.16	119.76
1	U	736	SER	CA-C-N	6.20	127.59	119.84
1	U	736	SER	C-N-CA	6.20	127.59	119.84
1	G	771	ILE	N-CA-C	6.20	117.95	108.71
1	O	210	GLU	N-CA-C	-6.20	106.36	114.04
2	X	23	CYS	CB-CA-C	-6.19	101.43	110.96
1	Q	403	GLY	N-CA-C	-6.18	103.12	112.89
2	H	267	VAL	N-CA-C	6.17	117.36	108.48
1	M	771	ILE	N-CA-C	6.17	117.90	108.71
1	K	325	SER	N-CA-C	6.14	120.85	113.23
1	U	507	THR	N-CA-C	6.14	123.88	110.80
1	K	465	GLY	N-CA-C	6.13	120.63	112.65
1	K	736	SER	CA-C-N	6.13	127.50	119.84
1	K	736	SER	C-N-CA	6.13	127.50	119.84
1	Q	393	VAL	CA-C-N	6.13	127.50	119.84
1	Q	393	VAL	C-N-CA	6.13	127.50	119.84
1	K	109	TYR	N-CA-C	6.12	119.69	109.95
2	P	109	CYS	CB-CA-C	-6.12	104.11	110.17
1	S	104	ASP	CA-C-N	6.12	125.34	118.97
1	S	104	ASP	C-N-CA	6.12	125.34	118.97
1	W	172	ASN	N-CA-C	-6.12	101.63	110.08
1	G	736	SER	CA-C-N	6.12	127.49	119.84
1	G	736	SER	C-N-CA	6.12	127.49	119.84
1	W	104	ASP	CA-C-N	6.12	125.60	119.24
1	W	104	ASP	C-N-CA	6.12	125.60	119.24
1	O	109	TYR	N-CA-C	6.12	119.50	109.72
2	B	23	CYS	N-CA-CB	6.11	118.87	110.01
1	W	109	TYR	N-CA-C	6.11	119.49	109.72
1	A	76	ILE	CA-C-N	6.08	125.64	119.19
1	A	76	ILE	C-N-CA	6.08	125.64	119.19
1	C	109	TYR	N-CA-C	6.08	119.46	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	109	TYR	N-CA-C	6.08	119.46	109.85
1	Q	736	SER	CA-C-N	6.07	127.43	119.84
1	Q	736	SER	C-N-CA	6.07	127.43	119.84
1	E	261	ASP	N-CA-C	-6.07	105.70	113.23
2	X	267	VAL	N-CA-C	6.07	117.21	108.48
1	O	76	ILE	CA-C-N	6.06	125.46	118.85
1	O	76	ILE	C-N-CA	6.06	125.46	118.85
1	W	261	ASP	N-CA-C	-6.06	106.05	113.50
1	M	403	GLY	N-CA-C	-6.05	103.34	112.89
1	I	736	SER	CA-C-N	6.04	127.39	119.84
1	I	736	SER	C-N-CA	6.04	127.39	119.84
1	Q	261	ASP	N-CA-C	-6.04	105.75	113.23
1	S	109	TYR	N-CA-C	6.04	119.39	109.85
1	A	227	ALA	N-CA-C	6.03	119.38	112.57
1	C	771	ILE	N-CA-C	6.02	117.69	108.71
1	A	273	ALA	N-CA-C	-6.02	104.80	111.36
2	L	126	CYS	CB-CA-C	-6.01	101.35	109.71
1	U	172	ASN	N-CA-C	-6.01	101.78	110.08
1	E	149	ASN	N-CA-C	6.01	117.50	111.07
1	C	224	GLY	N-CA-C	-6.00	98.96	113.18
1	U	858	ASN	N-CA-C	6.00	121.65	113.37
1	E	104	ASP	CA-C-N	5.99	125.47	119.24
1	E	104	ASP	C-N-CA	5.99	125.47	119.24
2	D	267	VAL	N-CA-C	5.99	116.56	108.17
1	E	857	ASN	N-CA-C	5.99	121.25	111.37
1	Q	200	ASP	N-CA-C	5.99	119.81	111.90
1	S	422	PHE	N-CA-C	5.98	117.47	111.07
1	I	109	TYR	N-CA-C	5.98	119.41	110.14
1	U	104	ASP	CA-C-N	5.96	125.44	119.24
1	U	104	ASP	C-N-CA	5.96	125.44	119.24
2	J	109	CYS	CB-CA-C	-5.95	103.07	109.85
1	G	149	ASN	N-CA-C	5.95	117.43	111.07
1	M	109	TYR	N-CA-C	5.94	119.24	109.85
1	E	17	PHE	N-CA-C	-5.93	99.58	109.24
1	O	149	ASN	N-CA-C	5.93	117.74	111.28
1	I	14	GLY	CA-C-N	5.92	125.83	119.85
1	I	14	GLY	C-N-CA	5.92	125.83	119.85
1	W	400	TYR	N-CA-C	5.92	118.17	108.52
1	M	176	TRP	N-CA-C	5.91	120.65	113.38
1	W	500	HIS	N-CA-C	5.91	119.31	111.75
1	E	730	TYR	CA-C-N	5.89	125.51	119.56
1	E	730	TYR	C-N-CA	5.89	125.51	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	771	ILE	N-CA-C	5.89	117.49	108.71
1	G	172	ASN	N-CA-C	-5.89	101.95	110.08
1	U	227	ALA	N-CA-C	5.89	120.04	112.26
2	F	267	VAL	N-CA-C	5.88	116.95	108.48
2	L	37	ALA	N-CA-C	-5.87	102.25	110.35
1	Q	771	ILE	N-CA-C	5.87	117.45	108.71
1	C	104	ASP	CA-C-N	5.87	125.34	119.24
1	C	104	ASP	C-N-CA	5.87	125.34	119.24
1	W	325	SER	N-CA-C	5.86	120.58	112.90
1	I	261	ASP	N-CA-C	-5.86	105.22	112.90
1	A	647	ASN	N-CA-C	5.86	120.42	113.16
1	S	149	ASN	N-CA-C	5.86	117.33	111.07
1	S	17	PHE	N-CA-C	-5.85	99.70	109.24
1	C	422	PHE	N-CA-C	5.84	117.65	111.28
2	B	109	CYS	CB-CA-C	-5.84	103.19	109.85
1	S	771	ILE	N-CA-C	5.83	117.40	108.71
2	L	27	HIS	N-CA-C	5.83	121.83	114.31
1	C	197	GLU	N-CA-C	-5.82	103.25	110.41
1	A	645	ASN	CA-C-N	5.82	125.96	119.32
1	A	645	ASN	C-N-CA	5.82	125.96	119.32
1	O	401	PHE	CA-C-N	5.82	125.77	119.78
1	O	401	PHE	C-N-CA	5.82	125.77	119.78
2	N	154	TYR	N-CA-C	5.81	119.29	109.76
1	C	227	ALA	N-CA-C	5.81	119.34	112.72
2	R	74	ALA	N-CA-C	5.80	118.00	109.42
1	E	176	TRP	N-CA-C	5.79	120.62	113.50
2	J	154	TYR	N-CA-C	5.79	119.53	110.32
1	A	858	ASN	N-CA-C	5.79	121.36	113.37
2	F	126	CYS	CB-CA-C	-5.79	101.67	109.71
1	A	143	SER	N-CA-C	5.79	118.05	111.11
1	E	647	ASN	N-CA-C	5.78	120.61	113.50
2	R	27	HIS	N-CA-C	5.78	121.37	113.97
1	M	400	TYR	N-CA-C	5.77	117.93	108.52
1	U	400	TYR	N-CA-C	5.77	117.93	108.52
2	B	154	TYR	N-CA-C	5.77	119.65	109.96
1	G	17	PHE	N-CA-C	-5.76	99.86	109.24
1	K	858	ASN	N-CA-C	5.75	121.31	113.37
1	M	858	ASN	N-CA-C	5.75	121.31	113.37
1	I	822	VAL	N-CA-C	5.74	116.38	107.99
2	T	37	ALA	N-CA-C	-5.74	102.43	110.35
1	U	143	SER	N-CA-C	5.73	117.20	111.07
1	A	771	ILE	N-CA-C	5.71	117.22	108.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	858	ASN	N-CA-C	5.70	121.24	113.37
1	G	824	ASP	CA-C-N	5.70	125.63	119.76
1	G	824	ASP	C-N-CA	5.70	125.63	119.76
1	S	133	GLY	CA-C-N	5.70	126.08	119.47
1	S	133	GLY	C-N-CA	5.70	126.08	119.47
1	U	500	HIS	N-CA-C	5.69	119.74	112.34
1	U	647	ASN	N-CA-C	5.69	120.22	113.28
1	U	273	ALA	N-CA-C	-5.69	105.16	111.36
1	U	645	ASN	CA-C-N	5.68	125.80	119.32
1	U	645	ASN	C-N-CA	5.68	125.80	119.32
1	A	17	PHE	N-CA-C	-5.68	99.98	109.24
1	K	771	ILE	N-CA-C	5.68	117.17	108.71
2	J	267	VAL	N-CA-C	5.67	116.65	108.48
1	G	143	SER	N-CA-C	5.67	117.91	111.11
2	H	232	PHE	N-CA-C	-5.67	105.95	112.92
1	O	325	SER	N-CA-C	5.67	120.47	113.50
1	U	793	TYR	N-CA-C	5.67	116.88	108.60
1	I	363	GLY	N-CA-C	5.66	119.74	112.83
1	M	17	PHE	N-CA-C	-5.66	100.01	109.24
1	W	218	ASP	CA-C-N	5.66	125.13	119.24
1	W	218	ASP	C-N-CA	5.66	125.13	119.24
1	A	403	GLY	N-CA-C	-5.66	103.94	112.89
2	R	267	VAL	N-CA-C	5.66	116.63	108.48
1	I	210	GLU	N-CA-C	-5.66	107.03	114.04
1	O	822	VAL	N-CA-C	5.66	116.00	107.80
2	P	154	TYR	N-CA-C	5.66	119.31	110.32
1	W	133	GLY	CA-C-N	5.66	125.50	119.28
1	W	133	GLY	C-N-CA	5.66	125.50	119.28
1	K	172	ASN	N-CA-C	-5.65	102.28	110.08
1	W	197	GLU	N-CA-C	-5.65	103.07	110.53
1	G	227	ALA	N-CA-C	5.64	119.15	112.72
2	J	74	ALA	N-CA-C	5.64	117.79	109.50
2	P	267	VAL	N-CA-C	5.64	116.60	108.48
2	H	154	TYR	N-CA-C	5.64	119.43	109.96
1	I	176	TRP	N-CA-C	5.64	120.27	113.17
1	Q	227	ALA	N-CA-C	5.63	119.69	112.26
1	W	210	GLU	N-CA-C	-5.63	107.06	114.04
2	H	45	TRP	N-CA-C	-5.63	105.15	111.28
2	T	149	CYS	CB-CA-C	-5.62	100.38	109.72
2	N	23	CYS	N-CA-CB	5.62	118.12	109.91
1	A	401	PHE	CA-C-N	5.62	125.55	119.76
1	A	401	PHE	C-N-CA	5.62	125.55	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	76	CYS	CB-CA-C	-5.61	99.25	110.42
1	A	400	TYR	N-CA-C	5.61	117.67	108.52
1	E	403	GLY	N-CA-C	-5.61	104.03	112.89
1	G	273	ALA	N-CA-C	-5.61	105.25	111.36
2	J	23	CYS	N-CA-CB	5.60	118.13	110.01
1	U	109	TYR	N-CA-C	5.60	118.70	109.85
2	H	37	ALA	N-CA-C	-5.59	102.63	110.35
1	M	730	TYR	CA-C-N	5.59	125.21	119.56
1	M	730	TYR	C-N-CA	5.59	125.21	119.56
1	S	325	SER	N-CA-C	5.59	120.38	113.50
1	W	771	ILE	N-CA-C	5.59	117.05	108.71
2	B	27	HIS	N-CA-C	5.59	121.53	114.31
1	E	200	ASP	N-CA-C	5.59	119.28	111.90
2	J	149	CYS	CB-CA-C	-5.59	99.75	109.64
2	F	232	PHE	N-CA-C	-5.59	106.05	112.92
1	S	858	ASN	N-CA-C	5.59	121.08	113.37
2	P	27	HIS	N-CA-C	5.58	121.51	114.31
1	I	645	ASN	CA-C-N	5.58	125.94	119.47
1	I	645	ASN	C-N-CA	5.58	125.94	119.47
1	A	433	PHE	CA-C-N	5.57	125.56	120.21
1	A	433	PHE	C-N-CA	5.57	125.56	120.21
2	T	145	CYS	CB-CA-C	-5.57	99.33	110.42
1	E	400	TYR	N-CA-C	5.57	117.59	108.52
1	G	400	TYR	N-CA-C	5.56	117.58	108.52
1	I	422	PHE	N-CA-C	5.56	117.34	111.28
1	K	227	ALA	N-CA-C	5.56	119.59	112.26
1	E	273	ALA	N-CA-C	-5.55	105.31	111.36
1	O	172	ASN	N-CA-C	-5.55	102.42	110.08
2	P	232	PHE	N-CA-C	-5.55	106.10	112.92
2	V	37	ALA	N-CA-C	-5.55	103.37	110.53
1	M	39	ALA	CA-C-N	5.54	125.49	119.78
1	M	39	ALA	C-N-CA	5.54	125.49	119.78
2	F	154	TYR	N-CA-C	5.54	119.13	110.32
1	O	17	PHE	N-CA-C	-5.54	100.20	109.24
1	U	771	ILE	N-CA-C	5.54	116.97	108.71
2	H	126	CYS	CB-CA-C	-5.53	102.99	109.80
1	W	858	ASN	N-CA-C	5.53	121.00	113.37
1	I	104	ASP	CA-C-N	5.52	124.98	119.24
1	I	104	ASP	C-N-CA	5.52	124.98	119.24
1	M	422	PHE	N-CA-C	5.52	117.74	111.11
1	E	822	VAL	N-CA-C	5.52	116.05	107.99
1	G	176	TRP	N-CA-C	5.52	120.17	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	824	ASP	CA-C-N	5.52	125.44	119.76
1	I	824	ASP	C-N-CA	5.52	125.44	119.76
1	U	863	GLU	N-CA-C	-5.52	100.68	109.23
2	B	37	ALA	N-CA-C	-5.51	102.74	110.35
1	Q	172	ASN	N-CA-C	-5.51	102.47	110.08
1	I	403	GLY	N-CA-C	-5.51	104.19	112.89
2	P	23	CYS	N-CA-CB	5.51	117.99	110.01
1	C	199	TYR	N-CA-C	5.50	118.00	110.24
1	G	822	VAL	N-CA-C	5.50	116.02	107.99
1	K	400	TYR	N-CA-C	5.50	117.48	108.52
1	M	200	ASP	N-CA-C	5.50	119.16	111.90
1	U	721	GLN	N-CA-C	5.50	118.19	111.82
1	I	771	ILE	N-CA-C	5.49	116.89	108.71
1	Q	422	PHE	N-CA-C	5.49	117.26	111.28
1	M	172	ASN	N-CA-C	-5.49	102.51	110.08
1	O	403	GLY	N-CA-C	-5.49	104.22	112.89
1	S	863	GLU	N-CA-C	-5.48	100.84	109.50
1	U	149	ASN	N-CA-C	5.48	117.25	111.28
2	V	109	CYS	N-CA-C	5.48	118.56	108.69
1	A	104	ASP	CA-C-N	5.48	124.94	119.24
1	A	104	ASP	C-N-CA	5.48	124.94	119.24
2	L	13	CYS	CB-CA-C	-5.48	101.12	109.89
1	G	645	ASN	CA-C-N	5.47	125.56	119.32
1	G	645	ASN	C-N-CA	5.47	125.56	119.32
1	O	200	ASP	N-CA-C	5.47	119.13	111.90
1	A	30	PRO	N-CA-C	-5.47	103.56	111.22
1	C	325	SER	N-CA-C	5.47	120.23	113.50
2	N	27	HIS	N-CA-C	5.47	121.37	114.31
1	A	736	SER	CA-C-N	5.47	126.68	119.84
1	A	736	SER	C-N-CA	5.47	126.68	119.84
1	M	822	VAL	N-CA-C	5.46	115.97	107.99
1	Q	433	PHE	CA-C-N	5.46	125.46	120.21
1	Q	433	PHE	C-N-CA	5.46	125.46	120.21
1	Q	17	PHE	N-CA-C	-5.46	100.34	109.24
1	S	227	ALA	N-CA-C	5.46	119.46	112.26
1	S	822	VAL	N-CA-C	5.46	115.95	107.99
1	S	731	PRO	N-CA-C	5.45	120.68	113.86
1	Q	176	TRP	N-CA-C	5.45	120.04	113.17
1	G	218	ASP	CA-C-N	5.45	125.53	119.32
1	G	218	ASP	C-N-CA	5.45	125.53	119.32
1	Q	208	HIS	N-CA-C	5.45	121.69	114.12
1	Q	273	ALA	N-CA-C	-5.45	105.42	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	267	VAL	N-CA-C	5.44	116.31	108.48
2	N	45	TRP	N-CA-C	-5.44	105.35	111.28
1	C	261	ASP	N-CA-C	-5.44	106.81	113.50
1	C	172	ASN	N-CA-C	-5.43	102.58	110.08
2	T	267	VAL	N-CA-C	5.43	116.30	108.48
2	L	23	CYS	N-CA-CB	5.43	117.88	110.01
2	N	232	PHE	N-CA-C	-5.42	106.25	112.92
1	W	645	ASN	CA-C-N	5.42	126.62	119.84
1	W	645	ASN	C-N-CA	5.42	126.62	119.84
1	K	647	ASN	N-CA-C	5.42	119.89	113.28
2	R	23	CYS	N-CA-CB	5.42	117.82	109.91
1	O	771	ILE	N-CA-C	5.40	116.76	108.71
1	Q	104	ASP	CA-C-N	5.40	124.86	119.24
1	Q	104	ASP	C-N-CA	5.40	124.86	119.24
2	D	37	ALA	N-CA-C	-5.40	102.90	110.35
1	E	565	TYR	N-CA-C	-5.40	106.53	113.01
1	U	199	TYR	N-CA-C	5.40	117.85	110.24
2	H	110	PRO	N-CA-C	-5.39	106.68	114.18
2	R	45	TRP	N-CA-C	-5.38	104.81	111.33
1	M	574	SER	N-CA-C	5.38	117.57	109.23
1	O	433	PHE	CA-C-N	5.38	125.38	120.21
1	O	433	PHE	C-N-CA	5.38	125.38	120.21
1	I	149	ASN	N-CA-C	5.37	117.13	111.28
1	S	144	HIS	N-CA-C	5.37	118.03	110.14
1	G	858	ASN	N-CA-C	5.37	120.78	113.37
1	A	176	TRP	N-CA-C	5.36	119.98	113.38
1	M	104	ASP	CA-C-N	5.36	124.82	119.24
1	M	104	ASP	C-N-CA	5.36	124.82	119.24
1	Q	400	TYR	N-CA-C	5.36	117.26	108.52
1	K	199	TYR	N-CA-C	5.36	117.80	110.24
1	M	691	ILE	N-CA-C	-5.35	98.22	106.72
2	T	154	TYR	N-CA-C	5.35	118.83	110.32
1	W	822	VAL	N-CA-C	5.34	115.79	107.99
1	I	858	ASN	N-CA-C	5.34	120.74	113.37
1	U	565	TYR	N-CA-C	-5.34	106.60	113.01
1	K	863	GLU	N-CA-C	-5.33	101.07	109.50
1	O	863	GLU	N-CA-C	-5.33	100.97	109.23
2	R	154	TYR	N-CA-C	5.33	118.80	110.32
1	C	403	GLY	N-CA-C	-5.33	102.39	112.51
1	M	227	ALA	N-CA-C	5.32	119.29	112.26
1	O	793	TYR	N-CA-C	5.32	116.36	108.60
1	S	199	TYR	N-CA-C	5.31	117.73	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	37	ALA	N-CA-C	-5.30	103.04	110.35
1	I	144	HIS	N-CA-C	5.30	117.93	110.14
1	Q	133	GLY	CA-C-N	5.30	125.61	119.47
1	Q	133	GLY	C-N-CA	5.30	125.61	119.47
1	K	822	VAL	N-CA-C	5.29	115.72	107.99
2	X	21	MET	N-CA-C	-5.29	105.63	111.71
1	I	574	SER	N-CA-C	5.29	117.43	109.23
1	M	133	GLY	CA-C-N	5.29	125.60	119.47
1	M	133	GLY	C-N-CA	5.29	125.60	119.47
2	N	149	CYS	N-CA-CB	5.28	117.80	109.83
1	U	210	GLU	N-CA-C	-5.28	107.50	114.04
1	E	30	PRO	N-CA-C	-5.27	103.84	111.22
1	G	565	TYR	N-CA-C	-5.27	106.68	113.01
1	S	793	TYR	N-CA-C	5.27	116.29	108.60
2	B	149	CYS	N-CA-CB	5.27	117.78	109.83
1	G	197	GLU	N-CA-C	-5.27	103.58	110.53
1	M	433	PHE	N-CA-C	5.27	118.17	109.58
1	M	144	HIS	N-CA-C	5.26	117.88	110.14
1	C	721	GLN	N-CA-C	5.26	117.76	111.71
2	J	37	ALA	N-CA-C	-5.26	103.09	110.35
1	A	386	MET	N-CA-C	-5.26	100.15	108.73
1	W	403	GLY	N-CA-C	-5.26	104.58	112.89
1	C	452	ILE	CB-CA-C	-5.26	108.70	113.70
1	C	736	SER	CA-C-N	5.26	126.41	119.84
1	C	736	SER	C-N-CA	5.26	126.41	119.84
1	S	200	ASP	N-CA-C	5.26	118.84	111.90
1	A	691	ILE	N-CA-C	-5.25	98.36	106.72
1	A	208	HIS	N-CA-C	5.25	121.09	114.31
1	E	736	SER	CA-C-N	5.25	126.41	119.84
1	E	736	SER	C-N-CA	5.25	126.41	119.84
1	K	273	ALA	N-CA-C	-5.25	105.63	111.36
2	L	149	CYS	N-CA-CB	5.25	117.73	109.69
1	C	393	VAL	CA-C-N	5.25	126.40	119.84
1	C	393	VAL	C-N-CA	5.25	126.40	119.84
1	O	735	LEU	N-CA-C	-5.25	100.84	109.40
1	S	273	ALA	N-CA-C	-5.25	105.64	111.36
1	Q	14	GLY	CA-C-N	5.24	125.14	119.85
1	Q	14	GLY	C-N-CA	5.24	125.14	119.85
1	U	822	VAL	N-CA-C	5.24	115.64	107.99
2	D	149	CYS	CB-CA-C	-5.24	101.26	109.70
1	W	149	ASN	N-CA-C	5.24	116.99	111.28
1	W	565	TYR	N-CA-C	-5.24	106.58	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	197	GLU	N-CA-C	-5.24	103.62	110.53
1	K	731	PRO	N-CA-C	5.23	120.40	113.86
1	O	721	GLN	N-CA-C	5.23	117.89	111.82
1	W	199	TYR	N-CA-C	5.23	117.62	110.24
1	K	17	PHE	N-CA-C	-5.23	100.72	109.24
1	E	143	SER	N-CA-C	5.22	116.66	111.07
1	E	210	GLU	N-CA-C	-5.22	107.57	114.04
1	Q	452	ILE	CB-CA-C	-5.22	108.82	114.35
1	S	403	GLY	N-CA-C	-5.22	104.64	112.89
1	W	736	SER	CA-C-N	5.22	126.36	119.84
1	W	736	SER	C-N-CA	5.22	126.36	119.84
2	F	45	TRP	N-CA-C	-5.22	105.59	111.28
1	I	259	VAL	N-CA-C	5.22	120.19	109.34
2	T	232	PHE	N-CA-C	-5.21	106.51	112.92
1	A	863	GLU	N-CA-C	-5.21	101.27	109.50
1	S	259	VAL	N-CA-C	5.21	120.17	109.34
1	A	200	ASP	N-CA-C	5.21	118.77	111.90
1	S	143	SER	N-CA-C	5.20	116.63	111.07
1	I	863	GLU	N-CA-C	-5.20	101.29	109.50
2	D	232	PHE	N-CA-C	-5.19	106.79	113.02
1	O	858	ASN	N-CA-C	5.19	120.54	113.37
2	L	241	ASP	N-CA-C	-5.19	103.54	110.55
1	E	841	ILE	N-CA-C	-5.19	104.60	111.09
1	E	721	GLN	N-CA-C	5.19	117.68	111.71
1	M	259	VAL	N-CA-C	5.19	120.13	109.34
2	B	74	ALA	N-CA-C	5.18	118.82	109.44
1	U	731	PRO	N-CA-C	5.18	120.34	113.86
2	X	232	PHE	N-CA-C	-5.18	106.55	112.92
1	K	452	ILE	CB-CA-C	-5.18	108.86	114.35
1	A	824	ASP	CA-C-N	5.18	125.10	119.76
1	A	824	ASP	C-N-CA	5.18	125.10	119.76
1	S	210	GLU	N-CA-C	-5.18	107.62	114.04
1	W	200	ASP	N-CA-C	5.18	118.74	111.90
1	Q	144	HIS	N-CA-C	5.18	117.75	110.14
1	C	144	HIS	N-CA-C	5.17	117.75	110.14
1	M	210	GLU	N-CA-C	-5.17	107.63	114.04
2	J	45	TRP	N-CA-C	-5.17	105.08	111.33
1	S	172	ASN	N-CA-C	-5.17	102.95	110.08
1	M	208	HIS	N-CA-C	5.16	120.97	114.31
1	K	176	TRP	N-CA-C	5.16	119.72	113.38
1	U	17	PHE	N-CA-C	-5.16	100.83	109.24
1	G	721	GLN	N-CA-C	5.16	117.80	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	793	TYR	N-CA-C	5.16	116.13	108.60
2	R	77	VAL	N-CA-C	-5.15	105.69	110.53
1	I	17	PHE	N-CA-C	-5.14	100.86	109.24
1	A	296	ASN	N-CA-C	5.14	119.51	112.88
1	I	474	SER	N-CA-C	5.14	119.53	113.16
2	R	232	PHE	N-CA-C	-5.13	106.71	113.17
1	U	200	ASP	N-CA-C	5.13	118.83	112.47
1	W	401	PHE	CA-C-N	5.13	125.06	119.78
1	W	401	PHE	C-N-CA	5.13	125.06	119.78
1	W	536	ALA	N-CA-C	5.13	117.47	110.55
1	G	647	ASN	N-CA-C	5.12	119.53	113.28
1	O	731	PRO	N-CA-C	5.12	120.26	113.86
1	I	172	ASN	N-CA-C	-5.12	103.01	110.08
1	M	53	PRO	N-CA-C	5.12	116.95	110.70
1	E	133	GLY	CA-C-N	5.12	125.41	119.47
1	E	133	GLY	C-N-CA	5.12	125.41	119.47
1	I	691	ILE	N-CA-C	-5.12	98.58	106.72
1	W	30	PRO	N-CA-C	-5.11	104.06	111.22
1	A	822	VAL	N-CA-C	5.11	115.45	107.99
2	N	95	ASP	CA-C-N	5.11	125.40	119.47
2	N	95	ASP	C-N-CA	5.11	125.40	119.47
1	W	176	TRP	N-CA-C	5.11	119.66	113.38
1	G	30	PRO	N-CA-C	-5.10	104.07	111.22
1	C	731	PRO	N-CA-C	5.10	120.23	113.86
1	W	39	ALA	N-CA-C	5.10	115.46	109.60
1	E	32	ASP	CA-C-O	-5.09	115.06	120.92
2	R	126	CYS	CB-CA-C	-5.09	102.20	109.84
1	M	197	GLU	N-CA-C	-5.09	103.81	110.53
1	O	218	ASP	CA-C-N	5.09	125.13	119.32
1	O	218	ASP	C-N-CA	5.09	125.13	119.32
1	O	227	ALA	N-CA-C	5.09	118.98	112.26
1	W	227	ALA	N-CA-C	5.09	118.98	112.26
1	M	325	SER	N-CA-C	5.08	119.75	113.50
1	K	200	ASP	N-CA-C	5.08	118.60	111.90
1	C	218	ASP	CA-C-N	5.07	125.10	119.32
1	C	218	ASP	C-N-CA	5.07	125.10	119.32
1	C	273	ALA	N-CA-C	-5.07	105.84	111.36
2	J	27	HIS	N-CA-C	5.06	120.84	114.31
1	I	689	GLU	N-CA-C	5.06	117.16	107.75
1	M	218	ASP	CA-C-N	5.05	125.08	119.32
1	M	218	ASP	C-N-CA	5.05	125.08	119.32
1	M	199	TYR	N-CA-C	5.04	117.35	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	143	SER	N-CA-C	5.04	117.43	111.33
1	I	401	PHE	CA-C-N	5.04	124.95	119.76
1	I	401	PHE	C-N-CA	5.04	124.95	119.76
2	F	149	CYS	N-CA-CB	5.04	117.70	109.69
1	Q	210	GLU	N-CA-C	-5.04	107.80	114.04
1	Q	39	ALA	CA-C-N	5.03	124.96	119.78
1	Q	39	ALA	C-N-CA	5.03	124.96	119.78
1	S	296	ASN	N-CA-C	5.03	119.37	112.88
1	E	863	GLU	N-CA-C	-5.03	101.55	109.50
1	I	200	ASP	N-CA-C	5.03	118.53	111.90
1	K	32	ASP	CA-C-O	-5.03	115.22	120.80
1	G	200	ASP	N-CA-C	5.02	118.53	111.90
1	I	841	ILE	N-CA-C	-5.02	104.81	111.09
1	M	721	GLN	N-CA-C	5.02	117.65	111.82
2	F	23	CYS	N-CA-CB	5.02	117.29	110.01
1	S	176	TRP	N-CA-C	5.02	119.55	113.38
1	U	144	HIS	N-CA-C	5.02	117.51	110.14
1	U	403	GLY	N-CA-C	-5.01	104.97	112.89
2	F	37	ALA	N-CA-C	-5.01	103.43	110.35
2	F	95	ASP	CA-C-N	5.01	125.28	119.47
2	F	95	ASP	C-N-CA	5.01	125.28	119.47
1	U	133	GLY	CA-C-N	5.01	125.03	119.32
1	U	133	GLY	C-N-CA	5.01	125.03	119.32
1	C	210	GLU	N-CA-C	-5.00	107.83	114.04
2	H	95	ASP	CA-C-N	5.00	125.27	119.47
2	H	95	ASP	C-N-CA	5.00	125.27	119.47
1	U	218	ASP	CA-C-N	5.00	125.02	119.32
1	U	218	ASP	C-N-CA	5.00	125.02	119.32

There are no chirality outliers.

There are no planarity outliers.

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	6998	0	6632	161	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6998	0	6632	169	0
1	E	6998	0	6632	151	0
1	G	6998	0	6632	154	0
1	I	6998	0	6632	155	0
1	K	6998	0	6632	153	0
1	M	6998	0	6632	160	0
1	O	6998	0	6632	157	1
1	Q	6998	0	6632	179	0
1	S	6998	0	6632	165	0
1	U	6998	0	6632	167	0
1	W	6998	0	6632	148	0
2	B	2182	0	2077	66	0
2	D	2182	0	2077	91	0
2	F	2182	0	2077	82	0
2	H	2182	0	2077	76	0
2	J	2182	0	2077	84	0
2	L	2182	0	2077	80	0
2	N	2182	0	2077	82	0
2	P	2182	0	2077	69	0
2	R	2182	0	2077	77	0
2	T	2182	0	2077	71	0
2	V	2182	0	2077	68	0
2	X	2182	0	2077	81	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	A	94	0	44	11	0
4	C	94	0	44	15	0
4	E	94	0	44	13	0
4	G	94	0	44	16	0
4	I	94	0	44	10	0
4	K	94	0	44	15	0
4	M	94	0	44	16	0
4	O	94	0	44	17	0
4	Q	94	0	44	16	0
4	S	94	0	44	11	0
4	U	94	0	44	15	0
4	W	94	0	44	14	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
5	M	1	0	0	0	0
5	O	1	0	0	0	0
5	Q	1	0	0	0	0
5	S	1	0	0	0	0
5	U	1	0	0	0	0
5	W	1	0	0	0	0
6	A	10	0	2	1	0
6	C	10	0	2	1	0
6	E	10	0	2	1	0
6	G	10	0	2	1	0
6	I	10	0	2	1	0
6	K	10	0	2	1	0
6	M	10	0	2	1	0
6	O	10	0	2	1	0
6	Q	10	0	2	1	0
6	S	10	0	2	1	0
6	U	10	0	2	1	0
6	W	10	0	2	1	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	4	0
7	F	24	0	0	4	0
7	H	24	0	0	4	0
7	J	24	0	0	4	0
7	L	24	0	0	4	0
7	N	24	0	0	5	0
7	P	24	0	0	4	0
7	R	24	0	0	4	0
7	T	24	0	0	4	0
7	V	24	0	0	4	0
7	X	24	0	0	4	0
8	A	681	0	0	13	2
8	B	169	0	0	3	0
8	C	684	0	0	10	0
8	D	162	0	0	1	0
8	E	688	0	0	14	0
8	F	160	0	0	0	0
8	G	682	0	0	9	0
8	H	161	0	0	2	0
8	I	671	0	0	7	0
8	J	168	0	0	2	0
8	K	681	0	0	7	0
8	L	165	0	0	3	0
8	M	682	0	0	12	0
8	N	160	0	0	2	0
8	O	675	0	0	12	1
8	P	160	0	0	2	0
8	Q	693	0	0	13	0
8	R	158	0	0	2	0
8	S	665	0	0	14	0
8	T	162	0	0	0	0
8	U	670	0	0	10	0
8	V	154	0	0	0	0
8	W	675	0	0	9	0
8	X	165	0	0	1	0
All	All	121823	0	105060	2775	2

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 13.

All (2775) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:MET:HE2	1:G:754:MET:HE1	1.30	1.13
1:I:356:GLY:N	4:I:903:MGD:O1B	1.86	1.09
1:C:356:GLY:N	4:C:903:MGD:O1B	1.86	1.09
1:C:557:CYS:H	1:C:564:ASN:HD21	1.08	1.00
2:D:19:CYS:HB3	2:D:145:CYS:HB3	1.44	1.00
1:S:356:GLY:N	4:S:903:MGD:O1B	1.94	0.99
1:I:557:CYS:H	1:I:564:ASN:HD21	1.11	0.99
1:A:69:MET:HE2	1:A:754:MET:HE1	1.44	0.99
1:K:557:CYS:H	1:K:564:ASN:HD21	1.05	0.98
2:R:68:CYS:HB2	2:R:126:CYS:HB3	1.46	0.98
1:M:211:MET:HE1	2:N:231:PHE:CZ	1.99	0.98
1:K:28:MET:HE1	1:K:66:PHE:HB3	1.45	0.97
2:V:46:MET:HE1	2:V:66:THR:N	1.77	0.97
2:F:68:CYS:HB2	2:F:126:CYS:HB3	1.44	0.97
1:M:557:CYS:H	1:M:564:ASN:HD21	1.08	0.97
1:Q:557:CYS:H	1:Q:564:ASN:HD21	1.06	0.97
2:B:46:MET:HE1	2:B:66:THR:N	1.80	0.97
2:N:68:CYS:HB2	2:N:126:CYS:HB3	1.45	0.97
1:S:69:MET:HE2	1:S:754:MET:HE1	1.47	0.97
1:C:69:MET:HE2	1:C:754:MET:HE1	1.46	0.96
2:N:207:GLY:HA2	1:S:728:VAL:HG12	1.49	0.95
1:O:557:CYS:H	1:O:564:ASN:HD21	1.11	0.95
2:P:2:GLU:HG2	2:P:158:LYS:HG2	1.48	0.95
2:L:46:MET:HE1	2:L:66:THR:N	1.80	0.95
2:H:142:MET:HE2	2:H:146:ALA:HB1	1.49	0.95
1:I:66:PHE:HZ	1:I:146:MET:HE1	1.29	0.94
1:W:557:CYS:H	1:W:564:ASN:HD21	1.14	0.94
1:I:426:MET:HA	1:I:426:MET:HE3	1.49	0.94
1:Q:69:MET:HE2	1:Q:754:MET:HE1	1.49	0.94
1:S:66:PHE:HA	1:S:69:MET:HE3	1.49	0.94
1:E:557:CYS:H	1:E:564:ASN:HD21	1.08	0.93
2:H:105:LEU:HB3	2:H:114:MET:HE1	1.49	0.93
2:B:46:MET:HE1	2:B:66:THR:H	1.34	0.92
1:Q:319:GLU:HG2	1:U:726:LEU:HD13	1.48	0.92
1:M:426:MET:HA	1:M:426:MET:HE3	1.51	0.92
1:U:557:CYS:H	1:U:564:ASN:HD21	1.10	0.92
1:M:319:GLU:HG2	1:S:726:LEU:HD13	1.52	0.92
2:N:142:MET:HE2	2:N:146:ALA:HB1	1.49	0.92
2:P:68:CYS:HB2	2:P:126:CYS:HB3	1.52	0.92
2:J:46:MET:HE1	2:J:66:THR:H	1.35	0.92
2:H:46:MET:HE1	2:H:66:THR:N	1.84	0.91
2:H:68:CYS:HB2	2:H:126:CYS:HB3	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:68:CYS:HB2	2:T:126:CYS:HB3	1.52	0.91
2:J:46:MET:HE1	2:J:66:THR:N	1.84	0.91
2:R:142:MET:HE2	2:R:146:ALA:HB1	1.51	0.91
1:U:69:MET:HE2	1:U:754:MET:HE1	1.51	0.91
1:E:211:MET:HE1	2:F:231:PHE:CZ	2.05	0.91
1:S:557:CYS:H	1:S:564:ASN:HD21	1.03	0.91
1:A:426:MET:HA	1:A:426:MET:HE3	1.53	0.90
2:D:68:CYS:HB2	2:D:126:CYS:HB3	1.53	0.90
1:W:426:MET:HA	1:W:426:MET:HE3	1.52	0.90
2:L:46:MET:HE1	2:L:66:THR:H	1.34	0.90
1:A:66:PHE:HA	1:A:69:MET:HE3	1.53	0.90
1:A:557:CYS:H	1:A:564:ASN:HD21	1.09	0.90
1:Q:211:MET:HE1	2:R:231:PHE:CZ	2.06	0.90
2:R:207:GLY:HA2	1:U:728:VAL:HG12	1.49	0.90
1:S:66:PHE:HZ	1:S:146:MET:HE1	1.37	0.90
1:S:426:MET:HE3	1:S:426:MET:HA	1.54	0.90
1:I:69:MET:HE2	1:I:754:MET:HE1	1.51	0.90
1:O:426:MET:HA	1:O:426:MET:HE3	1.50	0.90
2:B:68:CYS:HB2	2:B:126:CYS:CB	2.02	0.90
1:I:211:MET:HE1	2:J:231:PHE:CZ	2.06	0.90
1:Q:426:MET:HA	1:Q:426:MET:HE3	1.54	0.89
1:G:66:PHE:HA	1:G:69:MET:HE3	1.54	0.89
2:T:46:MET:HE1	2:T:66:THR:N	1.87	0.89
2:F:70:HIS:HD2	2:F:92:VAL:H	1.19	0.89
2:R:142:MET:HE2	2:R:146:ALA:CB	2.02	0.89
1:W:28:MET:HE1	1:W:66:PHE:HB3	1.51	0.89
2:N:105:LEU:HB3	2:N:114:MET:HE1	1.53	0.89
2:T:68:CYS:HB2	2:T:126:CYS:CB	2.03	0.89
1:W:69:MET:HE2	1:W:754:MET:HE1	1.55	0.89
1:Q:355:GLY:HA2	4:Q:903:MGD:O2B	1.71	0.89
1:C:211:MET:HE1	2:D:231:PHE:CZ	2.07	0.89
2:H:142:MET:HE2	2:H:146:ALA:CB	2.03	0.89
2:H:106:LEU:HD23	2:H:114:MET:HE2	1.54	0.88
2:L:68:CYS:HB2	2:L:126:CYS:CB	2.02	0.88
1:M:69:MET:HE2	1:M:754:MET:HE1	1.53	0.88
1:O:66:PHE:HA	1:O:69:MET:HE3	1.55	0.88
1:K:66:PHE:HZ	1:K:146:MET:HE1	1.39	0.88
2:N:70:HIS:HD2	2:N:92:VAL:H	1.18	0.88
2:T:2:GLU:HG2	2:T:158:LYS:HG2	1.54	0.88
1:U:426:MET:HE1	1:U:618:GLN:HG2	1.56	0.88
2:J:68:CYS:HB2	2:J:126:CYS:HB3	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:211:MET:HE1	2:P:231:PHE:CZ	2.08	0.88
2:R:46:MET:HE1	2:R:66:THR:N	1.89	0.88
1:K:146:MET:HE2	1:K:544:THR:HB	1.56	0.88
2:F:46:MET:HE1	2:F:66:THR:H	1.39	0.87
1:A:66:PHE:HZ	1:A:146:MET:HE1	1.38	0.87
1:G:355:GLY:HA2	4:G:903:MGD:O2B	1.75	0.87
1:I:28:MET:HE1	1:I:66:PHE:HB3	1.54	0.87
1:K:426:MET:HE3	1:K:426:MET:HA	1.54	0.87
2:N:142:MET:HE2	2:N:146:ALA:CB	2.03	0.87
2:B:70:HIS:HD2	2:B:92:VAL:H	1.16	0.87
1:E:426:MET:HA	1:E:426:MET:HE3	1.55	0.87
1:U:28:MET:HE1	1:U:66:PHE:HB3	1.56	0.87
2:V:68:CYS:HB2	2:V:126:CYS:HB3	1.57	0.87
1:G:557:CYS:H	1:G:564:ASN:HD21	1.14	0.87
2:J:68:CYS:HB2	2:J:126:CYS:CB	2.05	0.87
1:O:66:PHE:HZ	1:O:146:MET:HE1	1.39	0.87
2:B:68:CYS:HB2	2:B:126:CYS:HB3	1.53	0.87
1:G:211:MET:HE1	2:H:231:PHE:CZ	2.09	0.87
2:R:70:HIS:HD2	2:R:92:VAL:H	1.22	0.87
2:H:46:MET:HE1	2:H:66:THR:H	1.38	0.87
1:C:66:PHE:HZ	1:C:146:MET:HE1	1.40	0.86
1:E:66:PHE:HZ	1:E:146:MET:HE1	1.38	0.86
2:L:70:HIS:HD2	2:L:92:VAL:H	1.16	0.86
2:P:68:CYS:HB2	2:P:126:CYS:CB	2.03	0.86
1:I:66:PHE:HA	1:I:69:MET:HE3	1.55	0.86
1:K:66:PHE:HA	1:K:69:MET:HE3	1.57	0.86
1:K:69:MET:HE2	1:K:754:MET:HE1	1.57	0.86
1:C:360:ALA:HB1	1:C:859:THR:HG23	1.54	0.86
2:H:68:CYS:HB2	2:H:126:CYS:CB	2.06	0.86
2:R:46:MET:HE1	2:R:66:THR:H	1.41	0.86
1:E:69:MET:HE2	1:E:754:MET:HE1	1.56	0.86
1:S:211:MET:HE1	2:T:231:PHE:CZ	2.10	0.86
2:N:68:CYS:HB2	2:N:126:CYS:CB	2.05	0.86
1:G:28:MET:HE1	1:G:66:PHE:HB3	1.56	0.86
2:L:68:CYS:HB2	2:L:126:CYS:HB3	1.57	0.86
1:Q:69:MET:HE2	1:Q:754:MET:CE	2.05	0.86
1:A:28:MET:HE1	1:A:66:PHE:HB3	1.58	0.85
2:D:46:MET:HE1	2:D:66:THR:N	1.90	0.85
2:T:46:MET:HE1	2:T:66:THR:H	1.39	0.85
2:F:68:CYS:HB2	2:F:126:CYS:CB	2.05	0.85
1:O:69:MET:HE2	1:O:754:MET:HE1	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:46:MET:HE1	2:P:66:THR:N	1.90	0.85
2:R:68:CYS:HB2	2:R:126:CYS:CB	2.05	0.85
2:X:142:MET:HE2	2:X:146:ALA:HB1	1.57	0.85
1:G:141:PRO:HA	1:G:496:TYR:HB3	1.59	0.85
2:N:106:LEU:HD23	2:N:114:MET:HE2	1.57	0.85
2:J:70:HIS:HD2	2:J:92:VAL:H	1.22	0.85
1:S:360:ALA:HB1	1:S:859:THR:HG23	1.57	0.85
2:V:23:CYS:HB3	2:V:39:MET:HE1	1.57	0.85
1:K:146:MET:HE3	1:K:545:ASN:OD1	1.77	0.85
2:V:68:CYS:HB2	2:V:126:CYS:CB	2.07	0.85
1:O:28:MET:HE1	1:O:66:PHE:HB3	1.59	0.84
2:N:46:MET:HE1	2:N:66:THR:H	1.42	0.84
1:M:69:MET:HE2	1:M:754:MET:CE	2.07	0.84
1:C:426:MET:HE3	1:C:426:MET:HA	1.59	0.84
1:U:146:MET:HE3	1:U:545:ASN:OD1	1.78	0.84
2:X:46:MET:HE1	2:X:66:THR:N	1.92	0.84
2:P:70:HIS:HD2	2:P:92:VAL:H	1.26	0.84
1:U:66:PHE:HZ	1:U:146:MET:HE1	1.42	0.84
2:V:46:MET:HE1	2:V:66:THR:H	1.38	0.84
2:X:106:LEU:HD11	2:X:116:TRP:HB2	1.60	0.84
1:E:146:MET:HE3	1:E:545:ASN:OD1	1.78	0.84
1:U:146:MET:HE2	1:U:544:THR:HB	1.60	0.84
1:C:28:MET:HE1	1:C:66:PHE:HB3	1.58	0.83
2:X:46:MET:HE1	2:X:66:THR:H	1.43	0.83
1:U:211:MET:HE1	2:V:231:PHE:CZ	2.13	0.83
1:M:355:GLY:HA2	4:M:903:MGD:O1B	1.77	0.83
2:T:70:HIS:HD2	2:T:92:VAL:H	1.26	0.83
1:G:146:MET:HE3	1:G:545:ASN:OD1	1.78	0.83
1:S:753:TYR:HB3	2:T:24:MET:HE3	1.61	0.83
2:L:23:CYS:HB3	2:L:39:MET:HE1	1.61	0.83
1:O:695:LEU:O	1:O:699:GLU:HG2	1.79	0.83
2:P:19:CYS:HB3	2:P:145:CYS:HB3	1.61	0.83
1:C:610:LYS:NZ	1:C:618:GLN:HE22	1.77	0.83
2:N:46:MET:HE1	2:N:66:THR:N	1.93	0.83
2:R:40:GLN:HE22	2:R:118:GLU:H	1.24	0.83
1:A:360:ALA:HB1	1:A:859:THR:HG23	1.61	0.83
1:E:141:PRO:HA	1:E:496:TYR:HB3	1.61	0.82
2:H:70:HIS:HD2	2:H:92:VAL:H	1.26	0.82
1:A:141:PRO:HA	1:A:496:TYR:HB3	1.61	0.82
1:C:146:MET:HE3	1:C:545:ASN:OD1	1.79	0.82
1:K:695:LEU:O	1:K:699:GLU:HG2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:105:LEU:HB3	2:L:114:MET:HE1	1.60	0.82
1:Q:610:LYS:NZ	1:Q:618:GLN:HE22	1.77	0.82
1:C:66:PHE:HA	1:C:69:MET:HE3	1.59	0.82
1:A:69:MET:HE2	1:A:754:MET:CE	2.09	0.82
2:L:40:GLN:HE22	2:L:118:GLU:H	1.24	0.82
2:N:40:GLN:HE22	2:N:118:GLU:H	1.23	0.82
2:F:46:MET:HE1	2:F:66:THR:N	1.93	0.82
2:D:142:MET:HE2	2:D:146:ALA:HB1	1.62	0.82
1:E:426:MET:CE	1:E:618:GLN:HG2	2.09	0.81
1:Q:141:PRO:HA	1:Q:496:TYR:HB3	1.62	0.81
1:A:66:PHE:CZ	1:A:146:MET:HE1	2.15	0.81
1:C:141:PRO:HA	1:C:496:TYR:HB3	1.62	0.81
1:E:360:ALA:HB1	1:E:859:THR:HG23	1.63	0.81
1:U:360:ALA:HB1	1:U:859:THR:HG23	1.60	0.81
1:U:426:MET:CE	1:U:618:GLN:HG2	2.11	0.81
2:V:76:CYS:HB3	2:V:108:THR:OG1	1.80	0.81
1:W:66:PHE:HA	1:W:69:MET:HE3	1.62	0.81
1:A:211:MET:HE1	2:B:231:PHE:CZ	2.14	0.81
1:I:66:PHE:CZ	1:I:146:MET:HE1	2.14	0.81
1:A:146:MET:HE2	1:A:544:THR:HB	1.60	0.81
1:I:426:MET:CE	1:I:618:GLN:HG2	2.10	0.81
1:O:146:MET:HE3	1:O:545:ASN:OD1	1.81	0.81
1:E:66:PHE:CZ	1:E:146:MET:HE1	2.16	0.81
1:K:66:PHE:CZ	1:K:146:MET:HE1	2.16	0.80
1:G:426:MET:HA	1:G:426:MET:HE3	1.62	0.80
1:M:28:MET:HE1	1:M:66:PHE:HB3	1.64	0.80
1:E:426:MET:HE1	1:E:618:GLN:HG2	1.61	0.80
1:S:426:MET:CE	1:S:618:GLN:HG2	2.10	0.80
1:A:146:MET:HE3	1:A:545:ASN:OD1	1.82	0.80
1:E:28:MET:HE1	1:E:66:PHE:HB3	1.63	0.80
2:F:142:MET:HE2	2:F:146:ALA:HB1	1.64	0.80
1:G:629:MET:HE2	1:G:634:PHE:HA	1.64	0.80
1:M:66:PHE:HA	1:M:69:MET:HE3	1.61	0.80
1:S:426:MET:HE1	1:S:618:GLN:HG2	1.62	0.80
1:Q:66:PHE:HZ	1:Q:146:MET:HE1	1.44	0.80
2:X:23:CYS:HB3	2:X:39:MET:HE1	1.62	0.80
1:O:141:PRO:HA	1:O:496:TYR:HB3	1.64	0.80
1:U:356:GLY:N	4:U:903:MGD:O1B	2.13	0.80
2:F:40:GLN:HE22	2:F:118:GLU:H	1.27	0.79
1:W:141:PRO:HA	1:W:496:TYR:HB3	1.64	0.79
1:E:66:PHE:HA	1:E:69:MET:HE3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:LEU:HB3	2:F:114:MET:HE1	1.65	0.79
2:P:46:MET:HE1	2:P:66:THR:H	1.44	0.79
2:H:23:CYS:HB3	2:H:39:MET:HE1	1.62	0.79
1:K:69:MET:HE2	1:K:754:MET:CE	2.13	0.79
1:Q:610:LYS:HZ2	1:Q:618:GLN:HE22	1.28	0.79
1:U:695:LEU:O	1:U:699:GLU:HG2	1.83	0.79
2:P:23:CYS:HB3	2:P:39:MET:HE1	1.65	0.79
1:A:823:TYR:CZ	1:A:825:PRO:HG3	2.18	0.79
1:I:141:PRO:HA	1:I:496:TYR:HB3	1.64	0.79
1:E:216:SER:OG	4:E:903:MGD:H5'2	1.83	0.78
1:M:695:LEU:O	1:M:699:GLU:HG2	1.81	0.78
1:O:426:MET:CE	1:O:618:GLN:HG2	2.13	0.78
1:M:610:LYS:NZ	1:M:618:GLN:HE22	1.82	0.78
1:G:610:LYS:NZ	1:G:618:GLN:HE22	1.81	0.78
1:K:146:MET:CE	1:K:544:THR:HB	2.13	0.78
1:U:66:PHE:HA	1:U:69:MET:HE3	1.65	0.78
1:E:610:LYS:NZ	1:E:618:GLN:HE22	1.82	0.78
1:K:360:ALA:HB1	1:K:859:THR:HG23	1.66	0.78
1:M:426:MET:HE1	1:M:618:GLN:HG2	1.66	0.78
2:D:23:CYS:HB3	2:D:39:MET:HE1	1.64	0.78
1:U:426:MET:HA	1:U:426:MET:HE3	1.64	0.78
2:B:105:LEU:HB3	2:B:114:MET:HE1	1.65	0.78
1:K:426:MET:CE	1:K:618:GLN:HG2	2.13	0.78
1:O:823:TYR:CZ	1:O:825:PRO:HG3	2.18	0.78
2:D:70:HIS:HD2	2:D:92:VAL:H	1.30	0.77
1:E:786:ASN:HD22	1:E:805:VAL:H	1.30	0.77
1:Q:28:MET:HE1	1:Q:66:PHE:HB3	1.65	0.77
1:S:28:MET:HE1	1:S:66:PHE:HB3	1.66	0.77
1:C:695:LEU:O	1:C:699:GLU:HG2	1.81	0.77
1:I:211:MET:HE1	2:J:231:PHE:HZ	1.46	0.77
1:K:211:MET:HE1	2:L:231:PHE:CZ	2.19	0.77
1:O:66:PHE:CZ	1:O:146:MET:HE1	2.19	0.77
2:P:105:LEU:HB3	2:P:114:MET:HE1	1.66	0.77
1:I:360:ALA:HB1	1:I:859:THR:HG23	1.65	0.77
1:U:146:MET:CE	1:U:544:THR:HB	2.15	0.77
1:Q:146:MET:HE3	1:Q:545:ASN:OD1	1.85	0.77
2:F:23:CYS:HB3	2:F:39:MET:HE1	1.66	0.77
1:K:165:GLY:HA3	1:K:166:PHE:HB3	1.67	0.76
2:D:76:CYS:HB3	2:D:108:THR:OG1	1.85	0.76
1:G:823:TYR:CZ	1:G:825:PRO:HG3	2.20	0.76
1:A:629:MET:HE2	1:A:634:PHE:HA	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:PRO:HA	1:K:496:TYR:HB3	1.67	0.76
1:G:146:MET:HE2	1:G:544:THR:HB	1.67	0.76
1:Q:426:MET:CE	1:Q:618:GLN:HG2	2.14	0.76
2:L:46:MET:HE3	2:L:47:ASN:N	2.00	0.76
2:J:21:MET:HE2	2:J:24:MET:HE3	1.67	0.76
1:E:146:MET:HE2	1:E:544:THR:HB	1.66	0.76
1:I:146:MET:HE3	1:I:545:ASN:OD1	1.85	0.76
1:I:165:GLY:HA3	1:I:166:PHE:HB3	1.67	0.76
2:J:23:CYS:HB3	2:J:39:MET:HE1	1.67	0.76
2:P:128:MET:HA	7:P:303:SF4:S1	2.26	0.76
2:B:40:GLN:HE22	2:B:118:GLU:H	1.34	0.76
1:A:426:MET:CE	1:A:618:GLN:HG2	2.16	0.75
1:M:426:MET:CE	1:M:618:GLN:HG2	2.15	0.75
2:D:68:CYS:HB2	2:D:126:CYS:CB	2.16	0.75
2:F:40:GLN:NE2	2:F:118:GLU:H	1.83	0.75
1:G:69:MET:HE2	1:G:754:MET:CE	2.13	0.75
1:O:360:ALA:HB1	1:O:859:THR:HG23	1.68	0.75
1:S:69:MET:HE2	1:S:754:MET:CE	2.15	0.75
1:S:610:LYS:NZ	1:S:618:GLN:HE22	1.83	0.75
1:U:66:PHE:CZ	1:U:146:MET:HE1	2.21	0.75
1:C:146:MET:HE2	1:C:544:THR:HB	1.68	0.75
1:G:146:MET:CE	1:G:544:THR:HB	2.17	0.75
1:U:141:PRO:HA	1:U:496:TYR:HB3	1.66	0.75
2:R:23:CYS:HB3	2:R:39:MET:HE1	1.67	0.75
1:C:426:MET:CE	1:C:618:GLN:HG2	2.16	0.75
2:H:114:MET:HE3	2:H:123:ALA:HB1	1.67	0.75
1:C:69:MET:HE2	1:C:754:MET:CE	2.15	0.75
1:G:426:MET:CE	1:G:618:GLN:HG2	2.17	0.75
1:A:695:LEU:O	1:A:699:GLU:HG2	1.86	0.75
1:E:69:MET:HE2	1:E:754:MET:CE	2.15	0.75
1:K:823:TYR:CZ	1:K:825:PRO:HG3	2.20	0.75
2:V:19:CYS:HB3	2:V:145:CYS:HB3	1.68	0.74
1:W:69:MET:HE2	1:W:754:MET:CE	2.16	0.74
2:L:104:GLU:CD	2:L:104:GLU:H	1.95	0.74
1:Q:66:PHE:HA	1:Q:69:MET:HE3	1.67	0.74
1:A:786:ASN:HD22	1:A:805:VAL:H	1.34	0.74
2:D:2:GLU:HG2	2:D:158:LYS:HG2	1.67	0.74
1:U:69:MET:HE2	1:U:754:MET:CE	2.16	0.74
2:J:46:MET:HE3	2:J:47:ASN:N	2.02	0.74
1:Q:252:MET:HE3	1:Q:263:TRP:CE3	2.21	0.74
2:R:68:CYS:HB3	2:R:70:HIS:CE1	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:360:ALA:HB1	1:Q:859:THR:HG23	1.69	0.74
2:X:68:CYS:HB2	2:X:126:CYS:HB3	1.69	0.74
1:A:146:MET:CE	1:A:544:THR:HB	2.17	0.74
2:N:40:GLN:NE2	2:N:118:GLU:H	1.84	0.74
2:D:128:MET:HA	7:D:303:SF4:S1	2.26	0.74
1:W:360:ALA:HB1	1:W:859:THR:HG23	1.70	0.74
1:C:66:PHE:CZ	1:C:146:MET:HE1	2.21	0.74
1:U:610:LYS:NZ	1:U:618:GLN:HE22	1.86	0.74
2:V:128:MET:HA	7:V:303:SF4:S1	2.27	0.74
1:G:695:LEU:O	1:G:699:GLU:HG2	1.86	0.73
2:N:68:CYS:HB3	2:N:70:HIS:CE1	2.22	0.73
2:D:75:PRO:HD2	7:D:304:SF4:S4	2.27	0.73
2:T:128:MET:HA	7:T:303:SF4:S1	2.28	0.73
1:S:66:PHE:CZ	1:S:146:MET:HE1	2.22	0.73
1:W:610:LYS:NZ	1:W:618:GLN:HE22	1.86	0.73
2:T:142:MET:HE2	2:T:146:ALA:HB1	1.70	0.73
1:W:426:MET:CE	1:W:618:GLN:HG2	2.18	0.73
1:I:252:MET:HE3	1:I:263:TRP:CE3	2.22	0.73
1:S:557:CYS:N	1:S:564:ASN:HD21	1.85	0.73
1:S:823:TYR:CZ	1:S:825:PRO:HG3	2.23	0.73
2:T:76:CYS:HB3	2:T:108:THR:OG1	1.89	0.73
2:X:68:CYS:HB2	2:X:126:CYS:CB	2.17	0.73
1:I:695:LEU:O	1:I:699:GLU:HG2	1.89	0.73
1:A:211:MET:HE1	2:B:231:PHE:HZ	1.51	0.73
1:G:100:LEU:HD12	1:G:105:PRO:HG3	1.71	0.73
2:J:104:GLU:CD	2:J:104:GLU:H	1.97	0.73
1:M:141:PRO:HA	1:M:496:TYR:HB3	1.68	0.73
2:V:46:MET:HE3	2:V:47:ASN:N	2.03	0.73
1:A:610:LYS:NZ	1:A:618:GLN:HE22	1.86	0.72
2:R:40:GLN:NE2	2:R:118:GLU:H	1.86	0.72
1:W:252:MET:HE3	1:W:263:TRP:CE3	2.23	0.72
1:W:1:MET:H3	1:W:22:ASP:CG	1.97	0.72
2:B:114:MET:HE3	2:B:123:ALA:HB1	1.70	0.72
1:G:165:GLY:HA3	1:G:166:PHE:HB3	1.71	0.72
1:S:146:MET:HE3	1:S:545:ASN:OD1	1.90	0.72
2:P:142:MET:HE2	2:P:146:ALA:HB1	1.70	0.72
2:X:68:CYS:CB	2:X:126:CYS:HB3	2.19	0.72
2:B:40:GLN:NE2	2:B:118:GLU:H	1.86	0.72
2:D:69:MET:HB3	2:D:184:PRO:HB3	1.70	0.72
2:D:105:LEU:HB3	2:D:114:MET:HE1	1.72	0.72
1:S:141:PRO:HA	1:S:496:TYR:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:68:CYS:HB3	2:T:70:HIS:CE1	2.25	0.72
2:N:142:MET:CE	2:N:146:ALA:HB1	2.19	0.71
1:C:823:TYR:CZ	1:C:825:PRO:HG3	2.24	0.71
2:L:106:LEU:HD11	2:L:116:TRP:HB2	1.72	0.71
1:Q:165:GLY:HA3	1:Q:166:PHE:HB3	1.72	0.71
1:I:610:LYS:NZ	1:I:618:GLN:HE22	1.88	0.71
2:R:94:ILE:HD11	2:R:114:MET:HE3	1.72	0.71
2:X:128:MET:HA	7:X:303:SF4:S1	2.29	0.71
2:J:114:MET:HE3	2:J:123:ALA:HB1	1.71	0.71
1:W:695:LEU:O	1:W:699:GLU:HG2	1.88	0.71
1:Q:426:MET:HE1	1:Q:618:GLN:HG2	1.71	0.71
1:S:695:LEU:O	1:S:699:GLU:HG2	1.90	0.71
2:V:70:HIS:HD2	2:V:92:VAL:H	1.38	0.71
1:O:610:LYS:NZ	1:O:618:GLN:HE22	1.89	0.71
2:J:128:MET:HA	7:J:303:SF4:S1	2.30	0.71
1:E:394:PRO:HG3	8:E:1323:HOH:O	1.91	0.71
1:O:786:ASN:ND2	1:O:805:VAL:H	1.88	0.71
1:U:355:GLY:HA2	4:U:903:MGD:O1B	1.91	0.71
2:T:68:CYS:CB	2:T:126:CYS:HB3	2.21	0.71
2:D:142:MET:HE2	2:D:146:ALA:CB	2.20	0.71
2:P:68:CYS:HB3	2:P:70:HIS:CE1	2.26	0.71
1:A:561:ILE:HG22	1:A:564:ASN:HB3	1.72	0.70
2:B:68:CYS:HB3	2:B:70:HIS:CE1	2.26	0.70
1:E:100:LEU:HD12	1:E:105:PRO:HG3	1.73	0.70
2:J:68:CYS:HB3	2:J:70:HIS:CE1	2.26	0.70
2:L:166:LYS:O	2:L:170:GLU:HG3	1.92	0.70
1:M:823:TYR:CZ	1:M:825:PRO:HG3	2.26	0.70
1:O:426:MET:HE1	1:O:618:GLN:HG2	1.70	0.70
2:V:68:CYS:CB	2:V:126:CYS:HB3	2.20	0.70
1:W:645:ASN:ND2	1:W:648:ARG:HB3	2.06	0.70
2:L:5:TYR:HB2	2:L:157:LEU:CD1	2.20	0.70
2:N:23:CYS:HB3	2:N:39:MET:HE1	1.72	0.70
1:O:146:MET:CE	1:O:544:THR:HB	2.22	0.70
1:E:146:MET:CE	1:E:544:THR:HB	2.21	0.70
1:G:252:MET:HE3	1:G:263:TRP:CE3	2.26	0.70
2:J:40:GLN:NE2	2:J:118:GLU:H	1.90	0.70
2:T:46:MET:HE3	2:T:47:ASN:N	2.06	0.70
1:M:211:MET:HE1	2:N:231:PHE:HZ	1.53	0.70
2:N:114:MET:HE3	2:N:123:ALA:HB1	1.72	0.70
1:O:69:MET:HE2	1:O:754:MET:CE	2.22	0.70
1:Q:66:PHE:CZ	1:Q:146:MET:HE1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:PRO:HG3	8:C:1323:HOH:O	1.91	0.70
1:G:66:PHE:HZ	1:G:146:MET:HE1	1.57	0.70
1:Q:146:MET:CE	1:Q:544:THR:HB	2.21	0.70
2:L:68:CYS:HB2	2:L:126:CYS:HB2	1.71	0.70
1:G:360:ALA:HB1	1:G:859:THR:HG23	1.74	0.70
1:I:69:MET:HE2	1:I:754:MET:CE	2.20	0.70
2:J:71:CYS:HB2	2:J:182:THR:O	1.92	0.70
2:N:2:GLU:HG2	2:N:158:LYS:HG2	1.73	0.70
1:O:211:MET:HE1	2:P:231:PHE:HZ	1.53	0.70
1:Q:823:TYR:CZ	1:Q:825:PRO:HG3	2.27	0.70
1:U:823:TYR:CZ	1:U:825:PRO:HG3	2.26	0.70
2:F:76:CYS:HB3	2:F:108:THR:OG1	1.92	0.70
2:T:23:CYS:HB3	2:T:39:MET:HE1	1.72	0.70
1:A:165:GLY:HA3	1:A:166:PHE:HB3	1.71	0.70
1:I:823:TYR:CZ	1:I:825:PRO:HG3	2.27	0.70
1:K:146:MET:HE2	1:K:544:THR:CB	2.21	0.70
2:X:142:MET:HE2	2:X:146:ALA:CB	2.21	0.69
1:O:146:MET:HE2	1:O:544:THR:HB	1.74	0.69
1:O:394:PRO:HG3	8:O:1319:HOH:O	1.91	0.69
1:C:252:MET:HE3	1:C:263:TRP:CE3	2.27	0.69
1:K:249:ASP:OD1	4:K:903:MGD:H1'	1.92	0.69
1:M:360:ALA:HB1	1:M:859:THR:HG23	1.73	0.69
2:B:46:MET:HE3	2:B:47:ASN:N	2.07	0.69
1:C:426:MET:HE1	1:C:618:GLN:HG2	1.75	0.69
2:L:128:MET:HA	7:L:303:SF4:S1	2.32	0.69
2:B:23:CYS:HB3	2:B:39:MET:HE1	1.74	0.69
1:E:629:MET:HE2	1:E:634:PHE:HA	1.74	0.69
2:H:40:GLN:HE22	2:H:118:GLU:H	1.40	0.69
2:H:71:CYS:HB2	2:H:182:THR:O	1.92	0.69
2:J:68:CYS:CB	2:J:126:CYS:HB3	2.21	0.69
1:C:165:GLY:HA3	1:C:166:PHE:HB3	1.75	0.69
1:I:146:MET:CE	1:I:544:THR:HB	2.23	0.69
1:O:249:ASP:OD1	4:O:903:MGD:H1'	1.91	0.69
2:L:114:MET:HE3	2:L:123:ALA:HB1	1.73	0.69
1:M:252:MET:HE3	1:M:263:TRP:CE3	2.28	0.69
1:S:146:MET:HE2	1:S:544:THR:HB	1.73	0.69
1:S:561:ILE:HG22	1:S:564:ASN:HB3	1.73	0.69
1:U:211:MET:HE3	8:U:1453:HOH:O	1.92	0.69
1:W:644:ASP:OD1	1:W:646:PRO:HG3	1.93	0.69
2:B:68:CYS:HB2	2:B:126:CYS:HB2	1.75	0.69
2:B:71:CYS:HB2	2:B:182:THR:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:GLN:HE22	2:D:118:GLU:H	1.41	0.69
2:H:142:MET:CE	2:H:146:ALA:HB1	2.20	0.69
1:W:165:GLY:HA3	1:W:166:PHE:HB3	1.73	0.69
2:R:114:MET:HE2	2:R:123:ALA:HB1	1.75	0.69
2:J:21:MET:CE	2:J:24:MET:HE3	2.23	0.68
1:C:211:MET:HE1	2:D:231:PHE:HZ	1.57	0.68
2:D:68:CYS:CB	2:D:126:CYS:HB3	2.24	0.68
2:H:46:MET:HE3	2:H:47:ASN:N	2.08	0.68
2:H:68:CYS:HB3	2:H:70:HIS:CE1	2.28	0.68
2:P:104:GLU:H	2:P:104:GLU:CD	2.00	0.68
2:T:142:MET:HE2	2:T:146:ALA:CB	2.24	0.68
1:A:301:GLU:CD	1:A:301:GLU:H	2.00	0.68
1:W:356:GLY:N	4:W:903:MGD:O2B	2.26	0.68
1:C:146:MET:CE	1:C:544:THR:HB	2.23	0.68
2:J:5:TYR:HB2	2:J:157:LEU:CD1	2.23	0.68
1:Q:146:MET:HE2	1:Q:544:THR:HB	1.75	0.68
2:F:68:CYS:HB3	2:F:70:HIS:CE1	2.27	0.68
2:P:76:CYS:HB3	2:P:108:THR:OG1	1.93	0.68
1:U:146:MET:HE2	1:U:544:THR:CB	2.24	0.68
2:X:71:CYS:HA	2:X:184:PRO:HA	1.75	0.68
2:X:76:CYS:HB3	2:X:108:THR:OG1	1.94	0.68
1:I:426:MET:HE1	1:I:618:GLN:HG2	1.74	0.68
2:R:46:MET:HE3	2:R:47:ASN:N	2.09	0.68
1:W:561:ILE:HG22	1:W:564:ASN:HB3	1.75	0.68
1:E:695:LEU:O	1:E:699:GLU:HG2	1.94	0.67
1:K:426:MET:HE1	1:K:618:GLN:HG2	1.75	0.67
1:M:610:LYS:HZ3	1:M:618:GLN:HE22	1.40	0.67
2:D:46:MET:HE3	2:D:47:ASN:N	2.10	0.67
1:E:252:MET:HE3	1:E:263:TRP:CE3	2.29	0.67
1:G:146:MET:HE2	1:G:544:THR:CB	2.24	0.67
2:H:68:CYS:CB	2:H:126:CYS:HB3	2.23	0.67
1:K:74:LEU:HD12	1:K:750:LYS:HA	1.76	0.67
2:P:68:CYS:CB	2:P:126:CYS:HB3	2.22	0.67
2:R:68:CYS:CB	2:R:126:CYS:HB3	2.22	0.67
2:R:5:TYR:HB2	2:R:157:LEU:HD13	1.77	0.67
1:C:355:GLY:HA2	4:C:903:MGD:O1B	1.95	0.67
1:E:823:TYR:CZ	1:E:825:PRO:HG3	2.30	0.67
1:O:165:GLY:HA3	1:O:166:PHE:HB3	1.75	0.67
1:Q:695:LEU:O	1:Q:699:GLU:HG2	1.95	0.67
2:X:46:MET:HE3	2:X:47:ASN:N	2.10	0.67
1:C:1:MET:H3	1:C:22:ASP:CG	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:GLY:HA3	1:E:166:PHE:HB3	1.75	0.67
2:L:68:CYS:HB3	2:L:70:HIS:CE1	2.30	0.67
1:A:426:MET:HE1	1:A:618:GLN:HG2	1.76	0.66
1:K:301:GLU:H	1:K:301:GLU:CD	2.04	0.66
2:P:46:MET:HE3	2:P:47:ASN:N	2.09	0.66
1:W:610:LYS:HZ2	1:W:618:GLN:HE22	1.44	0.66
1:G:355:GLY:CA	4:G:903:MGD:O2B	2.43	0.66
2:L:69:MET:HB3	2:L:184:PRO:HB3	1.78	0.66
2:B:68:CYS:CB	2:B:126:CYS:HB3	2.24	0.66
1:A:216:SER:OG	4:A:903:MGD:H5'2	1.96	0.66
1:C:561:ILE:HG22	1:C:564:ASN:HB3	1.76	0.66
1:E:211:MET:HE1	2:F:231:PHE:HZ	1.60	0.66
2:F:5:TYR:HB2	2:F:157:LEU:HD11	1.77	0.66
2:J:40:GLN:HE22	2:J:118:GLU:H	1.42	0.66
1:S:146:MET:CE	1:S:544:THR:HB	2.25	0.66
2:B:75:PRO:HD2	7:B:304:SF4:S4	2.36	0.66
2:D:46:MET:HE1	2:D:66:THR:H	1.61	0.66
2:F:128:MET:HA	7:F:303:SF4:S1	2.36	0.66
1:G:32:ASP:OD2	8:G:1659:HOH:O	2.13	0.66
1:W:74:LEU:HD12	1:W:750:LYS:HA	1.76	0.66
1:E:630:THR:OG1	1:E:633:GLU:HG3	1.94	0.66
1:W:142:SER:HB3	4:W:902:MGD:H5'2	1.76	0.66
2:J:142:MET:HE2	2:J:146:ALA:HB1	1.77	0.66
1:S:138:LEU:HB2	1:S:490:ILE:HD12	1.78	0.66
1:A:142:SER:OG	4:A:902:MGD:O1A	2.13	0.65
2:D:68:CYS:HB3	2:D:70:HIS:CE1	2.30	0.65
1:G:356:GLY:N	4:G:903:MGD:O2B	2.28	0.65
1:K:610:LYS:NZ	1:K:618:GLN:HE22	1.95	0.65
1:M:165:GLY:HA3	1:M:166:PHE:HB3	1.77	0.65
1:M:74:LEU:HD12	1:M:750:LYS:HA	1.79	0.65
1:Q:134:PRO:HB2	1:Q:439:LEU:HD11	1.76	0.65
1:A:146:MET:HE2	1:A:544:THR:CB	2.26	0.65
2:R:104:GLU:CD	2:R:104:GLU:H	2.05	0.65
2:H:2:GLU:HG2	2:H:158:LYS:HG2	1.78	0.65
1:K:630:THR:OG1	1:K:633:GLU:HG3	1.97	0.65
1:S:1:MET:H3	1:S:22:ASP:CG	2.05	0.65
1:S:75:ARG:HH21	1:S:543:CYS:HA	1.62	0.65
1:C:696:LYS:HD3	8:C:1680:HOH:O	1.96	0.65
2:D:114:MET:HA	2:D:125:LYS:HB3	1.78	0.65
1:G:394:PRO:HG3	8:G:1321:HOH:O	1.97	0.65
2:L:71:CYS:HB2	2:L:182:THR:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:75:PRO:HD2	7:T:304:SF4:S4	2.37	0.65
2:X:69:MET:HB3	2:X:184:PRO:HB3	1.78	0.65
1:Q:211:MET:HE1	2:R:231:PHE:HZ	1.56	0.65
2:V:142:MET:HE2	2:V:146:ALA:C	2.21	0.65
1:A:394:PRO:HG3	8:A:1320:HOH:O	1.96	0.65
1:G:66:PHE:CZ	1:G:146:MET:HE1	2.31	0.65
1:O:355:GLY:HA2	4:O:903:MGD:O2B	1.96	0.65
2:B:128:MET:HA	7:B:303:SF4:S1	2.37	0.64
1:C:610:LYS:HZ2	1:C:618:GLN:HE22	1.43	0.64
1:C:644:ASP:C	1:C:646:PRO:HD3	2.22	0.64
2:J:106:LEU:HA	2:J:114:MET:HE2	1.79	0.64
2:N:142:MET:HE1	8:N:927:HOH:O	1.96	0.64
4:Q:903:MGD:O1B	4:Q:903:MGD:H4'	1.96	0.64
1:W:426:MET:HE1	1:W:618:GLN:HG2	1.79	0.64
1:I:478:HIS:HD2	8:I:1202:HOH:O	1.80	0.64
2:N:76:CYS:HB3	2:N:108:THR:OG1	1.97	0.64
2:R:128:MET:HA	7:R:303:SF4:S1	2.38	0.64
2:X:59:ASN:H	2:X:59:ASN:HD22	1.46	0.64
2:P:125:LYS:HD2	2:P:126:CYS:O	1.96	0.64
1:Q:394:PRO:HG3	8:Q:1320:HOH:O	1.96	0.64
2:N:68:CYS:CB	2:N:126:CYS:HB3	2.24	0.64
2:P:40:GLN:HE22	2:P:118:GLU:H	1.45	0.64
1:U:165:GLY:HA3	1:U:166:PHE:HB3	1.78	0.64
1:I:394:PRO:HG3	8:I:1318:HOH:O	1.98	0.64
1:K:478:HIS:HD2	8:K:1201:HOH:O	1.80	0.64
2:P:75:PRO:HD2	7:P:304:SF4:S4	2.37	0.64
2:N:128:MET:HA	7:N:303:SF4:S1	2.38	0.64
1:U:35:ASP:OD1	1:U:55:ARG:HD3	1.98	0.64
2:V:68:CYS:HB3	2:V:70:HIS:CE1	2.33	0.64
2:V:69:MET:HB3	2:V:184:PRO:HB3	1.79	0.64
2:P:69:MET:HB3	2:P:184:PRO:HB3	1.80	0.64
1:U:249:ASP:CG	4:U:903:MGD:H1'	2.23	0.64
2:D:71:CYS:HB2	2:D:182:THR:O	1.98	0.64
1:E:197:GLU:HG3	1:E:199:TYR:CD1	2.34	0.64
2:L:142:MET:HE2	2:L:146:ALA:HB1	1.80	0.64
2:R:157:LEU:H	2:R:157:LEU:HD12	1.62	0.64
1:K:561:ILE:HG22	1:K:564:ASN:HB3	1.80	0.63
1:K:629:MET:HE2	1:K:634:PHE:HA	1.79	0.63
1:M:561:ILE:HG22	1:M:564:ASN:HB3	1.79	0.63
1:M:100:LEU:HD12	1:M:105:PRO:HG3	1.80	0.63
2:T:68:CYS:HB2	2:T:126:CYS:HB2	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:LYS:HD3	8:A:1105:HOH:O	1.98	0.63
1:M:134:PRO:HB2	1:M:439:LEU:HD11	1.80	0.63
2:V:75:PRO:HD2	7:V:304:SF4:S4	2.38	0.63
1:E:146:MET:HE2	1:E:544:THR:CB	2.28	0.63
1:I:75:ARG:HH21	1:I:543:CYS:HA	1.63	0.63
2:L:68:CYS:CB	2:L:126:CYS:HB3	2.28	0.63
1:Q:114:TRP:CZ2	1:Q:541:PRO:HD2	2.33	0.63
1:S:249:ASP:CG	4:S:903:MGD:H1'	2.24	0.63
2:T:71:CYS:HB2	2:T:182:THR:O	1.99	0.63
1:U:561:ILE:HG22	1:U:564:ASN:HB3	1.80	0.63
2:F:21:MET:HA	2:F:21:MET:HE2	1.80	0.63
1:Q:100:LEU:HD13	1:Q:105:PRO:HG3	1.80	0.63
2:L:70:HIS:CD2	2:L:92:VAL:H	2.08	0.63
1:S:478:HIS:HD2	8:S:1205:HOH:O	1.82	0.63
1:S:165:GLY:HA3	1:S:166:PHE:HB3	1.80	0.63
2:X:2:GLU:HG2	2:X:158:LYS:HG2	1.79	0.63
1:G:426:MET:HE1	1:G:618:GLN:HG2	1.78	0.62
2:H:142:MET:HE1	8:H:429:HOH:O	1.98	0.62
1:E:800:ILE:HD12	1:E:800:ILE:N	2.15	0.62
1:I:146:MET:HE2	1:I:544:THR:HB	1.81	0.62
1:S:558:SER:H	1:S:564:ASN:ND2	1.97	0.62
2:X:59:ASN:H	2:X:59:ASN:ND2	1.96	0.62
2:D:7:VAL:HB	2:D:155:GLU:HB3	1.82	0.62
1:E:610:LYS:HZ2	1:E:618:GLN:HE22	1.46	0.62
1:G:249:ASP:OD1	4:G:903:MGD:H1'	1.99	0.62
2:J:20:PHE:CZ	2:J:24:MET:HE2	2.34	0.62
1:M:356:GLY:N	4:M:903:MGD:O1B	2.31	0.62
1:M:629:MET:HE2	1:M:634:PHE:HA	1.80	0.62
1:Q:333:ARG:NH1	1:U:729:LYS:HE3	2.14	0.62
2:N:69:MET:HB3	2:N:184:PRO:HB3	1.81	0.62
1:Q:249:ASP:OD1	4:Q:903:MGD:H1'	1.98	0.62
2:R:94:ILE:CD1	2:R:114:MET:HE3	2.28	0.62
1:U:138:LEU:HB2	1:U:490:ILE:HD12	1.80	0.62
1:A:252:MET:HE3	1:A:263:TRP:CE3	2.34	0.62
1:C:146:MET:HE2	1:C:544:THR:CB	2.28	0.62
2:J:75:PRO:HD2	7:J:304:SF4:S4	2.39	0.62
1:K:753:TYR:HB3	2:L:24:MET:HE3	1.82	0.62
1:Q:319:GLU:CG	1:U:726:LEU:HD13	2.27	0.62
1:W:311:THR:HG21	8:W:1499:HOH:O	1.98	0.62
2:F:104:GLU:H	2:F:104:GLU:CD	2.07	0.62
1:G:691:ILE:HD11	1:G:711:MET:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:311:THR:HG21	8:U:1502:HOH:O	2.00	0.62
2:X:143:PRO:HB3	7:X:303:SF4:S1	2.39	0.62
2:B:46:MET:CE	2:B:66:THR:H	2.09	0.62
1:S:753:TYR:HB3	2:T:24:MET:CE	2.29	0.62
2:V:46:MET:CE	2:V:66:THR:H	2.12	0.62
1:I:75:ARG:NH2	1:I:543:CYS:HA	2.15	0.62
1:O:146:MET:HE2	1:O:544:THR:CB	2.30	0.62
1:S:610:LYS:HZ2	1:S:618:GLN:HE22	1.46	0.62
1:M:725:PRO:HA	1:S:704:ILE:HG13	1.82	0.62
1:Q:708:ARG:HD2	8:Q:1043:HOH:O	1.98	0.62
1:U:478:HIS:HD2	8:U:1207:HOH:O	1.83	0.62
1:A:249:ASP:OD1	4:A:903:MGD:H1'	2.00	0.61
1:I:610:LYS:HZ2	1:I:618:GLN:HE22	1.46	0.61
2:V:2:GLU:HG2	2:V:158:LYS:HG2	1.82	0.61
2:X:125:LYS:HD2	2:X:126:CYS:O	2.00	0.61
1:G:301:GLU:H	1:G:301:GLU:CD	2.08	0.61
2:V:68:CYS:HB2	2:V:126:CYS:HB2	1.80	0.61
2:J:68:CYS:HB2	2:J:126:CYS:HB2	1.81	0.61
2:L:75:PRO:HD2	7:L:304:SF4:S4	2.41	0.61
2:P:68:CYS:HB2	2:P:126:CYS:HB2	1.79	0.61
1:S:81:LYS:HB2	1:S:112:ILE:HD13	1.82	0.61
2:B:205:VAL:HG13	2:B:254:LYS:NZ	2.16	0.61
1:S:252:MET:HE3	1:S:263:TRP:CE3	2.34	0.61
2:N:75:PRO:HD2	7:N:304:SF4:S4	2.41	0.61
4:A:903:MGD:O2B	4:A:903:MGD:O1A	2.18	0.61
1:E:561:ILE:HG22	1:E:564:ASN:HB3	1.82	0.61
1:G:162:ASN:HA	8:G:1364:HOH:O	1.99	0.61
2:F:68:CYS:CB	2:F:126:CYS:HB3	2.23	0.61
1:C:786:ASN:ND2	1:C:805:VAL:H	1.99	0.61
1:K:746:MET:HE2	4:K:902:MGD:O1B	2.01	0.61
2:F:5:TYR:HB2	2:F:157:LEU:CD1	2.30	0.61
2:N:71:CYS:HB2	2:N:182:THR:O	2.00	0.61
2:T:40:GLN:HE22	2:T:118:GLU:H	1.47	0.61
1:O:257:ARG:HD3	2:P:61:ILE:HG21	1.83	0.60
1:Q:696:LYS:O	1:Q:700:GLU:HG3	2.00	0.60
2:V:104:GLU:H	2:V:104:GLU:CD	2.09	0.60
2:B:21:MET:HE2	2:B:21:MET:HA	1.83	0.60
1:S:311:THR:HG21	8:S:1495:HOH:O	2.01	0.60
1:A:81:LYS:HB2	1:A:112:ILE:HD13	1.84	0.60
1:C:610:LYS:HZ3	1:C:618:GLN:HE22	1.48	0.60
2:H:128:MET:HA	7:H:303:SF4:S1	2.42	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1:MET:HG3	2:L:88:GLU:HB3	1.83	0.60
1:M:319:GLU:CG	1:S:726:LEU:HD13	2.30	0.60
1:M:696:LYS:O	1:M:700:GLU:HG3	2.01	0.60
1:O:557:CYS:N	1:O:564:ASN:HD21	1.93	0.60
1:Q:142:SER:OG	4:Q:902:MGD:O1A	2.15	0.60
2:X:252:ASP:C	2:X:254:LYS:H	2.09	0.60
2:D:143:PRO:HB3	7:D:303:SF4:S1	2.41	0.60
1:E:696:LYS:O	1:E:700:GLU:HG3	2.01	0.60
2:J:105:LEU:HB3	2:J:114:MET:HE1	1.83	0.60
4:K:903:MGD:O2B	4:K:903:MGD:O1A	2.18	0.60
2:L:59:ASN:H	2:L:59:ASN:ND2	1.99	0.60
1:O:74:LEU:HD12	1:O:750:LYS:HA	1.83	0.60
1:S:786:ASN:HD22	1:S:805:VAL:H	1.48	0.60
1:W:249:ASP:OD1	4:W:903:MGD:H1'	2.01	0.60
1:G:211:MET:HE1	2:H:231:PHE:HZ	1.64	0.60
1:K:216:SER:OG	4:K:903:MGD:H5'2	2.01	0.60
1:I:786:ASN:ND2	1:I:804:GLN:HA	2.16	0.60
2:J:76:CYS:O	2:J:80:GLY:N	2.35	0.60
1:Q:557:CYS:N	1:Q:564:ASN:HD21	1.88	0.60
2:R:125:LYS:HD2	2:R:126:CYS:O	2.02	0.60
1:U:301:GLU:H	1:U:301:GLU:CD	2.10	0.60
2:X:70:HIS:HD2	2:X:92:VAL:H	1.48	0.60
1:A:495:LYS:HD2	1:A:514:TYR:OH	2.01	0.60
1:G:610:LYS:HZ1	1:G:618:GLN:HE22	1.47	0.60
1:C:610:LYS:HB3	1:C:614:ALA:HB3	1.84	0.60
1:E:301:GLU:H	1:E:301:GLU:CD	2.09	0.60
2:F:46:MET:HE1	2:F:65:PRO:HA	1.84	0.60
2:H:21:MET:HE2	2:H:21:MET:HA	1.82	0.60
2:H:40:GLN:NE2	2:H:118:GLU:H	1.99	0.60
2:R:59:ASN:ND2	2:R:59:ASN:H	2.00	0.60
1:C:557:CYS:N	1:C:564:ASN:HD21	1.89	0.59
2:F:166:LYS:O	2:F:170:GLU:HG3	2.02	0.59
1:Q:800:ILE:HD12	1:Q:800:ILE:N	2.17	0.59
1:U:134:PRO:HB2	1:U:439:LEU:HD11	1.83	0.59
2:B:166:LYS:HG2	2:B:170:GLU:OE2	2.01	0.59
1:K:557:CYS:N	1:K:564:ASN:HD21	1.88	0.59
1:M:163:MET:HE1	1:M:606:PHE:HA	1.84	0.59
1:W:645:ASN:HD22	1:W:648:ARG:HB3	1.65	0.59
1:A:211:MET:HE3	1:A:244:ASP:HB2	1.84	0.59
1:C:249:ASP:CG	4:C:903:MGD:H1'	2.28	0.59
1:I:66:PHE:HA	1:I:69:MET:CE	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:356:GLY:H	4:M:903:MGD:H5'2	1.67	0.59
2:R:142:MET:CE	2:R:146:ALA:HB1	2.27	0.59
1:I:114:TRP:CZ2	1:I:541:PRO:HD2	2.36	0.59
1:K:211:MET:HE3	8:K:1446:HOH:O	2.01	0.59
1:Q:649:LYS:HE3	1:Q:651:THR:HG22	1.84	0.59
1:G:249:ASP:CG	4:G:903:MGD:H1'	2.28	0.59
1:G:629:MET:HE2	1:G:634:PHE:CA	2.32	0.59
1:G:786:ASN:HD22	1:G:805:VAL:H	1.50	0.59
2:H:201:ALA:HB2	2:H:269:LEU:HB2	1.84	0.59
1:I:426:MET:HE2	1:I:618:GLN:HG2	1.83	0.59
1:O:301:GLU:CD	1:O:301:GLU:H	2.10	0.59
2:R:142:MET:HE1	8:R:429:HOH:O	2.01	0.59
2:L:103:LYS:HE2	2:L:116:TRP:NE1	2.18	0.59
1:M:630:THR:OG1	1:M:633:GLU:HG3	2.02	0.59
1:M:800:ILE:HD12	1:M:800:ILE:N	2.17	0.59
1:A:15:PRO:HD2	8:A:1003:HOH:O	2.01	0.59
1:A:55:ARG:HD2	8:A:1637:HOH:O	2.03	0.59
2:F:46:MET:HE3	2:F:47:ASN:N	2.18	0.59
1:O:561:ILE:HG22	1:O:564:ASN:HB3	1.82	0.59
1:W:249:ASP:CG	4:W:903:MGD:H1'	2.27	0.59
1:W:708:ARG:HD2	8:W:1044:HOH:O	2.03	0.59
1:E:197:GLU:OE2	1:E:667:ASP:HB2	2.03	0.59
1:G:134:PRO:HB2	1:G:439:LEU:HD11	1.84	0.59
1:M:610:LYS:HB3	1:M:614:ALA:HB3	1.85	0.59
2:N:21:MET:HA	2:N:21:MET:HE2	1.85	0.59
1:Q:691:ILE:HD11	1:Q:711:MET:HE3	1.84	0.59
1:Q:823:TYR:CE2	1:Q:825:PRO:HG3	2.38	0.59
1:Q:871:LYS:HG2	8:Q:1230:HOH:O	2.02	0.59
1:W:35:ASP:OD1	1:W:55:ARG:HD3	2.03	0.59
2:B:70:HIS:CD2	2:B:92:VAL:H	2.09	0.58
1:C:478:HIS:HD2	8:C:1205:HOH:O	1.86	0.58
1:M:146:MET:HE3	1:M:544:THR:HA	1.85	0.58
2:X:5:TYR:HB2	2:X:157:LEU:CD1	2.33	0.58
1:G:144:HIS:HB2	4:G:902:MGD:O1B	2.03	0.58
1:G:610:LYS:HB3	1:G:614:ALA:HB3	1.84	0.58
1:Q:44:ILE:HD11	1:Q:394:PRO:HG2	1.85	0.58
2:B:114:MET:HA	2:B:125:LYS:HB3	1.85	0.58
1:C:726:LEU:HD23	8:C:1194:HOH:O	2.02	0.58
2:N:46:MET:HE1	2:N:65:PRO:HA	1.85	0.58
1:Q:55:ARG:HD2	8:Q:1636:HOH:O	2.02	0.58
1:Q:800:ILE:HD11	1:Q:833:ALA:HB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:146:MET:HG2	4:Q:902:MGD:N7	2.19	0.58
1:S:510:TYR:O	1:S:513:MET:HG2	2.03	0.58
2:D:106:LEU:HD23	2:D:114:MET:HE2	1.84	0.58
2:D:142:MET:HE1	8:D:927:HOH:O	2.03	0.58
1:K:311:THR:HG21	8:K:1495:HOH:O	2.02	0.58
1:K:400:TYR:CE1	1:K:421:LYS:HD2	2.39	0.58
1:M:249:ASP:CG	4:M:903:MGD:H1'	2.28	0.58
1:Q:291:GLU:CD	1:Q:291:GLU:H	2.11	0.58
1:U:85:PHE:CE2	1:U:87:PRO:HG3	2.38	0.58
2:F:205:VAL:HG13	2:F:254:LYS:NZ	2.18	0.58
1:O:138:LEU:HB2	1:O:490:ILE:HD12	1.85	0.58
2:X:7:VAL:HG21	2:X:167:LYS:HZ2	1.68	0.58
2:P:106:LEU:HD23	2:P:114:MET:HE2	1.85	0.58
1:Q:738:HIS:HE2	4:Q:902:MGD:H15	1.52	0.58
1:S:647:ASN:O	1:S:648:ARG:O	2.21	0.58
1:U:610:LYS:HZ2	1:U:618:GLN:HE22	1.51	0.58
1:C:785:LYS:HB2	1:C:785:LYS:NZ	2.18	0.58
2:D:114:MET:HE3	2:D:123:ALA:HB1	1.85	0.58
2:L:142:MET:HE2	2:L:146:ALA:CB	2.34	0.58
1:M:75:ARG:NH2	1:M:543:CYS:HA	2.18	0.58
1:O:696:LYS:O	1:O:700:GLU:HG3	2.02	0.58
1:O:786:ASN:ND2	1:O:804:GLN:HA	2.19	0.58
4:O:903:MGD:H4'	4:O:903:MGD:O1B	2.04	0.58
1:U:214:PHE:HA	1:U:347:ALA:HB3	1.86	0.58
1:U:753:TYR:HB3	2:V:24:MET:HE3	1.84	0.58
2:D:40:GLN:NE2	2:D:117:ASN:HA	2.18	0.58
1:I:494:TRP:HE1	1:I:525:GLN:HE21	1.52	0.58
2:N:21:MET:HE2	2:N:21:MET:CA	2.34	0.58
2:P:5:TYR:HB2	2:P:157:LEU:CD1	2.34	0.58
1:C:505:THR:O	1:C:506:ALA:C	2.46	0.58
2:D:70:HIS:CD2	2:D:92:VAL:H	2.16	0.58
1:G:870:ASP:HB3	1:G:872:TYR:CE1	2.39	0.58
2:T:114:MET:HE3	2:T:123:ALA:HB1	1.86	0.58
1:C:74:LEU:HD12	1:C:750:LYS:HA	1.85	0.57
1:G:114:TRP:CZ2	1:G:541:PRO:HD2	2.39	0.57
2:H:21:MET:HE2	2:H:24:MET:HE3	1.86	0.57
2:N:5:TYR:HB2	2:N:157:LEU:CD1	2.34	0.57
1:O:100:LEU:HD12	1:O:105:PRO:HG3	1.86	0.57
1:S:754:MET:HG3	8:S:1652:HOH:O	2.04	0.57
1:W:757:ILE:HD11	2:X:21:MET:HE3	1.86	0.57
1:C:823:TYR:CE2	1:C:825:PRO:HG3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:59:ASN:ND2	2:H:59:ASN:H	2.03	0.57
4:O:903:MGD:O2B	4:O:903:MGD:O1A	2.21	0.57
1:U:696:LYS:O	1:U:700:GLU:HG3	2.04	0.57
2:D:106:LEU:HD11	2:D:116:TRP:HB2	1.86	0.57
1:E:134:PRO:HB2	1:E:439:LEU:HD11	1.86	0.57
1:I:100:LEU:HD12	1:I:105:PRO:HG3	1.85	0.57
1:K:610:LYS:HB3	1:K:614:ALA:HB3	1.84	0.57
1:W:510:TYR:O	1:W:513:MET:HG2	2.05	0.57
2:X:75:PRO:HD2	7:X:304:SF4:S4	2.45	0.57
1:K:786:ASN:ND2	1:K:805:VAL:H	2.03	0.57
2:L:40:GLN:NE2	2:L:118:GLU:H	1.97	0.57
1:M:35:ASP:OD1	1:M:55:ARG:HD3	2.04	0.57
1:Q:100:LEU:CD1	1:Q:105:PRO:HG3	2.34	0.57
1:S:146:MET:HE2	1:S:544:THR:CB	2.35	0.57
2:T:166:LYS:HG2	2:T:170:GLU:OE2	2.04	0.57
1:C:355:GLY:C	4:C:903:MGD:O1B	2.47	0.57
1:K:823:TYR:CE2	1:K:825:PRO:HG3	2.40	0.57
1:M:146:MET:HE3	1:M:544:THR:CB	2.34	0.57
1:O:479:GLN:HG2	8:O:1176:HOH:O	2.04	0.57
1:Q:249:ASP:CG	4:Q:903:MGD:H1'	2.30	0.57
1:Q:753:TYR:HB3	2:R:24:MET:HE3	1.86	0.57
2:T:104:GLU:CD	2:T:104:GLU:H	2.12	0.57
1:A:426:MET:HA	1:A:426:MET:CE	2.32	0.57
1:E:800:ILE:HD11	1:E:833:ALA:HB1	1.86	0.57
1:I:557:CYS:N	1:I:564:ASN:HD21	1.92	0.57
2:J:19:CYS:HB3	2:J:145:CYS:HB3	1.86	0.57
1:S:140:THR:HB	1:S:169:ALA:HB3	1.86	0.57
2:X:19:CYS:HB3	2:X:145:CYS:HB3	1.85	0.57
2:N:46:MET:HE1	2:N:65:PRO:CA	2.35	0.57
2:N:70:HIS:CD2	2:N:92:VAL:H	2.10	0.57
2:N:104:GLU:H	2:N:104:GLU:CD	2.12	0.57
1:O:252:MET:HE3	1:O:263:TRP:CE3	2.39	0.57
2:P:114:MET:HE3	2:P:123:ALA:HB1	1.87	0.57
2:H:76:CYS:HB3	2:H:108:THR:OG1	2.05	0.57
2:J:106:LEU:HD11	2:J:116:TRP:HB2	1.87	0.57
1:M:823:TYR:CE2	1:M:825:PRO:HG3	2.39	0.57
1:Q:146:MET:HE2	1:Q:544:THR:CB	2.34	0.57
2:T:106:LEU:HD11	2:T:116:TRP:HB2	1.86	0.57
1:W:28:MET:HE2	8:W:1398:HOH:O	2.04	0.57
1:A:218:ASP:OD2	1:A:253:ASN:HB2	2.05	0.57
2:B:46:MET:HE1	2:B:65:PRO:C	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:ASP:OD1	4:E:903:MGD:H1'	2.04	0.57
2:F:69:MET:HB3	2:F:184:PRO:HB3	1.87	0.57
2:J:5:TYR:HB2	2:J:157:LEU:HD11	1.85	0.57
2:L:162:GLU:H	2:L:162:GLU:CD	2.13	0.57
1:O:823:TYR:CE2	1:O:825:PRO:HG3	2.40	0.57
2:P:142:MET:HE2	2:P:146:ALA:CB	2.35	0.57
1:Q:100:LEU:HD22	1:Q:534:PRO:HB2	1.87	0.57
1:Q:503:THR:HG21	4:Q:902:MGD:O2A	2.04	0.57
1:U:394:PRO:HG3	8:U:1322:HOH:O	2.04	0.57
1:C:100:LEU:HD12	1:C:105:PRO:HG3	1.87	0.57
1:E:114:TRP:CZ2	1:E:541:PRO:HD2	2.40	0.57
1:U:100:LEU:HD12	1:U:105:PRO:HG3	1.87	0.57
1:G:74:LEU:HD12	1:G:750:LYS:HA	1.87	0.56
1:M:211:MET:HE3	8:M:1451:HOH:O	2.05	0.56
2:R:70:HIS:CD2	2:R:92:VAL:H	2.13	0.56
2:B:59:ASN:ND2	2:B:59:ASN:H	2.02	0.56
1:I:708:ARG:HD2	8:I:1043:HOH:O	2.03	0.56
1:K:737:PRO:CG	4:K:903:MGD:H2'	2.35	0.56
2:V:142:MET:HE2	2:V:146:ALA:CB	2.35	0.56
4:E:903:MGD:O2B	8:E:1287:HOH:O	2.18	0.56
1:I:426:MET:HE1	1:I:618:GLN:O	2.05	0.56
2:J:46:MET:CE	2:J:66:THR:H	2.15	0.56
1:K:356:GLY:H	4:K:903:MGD:C5'	2.19	0.56
2:L:105:LEU:HB3	2:L:114:MET:CE	2.35	0.56
1:O:140:THR:HB	1:O:169:ALA:HB3	1.87	0.56
2:R:75:PRO:HD2	7:R:304:SF4:S4	2.45	0.56
1:S:211:MET:HE3	8:S:1447:HOH:O	2.06	0.56
2:X:68:CYS:HB3	2:X:70:HIS:CE1	2.40	0.56
4:E:903:MGD:O2B	4:E:903:MGD:O1A	2.24	0.56
1:G:378:GLY:O	1:G:381:LYS:HG2	2.04	0.56
2:H:75:PRO:HD2	7:H:304:SF4:S4	2.45	0.56
1:U:253:ASN:O	1:U:257:ARG:HG3	2.06	0.56
1:A:478:HIS:HD2	8:A:1203:HOH:O	1.87	0.56
1:A:610:LYS:HZ1	1:A:618:GLN:HE22	1.53	0.56
1:A:737:PRO:HG3	4:A:903:MGD:H2'	1.87	0.56
1:E:56:LYS:HG2	1:E:57:THR:O	2.05	0.56
1:G:426:MET:HE2	1:G:618:GLN:HG2	1.88	0.56
2:N:46:MET:HE3	2:N:47:ASN:N	2.19	0.56
1:Q:356:GLY:N	4:Q:903:MGD:O2B	2.38	0.56
1:U:76:ILE:HG22	1:U:541:PRO:HG3	1.88	0.56
2:V:40:GLN:HE22	2:V:118:GLU:H	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:140:THR:HB	1:W:169:ALA:HB3	1.88	0.56
1:C:757:ILE:HD11	2:D:21:MET:HE3	1.88	0.56
1:G:142:SER:OG	4:G:902:MGD:O1A	2.20	0.56
1:G:708:ARG:HD2	8:G:1044:HOH:O	2.05	0.56
1:I:249:ASP:CG	4:I:903:MGD:H1'	2.30	0.56
1:U:510:TYR:O	1:U:513:MET:HG2	2.06	0.56
1:W:696:LYS:O	1:W:700:GLU:HG3	2.06	0.56
2:X:40:GLN:HE22	2:X:118:GLU:H	1.53	0.56
2:D:125:LYS:HD2	2:D:126:CYS:O	2.05	0.56
1:E:510:TYR:O	1:E:513:MET:HG2	2.06	0.56
1:M:786:ASN:ND2	1:M:804:GLN:HA	2.21	0.56
1:O:478:HIS:HD2	8:O:1204:HOH:O	1.89	0.56
1:S:74:LEU:HD12	1:S:750:LYS:HA	1.86	0.56
1:S:142:SER:OG	4:S:902:MGD:O1A	2.20	0.56
1:A:630:THR:OG1	1:A:633:GLU:HG3	2.06	0.56
1:G:786:ASN:ND2	1:G:805:VAL:H	2.03	0.56
2:H:21:MET:CE	2:H:24:MET:HE3	2.36	0.56
1:S:696:LYS:O	1:S:700:GLU:HG3	2.05	0.56
1:I:146:MET:HE2	1:I:544:THR:CB	2.36	0.56
1:I:495:LYS:HD2	1:I:514:TYR:OH	2.06	0.56
1:M:478:HIS:HD2	8:M:1205:HOH:O	1.89	0.56
1:Q:478:HIS:HD2	8:Q:1203:HOH:O	1.88	0.56
2:R:166:LYS:HG2	2:R:170:GLU:OE2	2.06	0.56
1:W:610:LYS:HB3	1:W:614:ALA:HB3	1.87	0.56
1:C:725:PRO:HD2	8:C:1194:HOH:O	2.06	0.56
1:M:333:ARG:NH1	1:S:729:LYS:HE3	2.20	0.56
1:O:143:SER:N	4:O:902:MGD:O1A	2.39	0.56
2:X:95:ASP:HB3	2:X:98:LYS:HB2	1.88	0.56
2:F:46:MET:HE1	2:F:65:PRO:CA	2.36	0.55
2:F:70:HIS:CD2	2:F:92:VAL:H	2.10	0.55
2:J:69:MET:HB3	2:J:184:PRO:HB3	1.87	0.55
2:L:254:LYS:HD2	2:L:274:LEU:OXT	2.06	0.55
2:L:59:ASN:H	2:L:59:ASN:HD22	1.54	0.55
1:O:311:THR:HG21	8:O:1498:HOH:O	2.06	0.55
1:Q:319:GLU:HG2	1:U:726:LEU:CD1	2.30	0.55
1:Q:629:MET:HE2	1:Q:634:PHE:HA	1.88	0.55
2:R:142:MET:HE2	2:R:146:ALA:HB3	1.88	0.55
2:T:46:MET:CE	2:T:66:THR:H	2.16	0.55
1:W:557:CYS:N	1:W:564:ASN:HD21	1.95	0.55
1:I:644:ASP:C	1:I:646:PRO:HD3	2.32	0.55
1:E:146:MET:HG2	4:E:902:MGD:N7	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:629:MET:HE2	1:E:634:PHE:CA	2.36	0.55
1:G:66:PHE:CD1	1:G:69:MET:HE3	2.42	0.55
1:G:146:MET:HE2	1:G:544:THR:CA	2.36	0.55
2:L:114:MET:HA	2:L:125:LYS:HB3	1.87	0.55
1:O:753:TYR:HB3	2:P:24:MET:HE3	1.87	0.55
1:Q:1:MET:H3	1:Q:22:ASP:CG	2.14	0.55
1:Q:561:ILE:HG22	1:Q:564:ASN:HB3	1.87	0.55
2:R:46:MET:CE	2:R:66:THR:H	2.17	0.55
2:H:157:LEU:HD12	2:H:157:LEU:N	2.21	0.55
1:I:629:MET:HE2	1:I:634:PHE:HA	1.88	0.55
1:K:426:MET:HE2	1:K:618:GLN:HG2	1.87	0.55
2:R:68:CYS:HB2	2:R:126:CYS:HB2	1.88	0.55
2:R:207:GLY:CA	1:U:728:VAL:HG12	2.29	0.55
1:W:28:MET:HE1	1:W:66:PHE:CB	2.30	0.55
1:C:451:LYS:HG3	1:C:461:PHE:CE2	2.42	0.55
1:C:533:VAL:HB	1:C:534:PRO:HD3	1.88	0.55
1:G:146:MET:HE2	1:G:544:THR:HA	1.88	0.55
2:J:21:MET:HE2	2:J:21:MET:HA	1.88	0.55
1:Q:56:LYS:HG2	1:Q:57:THR:O	2.06	0.55
1:C:356:GLY:H	4:C:903:MGD:H5'2	1.70	0.55
2:F:46:MET:CE	2:F:66:THR:H	2.17	0.55
2:F:201:ALA:HB2	2:F:269:LEU:HB2	1.89	0.55
1:G:505:THR:O	1:G:506:ALA:C	2.50	0.55
1:Q:15:PRO:HD2	8:Q:1003:HOH:O	2.06	0.55
1:U:610:LYS:HB3	1:U:614:ALA:HB3	1.89	0.55
2:V:143:PRO:HB3	7:V:303:SF4:S1	2.47	0.55
1:W:770:TRP:HB3	1:W:801:LEU:HD23	1.89	0.55
2:X:68:CYS:HB2	2:X:126:CYS:HB2	1.86	0.55
1:E:823:TYR:CE2	1:E:825:PRO:HG3	2.42	0.55
2:L:166:LYS:HG2	2:L:170:GLU:OE2	2.07	0.55
1:M:800:ILE:HD11	1:M:833:ALA:HB1	1.89	0.55
1:S:855:MET:HB2	1:S:857:ASN:OD1	2.07	0.55
1:C:75:ARG:HH21	1:C:543:CYS:HA	1.72	0.55
1:C:355:GLY:CA	4:C:903:MGD:O1B	2.55	0.55
2:D:53:ARG:HB2	2:D:60:ASP:OD1	2.07	0.55
1:G:476:GLN:OE1	1:G:708:ARG:NH2	2.40	0.55
2:F:114:MET:HG2	2:F:125:LYS:HG2	1.89	0.54
2:H:20:PHE:CZ	2:H:24:MET:HE2	2.41	0.54
1:M:691:ILE:HD11	1:M:711:MET:HE3	1.89	0.54
1:O:563:ASP:O	1:O:566:GLN:HG2	2.07	0.54
1:O:855:MET:HB2	1:O:857:ASN:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:146:MET:HE3	1:W:544:THR:CB	2.37	0.54
1:M:394:PRO:HG3	8:M:1322:HOH:O	2.07	0.54
1:O:708:ARG:HD2	8:O:1043:HOH:O	2.07	0.54
2:B:104:GLU:CD	2:B:104:GLU:H	2.12	0.54
1:C:253:ASN:O	1:C:257:ARG:HG3	2.07	0.54
1:M:476:GLN:OE1	1:M:708:ARG:NH2	2.40	0.54
2:P:59:ASN:H	2:P:59:ASN:HD22	1.54	0.54
2:R:46:MET:HE2	2:R:48:ILE:HG13	1.88	0.54
2:J:114:MET:HA	2:J:125:LYS:HB3	1.88	0.54
1:K:1:MET:H3	1:K:22:ASP:CG	2.15	0.54
1:K:426:MET:HE3	1:K:622:ALA:HB2	1.89	0.54
1:K:426:MET:HA	1:K:426:MET:CE	2.33	0.54
2:L:21:MET:HE1	2:L:24:MET:CE	2.37	0.54
1:M:81:LYS:HB2	1:M:112:ILE:HD13	1.90	0.54
1:M:356:GLY:N	4:M:903:MGD:PB	2.80	0.54
1:S:563:ASP:O	1:S:566:GLN:HG2	2.07	0.54
1:G:141:PRO:CA	1:G:496:TYR:HB3	2.35	0.54
1:G:211:MET:HE1	2:H:231:PHE:CE1	2.43	0.54
1:I:175:SER:HB2	1:I:176:TRP:CE3	2.43	0.54
2:J:59:ASN:ND2	2:J:59:ASN:H	2.04	0.54
1:O:253:ASN:O	1:O:257:ARG:HG3	2.08	0.54
1:E:211:MET:HE1	2:F:231:PHE:CE1	2.43	0.54
1:G:800:ILE:HD12	1:G:800:ILE:N	2.23	0.54
2:H:21:MET:HA	2:H:21:MET:CE	2.38	0.54
1:I:800:ILE:HD12	1:I:800:ILE:N	2.23	0.54
1:Q:855:MET:HB2	1:Q:857:ASN:OD1	2.07	0.54
1:U:249:ASP:OD1	4:U:903:MGD:H1'	2.07	0.54
2:V:125:LYS:HD2	2:V:126:CYS:O	2.07	0.54
1:A:114:TRP:CZ2	1:A:541:PRO:HD2	2.43	0.54
2:B:5:TYR:HB2	2:B:157:LEU:CD1	2.37	0.54
1:G:730:TYR:CE1	1:G:794:ASN:HA	2.43	0.54
1:M:505:THR:O	1:M:506:ALA:C	2.50	0.54
2:P:59:ASN:H	2:P:59:ASN:ND2	2.05	0.54
1:Q:211:MET:HE1	2:R:231:PHE:CE1	2.43	0.54
2:R:157:LEU:HD12	2:R:157:LEU:N	2.23	0.54
1:A:505:THR:O	1:A:506:ALA:C	2.51	0.54
1:C:476:GLN:OE1	1:C:708:ARG:NH2	2.41	0.54
1:G:195:ASN:HD21	1:G:354:TRP:CD1	2.26	0.54
1:I:823:TYR:CE2	1:I:825:PRO:HG3	2.43	0.54
1:O:195:ASN:HD21	1:O:354:TRP:CD1	2.25	0.54
1:Q:355:GLY:CA	4:Q:903:MGD:O2B	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:786:ASN:HD22	1:Q:805:VAL:H	1.55	0.54
1:S:75:ARG:NH2	1:S:543:CYS:HA	2.23	0.54
1:S:505:THR:O	1:S:506:ALA:C	2.50	0.54
2:V:87:ARG:HG3	2:V:91:ILE:O	2.08	0.54
2:X:18:ASN:HB2	7:X:302:SF4:S1	2.48	0.54
1:C:871:LYS:HG2	8:C:1233:HOH:O	2.07	0.54
2:H:68:CYS:HB2	2:H:126:CYS:HB2	1.85	0.54
1:M:356:GLY:H	4:M:903:MGD:PB	2.31	0.54
2:R:21:MET:HE2	2:R:21:MET:CA	2.38	0.54
1:U:28:MET:HE1	1:U:66:PHE:CB	2.34	0.54
1:U:753:TYR:HB3	2:V:24:MET:CE	2.38	0.54
1:C:426:MET:HE1	1:C:618:GLN:O	2.08	0.54
1:E:673:ASN:HD22	1:E:673:ASN:H	1.56	0.54
2:R:5:TYR:O	2:R:157:LEU:HD12	2.07	0.54
1:A:387:TRP:CE2	1:A:389:THR:HA	2.43	0.53
2:D:164:MET:O	2:D:168:VAL:HG23	2.08	0.53
2:L:46:MET:HE1	2:L:65:PRO:C	2.33	0.53
1:M:28:MET:HE1	1:M:66:PHE:CB	2.38	0.53
2:P:46:MET:HE1	2:P:65:PRO:CA	2.39	0.53
2:P:216:VAL:HG13	2:P:223:GLU:HG3	1.89	0.53
1:E:737:PRO:CG	4:E:903:MGD:H2'	2.38	0.53
2:J:164:MET:O	2:J:168:VAL:HG23	2.09	0.53
2:N:5:TYR:HB2	2:N:157:LEU:HD11	1.89	0.53
1:Q:649:LYS:HE3	1:Q:651:THR:CG2	2.38	0.53
1:A:66:PHE:CD1	1:A:69:MET:HE3	2.43	0.53
1:A:476:GLN:OE1	1:A:708:ARG:NH2	2.41	0.53
1:E:478:HIS:HD2	8:E:1205:HOH:O	1.92	0.53
1:O:146:MET:HG2	4:O:902:MGD:N7	2.24	0.53
1:U:211:MET:HE1	2:V:231:PHE:CE1	2.43	0.53
2:B:142:MET:HE1	8:B:429:HOH:O	2.08	0.53
2:B:142:MET:HE2	2:B:146:ALA:HB1	1.89	0.53
1:C:81:LYS:HB2	1:C:112:ILE:HD13	1.91	0.53
1:C:85:PHE:CE2	1:C:87:PRO:HG3	2.43	0.53
1:G:66:PHE:HA	1:G:69:MET:CE	2.34	0.53
1:G:571:ARG:HB2	1:G:642:VAL:HB	1.91	0.53
2:H:211:GLU:HB2	2:H:231:PHE:HA	1.89	0.53
1:O:426:MET:HA	1:O:426:MET:CE	2.33	0.53
1:O:505:THR:O	1:O:506:ALA:C	2.52	0.53
1:Q:425:ARG:HD3	1:Q:622:ALA:O	2.08	0.53
1:S:35:ASP:OD1	1:S:55:ARG:HD3	2.08	0.53
1:W:75:ARG:NH2	1:W:543:CYS:HA	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:ILE:HD12	1:A:800:ILE:N	2.23	0.53
1:C:510:TYR:O	1:C:513:MET:HG2	2.08	0.53
1:K:644:ASP:C	1:K:646:PRO:HD3	2.33	0.53
2:L:46:MET:CE	2:L:66:THR:H	2.12	0.53
2:L:201:ALA:HB2	2:L:269:LEU:HB2	1.90	0.53
1:M:66:PHE:CD1	1:M:69:MET:HE3	2.44	0.53
1:U:140:THR:HB	1:U:169:ALA:HB3	1.89	0.53
1:W:218:ASP:OD2	1:W:253:ASN:HB2	2.08	0.53
2:F:203:ILE:HD12	2:F:203:ILE:N	2.24	0.53
1:O:825:PRO:HD2	8:O:1332:HOH:O	2.08	0.53
1:U:44:ILE:HD11	1:U:394:PRO:HG2	1.89	0.53
1:A:211:MET:HE2	1:A:246:VAL:HG23	1.91	0.53
2:B:203:ILE:HD12	2:B:203:ILE:N	2.24	0.53
1:C:15:PRO:HD3	1:C:554:PHE:CD1	2.43	0.53
2:F:75:PRO:HD2	7:F:304:SF4:S4	2.49	0.53
2:H:70:HIS:CD2	2:H:92:VAL:H	2.16	0.53
1:O:81:LYS:HB2	1:O:112:ILE:HD13	1.91	0.53
2:T:21:MET:HE2	2:T:21:MET:N	2.23	0.53
1:A:629:MET:HE2	1:A:634:PHE:CA	2.37	0.53
1:G:353:GLY:O	1:G:354:TRP:HB2	2.07	0.53
1:G:478:HIS:HD2	8:G:1203:HOH:O	1.91	0.53
2:H:46:MET:HE1	2:H:65:PRO:C	2.33	0.53
2:H:69:MET:HB3	2:H:184:PRO:HB3	1.90	0.53
2:J:143:PRO:HB3	7:J:303:SF4:S1	2.49	0.53
1:K:510:TYR:O	1:K:513:MET:HG2	2.09	0.53
1:U:252:MET:HE3	1:U:263:TRP:CE3	2.44	0.53
2:V:58:ARG:HD2	2:V:268:ASP:OD1	2.07	0.53
1:A:673:ASN:CG	8:A:1584:HOH:O	2.52	0.53
1:C:140:THR:HB	1:C:169:ALA:HB3	1.91	0.53
1:I:426:MET:HA	1:I:426:MET:CE	2.31	0.53
1:K:195:ASN:HD21	1:K:354:TRP:CD1	2.27	0.53
1:M:142:SER:CB	4:M:902:MGD:O1A	2.57	0.53
1:O:451:LYS:HG3	1:O:461:PHE:CE2	2.43	0.53
1:O:645:ASN:ND2	1:O:648:ARG:HB3	2.23	0.53
1:Q:460:LYS:HE2	8:Q:1022:HOH:O	2.09	0.53
2:R:46:MET:HE1	2:R:65:PRO:CA	2.39	0.53
2:R:203:ILE:N	2:R:203:ILE:HD12	2.24	0.53
1:U:291:GLU:H	1:U:291:GLU:CD	2.17	0.53
1:W:144:HIS:HB2	4:W:902:MGD:O1B	2.09	0.53
1:W:478:HIS:HD2	8:W:1206:HOH:O	1.92	0.53
2:X:87:ARG:HG3	2:X:91:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:203:ILE:HD12	2:X:203:ILE:N	2.23	0.53
1:A:426:MET:HE3	1:A:622:ALA:HB2	1.90	0.53
1:A:737:PRO:CG	4:A:903:MGD:H2'	2.39	0.53
1:C:587:MET:HE3	1:C:591:GLU:HB3	1.91	0.53
1:E:671:ARG:HB2	8:E:1099:HOH:O	2.09	0.53
1:I:510:TYR:O	1:I:513:MET:HG2	2.09	0.53
1:M:460:LYS:HE2	8:M:1023:HOH:O	2.09	0.53
1:M:730:TYR:CE1	1:M:794:ASN:HA	2.44	0.53
2:P:143:PRO:HB3	7:P:303:SF4:S1	2.49	0.53
1:S:163:MET:HE1	1:S:606:PHE:HA	1.90	0.53
1:S:610:LYS:HZ3	1:S:618:GLN:HE22	1.56	0.53
1:W:75:ARG:HH21	1:W:543:CYS:HA	1.74	0.53
1:W:426:MET:HA	1:W:426:MET:CE	2.34	0.53
1:C:138:LEU:HB2	1:C:490:ILE:HD12	1.91	0.52
1:M:557:CYS:N	1:M:564:ASN:HD21	1.92	0.52
1:S:528:TRP:CD2	1:S:750:LYS:HD3	2.44	0.52
2:T:59:ASN:H	2:T:59:ASN:ND2	2.07	0.52
1:U:610:LYS:HZ3	1:U:618:GLN:HE22	1.57	0.52
1:A:610:LYS:HZ3	1:A:618:GLN:HE22	1.57	0.52
2:H:46:MET:CE	2:H:66:THR:H	2.15	0.52
1:C:153:ARG:O	1:C:157:TYR:HB3	2.08	0.52
1:E:197:GLU:HG3	1:E:199:TYR:HD1	1.73	0.52
1:K:617:GLU:HG3	1:K:631:TRP:CG	2.44	0.52
1:K:708:ARG:HD2	8:K:1043:HOH:O	2.09	0.52
2:L:106:LEU:HD23	2:L:114:MET:HE2	1.91	0.52
2:N:59:ASN:ND2	2:N:59:ASN:H	2.06	0.52
2:P:201:ALA:HB2	2:P:269:LEU:HB2	1.90	0.52
2:R:46:MET:HE1	2:R:65:PRO:HA	1.91	0.52
1:S:823:TYR:CE2	1:S:825:PRO:HG3	2.44	0.52
1:C:387:TRP:CE2	1:C:389:THR:HA	2.44	0.52
1:C:630:THR:OG1	1:C:633:GLU:HG3	2.10	0.52
1:E:495:LYS:HD2	1:E:514:TYR:OH	2.10	0.52
2:F:1:MET:SD	2:F:88:GLU:HB3	2.49	0.52
1:I:855:MET:HB2	1:I:857:ASN:OD1	2.08	0.52
1:Q:175:SER:HB2	1:Q:176:TRP:CE3	2.45	0.52
1:S:786:ASN:ND2	1:S:805:VAL:H	2.08	0.52
2:T:69:MET:HB3	2:T:184:PRO:HB3	1.89	0.52
1:W:85:PHE:CE2	1:W:87:PRO:HG3	2.45	0.52
2:B:7:VAL:HB	2:B:155:GLU:HB3	1.92	0.52
1:C:378:GLY:O	1:C:381:LYS:HG2	2.09	0.52
1:G:182:GLY:HA3	1:G:364:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:753:TYR:HB3	2:H:24:MET:HE3	1.92	0.52
1:I:144:HIS:HB2	4:I:902:MGD:O1B	2.09	0.52
2:J:21:MET:CE	2:J:21:MET:HA	2.40	0.52
2:L:18:ASN:HB2	7:L:302:SF4:S1	2.50	0.52
1:M:400:TYR:CE1	1:M:421:LYS:HD2	2.44	0.52
1:O:610:LYS:HZ3	1:O:618:GLN:HE22	1.54	0.52
1:Q:825:PRO:HD2	8:Q:1334:HOH:O	2.10	0.52
1:A:753:TYR:HB3	2:B:24:MET:HE3	1.91	0.52
1:C:144:HIS:HB2	4:C:902:MGD:O1B	2.09	0.52
2:D:59:ASN:H	2:D:59:ASN:ND2	2.07	0.52
1:E:1:MET:H3	1:E:22:ASP:CG	2.17	0.52
1:E:55:ARG:HD2	8:E:1644:HOH:O	2.10	0.52
2:H:114:MET:HE3	2:H:123:ALA:CB	2.39	0.52
1:I:1:MET:H3	1:I:22:ASP:CG	2.17	0.52
1:I:143:SER:N	4:I:902:MGD:O1A	2.42	0.52
1:O:783:GLY:O	1:O:866:LYS:HD2	2.10	0.52
2:P:21:MET:HE1	2:P:24:MET:CE	2.40	0.52
2:P:46:MET:HE1	2:P:65:PRO:HA	1.92	0.52
2:V:201:ALA:HB2	2:V:269:LEU:HB2	1.90	0.52
1:E:66:PHE:CD1	1:E:69:MET:HE3	2.45	0.52
1:G:610:LYS:HZ3	1:G:618:GLN:HE22	1.54	0.52
1:M:146:MET:HE3	1:M:544:THR:HB	1.92	0.52
2:N:7:VAL:HB	2:N:155:GLU:HB3	1.92	0.52
1:O:134:PRO:HB2	1:O:439:LEU:HD11	1.91	0.52
1:Q:195:ASN:HD21	1:Q:354:TRP:CD1	2.28	0.52
2:V:46:MET:HE1	2:V:65:PRO:C	2.35	0.52
2:X:129:CYS:HB3	2:X:131:HIS:CE1	2.44	0.52
1:E:505:THR:O	1:E:506:ALA:C	2.53	0.52
1:E:610:LYS:HZ3	1:E:618:GLN:HE22	1.53	0.52
2:F:106:LEU:HD11	2:F:116:TRP:HB2	1.91	0.52
2:L:40:GLN:NE2	2:L:117:ASN:HA	2.24	0.52
2:L:58:ARG:HD2	2:L:268:ASP:OD1	2.10	0.52
1:Q:75:ARG:NH2	1:Q:543:CYS:HA	2.25	0.52
2:V:5:TYR:HB2	2:V:157:LEU:CD1	2.40	0.52
2:V:205:VAL:HG13	2:V:254:LYS:HZ2	1.75	0.52
1:A:291:GLU:CD	1:A:291:GLU:H	2.18	0.52
2:B:205:VAL:HG13	2:B:254:LYS:HZ2	1.74	0.52
1:C:495:LYS:HD2	1:C:514:TYR:OH	2.10	0.52
1:M:825:PRO:HD2	8:M:1336:HOH:O	2.09	0.52
1:O:356:GLY:H	4:O:903:MGD:C5'	2.22	0.52
1:U:146:MET:HG2	4:U:902:MGD:N7	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:143:SER:N	4:W:902:MGD:O1A	2.42	0.52
2:X:166:LYS:O	2:X:170:GLU:HG3	2.09	0.52
1:C:753:TYR:HB3	2:D:24:MET:HE3	1.91	0.52
2:D:201:ALA:HB2	2:D:269:LEU:HB2	1.91	0.52
1:E:426:MET:HE2	1:E:618:GLN:HG2	1.88	0.52
1:I:630:THR:OG1	1:I:633:GLU:HG3	2.10	0.52
1:K:610:LYS:HZ2	1:K:618:GLN:HE22	1.58	0.52
1:M:114:TRP:CZ2	1:M:541:PRO:HD2	2.45	0.52
2:N:72:GLU:HG2	2:N:185:ARG:NH2	2.25	0.52
2:P:2:GLU:CG	2:P:158:LYS:HG2	2.33	0.52
1:U:66:PHE:CD1	1:U:69:MET:HE3	2.45	0.52
2:X:68:CYS:HB3	2:X:126:CYS:HB3	1.91	0.52
1:A:195:ASN:HD21	1:A:354:TRP:CD1	2.27	0.51
2:D:103:LYS:HG2	2:D:116:TRP:CD2	2.45	0.51
1:E:387:TRP:CE2	1:E:389:THR:HA	2.46	0.51
1:G:644:ASP:C	1:G:646:PRO:HD3	2.34	0.51
1:S:134:PRO:HB2	1:S:439:LEU:HD11	1.91	0.51
1:S:717:ALA:HB3	1:S:720:SER:HB3	1.92	0.51
1:U:257:ARG:HD3	2:V:61:ILE:HG21	1.92	0.51
1:A:32:ASP:HB2	8:A:1658:HOH:O	2.10	0.51
2:B:76:CYS:O	2:B:80:GLY:N	2.43	0.51
1:C:426:MET:HE2	1:C:618:GLN:HG2	1.90	0.51
1:G:823:TYR:CE2	1:G:825:PRO:HG3	2.45	0.51
1:K:696:LYS:O	1:K:700:GLU:HG3	2.10	0.51
1:O:630:THR:OG1	1:O:633:GLU:HG3	2.11	0.51
1:S:253:ASN:O	1:S:257:ARG:HG3	2.09	0.51
1:S:617:GLU:HG3	1:S:631:TRP:CG	2.46	0.51
1:S:708:ARG:HD2	8:S:1046:HOH:O	2.11	0.51
2:T:125:LYS:HD2	2:T:126:CYS:O	2.10	0.51
2:T:167:LYS:HZ3	2:T:171:GLU:CD	2.18	0.51
2:V:71:CYS:HB2	2:V:182:THR:O	2.09	0.51
1:W:104:ASP:OD2	1:W:107:SER:HB3	2.10	0.51
1:W:644:ASP:C	1:W:646:PRO:HD3	2.35	0.51
1:C:563:ASP:O	1:C:566:GLN:HG2	2.11	0.51
2:D:166:LYS:HE2	2:D:170:GLU:OE2	2.10	0.51
1:G:56:LYS:HG2	1:G:57:THR:O	2.10	0.51
1:K:353:GLY:O	1:K:354:TRP:HB2	2.11	0.51
2:N:46:MET:CE	2:N:66:THR:H	2.19	0.51
1:S:146:MET:HG2	4:S:902:MGD:N7	2.25	0.51
2:T:203:ILE:N	2:T:203:ILE:HD12	2.24	0.51
1:E:195:ASN:HD21	1:E:354:TRP:CD1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:855:MET:HB2	1:G:857:ASN:OD1	2.10	0.51
1:K:146:MET:HG2	4:K:902:MGD:N7	2.25	0.51
1:K:211:MET:HE1	2:L:231:PHE:CE1	2.45	0.51
1:K:533:VAL:HB	1:K:534:PRO:HD3	1.93	0.51
2:L:27:HIS:HB2	2:L:39:MET:HE3	1.92	0.51
1:Q:100:LEU:CD2	1:Q:534:PRO:HB2	2.39	0.51
2:T:23:CYS:O	2:T:27:HIS:N	2.40	0.51
1:W:418:ALA:HB1	1:W:423:ALA:HB2	1.92	0.51
1:A:510:TYR:O	1:A:513:MET:HG2	2.10	0.51
1:A:644:ASP:C	1:A:646:PRO:HD3	2.36	0.51
1:C:155:SER:OG	1:C:409:ILE:HG12	2.09	0.51
1:I:81:LYS:HB2	1:I:112:ILE:HD13	1.93	0.51
2:J:211:GLU:HB2	2:J:231:PHE:HA	1.91	0.51
2:L:2:GLU:HG2	2:L:158:LYS:HG2	1.92	0.51
1:Q:66:PHE:CD1	1:Q:69:MET:HE3	2.46	0.51
1:Q:111:ARG:NH2	1:Q:585:GLU:OE2	2.37	0.51
1:S:144:HIS:HB2	4:S:902:MGD:O1B	2.10	0.51
1:U:187:TRP:CH2	1:U:196:PRO:HB3	2.46	0.51
1:U:353:GLY:O	1:U:354:TRP:HB2	2.11	0.51
1:W:426:MET:HE3	1:W:622:ALA:HB2	1.92	0.51
2:X:40:GLN:NE2	8:X:942:HOH:O	2.43	0.51
1:A:253:ASN:O	1:A:257:ARG:HG3	2.11	0.51
1:A:494:TRP:HE1	1:A:525:GLN:HE21	1.58	0.51
1:I:111:ARG:NH2	1:I:585:GLU:OE2	2.42	0.51
1:K:140:THR:HB	1:K:169:ALA:HB3	1.92	0.51
1:M:175:SER:OG	6:M:905:BTT:C5	2.59	0.51
2:P:71:CYS:HB2	2:P:182:THR:O	2.10	0.51
1:Q:649:LYS:HE2	8:Q:1459:HOH:O	2.10	0.51
1:Q:730:TYR:CE1	1:Q:794:ASN:HA	2.45	0.51
1:S:387:TRP:CE2	1:S:389:THR:HA	2.45	0.51
2:X:21:MET:HE2	2:X:21:MET:N	2.26	0.51
1:C:195:ASN:HD21	1:C:354:TRP:CD1	2.29	0.51
1:C:786:ASN:ND2	1:C:804:GLN:HA	2.26	0.51
2:F:71:CYS:HB2	2:F:182:THR:O	2.10	0.51
2:H:254:LYS:HD2	2:H:274:LEU:OXT	2.10	0.51
1:K:825:PRO:HD2	8:K:1330:HOH:O	2.10	0.51
2:L:162:GLU:CD	2:L:162:GLU:N	2.69	0.51
1:M:100:LEU:CD1	1:M:105:PRO:HG3	2.40	0.51
1:M:211:MET:HE1	2:N:231:PHE:CE1	2.44	0.51
2:N:68:CYS:HB2	2:N:126:CYS:HB2	1.90	0.51
1:S:644:ASP:C	1:S:646:PRO:HD3	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:797:GLY:HA2	1:S:875:TYR:CE2	2.45	0.51
2:T:143:PRO:HB3	7:T:303:SF4:S1	2.51	0.51
1:W:587:MET:HE2	1:W:592:ILE:HA	1.91	0.51
1:A:142:SER:CB	4:A:902:MGD:O1A	2.59	0.51
1:C:628:TYR:CE2	1:C:643:PRO:HG2	2.45	0.51
1:I:15:PRO:HD3	1:I:554:PHE:CD1	2.46	0.51
2:J:105:LEU:C	2:J:114:MET:HE2	2.36	0.51
2:P:46:MET:HE1	2:P:65:PRO:C	2.36	0.51
2:R:71:CYS:HB2	2:R:182:THR:O	2.11	0.51
1:S:426:MET:HE2	1:S:618:GLN:HG2	1.92	0.51
2:V:18:ASN:HB2	7:V:302:SF4:S1	2.51	0.51
1:E:644:ASP:C	1:E:646:PRO:HD3	2.36	0.51
1:I:47:ARG:HD2	1:I:241:LEU:HD22	1.91	0.51
1:K:451:LYS:HG3	1:K:461:PHE:CE2	2.46	0.51
1:K:673:ASN:HD22	1:K:673:ASN:H	1.59	0.51
1:O:510:TYR:O	1:O:513:MET:HG2	2.09	0.51
1:Q:138:LEU:HB2	1:Q:490:ILE:HD12	1.93	0.51
1:Q:505:THR:O	1:Q:506:ALA:C	2.53	0.51
2:X:4:TYR:CE2	2:X:158:LYS:HD2	2.45	0.51
1:A:644:ASP:O	1:A:646:PRO:HD3	2.11	0.51
1:I:44:ILE:HD11	1:I:394:PRO:HG2	1.92	0.51
1:I:66:PHE:CD1	1:I:69:MET:HE3	2.45	0.51
1:O:176:TRP:O	1:O:177:GLU:C	2.54	0.51
1:O:476:GLN:OE1	1:O:708:ARG:NH2	2.44	0.51
1:Q:510:TYR:O	1:Q:513:MET:HG2	2.11	0.51
1:W:56:LYS:HG2	1:W:57:THR:O	2.11	0.51
1:C:218:ASP:OD2	1:C:253:ASN:HB2	2.11	0.50
1:C:696:LYS:O	1:C:700:GLU:HG3	2.11	0.50
1:C:708:ARG:HD2	8:C:1044:HOH:O	2.11	0.50
1:C:753:TYR:HB3	2:D:24:MET:CE	2.42	0.50
2:D:104:GLU:CD	2:D:104:GLU:H	2.18	0.50
1:G:81:LYS:HB2	1:G:112:ILE:HD13	1.93	0.50
1:O:85:PHE:CE2	1:O:87:PRO:HG3	2.46	0.50
2:R:46:MET:HE1	2:R:65:PRO:C	2.36	0.50
1:A:855:MET:HB2	1:A:857:ASN:OD1	2.10	0.50
2:B:46:MET:HE1	2:B:65:PRO:CA	2.41	0.50
1:E:175:SER:OG	6:E:905:BTT:C5	2.59	0.50
1:G:146:MET:HE3	1:G:545:ASN:H	1.75	0.50
1:G:258:LEU:HG	1:G:259:VAL:HG13	1.93	0.50
1:M:75:ARG:HH21	1:M:543:CYS:HA	1.77	0.50
1:M:451:LYS:HG3	1:M:461:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:100:LEU:CD1	1:O:105:PRO:HG3	2.42	0.50
2:B:5:TYR:HB2	2:B:157:LEU:HD13	1.94	0.50
2:D:5:TYR:HB2	2:D:157:LEU:CD1	2.42	0.50
2:D:203:ILE:N	2:D:203:ILE:HD12	2.26	0.50
2:F:166:LYS:HG2	2:F:170:GLU:OE2	2.12	0.50
1:G:142:SER:CB	4:G:902:MGD:O1A	2.59	0.50
1:G:166:PHE:HD2	8:G:1364:HOH:O	1.94	0.50
2:J:203:ILE:HD12	2:J:203:ILE:N	2.27	0.50
1:K:100:LEU:HD12	1:K:105:PRO:HG3	1.93	0.50
1:K:716:PRO:HB3	1:K:723:HIS:CD2	2.46	0.50
1:Q:175:SER:OG	6:Q:905:BTT:C5	2.60	0.50
1:Q:296:ASN:HB3	1:Q:657:PHE:CZ	2.47	0.50
1:Q:451:LYS:HG3	1:Q:461:PHE:CE2	2.46	0.50
2:R:105:LEU:HB3	2:R:114:MET:HE1	1.93	0.50
1:S:195:ASN:HD21	1:S:354:TRP:CD1	2.29	0.50
1:U:56:LYS:HG2	1:U:57:THR:O	2.11	0.50
2:V:96:PRO:O	2:V:100:LYS:HG3	2.11	0.50
1:G:510:TYR:O	1:G:513:MET:HG2	2.10	0.50
1:I:134:PRO:HB2	1:I:439:LEU:HD11	1.92	0.50
1:I:387:TRP:CE2	1:I:389:THR:HA	2.46	0.50
1:K:387:TRP:CE2	1:K:389:THR:HA	2.46	0.50
1:O:387:TRP:CE2	1:O:389:THR:HA	2.46	0.50
1:Q:770:TRP:HB3	1:Q:801:LEU:HD23	1.93	0.50
1:S:142:SER:CB	4:S:902:MGD:O1A	2.59	0.50
1:W:353:GLY:O	1:W:354:TRP:HB2	2.11	0.50
1:W:400:TYR:CE1	1:W:421:LYS:HD2	2.47	0.50
1:E:786:ASN:ND2	1:E:805:VAL:H	2.04	0.50
1:G:630:THR:OG1	1:G:633:GLU:HG3	2.11	0.50
1:K:505:THR:O	1:K:506:ALA:C	2.55	0.50
1:M:166:PHE:N	1:M:439:LEU:HD12	2.27	0.50
1:O:75:ARG:NH2	1:O:543:CYS:HA	2.26	0.50
2:R:59:ASN:H	2:R:59:ASN:HD22	1.59	0.50
2:V:5:TYR:HB2	2:V:157:LEU:HD11	1.93	0.50
1:W:797:GLY:HA2	1:W:875:TYR:CE2	2.46	0.50
2:B:5:TYR:O	2:B:157:LEU:HD12	2.11	0.50
2:D:23:CYS:CB	2:D:39:MET:HE1	2.40	0.50
1:E:211:MET:HE3	8:E:1454:HOH:O	2.10	0.50
1:E:476:GLN:OE1	1:E:708:ARG:NH2	2.45	0.50
2:H:166:LYS:HG2	2:H:170:GLU:OE2	2.11	0.50
1:I:610:LYS:HB3	1:I:614:ALA:HB3	1.92	0.50
1:M:296:ASN:HB3	1:M:657:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:610:LYS:HB3	1:O:614:ALA:HB3	1.93	0.50
2:P:106:LEU:HD23	2:P:114:MET:CE	2.42	0.50
8:Q:1681:HOH:O	1:S:871:LYS:HE2	2.12	0.50
1:W:505:THR:O	1:W:506:ALA:C	2.54	0.50
1:C:35:ASP:OD1	1:C:55:ARG:HD3	2.11	0.50
2:F:68:CYS:HB2	2:F:126:CYS:HB2	1.91	0.50
2:F:142:MET:HE2	2:F:146:ALA:CB	2.36	0.50
1:G:561:ILE:HG22	1:G:564:ASN:HB3	1.93	0.50
1:K:56:LYS:HG2	1:K:57:THR:O	2.11	0.50
2:N:143:PRO:HB3	7:N:303:SF4:S1	2.52	0.50
1:S:729:LYS:HD2	8:S:1134:HOH:O	2.11	0.50
1:U:144:HIS:HB2	4:U:902:MGD:O1B	2.12	0.50
1:A:670:PRO:HG2	1:A:675:GLN:CD	2.37	0.50
1:E:144:HIS:HB2	4:E:902:MGD:O1B	2.12	0.50
1:E:187:TRP:CH2	1:E:196:PRO:HB3	2.46	0.50
2:H:166:LYS:O	2:H:170:GLU:HG3	2.11	0.50
1:M:510:TYR:O	1:M:513:MET:HG2	2.12	0.50
1:M:738:HIS:HE2	4:M:902:MGD:H15	1.60	0.50
1:O:501:LEU:HD13	1:O:823:TYR:CD2	2.47	0.50
1:O:737:PRO:HG3	4:O:903:MGD:H2'	1.94	0.50
2:P:18:ASN:HB2	7:P:302:SF4:S1	2.52	0.50
1:A:100:LEU:CD1	1:A:105:PRO:HG3	2.42	0.50
1:E:81:LYS:HB2	1:E:112:ILE:HD13	1.92	0.50
2:F:20:PHE:CZ	2:F:24:MET:HE2	2.47	0.50
2:F:68:CYS:HB3	2:F:70:HIS:ND1	2.27	0.50
2:F:216:VAL:HG13	2:F:223:GLU:HG3	1.93	0.50
1:I:356:GLY:H	4:I:903:MGD:H5'2	1.75	0.50
2:J:210:PHE:HD2	2:J:213:ALA:HB2	1.77	0.50
2:N:20:PHE:CZ	2:N:24:MET:HE2	2.47	0.50
2:N:114:MET:CE	2:N:123:ALA:HB1	2.42	0.50
1:O:426:MET:HE2	1:O:618:GLN:HG2	1.91	0.50
1:W:66:PHE:CD1	1:W:69:MET:HE3	2.47	0.50
1:A:356:GLY:H	4:A:903:MGD:C5'	2.23	0.49
1:A:823:TYR:CE2	1:A:825:PRO:HG3	2.46	0.49
1:C:800:ILE:N	1:C:800:ILE:HD12	2.27	0.49
1:I:505:THR:O	1:I:506:ALA:C	2.55	0.49
1:I:561:ILE:HG22	1:I:564:ASN:HB3	1.93	0.49
1:K:735:LEU:HD23	1:K:735:LEU:H	1.77	0.49
1:O:66:PHE:CD1	1:O:69:MET:HE3	2.47	0.49
1:U:557:CYS:N	1:U:564:ASN:HD21	1.93	0.49
1:A:708:ARG:HD2	8:A:1044:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:ASP:OD2	1:I:253:ASN:HB2	2.12	0.49
1:M:770:TRP:HB3	1:M:801:LEU:HD23	1.94	0.49
1:Q:144:HIS:HB2	4:Q:902:MGD:O1B	2.13	0.49
1:S:263:TRP:CZ2	1:S:265:SER:HB2	2.47	0.49
2:T:46:MET:HE2	2:T:48:ILE:HG13	1.94	0.49
1:U:81:LYS:HB2	1:U:112:ILE:HD13	1.94	0.49
1:U:176:TRP:O	1:U:177:GLU:C	2.53	0.49
2:V:21:MET:N	2:V:21:MET:HE2	2.27	0.49
1:A:696:LYS:O	1:A:700:GLU:HG3	2.11	0.49
1:E:140:THR:HB	1:E:169:ALA:HB3	1.93	0.49
1:G:377:GLN:O	1:G:381:LYS:HE2	2.12	0.49
1:K:141:PRO:CA	1:K:496:TYR:HB3	2.41	0.49
1:K:269:GLY:HA2	1:K:362:HIS:CE1	2.47	0.49
1:M:355:GLY:CA	4:M:903:MGD:O1B	2.56	0.49
1:O:21:LYS:HB3	1:O:26:ILE:HD11	1.93	0.49
1:Q:426:MET:HE2	1:Q:618:GLN:HG2	1.94	0.49
1:A:561:ILE:CG2	1:A:564:ASN:HB3	2.41	0.49
1:E:74:LEU:HD12	1:E:750:LYS:HA	1.94	0.49
1:O:142:SER:HB3	4:O:902:MGD:H5'2	1.95	0.49
1:W:753:TYR:HB3	2:X:24:MET:CE	2.41	0.49
1:A:75:ARG:NH2	1:A:543:CYS:HA	2.27	0.49
1:A:870:ASP:HB3	1:A:872:TYR:CE1	2.47	0.49
2:H:20:PHE:CE2	2:H:24:MET:HE2	2.47	0.49
1:I:355:GLY:C	4:I:903:MGD:O1B	2.53	0.49
2:J:46:MET:HE3	2:J:46:MET:C	2.38	0.49
1:K:28:MET:HE1	1:K:66:PHE:CB	2.30	0.49
1:M:617:GLU:HG3	1:M:631:TRP:CG	2.47	0.49
2:P:46:MET:CE	2:P:66:THR:H	2.18	0.49
1:S:176:TRP:O	1:S:177:GLU:C	2.56	0.49
1:S:738:HIS:HE2	4:S:902:MGD:H15	1.58	0.49
1:E:557:CYS:N	1:E:564:ASN:HD21	1.92	0.49
2:F:114:MET:CE	2:F:123:ALA:HB1	2.42	0.49
1:G:495:LYS:HD2	1:G:514:TYR:OH	2.12	0.49
1:M:767:TYR:HB3	1:M:769:TYR:CE1	2.47	0.49
2:N:46:MET:HE2	2:N:48:ILE:HG13	1.94	0.49
1:Q:214:PHE:HA	1:Q:347:ALA:HB3	1.95	0.49
1:S:700:GLU:HG2	8:S:1561:HOH:O	2.12	0.49
2:T:70:HIS:CD2	2:T:92:VAL:H	2.18	0.49
2:F:21:MET:HE2	2:F:21:MET:CA	2.43	0.49
1:G:165:GLY:HA3	1:G:166:PHE:CB	2.40	0.49
1:G:175:SER:OG	6:G:905:BTT:C5	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:656:TRP:CD2	1:G:663:LYS:HA	2.48	0.49
2:H:46:MET:HE1	2:H:65:PRO:CA	2.43	0.49
1:I:175:SER:OG	6:I:905:BTT:C5	2.60	0.49
1:K:2:GLY:O	1:K:21:LYS:HE3	2.13	0.49
1:K:786:ASN:ND2	1:K:804:GLN:HA	2.28	0.49
1:M:69:MET:HE2	1:M:754:MET:HE3	1.93	0.49
1:M:142:SER:HB3	4:M:902:MGD:O1A	2.12	0.49
1:S:21:LYS:HB3	1:S:26:ILE:HD11	1.94	0.49
1:U:182:GLY:HA3	1:U:364:ILE:HG23	1.95	0.49
1:U:629:MET:HE2	1:U:634:PHE:HA	1.93	0.49
2:V:71:CYS:HA	2:V:184:PRO:HA	1.95	0.49
2:V:211:GLU:HB2	2:V:231:PHE:HA	1.95	0.49
1:W:387:TRP:CE2	1:W:389:THR:HA	2.48	0.49
2:H:109:CYS:HB3	2:H:112:GLY:H	1.78	0.49
1:I:644:ASP:O	1:I:646:PRO:HD3	2.13	0.49
1:M:328:PRO:HB2	1:M:331:GLU:HG3	1.95	0.49
1:M:708:ARG:HD2	8:M:1044:HOH:O	2.12	0.49
1:O:211:MET:HE2	1:O:246:VAL:HG23	1.94	0.49
1:O:469:ALA:HA	8:O:1516:HOH:O	2.12	0.49
1:S:100:LEU:HD12	1:S:105:PRO:HG3	1.94	0.49
1:U:75:ARG:NH2	1:U:543:CYS:HA	2.28	0.49
1:U:114:TRP:CZ2	1:U:541:PRO:HD2	2.48	0.49
1:A:111:ARG:NH2	1:A:585:GLU:OE2	2.45	0.49
2:B:59:ASN:H	2:B:59:ASN:HD22	1.58	0.49
2:D:13:CYS:HB3	2:D:63:TYR:HB2	1.95	0.49
1:G:414:GLU:OE2	1:G:441:THR:HA	2.12	0.49
1:I:96:ARG:HD2	1:I:514:TYR:O	2.13	0.49
1:K:35:ASP:OD1	1:K:55:ARG:HD3	2.11	0.49
2:L:5:TYR:HB2	2:L:157:LEU:HD11	1.94	0.49
1:M:195:ASN:HD21	1:M:354:TRP:CD1	2.31	0.49
1:Q:378:GLY:O	1:Q:381:LYS:HG2	2.12	0.49
1:S:301:GLU:H	1:S:301:GLU:CD	2.20	0.49
2:T:94:ILE:O	2:T:96:PRO:HD3	2.13	0.49
1:W:253:ASN:O	1:W:257:ARG:HG3	2.12	0.49
1:W:561:ILE:CG2	1:W:564:ASN:HB3	2.41	0.49
1:C:176:TRP:O	1:C:177:GLU:C	2.56	0.49
1:I:147:TRP:CD1	1:I:552:SER:HG	2.31	0.49
1:M:400:TYR:CZ	1:M:421:LYS:HD2	2.48	0.49
2:N:46:MET:HE1	2:N:65:PRO:C	2.38	0.49
1:O:786:ASN:HD21	1:O:804:GLN:HA	1.77	0.49
1:W:195:ASN:HD21	1:W:354:TRP:CD1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:23:CYS:O	2:X:27:HIS:N	2.41	0.49
2:B:106:LEU:HD11	2:B:116:TRP:HB2	1.95	0.48
1:G:541:PRO:HB2	1:G:586:SER:HA	1.95	0.48
1:I:153:ARG:O	1:I:157:TYR:HB3	2.13	0.48
1:I:402:PRO:HG2	1:I:422:PHE:CE1	2.48	0.48
2:N:210:PHE:HD2	2:N:213:ALA:HB2	1.78	0.48
1:O:558:SER:H	1:O:564:ASN:ND2	2.11	0.48
2:P:46:MET:HE2	2:P:48:ILE:HG12	1.95	0.48
1:Q:630:THR:OG1	1:Q:633:GLU:HG3	2.13	0.48
1:C:355:GLY:N	4:C:903:MGD:O2A	2.43	0.48
1:E:395:LEU:HD13	1:E:571:ARG:HG3	1.95	0.48
1:E:400:TYR:CZ	1:E:421:LYS:HD2	2.49	0.48
1:I:452:ILE:HB	1:I:453:PRO:HD3	1.95	0.48
2:L:142:MET:HE1	8:L:430:HOH:O	2.12	0.48
1:Q:257:ARG:HD3	2:R:61:ILE:HG21	1.95	0.48
1:Q:452:ILE:HB	1:Q:453:PRO:HD3	1.95	0.48
1:S:56:LYS:HG2	1:S:57:THR:O	2.13	0.48
1:S:476:GLN:OE1	1:S:708:ARG:NH2	2.46	0.48
1:S:644:ASP:O	1:S:646:PRO:HD3	2.13	0.48
1:U:104:ASP:OD2	1:U:107:SER:HB3	2.12	0.48
1:U:505:THR:O	1:U:506:ALA:C	2.56	0.48
1:U:558:SER:H	1:U:564:ASN:ND2	2.11	0.48
1:U:801:LEU:HD11	1:U:839:ILE:HD11	1.95	0.48
2:X:7:VAL:HG21	2:X:167:LYS:NZ	2.27	0.48
1:A:146:MET:HG2	4:A:902:MGD:N7	2.27	0.48
1:A:377:GLN:O	1:A:381:LYS:HE2	2.14	0.48
1:A:673:ASN:H	1:A:673:ASN:HD22	1.61	0.48
1:K:426:MET:HE1	1:K:618:GLN:O	2.13	0.48
1:K:476:GLN:OE1	1:K:708:ARG:NH2	2.47	0.48
1:O:610:LYS:HZ2	1:O:618:GLN:HE22	1.61	0.48
1:U:563:ASP:O	1:U:566:GLN:HG2	2.13	0.48
1:U:708:ARG:HD2	8:U:1047:HOH:O	2.12	0.48
1:A:452:ILE:HB	1:A:453:PRO:HD3	1.95	0.48
1:E:737:PRO:HG3	4:E:903:MGD:H2'	1.95	0.48
2:H:106:LEU:CD2	2:H:114:MET:HB3	2.44	0.48
1:O:479:GLN:N	8:O:1176:HOH:O	2.37	0.48
1:O:725:PRO:HD2	8:O:1193:HOH:O	2.14	0.48
2:P:203:ILE:HD12	2:P:203:ILE:N	2.28	0.48
2:R:207:GLY:HA2	1:U:728:VAL:CG1	2.34	0.48
1:S:85:PHE:CE2	1:S:87:PRO:HG3	2.48	0.48
1:S:696:LYS:HD3	8:S:1660:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:716:PRO:HB3	1:S:723:HIS:CD2	2.49	0.48
1:U:15:PRO:HD3	1:U:554:PHE:CD1	2.48	0.48
1:W:696:LYS:HD3	8:W:1670:HOH:O	2.12	0.48
1:W:753:TYR:HB3	2:X:24:MET:HE3	1.93	0.48
1:A:175:SER:OG	6:A:905:BTT:C5	2.61	0.48
1:A:636:LYS:HE3	2:X:166:LYS:HE2	1.96	0.48
2:D:71:CYS:HA	2:D:184:PRO:HA	1.95	0.48
1:E:176:TRP:O	1:E:177:GLU:C	2.57	0.48
1:I:176:TRP:O	1:I:177:GLU:C	2.56	0.48
1:I:400:TYR:CE1	1:I:421:LYS:HD2	2.49	0.48
2:J:70:HIS:CD2	2:J:92:VAL:H	2.14	0.48
2:L:60:ASP:C	2:L:60:ASP:OD1	2.56	0.48
1:O:214:PHE:HA	1:O:347:ALA:HB3	1.95	0.48
1:O:218:ASP:OD2	1:O:253:ASN:HB2	2.13	0.48
1:A:176:TRP:O	1:A:177:GLU:C	2.56	0.48
1:E:353:GLY:O	1:E:354:TRP:HB2	2.14	0.48
2:F:210:PHE:HD2	2:F:213:ALA:HB2	1.79	0.48
2:J:46:MET:HE1	2:J:65:PRO:C	2.37	0.48
1:K:165:GLY:CA	1:K:166:PHE:HB3	2.41	0.48
1:M:797:GLY:HA2	1:M:875:TYR:CE2	2.49	0.48
2:N:68:CYS:HB3	2:N:70:HIS:ND1	2.29	0.48
1:O:35:ASP:OD1	1:O:55:ARG:HD3	2.13	0.48
1:Q:670:PRO:HB3	1:Q:682:GLN:HB2	1.96	0.48
1:W:451:LYS:HG3	1:W:461:PHE:CE2	2.48	0.48
2:B:10:VAL:HG13	2:B:63:TYR:O	2.14	0.48
2:F:46:MET:HE2	2:F:48:ILE:CG1	2.43	0.48
1:G:387:TRP:CE2	1:G:389:THR:HA	2.48	0.48
1:O:141:PRO:CA	1:O:496:TYR:HB3	2.41	0.48
2:P:40:GLN:HB3	2:P:43:HIS:CE1	2.48	0.48
2:P:166:LYS:O	2:P:170:GLU:HG3	2.13	0.48
1:S:561:ILE:CG2	1:S:564:ASN:HB3	2.42	0.48
1:S:870:ASP:HB3	1:S:872:TYR:CE1	2.48	0.48
2:T:18:ASN:HB2	7:T:302:SF4:S1	2.53	0.48
2:T:58:ARG:HD2	2:T:268:ASP:OD1	2.13	0.48
1:C:134:PRO:HB2	1:C:439:LEU:HD11	1.96	0.48
1:C:147:TRP:CD1	1:C:552:SER:HG	2.32	0.48
1:E:111:ARG:NH2	1:E:585:GLU:OE2	2.44	0.48
1:E:356:GLY:H	4:E:903:MGD:C5'	2.27	0.48
2:F:59:ASN:ND2	2:F:59:ASN:H	2.12	0.48
2:H:256:TYR:HB2	2:H:274:LEU:HD21	1.95	0.48
1:I:184:MET:HE2	1:I:190:SER:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:211:GLU:HB2	2:L:231:PHE:HA	1.95	0.48
1:M:153:ARG:O	1:M:157:TYR:HB3	2.14	0.48
1:M:452:ILE:N	1:M:453:PRO:CD	2.76	0.48
2:T:5:TYR:HB2	2:T:157:LEU:CD1	2.43	0.48
1:U:142:SER:CB	4:U:902:MGD:O1A	2.62	0.48
1:U:604:GLU:HB3	1:U:605:MET:HE3	1.94	0.48
1:U:823:TYR:CE2	1:U:825:PRO:HG3	2.48	0.48
1:U:825:PRO:HD2	8:U:1336:HOH:O	2.14	0.48
1:W:716:PRO:HB3	1:W:723:HIS:CD2	2.49	0.48
2:X:114:MET:HA	2:X:125:LYS:HB3	1.94	0.48
1:C:114:TRP:CZ2	1:C:541:PRO:HD2	2.49	0.48
1:E:257:ARG:HD3	2:F:61:ILE:HG21	1.96	0.48
1:G:176:TRP:O	1:G:177:GLU:C	2.57	0.48
2:H:106:LEU:HD22	2:H:114:MET:HB3	1.95	0.48
1:I:565:TYR:C	1:I:567:LEU:H	2.22	0.48
2:J:46:MET:HE2	2:J:48:ILE:HG13	1.95	0.48
1:K:134:PRO:HB2	1:K:439:LEU:HD11	1.96	0.48
2:P:49:GLU:HG3	2:P:64:ARG:NH2	2.29	0.48
1:Q:387:TRP:CE2	1:Q:389:THR:HA	2.49	0.48
1:U:644:ASP:C	1:U:646:PRO:HD3	2.39	0.48
1:W:563:ASP:O	1:W:566:GLN:HG2	2.14	0.48
1:E:142:SER:CB	4:E:902:MGD:O1A	2.62	0.48
1:E:730:TYR:CE1	1:E:794:ASN:HA	2.49	0.48
1:G:482:TYR:HA	1:G:483:PRO:C	2.39	0.48
1:S:291:GLU:H	1:S:291:GLU:CD	2.21	0.48
1:U:356:GLY:N	4:U:903:MGD:PB	2.86	0.48
1:U:716:PRO:HB3	1:U:723:HIS:CD2	2.49	0.48
2:X:205:VAL:HG11	2:X:252:ASP:OD1	2.14	0.48
1:A:753:TYR:HB3	2:B:24:MET:CE	2.44	0.47
2:D:58:ARG:HD2	2:D:268:ASP:OD1	2.14	0.47
1:G:175:SER:HB2	1:G:176:TRP:CE3	2.49	0.47
1:M:291:GLU:H	1:M:291:GLU:CD	2.22	0.47
1:Q:258:LEU:HG	1:Q:259:VAL:HG13	1.96	0.47
1:Q:753:TYR:HB3	2:R:24:MET:CE	2.43	0.47
1:S:587:MET:HE3	1:S:591:GLU:HB3	1.96	0.47
1:W:128:ILE:CD1	1:W:492:MET:HB2	2.43	0.47
1:W:347:ALA:CB	1:W:388:SER:HA	2.44	0.47
2:D:23:CYS:O	2:D:26:GLU:N	2.47	0.47
2:D:198:TYR:HB3	2:D:238:ASP:HA	1.95	0.47
1:E:175:SER:HB2	1:E:176:TRP:CE3	2.49	0.47
1:I:138:LEU:HB2	1:I:490:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:296:ASN:HB3	1:I:657:PHE:CZ	2.50	0.47
1:I:797:GLY:HA2	1:I:875:TYR:CE2	2.50	0.47
1:M:175:SER:HB2	1:M:176:TRP:CE3	2.48	0.47
1:M:831:LYS:HD3	8:M:1576:HOH:O	2.13	0.47
1:M:855:MET:HB2	1:M:857:ASN:OD1	2.14	0.47
2:N:19:CYS:O	2:N:22:GLY:N	2.48	0.47
2:N:203:ILE:HD12	2:N:203:ILE:N	2.28	0.47
1:Q:81:LYS:HB2	1:Q:112:ILE:HD13	1.95	0.47
1:U:855:MET:HB2	1:U:857:ASN:OD1	2.14	0.47
1:W:176:TRP:O	1:W:177:GLU:C	2.58	0.47
1:W:356:GLY:H	4:W:903:MGD:PB	2.37	0.47
2:X:69:MET:O	2:X:70:HIS:C	2.56	0.47
1:A:451:LYS:HG3	1:A:461:PHE:CE2	2.49	0.47
2:B:247:VAL:O	2:B:257:SER:HA	2.14	0.47
1:G:174:ASP:OD1	1:G:175:SER:N	2.47	0.47
1:I:617:GLU:HG3	1:I:631:TRP:CG	2.50	0.47
2:J:18:ASN:HB2	7:J:302:SF4:S1	2.54	0.47
2:N:106:LEU:HD22	2:N:114:MET:HB3	1.95	0.47
2:N:166:LYS:O	2:N:170:GLU:HG3	2.13	0.47
1:U:563:ASP:HA	1:U:565:TYR:CE1	2.48	0.47
1:W:439:LEU:HD21	1:W:487:TYR:CE2	2.49	0.47
1:A:258:LEU:HG	1:A:259:VAL:HG13	1.95	0.47
2:F:20:PHE:CE2	2:F:24:MET:HE2	2.49	0.47
1:G:44:ILE:HD11	1:G:394:PRO:HG2	1.97	0.47
1:I:146:MET:HE2	1:I:544:THR:HA	1.97	0.47
1:K:176:TRP:O	1:K:177:GLU:C	2.57	0.47
1:M:558:SER:H	1:M:564:ASN:ND2	2.13	0.47
1:M:677:CYS:C	1:M:678:ARG:HG2	2.39	0.47
1:O:56:LYS:HG2	1:O:57:THR:O	2.14	0.47
1:O:494:TRP:HE1	1:O:525:GLN:HE21	1.62	0.47
1:Q:153:ARG:O	1:Q:157:TYR:HB3	2.14	0.47
1:U:725:PRO:HD2	8:U:1197:HOH:O	2.15	0.47
2:V:114:MET:HA	2:V:125:LYS:HB3	1.96	0.47
1:W:146:MET:HE3	1:W:544:THR:HB	1.95	0.47
2:D:73:ASN:HB3	2:D:182:THR:HA	1.96	0.47
2:H:104:GLU:H	2:H:104:GLU:CD	2.22	0.47
1:I:56:LYS:HG2	1:I:57:THR:O	2.15	0.47
2:J:189:LYS:HD2	8:J:997:HOH:O	2.15	0.47
1:K:85:PHE:CE2	1:K:87:PRO:HG3	2.50	0.47
1:M:187:TRP:CH2	1:M:196:PRO:HB3	2.50	0.47
1:M:533:VAL:HB	1:M:534:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:164:MET:O	2:N:168:VAL:HG23	2.15	0.47
1:O:28:MET:HE1	1:O:66:PHE:CB	2.37	0.47
2:P:142:MET:HE1	8:P:428:HOH:O	2.14	0.47
1:Q:558:SER:H	1:Q:564:ASN:ND2	2.13	0.47
2:R:46:MET:HE2	2:R:48:ILE:CG1	2.43	0.47
1:W:146:MET:HE3	1:W:544:THR:HA	1.96	0.47
1:A:138:LEU:HB2	1:A:490:ILE:HD12	1.96	0.47
1:A:730:TYR:CE1	1:A:794:ASN:HA	2.49	0.47
1:C:717:ALA:HB3	1:C:720:SER:HB3	1.97	0.47
1:E:855:MET:HB2	1:E:857:ASN:OD1	2.14	0.47
1:G:296:ASN:HB3	1:G:657:PHE:CZ	2.49	0.47
1:I:291:GLU:CD	1:I:291:GLU:H	2.23	0.47
2:J:142:MET:HE2	2:J:146:ALA:CB	2.42	0.47
2:N:207:GLY:CA	1:S:728:VAL:HG12	2.31	0.47
1:O:738:HIS:HE2	4:O:902:MGD:H15	1.62	0.47
1:S:610:LYS:HB3	1:S:614:ALA:HB3	1.96	0.47
1:S:670:PRO:HG2	1:S:675:GLN:CD	2.39	0.47
2:V:203:ILE:HD12	2:V:203:ILE:N	2.29	0.47
1:W:476:GLN:OE1	1:W:708:ARG:NH2	2.48	0.47
1:C:146:MET:HG2	4:C:902:MGD:N7	2.29	0.47
1:C:571:ARG:HB2	1:C:642:VAL:HB	1.96	0.47
2:D:118:GLU:HB3	1:S:604:GLU:CD	2.40	0.47
2:D:213:ALA:O	2:D:228:GLU:HA	2.14	0.47
2:D:216:VAL:HG13	2:D:223:GLU:HG3	1.97	0.47
1:E:21:LYS:CB	1:E:26:ILE:HD11	2.44	0.47
2:J:20:PHE:CE2	2:J:24:MET:HE2	2.49	0.47
2:J:166:LYS:HG2	2:J:170:GLU:OE2	2.15	0.47
1:K:15:PRO:HD3	1:K:554:PHE:CD1	2.50	0.47
1:K:730:TYR:CE1	1:K:794:ASN:HA	2.50	0.47
1:M:56:LYS:HG2	1:M:57:THR:O	2.14	0.47
1:M:218:ASP:OD2	1:M:253:ASN:HB2	2.14	0.47
1:O:114:TRP:CZ2	1:O:541:PRO:HD2	2.50	0.47
1:Q:786:ASN:ND2	1:Q:804:GLN:HA	2.29	0.47
1:S:114:TRP:CZ2	1:S:541:PRO:HD2	2.49	0.47
1:S:214:PHE:HA	1:S:347:ALA:HB3	1.97	0.47
1:S:495:LYS:HD2	1:S:514:TYR:OH	2.15	0.47
2:V:68:CYS:CB	2:V:126:CYS:CB	2.84	0.47
1:W:146:MET:HG2	4:W:902:MGD:N7	2.29	0.47
1:W:673:ASN:H	1:W:673:ASN:HD22	1.61	0.47
1:W:730:TYR:CE1	1:W:794:ASN:HA	2.49	0.47
1:A:347:ALA:CB	1:A:388:SER:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:MET:HE1	1:A:618:GLN:O	2.14	0.47
1:G:426:MET:HE1	1:G:618:GLN:O	2.14	0.47
1:G:737:PRO:CG	4:G:903:MGD:H2'	2.45	0.47
1:K:118:THR:O	1:K:122:VAL:HG23	2.15	0.47
1:M:426:MET:HE3	1:M:426:MET:CA	2.35	0.47
2:N:216:VAL:HG13	2:N:223:GLU:HG3	1.96	0.47
1:O:44:ILE:HD11	1:O:394:PRO:HG2	1.97	0.47
2:P:70:HIS:CD2	2:P:92:VAL:H	2.17	0.47
1:Q:218:ASP:OD2	1:Q:253:ASN:HB2	2.14	0.47
1:S:55:ARG:HD2	8:S:1627:HOH:O	2.15	0.47
1:S:153:ARG:O	1:S:157:TYR:HB3	2.14	0.47
2:T:46:MET:HE1	2:T:65:PRO:CA	2.45	0.47
1:U:387:TRP:CE2	1:U:389:THR:HA	2.49	0.47
1:U:476:GLN:OE1	1:U:708:ARG:NH2	2.48	0.47
1:W:786:ASN:ND2	1:W:804:GLN:HA	2.30	0.47
1:C:66:PHE:CD1	1:C:69:MET:HE3	2.50	0.47
1:E:495:LYS:HD3	8:E:1107:HOH:O	2.15	0.47
1:E:617:GLU:HG3	1:E:631:TRP:CG	2.49	0.47
1:G:218:ASP:OD2	1:G:253:ASN:HB2	2.14	0.47
1:G:426:MET:HE3	1:G:622:ALA:HB2	1.96	0.47
1:I:457:MET:HE3	8:I:1506:HOH:O	2.15	0.47
2:J:166:LYS:O	2:J:170:GLU:HG3	2.14	0.47
2:N:46:MET:HE2	2:N:48:ILE:CG1	2.45	0.47
1:O:146:MET:HE2	1:O:544:THR:HA	1.97	0.47
1:Q:146:MET:HE2	1:Q:544:THR:HA	1.96	0.47
2:R:143:PRO:HB3	7:R:303:SF4:S1	2.55	0.47
1:W:361:SER:OG	1:W:717:ALA:HB1	2.15	0.47
1:C:56:LYS:HG2	1:C:57:THR:O	2.15	0.47
1:C:75:ARG:NH2	1:C:543:CYS:HA	2.30	0.47
1:G:395:LEU:HD12	1:G:566:GLN:HA	1.97	0.47
2:H:46:MET:HE1	2:H:65:PRO:HA	1.97	0.47
1:K:142:SER:HB3	4:K:902:MGD:O1A	2.14	0.47
1:M:495:LYS:HD2	1:M:514:TYR:OH	2.15	0.47
2:N:201:ALA:HB2	2:N:269:LEU:HB2	1.97	0.47
1:Q:75:ARG:HH21	1:Q:543:CYS:HA	1.80	0.47
2:V:142:MET:CE	2:V:146:ALA:HB1	2.45	0.47
1:W:499:PRO:HG3	4:W:902:MGD:O5'	2.15	0.47
1:W:870:ASP:HB3	1:W:872:TYR:CE1	2.50	0.47
1:A:100:LEU:HD12	1:A:105:PRO:HG3	1.97	0.46
2:B:105:LEU:HB3	2:B:114:MET:CE	2.42	0.46
1:C:452:ILE:HB	1:C:453:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:378:GLY:O	1:E:381:LYS:HG2	2.15	0.46
1:I:13:GLY:HA3	1:I:63:THR:OG1	2.15	0.46
1:I:738:HIS:HE2	4:I:902:MGD:H15	1.63	0.46
1:K:253:ASN:O	1:K:257:ARG:HG3	2.16	0.46
1:K:521:PHE:CE2	1:K:523:VAL:CG2	2.99	0.46
2:L:68:CYS:CB	2:L:126:CYS:CB	2.85	0.46
2:L:143:PRO:HB3	7:L:303:SF4:S1	2.55	0.46
1:M:656:TRP:CD2	1:M:663:LYS:HA	2.50	0.46
1:O:9:ASN:HA	1:O:576:GLN:HA	1.97	0.46
1:S:563:ASP:HA	1:S:565:TYR:CE1	2.49	0.46
2:T:46:MET:HE2	2:T:48:ILE:CG1	2.44	0.46
2:T:68:CYS:CB	2:T:126:CYS:CB	2.84	0.46
1:U:166:PHE:N	1:U:439:LEU:HD12	2.30	0.46
1:U:195:ASN:HD21	1:U:354:TRP:CD1	2.32	0.46
2:V:59:ASN:ND2	2:V:59:ASN:H	2.13	0.46
2:V:105:LEU:HB3	2:V:114:MET:HE1	1.96	0.46
1:W:800:ILE:HD12	1:W:800:ILE:N	2.30	0.46
1:A:139:SER:OG	1:A:161:MET:HE2	2.15	0.46
1:A:426:MET:HE2	1:A:618:GLN:HG2	1.98	0.46
1:E:9:ASN:HA	1:E:576:GLN:HA	1.96	0.46
1:I:495:LYS:CD	1:I:514:TYR:OH	2.63	0.46
2:J:10:VAL:HG13	2:J:63:TYR:O	2.15	0.46
2:J:216:VAL:HG13	2:J:223:GLU:HG3	1.96	0.46
1:K:66:PHE:CD1	1:K:69:MET:HE3	2.50	0.46
2:L:46:MET:HE1	2:L:65:PRO:CA	2.45	0.46
1:M:96:ARG:HD2	1:M:514:TYR:O	2.15	0.46
1:O:175:SER:OG	6:O:905:BTT:C5	2.64	0.46
2:P:5:TYR:HB2	2:P:157:LEU:HD11	1.97	0.46
1:Q:176:TRP:O	1:Q:177:GLU:C	2.58	0.46
2:R:21:MET:HE2	2:R:21:MET:N	2.31	0.46
1:U:604:GLU:HB3	1:U:605:MET:CE	2.45	0.46
2:B:21:MET:HE2	2:B:21:MET:CA	2.45	0.46
1:C:670:PRO:HG2	1:C:675:GLN:CD	2.40	0.46
1:E:15:PRO:HD3	1:E:554:PHE:CD1	2.50	0.46
2:F:2:GLU:HG2	2:F:158:LYS:HG2	1.98	0.46
1:O:249:ASP:CG	4:O:903:MGD:H1'	2.39	0.46
1:O:356:GLY:N	4:O:903:MGD:O5'	2.39	0.46
2:P:210:PHE:CE2	2:P:251:ALA:HB1	2.51	0.46
1:A:35:ASP:OD1	1:A:55:ARG:HD3	2.15	0.46
1:A:56:LYS:HG2	1:A:57:THR:O	2.16	0.46
1:C:644:ASP:O	1:C:646:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:MET:HG2	4:G:902:MGD:N7	2.30	0.46
1:I:214:PHE:HA	1:I:347:ALA:HB3	1.96	0.46
1:K:175:SER:OG	6:K:905:BTT:C5	2.63	0.46
1:M:426:MET:HA	1:M:426:MET:CE	2.34	0.46
1:Q:140:THR:HB	1:Q:169:ALA:HB3	1.97	0.46
1:S:656:TRP:CD2	1:S:663:LYS:HA	2.51	0.46
1:U:521:PHE:CE2	1:U:523:VAL:CG2	2.98	0.46
2:V:205:VAL:HG13	2:V:254:LYS:NZ	2.29	0.46
2:D:142:MET:CE	2:D:146:ALA:HB1	2.41	0.46
1:I:195:ASN:HD21	1:I:354:TRP:CD1	2.32	0.46
1:I:629:MET:HE2	1:I:634:PHE:CA	2.45	0.46
2:J:13:CYS:HB3	2:J:63:TYR:HB2	1.97	0.46
2:J:142:MET:HE1	8:J:928:HOH:O	2.16	0.46
2:J:162:GLU:CD	2:J:162:GLU:H	2.23	0.46
1:O:1:MET:H3	1:O:22:ASP:CG	2.22	0.46
1:O:165:GLY:HA3	1:O:166:PHE:CB	2.41	0.46
1:O:182:GLY:HA3	1:O:364:ILE:HG23	1.98	0.46
1:Q:610:LYS:NZ	1:Q:618:GLN:NE2	2.56	0.46
1:Q:670:PRO:HG2	1:Q:675:GLN:CD	2.40	0.46
2:R:76:CYS:O	2:R:80:GLY:N	2.49	0.46
1:S:501:LEU:HD13	1:S:823:TYR:CG	2.50	0.46
1:U:528:TRP:CD2	1:U:750:LYS:HD3	2.51	0.46
2:V:5:TYR:CD2	2:V:164:MET:HG2	2.51	0.46
1:W:165:GLY:HA3	1:W:166:PHE:CB	2.40	0.46
2:X:235:PHE:CD1	2:X:235:PHE:C	2.94	0.46
1:E:656:TRP:CD2	1:E:663:LYS:HA	2.51	0.46
2:H:59:ASN:H	2:H:59:ASN:HD22	1.64	0.46
1:I:253:ASN:O	1:I:257:ARG:HG3	2.14	0.46
1:K:155:SER:OG	1:K:409:ILE:HG12	2.16	0.46
1:K:499:PRO:HG3	4:K:902:MGD:O5'	2.14	0.46
2:L:203:ILE:N	2:L:203:ILE:HD12	2.30	0.46
1:M:144:HIS:HB2	4:M:902:MGD:O1B	2.16	0.46
1:M:301:GLU:H	1:M:301:GLU:CD	2.23	0.46
1:M:610:LYS:HZ1	1:M:618:GLN:HE22	1.59	0.46
2:N:114:MET:HE3	2:N:123:ALA:CB	2.43	0.46
4:Q:903:MGD:O1B	4:Q:903:MGD:C4'	2.62	0.46
2:T:205:VAL:HG13	2:T:254:LYS:NZ	2.30	0.46
1:U:617:GLU:HG3	1:U:631:TRP:CG	2.51	0.46
1:A:15:PRO:HD3	1:A:554:PHE:CD1	2.51	0.46
1:A:75:ARG:HH21	1:A:543:CYS:HA	1.80	0.46
1:C:28:MET:HE1	1:C:66:PHE:CB	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ARG:NH2	1:E:543:CYS:HA	2.30	0.46
1:E:400:TYR:CE1	1:E:421:LYS:HD2	2.51	0.46
1:I:12:THR:O	1:I:226:TYR:HA	2.16	0.46
1:O:144:HIS:HB2	4:O:902:MGD:O1B	2.15	0.46
1:Q:118:THR:O	1:Q:122:VAL:HG23	2.15	0.46
2:V:102:LYS:HB3	2:V:104:GLU:OE2	2.16	0.46
1:C:767:TYR:HB3	1:C:769:TYR:CE1	2.50	0.46
1:E:253:ASN:O	1:E:257:ARG:HG3	2.16	0.46
2:F:46:MET:HE1	2:F:65:PRO:C	2.41	0.46
1:G:738:HIS:HE2	4:G:902:MGD:H15	1.64	0.46
1:M:353:GLY:O	1:M:354:TRP:HB2	2.16	0.46
1:M:460:LYS:HG3	8:M:1232:HOH:O	2.16	0.46
1:O:353:GLY:O	1:O:354:TRP:HB2	2.16	0.46
1:Q:460:LYS:HG3	8:Q:1229:HOH:O	2.16	0.46
2:R:68:CYS:HB3	2:R:70:HIS:ND1	2.30	0.46
1:U:362:HIS:HB3	1:U:717:ALA:HB2	1.97	0.46
1:W:452:ILE:HB	1:W:453:PRO:HD3	1.98	0.46
2:B:176:ILE:HG22	2:B:177:LYS:HG3	1.97	0.46
1:C:561:ILE:CG2	1:C:564:ASN:HB3	2.45	0.46
2:D:70:HIS:HD2	2:D:92:VAL:N	2.08	0.46
1:E:561:ILE:CG2	1:E:564:ASN:HB3	2.46	0.46
1:E:670:PRO:HG2	1:E:675:GLN:CD	2.41	0.46
2:F:143:PRO:HB3	7:F:303:SF4:S1	2.56	0.46
1:G:565:TYR:C	1:G:567:LEU:H	2.24	0.46
2:J:46:MET:HE1	2:J:65:PRO:CA	2.45	0.46
1:K:142:SER:CB	4:K:902:MGD:O1A	2.64	0.46
1:K:495:LYS:HD2	1:K:514:TYR:OH	2.16	0.46
1:M:12:THR:O	1:M:226:TYR:HA	2.16	0.46
1:M:257:ARG:HD3	2:N:61:ILE:HG21	1.97	0.46
1:O:323:GLU:HB2	8:O:1569:HOH:O	2.15	0.46
1:Q:103:GLN:CD	1:Q:103:GLN:N	2.74	0.46
1:Q:353:GLY:O	1:Q:354:TRP:HB2	2.14	0.46
2:R:87:ARG:HG3	2:R:91:ILE:O	2.15	0.46
2:T:216:VAL:HG13	2:T:223:GLU:HG3	1.97	0.46
1:U:265:SER:O	1:U:810:GLN:NE2	2.49	0.46
1:W:460:LYS:HE3	8:W:1232:HOH:O	2.16	0.46
1:W:629:MET:HE2	1:W:634:PHE:HA	1.97	0.46
1:C:100:LEU:CD1	1:C:105:PRO:HG3	2.45	0.46
2:D:106:LEU:HD23	2:D:114:MET:CE	2.46	0.46
1:G:460:LYS:HE3	8:G:1230:HOH:O	2.16	0.46
4:G:903:MGD:O2B	4:G:903:MGD:O2A	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:139:SER:CB	1:I:161:MET:HE2	2.46	0.46
1:Q:328:PRO:HB2	1:Q:331:GLU:HG3	1.98	0.46
2:R:58:ARG:HD2	2:R:268:ASP:OD1	2.16	0.46
1:S:528:TRP:CG	1:S:750:LYS:HD3	2.51	0.46
1:U:452:ILE:N	1:U:453:PRO:CD	2.79	0.46
2:X:105:LEU:HB3	2:X:114:MET:HE1	1.98	0.46
1:A:13:GLY:HA3	1:A:63:THR:OG1	2.16	0.45
1:A:395:LEU:HD12	1:A:566:GLN:HA	1.98	0.45
1:C:408:GLY:HA2	1:C:619:TYR:HE1	1.80	0.45
2:D:252:ASP:C	2:D:254:LYS:H	2.23	0.45
1:E:13:GLY:HA3	1:E:63:THR:OG1	2.16	0.45
1:E:708:ARG:HD2	8:E:1044:HOH:O	2.16	0.45
2:F:162:GLU:H	2:F:162:GLU:CD	2.23	0.45
1:G:452:ILE:HB	1:G:453:PRO:HD3	1.98	0.45
1:I:211:MET:HE3	1:I:244:ASP:HB2	1.97	0.45
1:I:696:LYS:O	1:I:700:GLU:HG3	2.16	0.45
2:L:219:SER:C	2:L:221:GLY:H	2.25	0.45
1:M:670:PRO:HG2	1:M:675:GLN:CD	2.41	0.45
1:S:521:PHE:CE2	1:S:523:VAL:CG2	2.99	0.45
2:T:46:MET:HE1	2:T:65:PRO:C	2.37	0.45
1:U:12:THR:O	1:U:226:TYR:HA	2.16	0.45
1:U:561:ILE:CG2	1:U:564:ASN:HB3	2.46	0.45
1:U:738:HIS:HE2	4:U:902:MGD:H15	1.64	0.45
1:W:400:TYR:CZ	1:W:421:LYS:HD2	2.51	0.45
1:W:426:MET:HE2	1:W:618:GLN:HG2	1.94	0.45
1:W:780:GLU:CD	1:W:780:GLU:C	2.83	0.45
2:X:60:ASP:C	2:X:60:ASP:OD1	2.58	0.45
1:A:96:ARG:HD2	1:A:514:TYR:O	2.16	0.45
1:A:452:ILE:N	1:A:453:PRO:CD	2.80	0.45
1:A:825:PRO:HD2	8:A:1333:HOH:O	2.15	0.45
1:C:44:ILE:HD11	1:C:394:PRO:HG2	1.98	0.45
1:E:153:ARG:O	1:E:157:TYR:HB3	2.16	0.45
1:G:128:ILE:CD1	1:G:492:MET:HB2	2.46	0.45
2:H:210:PHE:HD2	2:H:213:ALA:HB2	1.81	0.45
1:I:452:ILE:N	1:I:453:PRO:CD	2.79	0.45
1:K:452:ILE:N	1:K:453:PRO:CD	2.79	0.45
1:K:501:LEU:HD13	1:K:823:TYR:CD2	2.52	0.45
1:K:610:LYS:HZ3	1:K:618:GLN:HE22	1.64	0.45
1:M:28:MET:HE2	8:M:1399:HOH:O	2.16	0.45
1:O:146:MET:HE2	1:O:544:THR:CA	2.47	0.45
1:Q:2:GLY:O	1:Q:21:LYS:HE3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:691:ILE:CD1	1:Q:711:MET:HE3	2.46	0.45
1:S:197:GLU:HG3	1:S:653:ALA:HB1	1.98	0.45
2:T:105:LEU:HB3	2:T:114:MET:HE1	1.99	0.45
1:U:498:GLY:N	1:U:499:PRO:HD3	2.31	0.45
1:A:378:GLY:O	1:A:381:LYS:HG2	2.16	0.45
2:B:68:CYS:CB	2:B:126:CYS:CB	2.84	0.45
2:B:112:GLY:HA2	8:B:519:HOH:O	2.16	0.45
1:C:418:ALA:HB1	1:C:423:ALA:HB2	1.97	0.45
2:D:46:MET:CE	2:D:66:THR:H	2.26	0.45
2:F:60:ASP:C	2:F:60:ASP:OD1	2.60	0.45
1:K:738:HIS:HE2	4:K:902:MGD:H15	1.64	0.45
1:M:730:TYR:CZ	1:M:794:ASN:HA	2.51	0.45
1:M:786:ASN:HD21	1:M:804:GLN:HA	1.80	0.45
2:N:2:GLU:CG	2:N:158:LYS:HG2	2.43	0.45
1:O:15:PRO:HD3	1:O:554:PHE:CD1	2.51	0.45
1:O:211:MET:HE1	2:P:231:PHE:CE1	2.50	0.45
1:O:870:ASP:HB3	1:O:872:TYR:CE1	2.51	0.45
1:U:13:GLY:HA3	1:U:63:THR:OG1	2.17	0.45
1:U:21:LYS:CB	1:U:26:ILE:HD11	2.45	0.45
1:U:356:GLY:H	4:U:903:MGD:PB	2.38	0.45
2:V:213:ALA:O	2:V:228:GLU:HA	2.16	0.45
2:X:68:CYS:CB	2:X:126:CYS:CB	2.87	0.45
2:X:97:GLU:OE2	2:X:100:LYS:HE2	2.16	0.45
2:X:99:ALA:HA	2:X:102:LYS:HD2	1.97	0.45
2:B:60:ASP:C	2:B:60:ASP:OD1	2.60	0.45
2:B:228:GLU:OE2	2:H:214:LYS:NZ	2.50	0.45
1:C:460:LYS:HE3	8:C:1232:HOH:O	2.16	0.45
1:E:2:GLY:N	1:E:22:ASP:OD1	2.50	0.45
1:I:402:PRO:HG2	1:I:422:PHE:CD1	2.51	0.45
1:K:187:TRP:CH2	1:K:196:PRO:HB3	2.51	0.45
1:K:218:ASP:OD2	1:K:253:ASN:HB2	2.16	0.45
1:M:587:MET:HG3	1:M:592:ILE:HG13	1.99	0.45
1:Q:533:VAL:HB	1:Q:534:PRO:HD3	1.98	0.45
1:Q:656:TRP:CD2	1:Q:663:LYS:HA	2.51	0.45
2:R:39:MET:HE2	2:R:45:TRP:CD2	2.52	0.45
1:S:100:LEU:CD1	1:S:105:PRO:HG3	2.46	0.45
2:T:5:TYR:HB2	2:T:157:LEU:HD12	1.99	0.45
1:W:134:PRO:HB2	1:W:439:LEU:HD11	1.98	0.45
1:W:855:MET:HB2	1:W:857:ASN:OD1	2.16	0.45
1:E:451:LYS:HG3	1:E:461:PHE:CE2	2.52	0.45
1:E:644:ASP:O	1:E:646:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:PHE:CD1	1:G:69:MET:CE	2.99	0.45
1:G:201:LEU:HD13	1:G:387:TRP:HB2	1.98	0.45
1:K:114:TRP:CZ2	1:K:541:PRO:HD2	2.52	0.45
1:K:138:LEU:HB2	1:K:490:ILE:HD12	1.98	0.45
1:M:184:MET:HE2	1:M:190:SER:HA	1.98	0.45
1:O:561:ILE:CG2	1:O:564:ASN:HB3	2.47	0.45
1:Q:408:GLY:HA2	1:Q:619:TYR:HE1	1.82	0.45
1:Q:482:TYR:HA	1:Q:483:PRO:C	2.42	0.45
2:T:40:GLN:HB3	2:T:43:HIS:CE1	2.51	0.45
2:T:145:CYS:HB2	2:T:146:ALA:H	1.33	0.45
1:U:9:ASN:HA	1:U:576:GLN:HA	1.98	0.45
1:U:21:LYS:HB3	1:U:26:ILE:HD11	1.97	0.45
1:U:722:LYS:HG2	8:U:1560:HOH:O	2.16	0.45
2:V:27:HIS:HB2	2:V:39:MET:HE3	1.98	0.45
2:B:210:PHE:HD2	2:B:213:ALA:HB2	1.81	0.45
1:C:142:SER:CB	4:C:902:MGD:O1A	2.65	0.45
1:C:501:LEU:HD13	1:C:823:TYR:CD2	2.51	0.45
2:F:106:LEU:HD23	2:F:114:MET:HE2	1.99	0.45
2:J:46:MET:HE1	2:J:65:PRO:HA	1.99	0.45
2:J:46:MET:HE2	2:J:48:ILE:CG1	2.47	0.45
1:K:737:PRO:HG2	4:K:903:MGD:H2'	1.98	0.45
2:N:46:MET:HE3	2:N:47:ASN:C	2.42	0.45
1:U:146:MET:HE2	1:U:544:THR:CA	2.47	0.45
1:U:649:LYS:O	1:U:649:LYS:HG3	2.16	0.45
2:V:19:CYS:O	2:V:22:GLY:N	2.50	0.45
1:W:498:GLY:N	1:W:499:PRO:HD3	2.31	0.45
1:C:670:PRO:HB3	1:C:682:GLN:HB2	1.99	0.45
1:E:825:PRO:HD2	8:E:1337:HOH:O	2.16	0.45
1:G:138:LEU:HB2	1:G:490:ILE:HD12	1.99	0.45
2:H:1:MET:HE2	2:H:88:GLU:OE2	2.16	0.45
2:J:74:ALA:HA	2:J:75:PRO:HD3	1.86	0.45
1:K:69:MET:HE2	1:K:754:MET:HE3	1.95	0.45
1:K:75:ARG:NH2	1:K:543:CYS:HA	2.32	0.45
1:M:250:PRO:HD3	4:M:903:MGD:C2	2.46	0.45
1:M:867:TRP:CD1	1:M:869:GLY:H	2.34	0.45
2:N:20:PHE:CE2	2:N:24:MET:HE2	2.52	0.45
1:O:395:LEU:HD12	1:O:566:GLN:HA	1.99	0.45
1:O:737:PRO:CG	4:O:903:MGD:H2'	2.46	0.45
1:Q:35:ASP:OD1	1:Q:55:ARG:HD3	2.17	0.45
2:R:46:MET:HE3	2:R:47:ASN:C	2.42	0.45
1:U:361:SER:OG	1:U:717:ALA:HB1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:571:ARG:HB2	1:U:642:VAL:HB	1.97	0.45
1:C:402:PRO:HG2	1:C:422:PHE:CE1	2.51	0.45
1:E:800:ILE:CD1	1:E:833:ALA:HB1	2.47	0.45
1:G:540:LEU:HA	1:G:541:PRO:HD3	1.79	0.45
1:G:696:LYS:O	1:G:700:GLU:HG3	2.17	0.45
2:J:247:VAL:O	2:J:257:SER:HA	2.17	0.45
1:K:855:MET:HB2	1:K:857:ASN:OD1	2.16	0.45
1:M:378:GLY:O	1:M:381:LYS:HG2	2.17	0.45
1:O:175:SER:HB2	1:O:176:TRP:CE3	2.52	0.45
1:Q:296:ASN:O	1:Q:687:LYS:HB3	2.16	0.45
1:S:211:MET:HE1	2:T:231:PHE:CE1	2.50	0.45
1:S:452:ILE:N	1:S:453:PRO:CD	2.80	0.45
1:S:630:THR:OG1	1:S:633:GLU:HG3	2.17	0.45
1:U:155:SER:OG	1:U:409:ILE:HG12	2.17	0.45
1:W:111:ARG:NH2	1:W:585:GLU:OE2	2.46	0.45
4:W:903:MGD:O2B	4:W:903:MGD:O2A	2.34	0.45
2:X:110:PRO:HB3	2:X:180:LEU:HD13	1.98	0.45
1:C:541:PRO:HB2	1:C:586:SER:HA	1.99	0.45
1:K:76:ILE:HG22	1:K:541:PRO:HG3	1.99	0.45
1:K:753:TYR:HB3	2:L:24:MET:CE	2.47	0.45
1:U:142:SER:OG	4:U:902:MGD:O1A	2.31	0.45
1:W:426:MET:HE1	1:W:618:GLN:O	2.16	0.45
1:C:12:THR:O	1:C:226:TYR:HA	2.17	0.45
1:C:177:GLU:OE2	1:C:177:GLU:HA	2.17	0.45
1:C:211:MET:HE3	1:C:244:ASP:HB2	1.98	0.45
2:D:177:LYS:C	2:D:179:GLU:OE1	2.60	0.45
2:J:2:GLU:HG3	2:J:159:THR:C	2.42	0.45
1:K:100:LEU:CD1	1:K:105:PRO:HG3	2.47	0.45
1:K:561:ILE:CG2	1:K:564:ASN:HB3	2.45	0.45
1:Q:617:GLU:HG3	1:Q:631:TRP:CG	2.52	0.45
1:S:21:LYS:CB	1:S:26:ILE:HD11	2.47	0.45
1:S:730:TYR:CE1	1:S:794:ASN:HA	2.52	0.45
1:U:587:MET:HE2	1:U:592:ILE:HA	1.98	0.45
1:W:847:TYR:CZ	1:W:853:CYS:HB3	2.52	0.45
2:X:46:MET:HE1	2:X:65:PRO:CA	2.47	0.45
1:C:503:THR:O	1:C:504:MET:HE2	2.17	0.44
2:D:4:TYR:CE2	2:D:158:LYS:HD2	2.51	0.44
1:I:21:LYS:CB	1:I:26:ILE:HD11	2.46	0.44
1:I:656:TRP:CD2	1:I:663:LYS:HA	2.52	0.44
2:J:59:ASN:H	2:J:59:ASN:HD22	1.64	0.44
1:K:656:TRP:CD2	1:K:663:LYS:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:55:ARG:HD2	8:O:1636:HOH:O	2.17	0.44
2:R:21:MET:HE2	2:R:21:MET:HA	1.98	0.44
1:S:366:TRP:O	1:S:370:MET:HG2	2.16	0.44
2:X:70:HIS:CD2	2:X:92:VAL:H	2.32	0.44
1:A:565:TYR:C	1:A:567:LEU:H	2.25	0.44
1:A:738:HIS:HE2	4:A:902:MGD:H15	1.64	0.44
2:D:23:CYS:O	2:D:27:HIS:N	2.40	0.44
2:D:94:ILE:O	2:D:96:PRO:HD3	2.17	0.44
1:E:347:ALA:CB	1:E:388:SER:HA	2.47	0.44
1:E:521:PHE:CE2	1:E:523:VAL:CG2	3.00	0.44
2:F:205:VAL:HG13	2:F:254:LYS:HZ1	1.82	0.44
2:H:203:ILE:HD12	2:H:203:ILE:N	2.32	0.44
1:I:825:PRO:HD2	8:I:1332:HOH:O	2.17	0.44
2:J:256:TYR:HB2	2:J:274:LEU:HD21	1.98	0.44
1:M:501:LEU:HD13	1:M:823:TYR:CD2	2.52	0.44
2:P:5:TYR:HB2	2:P:157:LEU:HD12	1.98	0.44
1:Q:265:SER:O	1:Q:810:GLN:NE2	2.50	0.44
1:S:783:GLY:O	1:S:866:LYS:HD2	2.18	0.44
1:U:356:GLY:H	4:U:903:MGD:H5'2	1.83	0.44
1:U:735:LEU:HD23	1:U:735:LEU:H	1.81	0.44
1:W:301:GLU:CD	1:W:301:GLU:H	2.24	0.44
2:X:201:ALA:HB2	2:X:269:LEU:HB2	1.99	0.44
1:C:770:TRP:HB3	1:C:801:LEU:HD23	1.99	0.44
1:E:494:TRP:HE1	1:E:525:GLN:HE21	1.65	0.44
1:I:211:MET:HE2	1:I:246:VAL:HG23	1.98	0.44
1:I:501:LEU:HD13	1:I:823:TYR:CD2	2.51	0.44
2:J:106:LEU:CA	2:J:114:MET:HE2	2.44	0.44
2:N:60:ASP:C	2:N:60:ASP:OD1	2.61	0.44
1:O:177:GLU:HA	1:O:177:GLU:OE2	2.16	0.44
1:O:571:ARG:HB2	1:O:642:VAL:HB	1.99	0.44
1:O:656:TRP:CD2	1:O:663:LYS:HA	2.53	0.44
1:U:163:MET:HE1	1:U:606:PHE:HA	2.00	0.44
1:U:218:ASP:OD2	1:U:253:ASN:HB2	2.17	0.44
1:U:786:ASN:HD22	1:U:805:VAL:H	1.64	0.44
1:A:74:LEU:HD12	1:A:750:LYS:HA	2.00	0.44
1:C:870:ASP:HB3	1:C:872:TYR:CE1	2.53	0.44
2:D:91:ILE:HG22	2:D:93:LEU:HG	1.98	0.44
2:F:46:MET:HE3	2:F:47:ASN:C	2.41	0.44
2:F:166:LYS:HE2	2:F:170:GLU:OE2	2.17	0.44
2:H:5:TYR:CD2	2:H:164:MET:HG2	2.52	0.44
1:I:670:PRO:HG2	1:I:675:GLN:CD	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:106:LEU:N	2:J:114:MET:HE2	2.32	0.44
1:K:21:LYS:HB3	1:K:26:ILE:HD11	1.98	0.44
1:K:362:HIS:HB3	1:K:717:ALA:HB2	1.98	0.44
1:M:9:ASN:HA	1:M:576:GLN:HA	1.98	0.44
2:P:43:HIS:ND1	8:P:404:HOH:O	2.36	0.44
1:S:540:LEU:HA	1:S:541:PRO:HD3	1.79	0.44
1:S:647:ASN:O	1:S:648:ARG:HG2	2.18	0.44
1:U:505:THR:HG22	1:U:857:ASN:ND2	2.33	0.44
2:X:46:MET:HE1	2:X:65:PRO:HA	1.98	0.44
1:C:656:TRP:CD2	1:C:663:LYS:HA	2.53	0.44
2:D:166:LYS:HG2	2:D:170:GLU:OE2	2.17	0.44
1:E:138:LEU:HD12	1:E:167:THR:O	2.17	0.44
1:E:671:ARG:HD2	8:E:1099:HOH:O	2.17	0.44
1:G:139:SER:CB	1:G:161:MET:HE2	2.48	0.44
1:I:521:PHE:CE2	1:I:523:VAL:HG22	2.53	0.44
2:L:103:LYS:HE2	2:L:116:TRP:CE2	2.53	0.44
1:M:139:SER:CB	1:M:161:MET:HE2	2.47	0.44
1:M:347:ALA:CB	1:M:388:SER:HA	2.48	0.44
1:Q:15:PRO:HD3	1:Q:554:PHE:CD1	2.52	0.44
1:Q:253:ASN:O	1:Q:257:ARG:HG3	2.17	0.44
2:R:210:PHE:HD2	2:R:213:ALA:HB2	1.82	0.44
1:W:114:TRP:CZ2	1:W:541:PRO:HD2	2.51	0.44
1:A:28:MET:HE1	1:A:66:PHE:CB	2.39	0.44
1:A:153:ARG:O	1:A:157:TYR:HB3	2.18	0.44
2:B:74:ALA:HA	2:B:75:PRO:HD3	1.86	0.44
1:C:797:GLY:HA2	1:C:875:TYR:CE2	2.52	0.44
2:D:103:LYS:HE2	2:D:116:TRP:NE1	2.33	0.44
8:E:1394:HOH:O	2:F:60:ASP:HB2	2.17	0.44
2:F:21:MET:CA	2:F:21:MET:CE	2.95	0.44
2:F:46:MET:HB2	7:F:303:SF4:S2	2.58	0.44
1:I:772:MET:HB2	1:I:801:LEU:HD13	1.99	0.44
1:I:871:LYS:HE2	8:I:1230:HOH:O	2.18	0.44
2:L:1:MET:HE2	2:L:88:GLU:CG	2.48	0.44
2:L:10:VAL:HG13	2:L:63:TYR:O	2.18	0.44
1:O:1:MET:N	1:O:22:ASP:OD1	2.44	0.44
1:Q:620:PHE:CZ	1:Q:625:MET:HB3	2.52	0.44
1:U:17:PHE:CE2	1:U:31:MET:HE3	2.53	0.44
2:X:135:ASP:OD1	2:X:137:SER:HB2	2.17	0.44
2:B:76:CYS:HB2	2:B:84:VAL:HG11	1.99	0.44
1:C:214:PHE:HA	1:C:347:ALA:HB3	1.99	0.44
2:D:18:ASN:HB2	7:D:302:SF4:S1	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:MET:HE1	2:D:65:PRO:C	2.43	0.44
1:I:146:MET:HG2	4:I:902:MGD:N7	2.33	0.44
1:I:165:GLY:CA	1:I:166:PHE:HB3	2.44	0.44
2:J:60:ASP:C	2:J:60:ASP:OD1	2.60	0.44
1:K:629:MET:HE2	1:K:634:PHE:CA	2.44	0.44
1:M:610:LYS:NZ	1:M:618:GLN:NE2	2.60	0.44
1:Q:401:PHE:HA	1:Q:402:PRO:HD3	1.82	0.44
1:U:142:SER:HB3	4:U:902:MGD:O1A	2.18	0.44
1:W:76:ILE:HG22	1:W:541:PRO:HG3	1.99	0.44
1:W:452:ILE:N	1:W:453:PRO:CD	2.81	0.44
2:X:46:MET:HE2	2:X:48:ILE:HG12	2.00	0.44
1:A:66:PHE:CD1	1:A:69:MET:CE	3.01	0.44
1:E:75:ARG:HH21	1:E:543:CYS:HA	1.83	0.44
1:E:177:GLU:HA	1:E:177:GLU:OE2	2.17	0.44
1:E:482:TYR:HA	1:E:483:PRO:C	2.43	0.44
1:E:498:GLY:N	1:E:499:PRO:HD3	2.33	0.44
1:E:610:LYS:NZ	1:E:618:GLN:NE2	2.58	0.44
1:E:610:LYS:HZ3	1:E:618:GLN:NE2	2.16	0.44
1:G:737:PRO:HG2	4:G:903:MGD:H2'	1.99	0.44
1:G:767:TYR:HB3	1:G:769:TYR:CE1	2.53	0.44
4:G:903:MGD:O1B	4:G:903:MGD:H4'	2.16	0.44
1:I:870:ASP:HB3	1:I:872:TYR:CE1	2.52	0.44
2:J:201:ALA:HB2	2:J:269:LEU:HB2	1.99	0.44
1:K:165:GLY:HA3	1:K:166:PHE:CB	2.37	0.44
1:K:563:ASP:O	1:K:566:GLN:HG2	2.18	0.44
1:K:571:ARG:HB2	1:K:642:VAL:HB	2.00	0.44
1:M:176:TRP:O	1:M:177:GLU:C	2.59	0.44
1:Q:629:MET:HE2	1:Q:634:PHE:CA	2.48	0.44
2:R:7:VAL:HB	2:R:155:GLU:HB3	2.00	0.44
1:S:218:ASP:OD2	1:S:253:ASN:HB2	2.18	0.44
1:U:74:LEU:HD12	1:U:750:LYS:HA	1.99	0.44
1:U:128:ILE:CD1	1:U:492:MET:HB2	2.48	0.44
1:W:214:PHE:HA	1:W:347:ALA:HB3	2.00	0.44
1:A:10:SER:HA	1:A:15:PRO:HA	2.00	0.44
1:A:177:GLU:HA	1:A:177:GLU:OE2	2.18	0.44
1:A:460:LYS:HG3	8:A:1230:HOH:O	2.18	0.44
1:C:262:LYS:HG2	2:D:232:PHE:CE1	2.53	0.44
1:E:426:MET:HE3	1:E:426:MET:CA	2.39	0.44
1:G:211:MET:HE3	1:G:244:ASP:HB2	1.98	0.44
2:J:105:LEU:HB3	2:J:114:MET:CE	2.48	0.44
1:M:47:ARG:HD2	1:M:241:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:166:LYS:HE2	2:P:170:GLU:OE2	2.18	0.44
1:Q:187:TRP:CH2	1:Q:196:PRO:HB3	2.53	0.44
1:Q:426:MET:HE3	1:Q:426:MET:CA	2.38	0.44
1:Q:786:ASN:ND2	1:Q:805:VAL:H	2.16	0.44
1:S:12:THR:O	1:S:226:TYR:HA	2.18	0.44
1:S:451:LYS:HG3	1:S:461:PHE:CE2	2.52	0.44
2:T:201:ALA:HB2	2:T:269:LEU:HB2	2.00	0.44
1:U:146:MET:HE2	1:U:544:THR:HA	2.00	0.44
1:U:494:TRP:HE1	1:U:525:GLN:HE21	1.64	0.44
1:U:649:LYS:HE3	1:U:651:THR:CG2	2.48	0.44
2:V:94:ILE:O	2:V:96:PRO:HD3	2.17	0.44
1:W:257:ARG:HD3	2:X:61:ILE:HG21	1.99	0.44
1:W:322:GLU:HG3	1:W:327:VAL:O	2.17	0.44
2:X:46:MET:HE1	2:X:65:PRO:C	2.42	0.44
2:X:80:GLY:O	2:X:81:ASN:HB3	2.18	0.44
1:C:557:CYS:H	1:C:564:ASN:ND2	1.93	0.43
1:C:786:ASN:HD22	1:C:786:ASN:HA	1.57	0.43
2:F:21:MET:HA	2:F:21:MET:CE	2.48	0.43
2:F:211:GLU:HB2	2:F:231:PHE:HA	2.00	0.43
1:I:353:GLY:O	1:I:354:TRP:HB2	2.18	0.43
1:I:451:LYS:HA	1:I:454:GLU:OE1	2.17	0.43
1:I:610:LYS:HZ3	1:I:618:GLN:HE22	1.65	0.43
2:J:204:LEU:HD23	2:J:209:CYS:HA	2.00	0.43
1:K:716:PRO:HB3	1:K:723:HIS:CG	2.53	0.43
2:L:213:ALA:O	2:L:228:GLU:HA	2.18	0.43
1:O:162:ASN:CG	1:O:437:SER:HB2	2.43	0.43
1:Q:347:ALA:CB	1:Q:388:SER:HA	2.48	0.43
1:Q:737:PRO:CG	4:Q:903:MGD:H2'	2.48	0.43
1:Q:767:TYR:HB3	1:Q:769:TYR:CE1	2.52	0.43
1:S:32:ASP:HB2	8:S:1643:HOH:O	2.16	0.43
1:S:141:PRO:CA	1:S:496:TYR:HB3	2.43	0.43
1:S:187:TRP:CH2	1:S:196:PRO:HB3	2.53	0.43
1:S:249:ASP:OD1	4:S:903:MGD:H1'	2.18	0.43
1:S:427:PHE:CG	1:S:434:PRO:HG3	2.53	0.43
2:T:46:MET:HE1	2:T:65:PRO:HA	2.00	0.43
2:T:59:ASN:H	2:T:59:ASN:HD22	1.65	0.43
2:T:60:ASP:C	2:T:60:ASP:OD1	2.61	0.43
1:U:451:LYS:HG3	1:U:461:PHE:CE2	2.53	0.43
1:W:725:PRO:HD2	8:W:1195:HOH:O	2.18	0.43
2:X:252:ASP:C	2:X:254:LYS:N	2.75	0.43
1:A:272:HIS:O	1:A:276:PHE:HD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:CYS:HB3	2:B:70:HIS:ND1	2.33	0.43
1:C:30:PRO:HG3	1:C:59:ILE:HG12	1.99	0.43
1:C:673:ASN:HD22	1:C:673:ASN:H	1.65	0.43
1:E:100:LEU:CD1	1:E:105:PRO:HG3	2.46	0.43
1:E:377:GLN:O	1:E:381:LYS:HE2	2.17	0.43
1:I:83:LYS:HE3	1:I:109:TYR:O	2.18	0.43
1:I:716:PRO:HB3	1:I:723:HIS:CD2	2.53	0.43
2:J:21:MET:CE	2:J:21:MET:CA	2.96	0.43
1:M:146:MET:HE3	1:M:544:THR:CA	2.46	0.43
1:Q:494:TRP:HE1	1:Q:525:GLN:HE21	1.66	0.43
1:Q:571:ARG:HB2	1:Q:642:VAL:HB	1.99	0.43
1:Q:797:GLY:HA2	1:Q:875:TYR:CE2	2.53	0.43
2:R:247:VAL:O	2:R:257:SER:HA	2.18	0.43
1:U:729:LYS:HD2	8:U:1134:HOH:O	2.18	0.43
1:W:263:TRP:CZ2	1:W:265:SER:HB2	2.53	0.43
2:X:39:MET:HG2	2:X:40:GLN:N	2.32	0.43
1:C:249:ASP:OD1	4:C:903:MGD:H1'	2.19	0.43
1:C:356:GLY:N	4:C:903:MGD:PB	2.88	0.43
1:C:558:SER:H	1:C:564:ASN:ND2	2.15	0.43
1:C:785:LYS:HB2	1:C:785:LYS:HZ3	1.83	0.43
1:G:21:LYS:HB3	1:G:26:ILE:HD11	2.00	0.43
1:G:426:MET:HA	1:G:426:MET:CE	2.42	0.43
1:K:21:LYS:CB	1:K:26:ILE:HD11	2.49	0.43
1:K:96:ARG:HD2	1:K:514:TYR:O	2.17	0.43
1:M:66:PHE:CD1	1:M:69:MET:CE	3.02	0.43
1:M:146:MET:HG2	4:M:902:MGD:N7	2.33	0.43
1:O:216:SER:OG	4:O:903:MGD:H5'2	2.18	0.43
1:O:291:GLU:CD	1:O:291:GLU:H	2.27	0.43
1:Q:21:LYS:HB3	1:Q:26:ILE:HD11	2.00	0.43
1:Q:540:LEU:HA	1:Q:541:PRO:HD3	1.84	0.43
1:Q:725:PRO:HA	1:U:704:ILE:HG13	2.00	0.43
1:S:142:SER:HB3	4:S:902:MGD:O1A	2.18	0.43
1:S:175:SER:HB2	1:S:176:TRP:CE3	2.53	0.43
2:T:176:ILE:HG22	2:T:177:LYS:HG3	2.01	0.43
1:W:716:PRO:HB3	1:W:723:HIS:CG	2.54	0.43
2:X:1:MET:HE2	2:X:88:GLU:HB3	2.00	0.43
1:A:871:LYS:HE2	8:A:1231:HOH:O	2.18	0.43
1:C:503:THR:C	1:C:504:MET:HE2	2.43	0.43
1:C:816:SER:OG	1:C:839:ILE:HG13	2.18	0.43
2:D:121:ASN:CG	1:S:608:GLU:O	2.61	0.43
1:G:15:PRO:HD3	1:G:554:PHE:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:378:GLY:O	1:I:381:LYS:HG2	2.17	0.43
2:J:70:HIS:HD2	2:J:92:VAL:N	2.03	0.43
1:K:767:TYR:HB3	1:K:769:TYR:CE1	2.53	0.43
1:M:111:ARG:NH2	1:M:585:GLU:OE2	2.44	0.43
1:O:12:THR:O	1:O:226:TYR:HA	2.19	0.43
1:O:716:PRO:HB3	1:O:723:HIS:CD2	2.53	0.43
1:Q:69:MET:HE2	1:Q:754:MET:HE3	1.91	0.43
2:R:5:TYR:CD2	2:R:164:MET:HG2	2.53	0.43
2:R:19:CYS:O	2:R:22:GLY:N	2.52	0.43
2:R:159:THR:OG1	2:R:160:THR:N	2.51	0.43
1:S:175:SER:OG	6:S:905:BTT:C5	2.66	0.43
1:U:656:TRP:CD2	1:U:663:LYS:HA	2.53	0.43
2:V:46:MET:HE3	2:V:46:MET:C	2.42	0.43
1:W:673:ASN:H	1:W:673:ASN:ND2	2.17	0.43
1:A:66:PHE:HA	1:A:69:MET:CE	2.37	0.43
1:A:587:MET:HE3	1:A:591:GLU:HB3	2.00	0.43
1:A:770:TRP:HB3	1:A:801:LEU:HD23	2.01	0.43
2:B:69:MET:HB3	2:B:184:PRO:HB3	1.99	0.43
1:C:146:MET:HE2	1:C:544:THR:CA	2.49	0.43
2:D:176:ILE:HG22	2:D:177:LYS:HG3	2.01	0.43
1:E:871:LYS:HE2	8:E:1233:HOH:O	2.19	0.43
2:F:46:MET:HE2	2:F:48:ILE:HG12	2.00	0.43
2:F:247:VAL:O	2:F:257:SER:HA	2.19	0.43
1:G:35:ASP:OD1	1:G:55:ARG:HD3	2.19	0.43
1:G:75:ARG:NH2	1:G:543:CYS:HA	2.33	0.43
1:G:772:MET:HB2	1:G:801:LEU:HD13	1.99	0.43
2:H:21:MET:CE	2:H:21:MET:CA	2.96	0.43
1:K:494:TRP:HE1	1:K:525:GLN:HE21	1.67	0.43
1:M:15:PRO:HD3	1:M:554:PHE:CD1	2.53	0.43
1:M:141:PRO:CA	1:M:496:TYR:HB3	2.43	0.43
1:M:143:SER:N	4:M:902:MGD:O1A	2.52	0.43
2:N:91:ILE:HG22	2:N:93:LEU:HG	2.01	0.43
1:O:165:GLY:CA	1:O:166:PHE:HB3	2.46	0.43
1:Q:74:LEU:HD12	1:Q:750:LYS:HA	2.01	0.43
1:S:825:PRO:HD2	8:S:1331:HOH:O	2.19	0.43
2:T:122:VAL:HG22	2:T:123:ALA:N	2.34	0.43
1:W:39:ALA:HA	1:W:40:PRO:HD3	1.88	0.43
1:W:262:LYS:HG2	2:X:232:PHE:CE1	2.53	0.43
1:W:355:GLY:HA2	4:W:903:MGD:O1B	2.18	0.43
1:W:528:TRP:CD2	1:W:750:LYS:HD3	2.54	0.43
2:X:73:ASN:O	2:X:75:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HE2	1:A:190:SER:HA	2.00	0.43
1:C:512:LYS:HE3	1:C:830:GLY:O	2.18	0.43
1:E:139:SER:CB	1:E:161:MET:HE2	2.48	0.43
1:E:301:GLU:CD	1:E:301:GLU:N	2.77	0.43
2:F:176:ILE:HG22	2:F:177:LYS:HG3	2.00	0.43
1:G:142:SER:HB3	4:G:902:MGD:O1A	2.18	0.43
1:G:670:PRO:HG2	1:G:675:GLN:CD	2.42	0.43
2:H:19:CYS:O	2:H:22:GLY:N	2.51	0.43
1:I:558:SER:H	1:I:564:ASN:ND2	2.16	0.43
2:N:23:CYS:O	2:N:27:HIS:N	2.49	0.43
1:O:587:MET:HE3	1:O:591:GLU:HB3	2.00	0.43
1:Q:146:MET:HE2	1:Q:544:THR:CA	2.49	0.43
1:Q:166:PHE:N	1:Q:439:LEU:HD12	2.34	0.43
1:Q:452:ILE:N	1:Q:453:PRO:CD	2.81	0.43
1:S:501:LEU:HD13	1:S:823:TYR:CD2	2.53	0.43
1:A:141:PRO:CA	1:A:496:TYR:HB3	2.39	0.43
1:A:400:TYR:CE1	1:A:421:LYS:HD2	2.54	0.43
1:G:9:ASN:HA	1:G:576:GLN:HA	2.01	0.43
2:H:143:PRO:HB3	7:H:303:SF4:S1	2.58	0.43
1:K:378:GLY:O	1:K:381:LYS:HG2	2.17	0.43
2:L:106:LEU:HD23	2:L:114:MET:CE	2.49	0.43
2:P:68:CYS:CB	2:P:126:CYS:CB	2.85	0.43
1:Q:356:GLY:H	4:Q:903:MGD:H5'2	1.84	0.43
1:S:139:SER:CB	1:S:161:MET:HE2	2.49	0.43
2:T:49:GLU:HG3	2:T:64:ARG:NH2	2.33	0.43
1:U:139:SER:CB	1:U:161:MET:HE2	2.49	0.43
1:W:347:ALA:HB1	1:W:388:SER:HA	2.01	0.43
1:W:533:VAL:HB	1:W:534:PRO:HD3	1.99	0.43
2:X:247:VAL:O	2:X:257:SER:HA	2.19	0.43
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.84	0.43
1:A:144:HIS:HB2	4:A:902:MGD:O1B	2.18	0.43
1:C:9:ASN:HA	1:C:576:GLN:HA	1.99	0.43
1:C:175:SER:OG	6:C:905:BTT:C5	2.66	0.43
1:C:495:LYS:CD	1:C:514:TYR:OH	2.67	0.43
1:E:15:PRO:HD2	8:E:1003:HOH:O	2.17	0.43
1:E:857:ASN:HB3	4:E:902:MGD:N19	2.34	0.43
2:H:166:LYS:HE2	2:H:170:GLU:OE2	2.19	0.43
1:I:629:MET:HE2	1:I:634:PHE:N	2.34	0.43
1:K:670:PRO:HG2	1:K:675:GLN:CD	2.44	0.43
1:S:39:ALA:HA	1:S:40:PRO:HD3	1.87	0.43
1:U:100:LEU:CD1	1:U:105:PRO:HG3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:565:TYR:C	1:W:567:LEU:H	2.26	0.43
1:A:557:CYS:N	1:A:564:ASN:HD21	1.93	0.43
1:A:571:ARG:HA	8:A:1026:HOH:O	2.18	0.43
1:C:165:GLY:CA	1:C:166:PHE:HB3	2.46	0.43
1:E:452:ILE:N	1:E:453:PRO:CD	2.81	0.43
1:G:825:PRO:HD2	8:G:1335:HOH:O	2.19	0.43
2:H:58:ARG:HD2	2:H:268:ASP:OD1	2.19	0.43
2:H:60:ASP:C	2:H:60:ASP:OD1	2.62	0.43
1:I:74:LEU:HD12	1:I:750:LYS:HA	2.00	0.43
2:J:5:TYR:HB2	2:J:157:LEU:HD12	1.98	0.43
2:J:175:VAL:HG23	2:J:178:PRO:HG3	2.00	0.43
1:K:722:LYS:HE3	1:K:722:LYS:HB2	1.86	0.43
1:O:378:GLY:O	1:O:381:LYS:HG2	2.19	0.43
1:O:540:LEU:HA	1:O:541:PRO:HD3	1.82	0.43
2:P:87:ARG:HD3	2:P:93:LEU:HD12	2.01	0.43
2:P:106:LEU:HA	2:P:114:MET:HE2	1.99	0.43
1:Q:433:PHE:HA	1:Q:434:PRO:HD3	1.84	0.43
2:R:60:ASP:C	2:R:60:ASP:OD1	2.61	0.43
1:W:81:LYS:HB2	1:W:112:ILE:HD13	2.00	0.43
2:B:72:GLU:HG2	2:B:185:ARG:NH2	2.34	0.43
2:B:189:LYS:HD2	8:B:499:HOH:O	2.19	0.43
1:C:146:MET:HE2	1:C:544:THR:HA	2.01	0.43
1:E:558:SER:H	1:E:564:ASN:ND2	2.17	0.43
2:F:46:MET:HE2	2:F:48:ILE:HG13	2.01	0.43
1:G:482:TYR:CD1	1:G:483:PRO:HA	2.54	0.43
2:H:114:MET:HA	2:H:125:LYS:HB3	2.01	0.43
1:I:35:ASP:OD1	1:I:55:ARG:HD3	2.19	0.43
1:I:476:GLN:OE1	1:I:708:ARG:NH2	2.52	0.43
1:M:142:SER:OG	4:M:902:MGD:O1A	2.31	0.43
1:M:691:ILE:CG1	1:M:711:MET:HE3	2.49	0.43
2:N:166:LYS:HG2	2:N:170:GLU:OE2	2.18	0.43
1:S:454:GLU:CD	1:S:454:GLU:H	2.26	0.43
1:U:177:GLU:HA	1:U:177:GLU:OE2	2.18	0.43
1:U:770:TRP:HB3	1:U:801:LEU:HD23	2.01	0.43
1:W:677:CYS:C	1:W:678:ARG:HG2	2.43	0.43
2:D:5:TYR:HB2	2:D:157:LEU:HD11	2.01	0.42
1:G:505:THR:HG22	1:G:857:ASN:ND2	2.35	0.42
2:H:68:CYS:HB3	2:H:70:HIS:ND1	2.34	0.42
1:K:459:GLY:O	1:K:489:LYS:HE2	2.19	0.42
1:M:21:LYS:CB	1:M:26:ILE:HD11	2.49	0.42
1:O:263:TRP:CZ2	1:O:265:SER:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:401:PHE:HA	1:O:402:PRO:HD3	1.83	0.42
1:O:452:ILE:N	1:O:453:PRO:CD	2.81	0.42
2:P:53:ARG:HB2	2:P:60:ASP:OD1	2.19	0.42
1:Q:147:TRP:CD1	1:Q:552:SER:HG	2.37	0.42
1:U:393:VAL:HA	1:U:394:PRO:HD3	1.84	0.42
1:W:356:GLY:N	4:W:903:MGD:PB	2.91	0.42
1:A:128:ILE:CD1	1:A:492:MET:HB2	2.49	0.42
1:A:521:PHE:CE2	1:A:523:VAL:CG2	3.01	0.42
1:A:867:TRP:CD1	1:A:869:GLY:H	2.36	0.42
1:C:165:GLY:HA3	1:C:166:PHE:CB	2.42	0.42
1:C:296:ASN:HB3	1:C:657:PHE:CZ	2.55	0.42
1:C:724:SER:HA	1:C:725:PRO:HD3	1.94	0.42
2:D:109:CYS:HA	2:D:110:PRO:HD3	1.89	0.42
1:E:61:PRO:HG3	2:F:16:CYS:HB2	2.01	0.42
1:E:103:GLN:CD	1:E:103:GLN:N	2.78	0.42
1:E:629:MET:HE2	1:E:634:PHE:N	2.34	0.42
1:G:177:GLU:HA	1:G:177:GLU:OE2	2.19	0.42
1:G:347:ALA:CB	1:G:388:SER:HA	2.50	0.42
1:G:494:TRP:HE1	1:G:525:GLN:HE21	1.66	0.42
2:H:177:LYS:N	2:H:178:PRO:HD3	2.33	0.42
1:I:76:ILE:HA	1:I:77:PRO:HD3	1.78	0.42
1:I:165:GLY:HA3	1:I:166:PHE:CB	2.37	0.42
1:K:9:ASN:HA	1:K:576:GLN:HA	2.01	0.42
1:K:786:ASN:HD22	1:K:786:ASN:HA	1.58	0.42
2:N:2:GLU:HB3	2:N:158:LYS:HE2	2.01	0.42
2:N:74:ALA:HA	2:N:75:PRO:HD3	1.86	0.42
1:O:587:MET:HE2	1:O:592:ILE:HA	2.01	0.42
1:O:717:ALA:HB3	1:O:720:SER:HB3	2.00	0.42
2:P:10:VAL:HG13	2:P:63:TYR:O	2.19	0.42
2:P:46:MET:HE2	2:P:48:ILE:CG1	2.49	0.42
2:V:177:LYS:N	2:V:178:PRO:HD3	2.34	0.42
2:V:219:SER:C	2:V:221:GLY:H	2.26	0.42
1:W:291:GLU:CD	1:W:291:GLU:H	2.27	0.42
1:W:521:PHE:CE2	1:W:523:VAL:CG2	3.01	0.42
1:A:540:LEU:HA	1:A:541:PRO:HD3	1.77	0.42
1:C:347:ALA:CB	1:C:388:SER:HA	2.48	0.42
1:C:521:PHE:CE2	1:C:523:VAL:CG2	3.03	0.42
2:D:60:ASP:OD1	2:D:60:ASP:C	2.61	0.42
1:I:155:SER:OG	1:I:409:ILE:HG12	2.19	0.42
1:K:772:MET:HB2	1:K:801:LEU:HD13	2.01	0.42
1:M:319:GLU:HG2	1:S:726:LEU:CD1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:629:MET:HE2	1:M:634:PHE:CA	2.49	0.42
2:N:19:CYS:HB2	2:N:20:PHE:H	1.51	0.42
2:N:114:MET:HA	2:N:125:LYS:HB3	2.00	0.42
1:Q:250:PRO:HD3	4:Q:903:MGD:C2	2.49	0.42
1:Q:356:GLY:H	4:Q:903:MGD:C5'	2.32	0.42
2:R:27:HIS:HE1	8:R:469:HOH:O	2.01	0.42
2:R:106:LEU:HD11	2:R:116:TRP:HB2	2.01	0.42
1:S:725:PRO:HD2	8:S:1195:HOH:O	2.20	0.42
1:S:770:TRP:HB3	1:S:801:LEU:HD23	2.01	0.42
1:U:269:GLY:HA2	1:U:362:HIS:CE1	2.54	0.42
1:W:554:PHE:HB3	8:W:1025:HOH:O	2.19	0.42
2:X:80:GLY:C	2:X:82:GLY:H	2.27	0.42
1:A:361:SER:OG	1:A:717:ALA:HB1	2.20	0.42
2:B:13:CYS:HB3	2:B:63:TYR:HB2	2.01	0.42
1:C:182:GLY:HA3	1:C:364:ILE:HG23	2.01	0.42
1:C:855:MET:HB2	1:C:857:ASN:OD1	2.20	0.42
2:D:179:GLU:OE1	2:D:179:GLU:N	2.52	0.42
2:F:69:MET:O	2:F:70:HIS:C	2.62	0.42
1:K:262:LYS:HG2	2:L:232:PHE:CE1	2.53	0.42
1:K:557:CYS:H	1:K:564:ASN:ND2	1.90	0.42
2:P:7:VAL:HB	2:P:155:GLU:HB3	2.02	0.42
1:Q:495:LYS:HD2	1:Q:514:TYR:OH	2.20	0.42
1:Q:818:GLU:CD	1:Q:819:SER:OG	2.63	0.42
1:U:250:PRO:HD3	4:U:903:MGD:C2	2.50	0.42
1:A:610:LYS:HB3	1:A:614:ALA:HB3	2.01	0.42
1:C:65:GLY:HA3	2:D:21:MET:HG3	2.01	0.42
1:E:495:LYS:HE3	1:E:497:GLY:O	2.19	0.42
2:F:114:MET:HA	2:F:125:LYS:HB3	2.02	0.42
2:F:138:TRP:CD2	2:F:140:PRO:HD2	2.54	0.42
2:F:177:LYS:N	2:F:178:PRO:HD3	2.35	0.42
1:G:521:PHE:CE2	1:G:523:VAL:CG2	3.02	0.42
2:H:191:LEU:HG	2:H:195:GLU:HG3	2.01	0.42
1:I:100:LEU:CD1	1:I:105:PRO:HG3	2.49	0.42
1:K:76:ILE:HA	1:K:77:PRO:HD3	1.76	0.42
1:K:433:PHE:HA	1:K:434:PRO:HD3	1.79	0.42
1:M:561:ILE:CG2	1:M:564:ASN:HB3	2.47	0.42
1:O:521:PHE:CE2	1:O:523:VAL:CG2	3.02	0.42
1:Q:21:LYS:CB	1:Q:26:ILE:HD11	2.49	0.42
1:Q:141:PRO:CA	1:Q:496:TYR:HB3	2.40	0.42
1:S:76:ILE:HG22	1:S:541:PRO:HG3	2.02	0.42
1:U:426:MET:HE1	1:U:618:GLN:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:40:GLN:NE2	2:V:118:GLU:H	2.17	0.42
2:V:210:PHE:HD2	2:V:213:ALA:HB2	1.85	0.42
1:A:347:ALA:HB1	1:A:388:SER:HA	2.01	0.42
1:E:322:GLU:HG3	1:E:327:VAL:O	2.20	0.42
1:G:21:LYS:CB	1:G:26:ILE:HD11	2.50	0.42
1:I:301:GLU:CD	1:I:301:GLU:H	2.27	0.42
1:I:517:ASP:HB3	8:I:1203:HOH:O	2.19	0.42
1:M:146:MET:CE	1:M:544:THR:HG22	2.49	0.42
1:M:347:ALA:HB1	1:M:388:SER:HA	2.01	0.42
2:N:106:LEU:CD2	2:N:114:MET:HB3	2.50	0.42
1:O:114:TRP:CZ2	1:O:587:MET:HG2	2.55	0.42
1:S:362:HIS:HB3	1:S:717:ALA:HB2	2.01	0.42
1:U:355:GLY:CA	4:U:903:MGD:O1B	2.64	0.42
1:A:291:GLU:CD	1:A:291:GLU:N	2.77	0.42
1:A:296:ASN:HB3	1:A:657:PHE:CZ	2.55	0.42
2:B:46:MET:HE1	2:B:65:PRO:HA	2.01	0.42
1:C:257:ARG:HD3	2:D:61:ILE:HG21	2.01	0.42
1:C:353:GLY:O	1:C:354:TRP:HB2	2.19	0.42
2:D:19:CYS:HB2	2:D:46:MET:HG2	2.01	0.42
1:E:142:SER:OG	4:E:902:MGD:O1A	2.29	0.42
1:E:673:ASN:H	1:E:673:ASN:ND2	2.17	0.42
2:F:21:MET:CE	2:F:24:MET:HE3	2.49	0.42
1:G:103:GLN:N	1:G:103:GLN:CD	2.78	0.42
1:G:165:GLY:CA	1:G:166:PHE:HB3	2.46	0.42
1:G:495:LYS:CD	1:G:514:TYR:OH	2.68	0.42
1:G:644:ASP:OD1	1:G:646:PRO:HG3	2.20	0.42
1:I:426:MET:HE3	1:I:622:ALA:HB2	2.02	0.42
1:K:426:MET:HE3	1:K:426:MET:CA	2.39	0.42
2:L:76:CYS:O	2:L:80:GLY:N	2.52	0.42
2:L:119:GLU:HB2	8:L:442:HOH:O	2.19	0.42
2:L:247:VAL:O	2:L:257:SER:HA	2.19	0.42
1:M:140:THR:HB	1:M:169:ALA:HB3	2.01	0.42
1:O:146:MET:HE3	1:O:545:ASN:H	1.85	0.42
1:Q:291:GLU:CD	1:Q:291:GLU:N	2.76	0.42
1:Q:476:GLN:OE1	1:Q:708:ARG:NH2	2.52	0.42
1:Q:501:LEU:HD13	1:Q:823:TYR:CD2	2.54	0.42
1:Q:565:TYR:C	1:Q:567:LEU:H	2.27	0.42
2:T:177:LYS:N	2:T:178:PRO:HD3	2.34	0.42
1:U:630:THR:OG1	1:U:633:GLU:HG3	2.20	0.42
1:W:356:GLY:H	4:W:903:MGD:H5'2	1.83	0.42
1:A:673:ASN:H	1:A:673:ASN:ND2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:PHE:CE2	2:B:24:MET:HE2	2.55	0.42
2:B:106:LEU:HA	2:B:114:MET:HE2	2.01	0.42
1:C:142:SER:HB3	4:C:902:MGD:O1A	2.20	0.42
1:C:735:LEU:HD23	1:C:735:LEU:H	1.85	0.42
1:G:263:TRP:CZ2	1:G:265:SER:HB2	2.55	0.42
1:I:66:PHE:CD1	1:I:69:MET:CE	3.03	0.42
1:I:730:TYR:CE1	1:I:794:ASN:HA	2.54	0.42
2:J:19:CYS:O	2:J:22:GLY:N	2.53	0.42
2:J:162:GLU:CD	2:J:162:GLU:N	2.78	0.42
1:M:401:PHE:HA	1:M:402:PRO:HD3	1.87	0.42
1:M:670:PRO:HB3	1:M:682:GLN:HB2	2.02	0.42
1:O:322:GLU:HG3	1:O:327:VAL:O	2.19	0.42
2:P:46:MET:HE3	2:P:47:ASN:C	2.44	0.42
1:Q:139:SER:CB	1:Q:161:MET:HE2	2.49	0.42
1:Q:426:MET:HE1	1:Q:618:GLN:O	2.20	0.42
1:Q:780:GLU:C	1:Q:780:GLU:CD	2.86	0.42
2:T:4:TYR:CE2	2:T:158:LYS:HD2	2.55	0.42
2:T:162:GLU:H	2:T:162:GLU:CD	2.28	0.42
1:U:76:ILE:CG2	1:U:541:PRO:HG3	2.47	0.42
2:V:4:TYR:CE2	2:V:158:LYS:HD2	2.55	0.42
1:A:15:PRO:HD3	1:A:554:PHE:CE1	2.54	0.42
1:A:139:SER:CB	1:A:161:MET:HE2	2.49	0.42
1:A:786:ASN:ND2	1:A:805:VAL:H	2.10	0.42
2:B:69:MET:O	2:B:70:HIS:C	2.63	0.42
1:C:738:HIS:HE2	4:C:902:MGD:H15	1.68	0.42
2:D:3:GLN:O	2:D:158:LYS:HA	2.20	0.42
1:G:111:ARG:NH2	1:G:585:GLU:OE2	2.45	0.42
1:G:452:ILE:N	1:G:453:PRO:CD	2.83	0.42
2:H:18:ASN:HB2	7:H:302:SF4:S1	2.60	0.42
1:K:296:ASN:HB3	1:K:657:PHE:CZ	2.54	0.42
1:M:495:LYS:CD	1:M:514:TYR:OH	2.67	0.42
2:N:5:TYR:HB2	2:N:157:LEU:HD12	2.02	0.42
2:N:162:GLU:H	2:N:162:GLU:CD	2.28	0.42
1:O:15:PRO:HD3	1:O:554:PHE:CE1	2.55	0.42
1:Q:498:GLY:N	1:Q:499:PRO:HD3	2.34	0.42
1:Q:677:CYS:C	1:Q:678:ARG:HG2	2.44	0.42
2:R:176:ILE:HG22	2:R:177:LYS:HG3	2.02	0.42
1:S:257:ARG:HD3	2:T:61:ILE:HG21	2.02	0.42
1:S:691:ILE:HD11	1:S:711:MET:HE3	2.02	0.42
1:U:395:LEU:HD12	1:U:566:GLN:HA	2.01	0.42
1:U:426:MET:HE2	1:U:618:GLN:HG2	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:797:GLY:HA2	1:U:875:TYR:CE2	2.54	0.42
1:W:9:ASN:HA	1:W:576:GLN:HA	2.01	0.42
1:W:187:TRP:CH2	1:W:196:PRO:HB3	2.54	0.42
2:X:46:MET:HE3	2:X:47:ASN:C	2.45	0.42
1:C:565:TYR:C	1:C:567:LEU:H	2.28	0.42
2:D:210:PHE:HD2	2:D:213:ALA:HB2	1.85	0.42
1:E:218:ASP:OD2	1:E:253:ASN:HB2	2.19	0.42
1:G:501:LEU:HD13	1:G:823:TYR:CD2	2.55	0.42
1:I:263:TRP:CZ2	1:I:265:SER:HB2	2.55	0.42
1:K:15:PRO:HD2	8:K:1003:HOH:O	2.19	0.42
1:K:143:SER:N	4:K:902:MGD:O1A	2.52	0.42
1:K:797:GLY:HA2	1:K:875:TYR:CE2	2.55	0.42
1:O:75:ARG:HH21	1:O:543:CYS:HA	1.85	0.42
1:Q:610:LYS:HB3	1:Q:614:ALA:HB3	2.01	0.42
2:R:18:ASN:HB2	7:R:302:SF4:S1	2.59	0.42
2:R:70:HIS:HD2	2:R:92:VAL:N	2.02	0.42
2:R:177:LYS:N	2:R:178:PRO:HD3	2.34	0.42
1:U:396:ASP:OD2	1:U:398:GLU:HB2	2.20	0.42
2:D:19:CYS:O	2:D:22:GLY:N	2.53	0.41
2:F:21:MET:HE2	2:F:24:MET:HE3	2.01	0.41
1:G:291:GLU:CD	1:G:291:GLU:H	2.28	0.41
2:H:19:CYS:HB2	2:H:20:PHE:H	1.38	0.41
1:I:77:PRO:HB2	1:I:78:TYR:CD2	2.54	0.41
1:I:257:ARG:HD3	2:J:61:ILE:HG21	2.02	0.41
1:I:418:ALA:HB1	1:I:423:ALA:HB2	2.01	0.41
1:K:75:ARG:HH22	1:K:547:GLU:CD	2.27	0.41
1:K:175:SER:HB2	1:K:176:TRP:CE3	2.55	0.41
1:K:177:GLU:HA	1:K:177:GLU:OE2	2.20	0.41
2:N:13:CYS:HB3	2:N:63:TYR:HB2	2.02	0.41
2:N:18:ASN:HB2	7:N:302:SF4:S1	2.60	0.41
1:O:153:ARG:O	1:O:157:TYR:HB3	2.20	0.41
1:O:772:MET:HB2	1:O:801:LEU:HD13	2.00	0.41
2:P:60:ASP:OD1	2:P:60:ASP:C	2.63	0.41
1:S:353:GLY:O	1:S:354:TRP:HB2	2.20	0.41
2:T:39:MET:HE2	2:T:45:TRP:CD2	2.55	0.41
2:V:105:LEU:HB3	2:V:114:MET:CE	2.50	0.41
1:A:1:MET:H3	1:A:22:ASP:CG	2.26	0.41
1:A:670:PRO:HB3	1:A:682:GLN:HB2	2.03	0.41
1:C:143:SER:N	4:C:902:MGD:O1A	2.53	0.41
1:E:17:PHE:CE2	1:E:31:MET:HE3	2.55	0.41
2:H:10:VAL:HG13	2:H:63:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:CYS:CB	2:H:126:CYS:CB	2.88	0.41
1:I:74:LEU:HD23	1:I:74:LEU:HA	1.90	0.41
1:I:142:SER:CB	4:I:902:MGD:O1A	2.68	0.41
1:I:201:LEU:HD13	1:I:387:TRP:HB2	2.01	0.41
2:J:177:LYS:N	2:J:178:PRO:HD3	2.35	0.41
1:O:21:LYS:CB	1:O:26:ILE:HD11	2.50	0.41
1:O:855:MET:HE2	1:O:857:ASN:OD1	2.20	0.41
2:R:13:CYS:HB3	2:R:63:TYR:HB2	2.01	0.41
1:U:722:LYS:HE3	1:U:722:LYS:HB2	1.88	0.41
2:V:9:ASP:HA	2:V:189:LYS:HB3	2.02	0.41
1:W:138:LEU:HB2	1:W:490:ILE:HD12	2.03	0.41
1:W:165:GLY:CA	1:W:166:PHE:HB3	2.45	0.41
1:A:165:GLY:HA3	1:A:166:PHE:CB	2.40	0.41
1:A:211:MET:HE3	1:A:244:ASP:CB	2.49	0.41
1:C:498:GLY:N	1:C:499:PRO:HD3	2.35	0.41
2:D:56:TYR:HA	2:D:59:ASN:HD22	1.85	0.41
1:E:142:SER:HB3	4:E:902:MGD:O1A	2.20	0.41
1:G:140:THR:HB	1:G:169:ALA:HB3	2.02	0.41
2:H:4:TYR:CE2	2:H:158:LYS:HD2	2.55	0.41
1:I:139:SER:OG	1:I:161:MET:HE2	2.20	0.41
1:I:250:PRO:HD3	4:I:903:MGD:C2	2.51	0.41
2:L:216:VAL:HG13	2:L:223:GLU:HG3	2.02	0.41
2:L:218:LYS:HG2	2:L:223:GLU:HA	2.03	0.41
2:N:39:MET:HE2	2:N:45:TRP:CD2	2.56	0.41
1:Q:174:ASP:OD1	1:Q:175:SER:N	2.49	0.41
1:Q:867:TRP:CD1	1:Q:869:GLY:H	2.39	0.41
1:S:400:TYR:CE1	1:S:421:LYS:HD2	2.55	0.41
1:S:495:LYS:CD	1:S:514:TYR:OH	2.68	0.41
1:U:482:TYR:HA	1:U:483:PRO:C	2.45	0.41
1:E:15:PRO:HD3	1:E:554:PHE:CE1	2.55	0.41
1:E:21:LYS:HB2	1:E:26:ILE:HD11	2.03	0.41
1:E:76:ILE:HA	1:E:77:PRO:HD3	1.80	0.41
1:E:657:PHE:CE1	1:E:681:LEU:HG	2.54	0.41
1:E:753:TYR:HB3	2:F:24:MET:HE3	2.02	0.41
1:G:724:SER:HA	1:G:725:PRO:HD3	1.91	0.41
1:I:800:ILE:CD1	1:I:833:ALA:HB1	2.50	0.41
2:J:104:GLU:CD	2:J:104:GLU:N	2.74	0.41
2:P:179:GLU:OE1	2:P:179:GLU:N	2.45	0.41
1:Q:361:SER:OG	1:Q:717:ALA:HB1	2.20	0.41
1:Q:495:LYS:HD3	8:Q:1105:HOH:O	2.19	0.41
1:S:395:LEU:HD12	1:S:566:GLN:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:677:CYS:C	1:S:678:ARG:HG2	2.44	0.41
1:S:786:ASN:ND2	1:S:804:GLN:HA	2.34	0.41
1:A:85:PHE:CE2	1:A:87:PRO:HG3	2.56	0.41
1:A:140:THR:HB	1:A:169:ALA:HB3	2.01	0.41
1:C:66:PHE:HA	1:C:69:MET:CE	2.41	0.41
1:C:426:MET:HE3	1:C:426:MET:CA	2.41	0.41
1:C:868:ASP:OD1	1:C:870:ASP:HB2	2.20	0.41
1:E:165:GLY:HA3	1:E:166:PHE:CB	2.43	0.41
1:E:540:LEU:HA	1:E:541:PRO:HD3	1.84	0.41
1:G:355:GLY:C	4:G:903:MGD:O2B	2.63	0.41
2:H:114:MET:CE	2:H:123:ALA:HB1	2.43	0.41
1:I:21:LYS:HB2	1:I:26:ILE:HD11	2.02	0.41
1:K:263:TRP:HZ3	2:L:59:ASN:HD21	1.68	0.41
1:K:857:ASN:HB3	4:K:902:MGD:N19	2.35	0.41
2:L:40:GLN:HE21	2:L:117:ASN:HA	1.85	0.41
2:L:46:MET:HE1	2:L:65:PRO:HA	2.01	0.41
1:M:322:GLU:HG3	1:M:327:VAL:O	2.20	0.41
1:M:387:TRP:CE2	1:M:389:THR:HA	2.55	0.41
1:M:786:ASN:ND2	1:M:805:VAL:H	2.18	0.41
1:O:262:LYS:HG2	2:P:232:PHE:CE1	2.55	0.41
1:Q:402:PRO:HG2	1:Q:422:PHE:CE1	2.56	0.41
1:S:452:ILE:HB	1:S:453:PRO:HD3	2.03	0.41
1:S:868:ASP:HA	8:S:1002:HOH:O	2.21	0.41
1:U:625:MET:N	1:U:626:PRO:CD	2.83	0.41
1:W:495:LYS:HD2	1:W:514:TYR:OH	2.20	0.41
2:X:19:CYS:O	2:X:22:GLY:N	2.54	0.41
1:A:124:GLU:HG3	1:A:521:PHE:CD2	2.55	0.41
1:A:558:SER:H	1:A:564:ASN:ND2	2.19	0.41
1:C:53:PRO:HA	1:C:54:PRO:HD3	1.91	0.41
1:C:825:PRO:HD2	8:C:1337:HOH:O	2.21	0.41
2:D:69:MET:O	2:D:70:HIS:C	2.61	0.41
2:F:205:VAL:HG13	2:F:254:LYS:HZ2	1.82	0.41
1:G:162:ASN:CG	1:G:437:SER:HB2	2.46	0.41
1:G:501:LEU:HA	1:G:507:THR:HB	2.03	0.41
1:I:174:ASP:OD1	1:I:175:SER:N	2.50	0.41
2:J:72:GLU:HG2	2:J:185:ARG:NH2	2.36	0.41
1:K:301:GLU:CD	1:K:301:GLU:N	2.76	0.41
1:K:558:SER:H	1:K:564:ASN:ND2	2.18	0.41
1:K:673:ASN:H	1:K:673:ASN:ND2	2.18	0.41
2:L:256:TYR:HB2	2:L:274:LEU:HD21	2.01	0.41
1:M:1:MET:H3	1:M:22:ASP:CG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:15:PRO:HD2	8:M:1003:HOH:O	2.20	0.41
1:M:404:TYR:CD1	1:M:404:TYR:C	2.99	0.41
1:M:421:LYS:HA	1:M:424:TRP:HD1	1.86	0.41
2:N:142:MET:HE2	2:N:146:ALA:C	2.45	0.41
1:O:211:MET:HE3	1:O:244:ASP:HB2	2.02	0.41
1:O:498:GLY:N	1:O:499:PRO:HD3	2.36	0.41
2:P:23:CYS:O	2:P:27:HIS:N	2.45	0.41
2:R:95:ASP:HB3	2:R:98:LYS:HB2	2.03	0.41
1:S:625:MET:N	1:S:626:PRO:CD	2.83	0.41
1:S:857:ASN:HB3	4:S:902:MGD:N19	2.35	0.41
1:U:66:PHE:CD1	1:U:69:MET:CE	3.03	0.41
1:U:184:MET:HE2	1:U:190:SER:HA	2.01	0.41
1:U:610:LYS:NZ	1:U:618:GLN:NE2	2.64	0.41
1:W:2:GLY:N	1:W:22:ASP:OD1	2.53	0.41
1:W:296:ASN:HB3	1:W:657:PHE:CZ	2.55	0.41
1:W:563:ASP:HA	1:W:565:TYR:CE1	2.56	0.41
2:X:46:MET:HE2	2:X:48:ILE:CG1	2.50	0.41
2:X:210:PHE:CE2	2:X:251:ALA:HB1	2.55	0.41
1:A:39:ALA:HA	1:A:40:PRO:HD3	1.90	0.41
1:A:649:LYS:O	1:A:649:LYS:HG3	2.21	0.41
1:C:629:MET:HE2	1:C:634:PHE:HA	2.01	0.41
2:D:56:TYR:HA	2:D:59:ASN:ND2	2.36	0.41
1:E:21:LYS:HB3	1:E:26:ILE:HD11	2.03	0.41
1:I:175:SER:HB2	1:I:176:TRP:CZ3	2.56	0.41
1:I:451:LYS:HG3	1:I:461:PHE:CE2	2.54	0.41
1:I:521:PHE:CE2	1:I:523:VAL:CG2	3.04	0.41
1:K:269:GLY:HA2	1:K:362:HIS:CG	2.55	0.41
1:K:277:ALA:HB2	1:K:321:ALA:HB2	2.03	0.41
1:K:401:PHE:HA	1:K:402:PRO:HD3	1.90	0.41
1:M:165:GLY:CA	1:M:166:PHE:HB3	2.48	0.41
1:M:571:ARG:HB2	1:M:642:VAL:HB	2.03	0.41
1:Q:32:ASP:HB2	8:Q:1658:HOH:O	2.21	0.41
1:Q:736:SER:HA	1:Q:816:SER:O	2.21	0.41
1:S:328:PRO:HB2	1:S:331:GLU:HG3	2.03	0.41
1:S:816:SER:OG	1:S:839:ILE:HG13	2.19	0.41
2:T:10:VAL:HG13	2:T:63:TYR:O	2.20	0.41
1:W:541:PRO:HB2	1:W:586:SER:HA	2.02	0.41
1:A:818:GLU:CD	1:A:819:SER:OG	2.64	0.41
2:D:87:ARG:HG3	2:D:91:ILE:O	2.21	0.41
2:D:139:ALA:HB3	2:D:140:PRO:HD3	2.02	0.41
1:E:155:SER:OG	1:E:409:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:74:ALA:HA	2:F:75:PRO:HD3	1.85	0.41
2:F:162:GLU:CD	2:F:162:GLU:N	2.79	0.41
2:F:175:VAL:HG23	2:F:178:PRO:HG3	2.02	0.41
1:G:66:PHE:HD1	1:G:69:MET:CE	2.34	0.41
1:G:118:THR:O	1:G:122:VAL:HG23	2.21	0.41
2:H:64:ARG:NH1	8:H:417:HOH:O	2.48	0.41
1:I:393:VAL:HA	1:I:394:PRO:HD3	1.83	0.41
2:J:69:MET:O	2:J:70:HIS:C	2.64	0.41
1:M:66:PHE:HZ	1:M:146:MET:HE1	1.86	0.41
1:M:138:LEU:HB2	1:M:490:ILE:HD12	2.03	0.41
8:N:1045:HOH:O	1:S:729:LYS:HE2	2.20	0.41
1:O:39:ALA:HA	1:O:40:PRO:HD3	1.90	0.41
1:O:753:TYR:HB3	2:P:24:MET:CE	2.51	0.41
1:S:454:GLU:CD	1:S:454:GLU:N	2.79	0.41
1:S:701:GLN:HG3	8:S:1644:HOH:O	2.19	0.41
1:S:738:HIS:ND1	4:S:903:MGD:N15	2.65	0.41
2:T:139:ALA:HB3	2:T:140:PRO:HD3	2.01	0.41
2:T:162:GLU:CD	2:T:162:GLU:N	2.79	0.41
1:W:269:GLY:HA2	1:W:362:HIS:CG	2.56	0.41
1:W:571:ARG:HA	8:W:1025:HOH:O	2.20	0.41
1:W:670:PRO:HG2	1:W:675:GLN:CD	2.46	0.41
1:A:408:GLY:HA2	1:A:619:TYR:HE1	1.86	0.41
1:A:776:SER:HA	1:A:805:VAL:HG13	2.02	0.41
2:B:2:GLU:HG2	2:B:158:LYS:HG2	2.02	0.41
1:C:128:ILE:CD1	1:C:492:MET:HB2	2.51	0.41
1:C:163:MET:HE1	1:C:606:PHE:HA	2.02	0.41
1:C:395:LEU:HD13	1:C:571:ARG:CG	2.50	0.41
1:E:565:TYR:C	1:E:567:LEU:H	2.28	0.41
1:E:800:ILE:N	1:E:800:ILE:CD1	2.84	0.41
2:F:201:ALA:HB3	2:F:235:PHE:CE2	2.56	0.41
1:G:134:PRO:HB2	1:G:439:LEU:CD1	2.51	0.41
1:G:277:ALA:HB2	1:G:321:ALA:HB2	2.02	0.41
1:I:146:MET:HE2	1:I:544:THR:CA	2.51	0.41
1:I:677:CYS:C	1:I:678:ARG:HG2	2.46	0.41
1:K:75:ARG:HH21	1:K:543:CYS:HA	1.86	0.41
1:K:128:ILE:CD1	1:K:492:MET:HB2	2.51	0.41
1:K:134:PRO:HD2	8:K:1354:HOH:O	2.20	0.41
1:K:737:PRO:HG3	4:K:903:MGD:H2'	2.03	0.41
2:L:74:ALA:HA	2:L:75:PRO:HD3	1.92	0.41
2:L:110:PRO:HB2	2:L:180:LEU:HD13	2.02	0.41
1:M:55:ARG:HD2	8:M:1638:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:76:ILE:HG22	1:M:541:PRO:HG3	2.03	0.41
1:M:323:GLU:HB3	8:M:1109:HOH:O	2.21	0.41
1:M:418:ALA:HB1	1:M:423:ALA:HB2	2.03	0.41
4:O:903:MGD:O1B	4:O:903:MGD:C4'	2.68	0.41
1:Q:66:PHE:CD1	1:Q:69:MET:CE	3.03	0.41
1:Q:74:LEU:HD23	1:Q:74:LEU:HA	1.91	0.41
1:Q:426:MET:HA	1:Q:426:MET:CE	2.37	0.41
1:S:494:TRP:HE1	1:S:525:GLN:HE21	1.69	0.41
2:T:114:MET:HA	2:T:125:LYS:HB3	2.02	0.41
1:U:2:GLY:O	1:U:21:LYS:HE3	2.21	0.41
1:U:15:PRO:HD2	8:U:1006:HOH:O	2.20	0.41
1:U:175:SER:OG	6:U:905:BTT:C5	2.68	0.41
2:V:19:CYS:CB	2:V:145:CYS:HB3	2.46	0.41
1:W:175:SER:OG	6:W:905:BTT:C5	2.69	0.41
1:W:250:PRO:HD3	4:W:903:MGD:C2	2.51	0.41
1:W:402:PRO:HG2	1:W:422:PHE:CE1	2.56	0.41
1:W:656:TRP:CD2	1:W:663:LYS:HA	2.56	0.41
2:X:71:CYS:HB2	2:X:182:THR:O	2.20	0.41
1:A:495:LYS:CD	1:A:514:TYR:OH	2.68	0.41
2:D:114:MET:HB3	2:D:125:LYS:HG2	2.02	0.41
1:E:425:ARG:HD3	1:E:622:ALA:O	2.21	0.41
2:F:58:ARG:HD2	2:F:268:ASP:OD1	2.20	0.41
1:I:197:GLU:HG3	1:I:653:ALA:HB1	2.03	0.41
1:I:800:ILE:N	1:I:800:ILE:CD1	2.84	0.41
1:I:867:TRP:CD1	1:I:869:GLY:H	2.38	0.41
2:L:119:GLU:O	2:L:119:GLU:HG2	2.21	0.41
2:L:164:MET:O	2:L:168:VAL:HG23	2.21	0.41
2:N:177:LYS:N	2:N:178:PRO:HD3	2.36	0.41
1:O:425:ARG:NH2	8:O:1082:HOH:O	2.51	0.41
1:S:15:PRO:HD3	1:S:554:PHE:CD1	2.56	0.41
1:S:177:GLU:HA	1:S:177:GLU:OE2	2.21	0.41
1:U:757:ILE:HD11	2:V:21:MET:HE3	2.03	0.41
2:V:87:ARG:HB2	2:V:89:ASP:OD2	2.21	0.41
1:W:118:THR:O	1:W:122:VAL:HG23	2.21	0.41
1:W:272:HIS:ND1	1:W:272:HIS:N	2.69	0.41
1:A:533:VAL:HB	1:A:534:PRO:HD3	2.03	0.40
2:B:21:MET:CA	2:B:21:MET:CE	2.99	0.40
1:C:730:TYR:CE1	1:C:794:ASN:HA	2.56	0.40
1:I:533:VAL:HB	1:I:534:PRO:HD3	2.03	0.40
1:K:103:GLN:N	1:K:103:GLN:CD	2.79	0.40
2:L:103:LYS:HG2	2:L:116:TRP:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:11:SER:HA	1:O:147:TRP:HB2	2.03	0.40
1:O:144:HIS:CG	1:O:743:MET:HE1	2.55	0.40
1:O:362:HIS:HB3	1:O:717:ALA:HB2	2.02	0.40
1:O:402:PRO:HG2	1:O:422:PHE:CE1	2.56	0.40
1:O:670:PRO:HG2	1:O:675:GLN:CD	2.46	0.40
1:S:322:GLU:HG3	1:S:327:VAL:O	2.21	0.40
2:T:142:MET:CE	2:T:146:ALA:HB1	2.46	0.40
1:U:408:GLY:HA2	1:U:619:TYR:HE1	1.85	0.40
1:W:277:ALA:HB2	1:W:321:ALA:HB2	2.02	0.40
1:W:362:HIS:HB3	1:W:717:ALA:HB2	2.03	0.40
1:W:378:GLY:O	1:W:381:LYS:HG2	2.21	0.40
1:W:540:LEU:HA	1:W:541:PRO:HD3	1.82	0.40
2:X:53:ARG:HB2	2:X:60:ASP:OD1	2.22	0.40
1:A:165:GLY:CA	1:A:166:PHE:HB3	2.45	0.40
1:A:495:LYS:HE3	1:A:495:LYS:HB3	1.90	0.40
1:C:175:SER:HB2	1:C:176:TRP:CE3	2.56	0.40
1:C:436:PRO:HG3	8:C:1460:HOH:O	2.21	0.40
1:C:560:TYR:C	1:C:562:PRO:HD3	2.46	0.40
1:C:564:ASN:HD22	1:C:564:ASN:H	1.69	0.40
2:D:68:CYS:HB2	2:D:126:CYS:HB2	2.02	0.40
1:E:571:ARG:HA	8:E:1026:HOH:O	2.22	0.40
1:G:433:PHE:CD1	1:G:433:PHE:N	2.89	0.40
1:G:649:LYS:HE3	1:G:651:THR:CG2	2.51	0.40
1:G:845:ASP:OD2	1:G:845:ASP:N	2.51	0.40
1:I:15:PRO:HD3	1:I:554:PHE:CE1	2.56	0.40
1:I:414:GLU:O	1:I:414:GLU:HG3	2.21	0.40
1:M:44:ILE:HD11	1:M:394:PRO:CG	2.51	0.40
2:N:9:ASP:HA	2:N:189:LYS:HB3	2.02	0.40
1:O:17:PHE:CE2	1:O:31:MET:HE3	2.55	0.40
1:O:426:MET:HE3	1:O:426:MET:CA	2.35	0.40
1:Q:501:LEU:HD13	1:Q:823:TYR:CG	2.56	0.40
1:Q:870:ASP:HB3	1:Q:872:TYR:CE1	2.56	0.40
2:R:69:MET:HB3	2:R:184:PRO:HB3	2.04	0.40
1:S:565:TYR:C	1:S:567:LEU:H	2.29	0.40
2:T:142:MET:HE2	2:T:146:ALA:HB3	2.03	0.40
1:U:114:TRP:CZ2	1:U:587:MET:HG2	2.56	0.40
1:U:322:GLU:HG3	1:U:327:VAL:O	2.22	0.40
1:U:673:ASN:HD22	1:U:673:ASN:H	1.69	0.40
1:U:786:ASN:ND2	1:U:805:VAL:H	2.19	0.40
1:W:839:ILE:HD13	1:W:839:ILE:HA	1.96	0.40
2:X:218:LYS:HG2	2:X:223:GLU:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LYS:HD3	8:A:1677:HOH:O	2.20	0.40
1:A:800:ILE:N	1:A:800:ILE:CD1	2.83	0.40
2:B:143:PRO:HB3	7:B:303:SF4:S1	2.61	0.40
1:C:76:ILE:HG22	1:C:541:PRO:HG3	2.02	0.40
1:C:251:HIS:HA	1:C:809:LEU:HD23	2.04	0.40
1:C:395:LEU:HD13	1:C:571:ARG:HG2	2.03	0.40
1:G:15:PRO:HD2	8:G:1003:HOH:O	2.20	0.40
2:J:7:VAL:HB	2:J:155:GLU:HB3	2.03	0.40
1:K:12:THR:O	1:K:226:TYR:HA	2.21	0.40
1:M:391:GLN:HG2	1:M:567:LEU:HD23	2.03	0.40
1:M:736:SER:O	4:M:902:MGD:N18	2.54	0.40
1:O:142:SER:CB	4:O:902:MGD:O1A	2.70	0.40
1:Q:9:ASN:HA	1:Q:576:GLN:HA	2.03	0.40
1:Q:397:TYR:HA	1:Q:565:TYR:OH	2.21	0.40
1:S:76:ILE:HA	1:S:77:PRO:HD3	1.79	0.40
2:T:53:ARG:HB2	2:T:60:ASP:OD1	2.22	0.40
2:T:139:ALA:O	2:T:141:LYS:HG3	2.20	0.40
2:V:60:ASP:OD1	2:V:60:ASP:C	2.64	0.40
2:V:122:VAL:HG22	2:V:123:ALA:N	2.36	0.40
1:W:227:ALA:O	1:W:228:GLY:C	2.64	0.40
1:A:134:PRO:HG2	1:A:439:LEU:HD11	2.03	0.40
1:A:393:VAL:HA	1:A:394:PRO:HD3	1.80	0.40
1:C:387:TRP:CZ2	1:C:389:THR:HA	2.56	0.40
2:D:21:MET:N	2:D:21:MET:HE2	2.37	0.40
2:D:124:GLN:O	2:D:125:LYS:HB3	2.21	0.40
2:J:68:CYS:CB	2:J:126:CYS:CB	2.85	0.40
1:K:396:ASP:OD2	1:K:398:GLU:HB2	2.21	0.40
1:K:540:LEU:HA	1:K:541:PRO:HD3	1.81	0.40
2:N:139:ALA:HB3	2:N:140:PRO:HD3	2.03	0.40
2:N:198:TYR:HB3	2:N:238:ASP:HA	2.04	0.40
1:O:76:ILE:HD13	1:O:539:ILE:CG2	2.51	0.40
1:O:560:TYR:C	1:O:562:PRO:HD3	2.47	0.40
1:O:677:CYS:C	1:O:678:ARG:HG2	2.47	0.40
1:O:730:TYR:CE1	1:O:794:ASN:HA	2.57	0.40
1:Q:263:TRP:CZ2	1:Q:265:SER:HB2	2.57	0.40
1:U:141:PRO:CA	1:U:496:TYR:HB3	2.43	0.40
1:U:767:TYR:HB3	1:U:769:TYR:CE1	2.57	0.40
2:V:69:MET:O	2:V:70:HIS:C	2.65	0.40
1:W:12:THR:O	1:W:226:TYR:HA	2.22	0.40
1:W:719:GLU:HG2	1:W:859:THR:O	2.21	0.40
2:X:40:GLN:NE2	2:X:117:ASN:HA	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:46:MET:HE3	2:X:46:MET:C	2.47	0.40
2:X:159:THR:OG1	2:X:160:THR:N	2.53	0.40
1:A:397:TYR:HA	1:A:565:TYR:OH	2.22	0.40
1:A:498:GLY:N	1:A:499:PRO:HD3	2.37	0.40
1:A:756:TYR:CE2	1:A:768:LYS:HE2	2.57	0.40
2:D:177:LYS:N	2:D:178:PRO:HD3	2.37	0.40
1:E:32:ASP:OD2	1:E:32:ASP:N	2.54	0.40
1:E:45:GLU:OE2	1:E:45:GLU:N	2.55	0.40
1:E:587:MET:HE3	1:E:591:GLU:HB3	2.04	0.40
1:E:845:ASP:OD2	1:E:845:ASP:N	2.53	0.40
2:F:19:CYS:O	2:F:22:GLY:N	2.55	0.40
1:G:153:ARG:O	1:G:157:TYR:HB3	2.22	0.40
1:G:800:ILE:CD1	1:G:833:ALA:HB1	2.51	0.40
1:G:801:LEU:HD11	1:G:839:ILE:HD11	2.03	0.40
1:I:571:ARG:HB2	1:I:642:VAL:HB	2.03	0.40
1:K:400:TYR:CZ	1:K:421:LYS:HD2	2.56	0.40
2:L:27:HIS:HE1	8:L:473:HOH:O	2.04	0.40
2:L:128:MET:O	2:L:129:CYS:C	2.64	0.40
1:M:214:PHE:HA	1:M:347:ALA:HB3	2.03	0.40
2:N:46:MET:HB2	7:N:303:SF4:S2	2.62	0.40
1:Q:45:GLU:OE2	1:Q:45:GLU:N	2.55	0.40
1:Q:784:ILE:HD13	1:Q:790:ILE:HG21	2.04	0.40
2:R:201:ALA:HB2	2:R:269:LEU:HB2	2.04	0.40
1:S:498:GLY:N	1:S:499:PRO:HD3	2.36	0.40
1:S:772:MET:HB2	1:S:801:LEU:HD13	2.04	0.40
1:W:495:LYS:CD	1:W:514:TYR:OH	2.70	0.40
2:X:59:ASN:HD22	2:X:59:ASN:N	2.17	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1584:HOH:O	8:O:1361:HOH:O[1_644]	2.06	0.14
1:O:162:ASN:O	8:A:1584:HOH:O[1_466]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	873/875 (100%)	827 (95%)	44 (5%)	2 (0%)	43	42
1	C	873/875 (100%)	833 (95%)	37 (4%)	3 (0%)	36	35
1	E	873/875 (100%)	832 (95%)	39 (4%)	2 (0%)	43	42
1	G	873/875 (100%)	833 (95%)	37 (4%)	3 (0%)	36	35
1	I	873/875 (100%)	826 (95%)	44 (5%)	3 (0%)	36	35
1	K	873/875 (100%)	831 (95%)	39 (4%)	3 (0%)	36	35
1	M	873/875 (100%)	829 (95%)	41 (5%)	3 (0%)	36	35
1	O	873/875 (100%)	827 (95%)	43 (5%)	3 (0%)	36	35
1	Q	873/875 (100%)	835 (96%)	35 (4%)	3 (0%)	36	35
1	S	873/875 (100%)	826 (95%)	43 (5%)	4 (0%)	24	21
1	U	873/875 (100%)	829 (95%)	41 (5%)	3 (0%)	36	35
1	W	873/875 (100%)	826 (95%)	44 (5%)	3 (0%)	36	35
2	B	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	27
2	D	272/274 (99%)	259 (95%)	12 (4%)	1 (0%)	30	27
2	F	272/274 (99%)	259 (95%)	11 (4%)	2 (1%)	18	14
2	H	272/274 (99%)	258 (95%)	12 (4%)	2 (1%)	18	14
2	J	272/274 (99%)	261 (96%)	10 (4%)	1 (0%)	30	27
2	L	272/274 (99%)	259 (95%)	11 (4%)	2 (1%)	18	14
2	N	272/274 (99%)	262 (96%)	9 (3%)	1 (0%)	30	27
2	P	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	27
2	R	272/274 (99%)	260 (96%)	10 (4%)	2 (1%)	18	14
2	T	272/274 (99%)	259 (95%)	11 (4%)	2 (1%)	18	14
2	V	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	30	27
2	X	272/274 (99%)	252 (93%)	18 (7%)	2 (1%)	18	14
All	All	13740/13788 (100%)	13061 (95%)	626 (5%)	53 (0%)	30	27

All (53) 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	K	177	GLU
1	M	177	GLU
1	O	177	GLU
1	S	177	GLU
1	S	648	ARG
1	U	177	GLU
1	W	177	GLU
1	E	141	PRO
1	I	177	GLU
1	Q	177	GLU
1	A	141	PRO
1	C	141	PRO
1	G	141	PRO
1	I	141	PRO
1	K	141	PRO
1	M	141	PRO
1	O	141	PRO
1	Q	141	PRO
1	S	141	PRO
2	T	145	CYS
1	U	141	PRO
1	W	141	PRO
2	X	221	GLY
2	L	145	CYS
1	C	225	ILE
2	D	67	PRO
2	F	19	CYS
2	H	67	PRO
2	L	67	PRO
2	N	67	PRO
2	R	145	CYS
2	V	67	PRO
2	X	67	PRO
2	F	67	PRO
1	G	354	TRP
2	H	19	CYS
2	J	67	PRO
1	M	225	ILE

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Mol	Chain	Res	Type
2	P	67	PRO
2	R	67	PRO
2	T	67	PRO
2	B	67	PRO
1	K	225	ILE
1	O	225	ILE
1	S	225	ILE
1	I	225	ILE
1	U	225	ILE
1	W	225	ILE
1	Q	225	ILE

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	729/729 (100%)	720 (99%)	9 (1%)	63	70
1	C	729/729 (100%)	719 (99%)	10 (1%)	59	66
1	E	729/729 (100%)	722 (99%)	7 (1%)	68	75
1	G	729/729 (100%)	721 (99%)	8 (1%)	65	73
1	I	729/729 (100%)	719 (99%)	10 (1%)	59	66
1	K	729/729 (100%)	720 (99%)	9 (1%)	63	70
1	M	729/729 (100%)	721 (99%)	8 (1%)	65	73
1	O	729/729 (100%)	718 (98%)	11 (2%)	57	64
1	Q	729/729 (100%)	720 (99%)	9 (1%)	63	70
1	S	729/729 (100%)	721 (99%)	8 (1%)	65	73
1	U	729/729 (100%)	722 (99%)	7 (1%)	68	75
1	W	729/729 (100%)	720 (99%)	9 (1%)	63	70
2	B	235/235 (100%)	226 (96%)	9 (4%)	29	29
2	D	235/235 (100%)	223 (95%)	12 (5%)	21	19
2	F	235/235 (100%)	227 (97%)	8 (3%)	32	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	235/235 (100%)	227 (97%)	8 (3%)	32	33
2	J	235/235 (100%)	225 (96%)	10 (4%)	26	25
2	L	235/235 (100%)	227 (97%)	8 (3%)	32	33
2	N	235/235 (100%)	225 (96%)	10 (4%)	26	25
2	P	235/235 (100%)	224 (95%)	11 (5%)	23	22
2	R	235/235 (100%)	225 (96%)	10 (4%)	26	25
2	T	235/235 (100%)	225 (96%)	10 (4%)	26	25
2	V	235/235 (100%)	224 (95%)	11 (5%)	23	22
2	X	235/235 (100%)	225 (96%)	10 (4%)	26	25
All	All	11568/11568 (100%)	11346 (98%)	222 (2%)	50	56

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	SER
1	A	373	LEU
1	A	426	MET
1	A	499	PRO
1	A	564	ASN
1	A	605	MET
1	A	726	LEU
1	A	743	MET
1	A	818	GLU
2	B	19	CYS
2	B	21	MET
2	B	23	CYS
2	B	71	CYS
2	B	76	CYS
2	B	109	CYS
2	B	126	CYS
2	B	149	CYS
2	B	157	LEU
1	C	142	SER
1	C	373	LEU
1	C	426	MET
1	C	499	PRO
1	C	564	ASN
1	C	605	MET
1	C	743	MET

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Mol	Chain	Res	Type
1	C	786	ASN
1	C	801	LEU
1	C	818	GLU
2	D	13	CYS
2	D	19	CYS
2	D	21	MET
2	D	71	CYS
2	D	76	CYS
2	D	104	GLU
2	D	109	CYS
2	D	121	ASN
2	D	129	CYS
2	D	145	CYS
2	D	149	CYS
2	D	179	GLU
1	E	142	SER
1	E	499	PRO
1	E	560	TYR
1	E	564	ASN
1	E	678	ARG
1	E	743	MET
1	E	818	GLU
2	F	13	CYS
2	F	21	MET
2	F	57	PRO
2	F	71	CYS
2	F	76	CYS
2	F	109	CYS
2	F	129	CYS
2	F	149	CYS
1	G	142	SER
1	G	163	MET
1	G	373	LEU
1	G	426	MET
1	G	499	PRO
1	G	564	ASN
1	G	743	MET
1	G	818	GLU
2	H	21	MET
2	H	24	MET
2	H	71	CYS
2	H	76	CYS

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Mol	Chain	Res	Type
2	H	109	CYS
2	H	129	CYS
2	H	149	CYS
2	H	157	LEU
1	I	142	SER
1	I	373	LEU
1	I	426	MET
1	I	499	PRO
1	I	560	TYR
1	I	564	ASN
1	I	605	MET
1	I	726	LEU
1	I	743	MET
1	I	818	GLU
2	J	19	CYS
2	J	21	MET
2	J	71	CYS
2	J	76	CYS
2	J	104	GLU
2	J	109	CYS
2	J	129	CYS
2	J	145	CYS
2	J	149	CYS
2	J	157	LEU
1	K	142	SER
1	K	373	LEU
1	K	426	MET
1	K	499	PRO
1	K	564	ASN
1	K	726	LEU
1	K	743	MET
1	K	786	ASN
1	K	818	GLU
2	L	19	CYS
2	L	71	CYS
2	L	76	CYS
2	L	109	CYS
2	L	126	CYS
2	L	129	CYS
2	L	149	CYS
2	L	157	LEU
1	M	142	SER

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Mol	Chain	Res	Type
1	M	358	CYS
1	M	426	MET
1	M	499	PRO
1	M	564	ASN
1	M	726	LEU
1	M	743	MET
1	M	786	ASN
2	N	2	GLU
2	N	13	CYS
2	N	19	CYS
2	N	21	MET
2	N	71	CYS
2	N	76	CYS
2	N	109	CYS
2	N	129	CYS
2	N	145	CYS
2	N	149	CYS
1	O	142	SER
1	O	426	MET
1	O	499	PRO
1	O	560	TYR
1	O	564	ASN
1	O	605	MET
1	O	699	GLU
1	O	726	LEU
1	O	743	MET
1	O	786	ASN
1	O	818	GLU
2	P	13	CYS
2	P	19	CYS
2	P	57	PRO
2	P	71	CYS
2	P	73	ASN
2	P	76	CYS
2	P	104	GLU
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

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Mol	Chain	Res	Type
1	Q	426	MET
1	Q	499	PRO
1	Q	564	ASN
1	Q	605	MET
1	Q	743	MET
1	Q	818	GLU
2	R	2	GLU
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	149	CYS
2	R	157	LEU
1	S	142	SER
1	S	492	MET
1	S	499	PRO
1	S	564	ASN
1	S	605	MET
1	S	726	LEU
1	S	743	MET
1	S	818	GLU
2	T	13	CYS
2	T	19	CYS
2	T	21	MET
2	T	71	CYS
2	T	76	CYS
2	T	104	GLU
2	T	109	CYS
2	T	129	CYS
2	T	149	CYS
2	T	157	LEU
1	U	142	SER
1	U	414	GLU
1	U	499	PRO
1	U	564	ASN
1	U	605	MET
1	U	726	LEU
1	U	743	MET
2	V	13	CYS

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Mol	Chain	Res	Type
2	V	19	CYS
2	V	21	MET
2	V	71	CYS
2	V	73	ASN
2	V	76	CYS
2	V	104	GLU
2	V	109	CYS
2	V	129	CYS
2	V	145	CYS
2	V	149	CYS
1	W	142	SER
1	W	373	LEU
1	W	426	MET
1	W	499	PRO
1	W	564	ASN
1	W	605	MET
1	W	743	MET
1	W	786	ASN
1	W	818	GLU
2	X	13	CYS
2	X	19	CYS
2	X	21	MET
2	X	59	ASN
2	X	71	CYS
2	X	109	CYS
2	X	129	CYS
2	X	145	CYS
2	X	149	CYS
2	X	157	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (257) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	162	ASN
1	A	171	HIS
1	A	391	GLN
1	A	478	HIS
1	A	479	GLN
1	A	525	GLN
1	A	564	ASN
1	A	576	GLN

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Mol	Chain	Res	Type
1	A	618	GLN
1	A	647	ASN
1	A	673	ASN
1	A	674	ASN
1	A	697	ASN
1	A	701	GLN
1	A	721	GLN
1	A	786	ASN
2	B	18	ASN
2	B	27	HIS
2	B	40	GLN
2	B	59	ASN
2	B	70	HIS
2	B	73	ASN
1	C	88	ASN
1	C	162	ASN
1	C	171	HIS
1	C	391	GLN
1	C	440	ASN
1	C	462	GLN
1	C	478	HIS
1	C	525	GLN
1	C	564	ASN
1	C	576	GLN
1	C	618	GLN
1	C	673	ASN
1	C	674	ASN
1	C	697	ASN
1	C	701	GLN
1	C	786	ASN
1	C	810	GLN
2	D	27	HIS
2	D	40	GLN
2	D	59	ASN
2	D	70	HIS
2	D	73	ASN
2	D	190	ASN
1	E	162	ASN
1	E	171	HIS
1	E	391	GLN
1	E	440	ASN
1	E	462	GLN

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Mol	Chain	Res	Type
1	E	478	HIS
1	E	525	GLN
1	E	564	ASN
1	E	576	GLN
1	E	618	GLN
1	E	673	ASN
1	E	674	ASN
1	E	697	ASN
1	E	701	GLN
1	E	786	ASN
1	E	810	GLN
2	F	40	GLN
2	F	59	ASN
2	F	70	HIS
2	F	73	ASN
2	F	81	ASN
2	F	190	ASN
1	G	162	ASN
1	G	171	HIS
1	G	440	ASN
1	G	462	GLN
1	G	478	HIS
1	G	525	GLN
1	G	564	ASN
1	G	576	GLN
1	G	618	GLN
1	G	647	ASN
1	G	673	ASN
1	G	674	ASN
1	G	697	ASN
1	G	701	GLN
1	G	786	ASN
1	G	810	GLN
2	H	40	GLN
2	H	59	ASN
2	H	70	HIS
2	H	73	ASN
1	I	88	ASN
1	I	162	ASN
1	I	171	HIS
1	I	391	GLN
1	I	462	GLN

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Mol	Chain	Res	Type
1	I	478	HIS
1	I	525	GLN
1	I	564	ASN
1	I	576	GLN
1	I	618	GLN
1	I	674	ASN
1	I	697	ASN
1	I	701	GLN
1	I	786	ASN
2	J	40	GLN
2	J	59	ASN
2	J	70	HIS
2	J	73	ASN
2	J	81	ASN
2	J	190	ASN
1	K	88	ASN
1	K	162	ASN
1	K	171	HIS
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	18	ASN
2	L	40	GLN
2	L	59	ASN
2	L	70	HIS
2	L	73	ASN
2	L	81	ASN
2	L	190	ASN
1	M	162	ASN
1	M	171	HIS
1	M	222	ASN
1	M	462	GLN
1	M	478	HIS

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Mol	Chain	Res	Type
1	M	525	GLN
1	M	564	ASN
1	M	576	GLN
1	M	618	GLN
1	M	673	ASN
1	M	674	ASN
1	M	697	ASN
1	M	701	GLN
1	M	786	ASN
2	N	40	GLN
2	N	59	ASN
2	N	70	HIS
2	N	73	ASN
2	N	81	ASN
2	N	121	ASN
1	O	162	ASN
1	O	171	HIS
1	O	222	ASN
1	O	440	ASN
1	O	462	GLN
1	O	478	HIS
1	O	525	GLN
1	O	564	ASN
1	O	576	GLN
1	O	618	GLN
1	O	673	ASN
1	O	674	ASN
1	O	697	ASN
1	O	701	GLN
1	O	786	ASN
2	P	17	ASN
2	P	18	ASN
2	P	40	GLN
2	P	59	ASN
2	P	70	HIS
2	P	81	ASN
1	Q	88	ASN
1	Q	162	ASN
1	Q	171	HIS
1	Q	440	ASN
1	Q	462	GLN
1	Q	478	HIS

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Mol	Chain	Res	Type
1	Q	525	GLN
1	Q	564	ASN
1	Q	576	GLN
1	Q	618	GLN
1	Q	674	ASN
1	Q	697	ASN
1	Q	701	GLN
1	Q	786	ASN
1	Q	810	GLN
2	R	27	HIS
2	R	30	ASN
2	R	40	GLN
2	R	59	ASN
2	R	70	HIS
2	R	73	ASN
1	S	88	ASN
1	S	162	ASN
1	S	171	HIS
1	S	462	GLN
1	S	478	HIS
1	S	525	GLN
1	S	564	ASN
1	S	576	GLN
1	S	618	GLN
1	S	673	ASN
1	S	674	ASN
1	S	697	ASN
1	S	701	GLN
1	S	786	ASN
2	T	17	ASN
2	T	18	ASN
2	T	40	GLN
2	T	59	ASN
2	T	70	HIS
2	T	73	ASN
1	U	162	ASN
1	U	171	HIS
1	U	232	ASN
1	U	391	GLN
1	U	462	GLN
1	U	478	HIS
1	U	525	GLN

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Mol	Chain	Res	Type
1	U	564	ASN
1	U	576	GLN
1	U	618	GLN
1	U	647	ASN
1	U	673	ASN
1	U	674	ASN
1	U	697	ASN
1	U	701	GLN
1	U	721	GLN
1	U	786	ASN
2	V	40	GLN
2	V	59	ASN
2	V	70	HIS
2	V	73	ASN
2	V	81	ASN
1	W	162	ASN
1	W	171	HIS
1	W	232	ASN
1	W	478	HIS
1	W	479	GLN
1	W	525	GLN
1	W	564	ASN
1	W	576	GLN
1	W	618	GLN
1	W	645	ASN
1	W	673	ASN
1	W	674	ASN
1	W	697	ASN
1	W	701	GLN
1	W	721	GLN
1	W	786	ASN
2	X	17	ASN
2	X	18	ASN
2	X	40	GLN
2	X	59	ASN
2	X	70	HIS
2	X	73	ASN
2	X	121	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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
6	BTT	U	905	5	10,10,10	8.66	6 (60%)	14,14,14	2.20	3 (21%)
6	BTT	G	905	5	10,10,10	8.67	6 (60%)	14,14,14	2.10	3 (21%)
7	SF4	N	304	2	0,12,12	-	-	-		
7	SF4	N	302	2	0,12,12	-	-	-		
4	MGD	M	903	5	47,52,52	2.11	14 (29%)	58,81,81	2.07	6 (10%)
4	MGD	S	902	5	47,52,52	1.88	11 (23%)	58,81,81	2.02	8 (13%)
7	SF4	F	303	2	0,12,12	-	-	-		
7	SF4	J	303	2	0,12,12	-	-	-		
7	SF4	X	303	2	0,12,12	-	-	-		
6	BTT	S	905	5	10,10,10	8.70	6 (60%)	14,14,14	2.17	3 (21%)
4	MGD	I	902	5	47,52,52	1.76	10 (21%)	58,81,81	2.03	9 (15%)
7	SF4	D	304	2	0,12,12	-	-	-		
4	MGD	W	903	5	47,52,52	2.17	16 (34%)	58,81,81	1.98	9 (15%)
7	SF4	L	302	2	0,12,12	-	-	-		
4	MGD	M	902	5	47,52,52	1.81	9 (19%)	58,81,81	2.05	9 (15%)
7	SF4	H	302	2	0,12,12	-	-	-		
4	MGD	E	903	5	47,52,52	2.46	12 (25%)	58,81,81	2.10	8 (13%)
4	MGD	I	903	5	47,52,52	2.17	14 (29%)	58,81,81	1.84	6 (10%)
6	BTT	M	905	5	10,10,10	8.62	6 (60%)	14,14,14	2.13	3 (21%)
7	SF4	J	304	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MGD	U	903	5	47,52,52	2.04	13 (27%)	58,81,81	1.95	6 (10%)
7	SF4	T	304	2	0,12,12	-	-	-		
7	SF4	F	302	2	0,12,12	-	-	-		
4	MGD	W	902	5	47,52,52	1.93	13 (27%)	58,81,81	2.02	8 (13%)
7	SF4	T	302	2	0,12,12	-	-	-		
7	SF4	X	304	2	0,12,12	-	-	-		
4	MGD	Q	902	5	47,52,52	1.92	11 (23%)	58,81,81	2.13	9 (15%)
4	MGD	G	902	5	47,52,52	1.90	9 (19%)	58,81,81	2.07	8 (13%)
6	BTT	O	905	5	10,10,10	8.66	6 (60%)	14,14,14	2.17	3 (21%)
4	MGD	O	902	5	47,52,52	1.93	13 (27%)	58,81,81	1.97	8 (13%)
7	SF4	V	304	2	0,12,12	-	-	-		
7	SF4	R	302	2	0,12,12	-	-	-		
4	MGD	G	903	5	47,52,52	2.17	16 (34%)	58,81,81	2.27	11 (18%)
7	SF4	J	302	2	0,12,12	-	-	-		
4	MGD	Q	903	5	47,52,52	2.26	13 (27%)	58,81,81	2.24	11 (18%)
7	SF4	F	304	2	0,12,12	-	-	-		
6	BTT	W	905	5	10,10,10	8.65	6 (60%)	14,14,14	2.17	3 (21%)
7	SF4	P	302	2	0,12,12	-	-	-		
7	SF4	B	303	2	0,12,12	-	-	-		
6	BTT	E	905	5	10,10,10	8.71	6 (60%)	14,14,14	2.11	3 (21%)
7	SF4	B	302	2	0,12,12	-	-	-		
6	BTT	A	905	5	10,10,10	8.65	6 (60%)	14,14,14	2.13	3 (21%)
7	SF4	R	303	2	0,12,12	-	-	-		
7	SF4	H	303	2	0,12,12	-	-	-		
4	MGD	A	902	5	47,52,52	1.83	9 (19%)	58,81,81	2.10	8 (13%)
6	BTT	K	905	5	10,10,10	8.66	6 (60%)	14,14,14	2.19	3 (21%)
7	SF4	P	304	2	0,12,12	-	-	-		
4	MGD	A	903	5	47,52,52	2.57	15 (31%)	58,81,81	2.17	10 (17%)
4	MGD	S	903	5	47,52,52	2.07	15 (31%)	58,81,81	1.81	4 (6%)
6	BTT	Q	905	5	10,10,10	8.66	6 (60%)	14,14,14	2.12	3 (21%)
7	SF4	B	304	2	0,12,12	-	-	-		
7	SF4	H	304	2	0,12,12	-	-	-		
6	BTT	C	905	5	10,10,10	8.68	6 (60%)	14,14,14	2.18	3 (21%)
7	SF4	V	303	2	0,12,12	-	-	-		
7	SF4	P	303	2	0,12,12	-	-	-		
4	MGD	O	903	5	47,52,52	2.41	14 (29%)	58,81,81	2.25	11 (18%)
7	SF4	L	303	2	0,12,12	-	-	-		
4	MGD	E	902	5	47,52,52	1.85	10 (21%)	58,81,81	2.02	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MGD	U	902	5	47,52,52	1.91	11 (23%)	58,81,81	2.06	8 (13%)
7	SF4	L	304	2	0,12,12	-	-	-	-	-
4	MGD	K	903	5	47,52,52	2.46	16 (34%)	58,81,81	2.12	10 (17%)
7	SF4	N	303	2	0,12,12	-	-	-	-	-
7	SF4	X	302	2	0,12,12	-	-	-	-	-
7	SF4	V	302	2	0,12,12	-	-	-	-	-
7	SF4	D	302	2	0,12,12	-	-	-	-	-
7	SF4	D	303	2	0,12,12	-	-	-	-	-
7	SF4	R	304	2	0,12,12	-	-	-	-	-
7	SF4	T	303	2	0,12,12	-	-	-	-	-
4	MGD	C	903	5	47,52,52	2.28	15 (31%)	58,81,81	1.80	4 (6%)
4	MGD	K	902	5	47,52,52	1.95	9 (19%)	58,81,81	2.04	7 (12%)
6	BTT	I	905	5	10,10,10	8.64	6 (60%)	14,14,14	2.17	3 (21%)
4	MGD	C	902	5	47,52,52	1.90	10 (21%)	58,81,81	2.04	9 (15%)

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
6	BTT	U	905	5	-	-	0/1/1/1
6	BTT	G	905	5	-	-	0/1/1/1
7	SF4	N	304	2	-	-	0/6/5/5
7	SF4	N	302	2	-	-	0/6/5/5
4	MGD	M	903	5	-	5/22/66/66	0/6/6/6
4	MGD	S	902	5	-	7/22/66/66	0/6/6/6
7	SF4	F	303	2	-	-	0/6/5/5
7	SF4	J	303	2	-	-	0/6/5/5
7	SF4	X	303	2	-	-	0/6/5/5
6	BTT	S	905	5	-	-	0/1/1/1
4	MGD	I	902	5	-	7/22/66/66	0/6/6/6
7	SF4	D	304	2	-	-	0/6/5/5
4	MGD	W	903	5	-	5/22/66/66	0/6/6/6
7	SF4	L	302	2	-	-	0/6/5/5
4	MGD	M	902	5	-	7/22/66/66	0/6/6/6
7	SF4	H	302	2	-	-	0/6/5/5
4	MGD	E	903	5	-	10/22/66/66	0/6/6/6
4	MGD	I	903	5	-	3/22/66/66	0/6/6/6
6	BTT	M	905	5	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	J	304	2	-	-	0/6/5/5
4	MGD	U	903	5	-	4/22/66/66	0/6/6/6
7	SF4	T	304	2	-	-	0/6/5/5
7	SF4	F	302	2	-	-	0/6/5/5
4	MGD	W	902	5	-	8/22/66/66	0/6/6/6
7	SF4	T	302	2	-	-	0/6/5/5
7	SF4	X	304	2	-	-	0/6/5/5
4	MGD	Q	902	5	-	7/22/66/66	0/6/6/6
4	MGD	G	902	5	-	7/22/66/66	0/6/6/6
6	BTT	O	905	5	-	-	0/1/1/1
4	MGD	O	902	5	-	7/22/66/66	0/6/6/6
7	SF4	V	304	2	-	-	0/6/5/5
7	SF4	R	302	2	-	-	0/6/5/5
4	MGD	G	903	5	-	5/22/66/66	0/6/6/6
7	SF4	J	302	2	-	-	0/6/5/5
4	MGD	Q	903	5	-	5/22/66/66	0/6/6/6
7	SF4	F	304	2	-	-	0/6/5/5
6	BTT	W	905	5	-	-	0/1/1/1
7	SF4	P	302	2	-	-	0/6/5/5
7	SF4	B	303	2	-	-	0/6/5/5
6	BTT	E	905	5	-	-	0/1/1/1
7	SF4	B	302	2	-	-	0/6/5/5
6	BTT	A	905	5	-	-	0/1/1/1
7	SF4	R	303	2	-	-	0/6/5/5
7	SF4	H	303	2	-	-	0/6/5/5
4	MGD	A	902	5	-	7/22/66/66	0/6/6/6
6	BTT	K	905	5	-	-	0/1/1/1
7	SF4	P	304	2	-	-	0/6/5/5
4	MGD	A	903	5	-	9/22/66/66	0/6/6/6
4	MGD	S	903	5	-	3/22/66/66	0/6/6/6
6	BTT	Q	905	5	-	-	0/1/1/1
7	SF4	B	304	2	-	-	0/6/5/5
7	SF4	H	304	2	-	-	0/6/5/5
6	BTT	C	905	5	-	-	0/1/1/1
7	SF4	V	303	2	-	-	0/6/5/5
7	SF4	P	303	2	-	-	0/6/5/5
4	MGD	O	903	5	-	7/22/66/66	0/6/6/6
7	SF4	L	303	2	-	-	0/6/5/5
4	MGD	E	902	5	-	7/22/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MGD	U	902	5	-	7/22/66/66	0/6/6/6
7	SF4	L	304	2	-	-	0/6/5/5
4	MGD	K	903	5	-	9/22/66/66	0/6/6/6
7	SF4	N	303	2	-	-	0/6/5/5
7	SF4	X	302	2	-	-	0/6/5/5
7	SF4	V	302	2	-	-	0/6/5/5
7	SF4	D	302	2	-	-	0/6/5/5
7	SF4	D	303	2	-	-	0/6/5/5
7	SF4	R	304	2	-	-	0/6/5/5
7	SF4	T	303	2	-	-	0/6/5/5
4	MGD	C	903	5	-	3/22/66/66	0/6/6/6
4	MGD	K	902	5	-	9/22/66/66	0/6/6/6
6	BTT	I	905	5	-	-	0/1/1/1
4	MGD	C	902	5	-	7/22/66/66	0/6/6/6

All (370) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	905	BTT	C3-C2	15.82	1.61	1.38
6	A	905	BTT	C3-C2	15.78	1.61	1.38
6	S	905	BTT	C3-C2	15.77	1.61	1.38
6	K	905	BTT	C3-C2	15.75	1.61	1.38
6	G	905	BTT	C3-C2	15.65	1.61	1.38
6	O	905	BTT	C3-C2	15.58	1.61	1.38
6	Q	905	BTT	C3-C2	15.57	1.61	1.38
6	C	905	BTT	C3-C2	15.52	1.60	1.38
6	W	905	BTT	C3-C2	15.49	1.60	1.38
6	M	905	BTT	C3-C2	15.48	1.60	1.38
6	U	905	BTT	C3-C2	15.48	1.60	1.38
6	I	905	BTT	C3-C2	15.44	1.60	1.38
6	E	905	BTT	C6-C5	14.48	1.59	1.38
6	G	905	BTT	C6-C5	14.47	1.59	1.38
6	M	905	BTT	C6-C5	14.41	1.59	1.38
6	W	905	BTT	C6-C5	14.40	1.59	1.38
6	Q	905	BTT	C6-C5	14.35	1.59	1.38
6	A	905	BTT	C6-C5	14.28	1.59	1.38
6	S	905	BTT	C6-C5	14.20	1.59	1.38
6	K	905	BTT	C6-C5	14.19	1.59	1.38
6	C	905	BTT	C6-C5	14.17	1.59	1.38
6	O	905	BTT	C6-C5	14.15	1.59	1.38
6	I	905	BTT	C6-C5	14.10	1.58	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	905	BTT	C6-C5	14.09	1.58	1.38
6	C	905	BTT	C2-C1	11.46	1.59	1.40
6	U	905	BTT	C2-C1	11.40	1.59	1.40
6	I	905	BTT	C2-C1	11.37	1.59	1.40
6	S	905	BTT	C2-C1	11.35	1.59	1.40
6	O	905	BTT	C2-C1	11.31	1.59	1.40
6	Q	905	BTT	C2-C1	11.29	1.59	1.40
6	E	905	BTT	C2-C1	11.29	1.59	1.40
6	K	905	BTT	C2-C1	11.22	1.59	1.40
6	G	905	BTT	C2-C1	11.20	1.58	1.40
6	A	905	BTT	C2-C1	11.16	1.58	1.40
6	M	905	BTT	C2-C1	11.13	1.58	1.40
6	W	905	BTT	C2-C1	11.08	1.58	1.40
6	U	905	BTT	C5-C4	9.40	1.55	1.40
6	O	905	BTT	C5-C4	9.29	1.55	1.40
6	C	905	BTT	C5-C4	9.27	1.55	1.40
6	I	905	BTT	O2-C2	-9.18	1.17	1.36
6	W	905	BTT	C5-C4	9.18	1.55	1.40
6	I	905	BTT	C5-C4	9.14	1.55	1.40
6	S	905	BTT	C5-C4	9.10	1.55	1.40
6	W	905	BTT	O2-C2	-9.06	1.18	1.36
6	G	905	BTT	O2-C2	-9.05	1.18	1.36
6	Q	905	BTT	C5-C4	9.05	1.55	1.40
6	C	905	BTT	O2-C2	-9.04	1.18	1.36
6	M	905	BTT	O2-C2	-8.99	1.18	1.36
6	A	905	BTT	O2-C2	-8.99	1.18	1.36
6	O	905	BTT	O2-C2	-8.98	1.18	1.36
6	Q	905	BTT	O2-C2	-8.96	1.18	1.36
6	S	905	BTT	O2-C2	-8.95	1.18	1.36
6	K	905	BTT	C5-C4	8.95	1.55	1.40
6	K	905	BTT	O2-C2	-8.94	1.18	1.36
6	E	905	BTT	O2-C2	-8.93	1.18	1.36
6	M	905	BTT	C5-C4	8.93	1.55	1.40
6	U	905	BTT	O2-C2	-8.93	1.18	1.36
6	E	905	BTT	C5-C4	8.92	1.55	1.40
6	G	905	BTT	C5-C4	8.89	1.55	1.40
6	A	905	BTT	C5-C4	8.89	1.55	1.40
4	E	903	MGD	PB-O3B	8.53	1.68	1.59
4	A	903	MGD	PB-O3B	7.92	1.68	1.59
4	K	903	MGD	PB-O3B	7.87	1.68	1.59
4	A	903	MGD	C14-N15	7.10	1.54	1.46
4	Q	903	MGD	C14-N15	7.02	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	903	MGD	C14-N15	7.00	1.54	1.46
4	K	903	MGD	C14-N15	6.88	1.54	1.46
4	C	903	MGD	C14-N15	6.84	1.54	1.46
4	G	903	MGD	C14-N15	6.83	1.54	1.46
4	I	903	MGD	C14-N15	6.83	1.54	1.46
4	O	903	MGD	C14-N15	6.80	1.54	1.46
4	U	903	MGD	C14-N15	6.72	1.54	1.46
4	M	903	MGD	C14-N15	6.65	1.54	1.46
4	W	903	MGD	C14-N15	6.61	1.53	1.46
4	E	903	MGD	C14-N15	6.48	1.53	1.46
4	O	903	MGD	PA-O3B	6.30	1.66	1.59
4	A	903	MGD	C21-N22	6.09	1.41	1.35
4	C	902	MGD	C23-C14	6.08	1.58	1.53
4	E	903	MGD	C21-N22	6.00	1.41	1.35
4	W	903	MGD	C21-N22	5.91	1.41	1.35
4	K	902	MGD	C23-C14	5.88	1.58	1.53
4	G	902	MGD	C23-C14	5.80	1.58	1.53
4	C	903	MGD	C21-N22	5.74	1.41	1.35
4	O	903	MGD	PB-O3B	5.69	1.65	1.59
4	U	902	MGD	C23-C14	5.69	1.58	1.53
4	O	902	MGD	C23-C14	5.64	1.58	1.53
4	Q	903	MGD	PA-O3B	5.62	1.65	1.59
4	M	902	MGD	C23-C14	5.57	1.58	1.53
4	A	902	MGD	C23-C14	5.54	1.58	1.53
4	I	903	MGD	C21-N22	5.49	1.41	1.35
4	K	903	MGD	C21-N22	5.49	1.41	1.35
4	E	902	MGD	C23-C14	5.47	1.58	1.53
4	G	902	MGD	C21-N22	5.45	1.41	1.35
4	G	903	MGD	C21-N22	5.43	1.41	1.35
4	W	902	MGD	C21-N22	5.41	1.41	1.35
4	S	902	MGD	C21-N22	5.37	1.41	1.35
4	C	903	MGD	PB-O3B	-5.32	1.53	1.59
4	O	902	MGD	C21-N22	5.30	1.41	1.35
4	Q	903	MGD	C21-N22	5.29	1.41	1.35
4	A	903	MGD	PA-O3B	5.27	1.65	1.59
4	W	902	MGD	C23-C14	5.21	1.57	1.53
4	O	903	MGD	C21-N22	5.21	1.41	1.35
4	U	903	MGD	C21-N22	5.20	1.41	1.35
4	C	902	MGD	C21-N22	5.14	1.40	1.35
4	I	902	MGD	C23-C14	5.12	1.57	1.53
4	U	902	MGD	C21-N22	5.02	1.40	1.35
4	Q	902	MGD	C21-N22	4.97	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	903	MGD	C21-N22	4.91	1.40	1.35
4	E	903	MGD	C23-C14	4.91	1.57	1.53
4	S	903	MGD	C21-N22	4.85	1.40	1.35
4	C	903	MGD	C23-C14	4.75	1.57	1.53
4	E	902	MGD	C21-N22	4.74	1.40	1.35
4	Q	903	MGD	C23-C14	4.72	1.57	1.53
4	Q	902	MGD	C23-C14	4.70	1.57	1.53
4	K	902	MGD	C21-N22	4.64	1.40	1.35
4	O	903	MGD	C23-C14	4.54	1.57	1.53
4	S	902	MGD	C23-C14	4.52	1.57	1.53
4	G	903	MGD	C23-C14	4.49	1.57	1.53
4	M	903	MGD	C23-C14	4.47	1.57	1.53
4	K	903	MGD	PA-O3B	4.47	1.64	1.59
4	U	903	MGD	C23-C14	4.45	1.57	1.53
4	M	902	MGD	C21-N22	4.44	1.40	1.35
4	A	903	MGD	C23-C14	4.43	1.57	1.53
4	K	903	MGD	C23-C14	4.42	1.57	1.53
4	A	902	MGD	C21-N22	4.37	1.40	1.35
4	S	902	MGD	C14-N15	4.27	1.51	1.46
4	I	902	MGD	C21-N22	4.27	1.40	1.35
4	I	903	MGD	C23-C14	4.25	1.57	1.53
4	G	902	MGD	C14-N15	4.24	1.51	1.46
4	Q	902	MGD	C14-N15	4.19	1.51	1.46
4	M	903	MGD	PB-O3B	-4.14	1.55	1.59
4	W	903	MGD	C23-C14	4.07	1.56	1.53
4	E	902	MGD	C14-N15	4.07	1.51	1.46
4	O	902	MGD	C14-N15	4.03	1.51	1.46
4	O	903	MGD	C16-N15	4.03	1.47	1.37
4	A	902	MGD	C16-N15	4.00	1.47	1.37
4	C	903	MGD	C16-N15	3.99	1.47	1.37
4	A	903	MGD	C16-N15	3.97	1.47	1.37
4	Q	903	MGD	C16-N15	3.95	1.47	1.37
4	M	903	MGD	C16-N15	3.95	1.47	1.37
4	U	902	MGD	C14-N15	3.95	1.50	1.46
4	I	903	MGD	C16-N15	3.94	1.47	1.37
4	S	903	MGD	C23-C14	3.93	1.56	1.53
4	G	902	MGD	C16-N15	3.92	1.47	1.37
4	S	902	MGD	C16-N15	3.91	1.47	1.37
4	G	903	MGD	C16-N15	3.91	1.47	1.37
4	K	903	MGD	C16-N15	3.88	1.47	1.37
4	W	903	MGD	C16-N15	3.86	1.46	1.37
4	A	902	MGD	C14-N15	3.85	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	902	MGD	C16-N15	3.81	1.46	1.37
4	W	902	MGD	C14-N15	3.80	1.50	1.46
4	E	903	MGD	C16-N15	3.80	1.46	1.37
4	Q	902	MGD	O11-C11	3.79	1.50	1.43
4	M	902	MGD	C14-N15	3.78	1.50	1.46
4	U	902	MGD	C16-N15	3.74	1.46	1.37
4	K	902	MGD	C16-N15	3.68	1.46	1.37
4	G	903	MGD	PA-O3B	3.67	1.63	1.59
4	U	903	MGD	C16-N15	3.66	1.46	1.37
4	S	903	MGD	C16-N15	3.65	1.46	1.37
4	O	902	MGD	C16-N15	3.60	1.46	1.37
4	E	902	MGD	C16-N15	3.60	1.46	1.37
4	M	902	MGD	C16-N15	3.54	1.46	1.37
4	I	902	MGD	C16-N15	3.54	1.46	1.37
4	W	902	MGD	C16-N15	3.53	1.46	1.37
4	C	902	MGD	C16-N15	3.50	1.46	1.37
4	K	902	MGD	PA-O3B	3.44	1.63	1.59
6	S	905	BTT	O5-C5	-3.44	1.29	1.36
4	W	903	MGD	PB-O3B	-3.43	1.55	1.59
4	E	902	MGD	O11-C11	3.38	1.50	1.43
6	U	905	BTT	O5-C5	-3.37	1.29	1.36
4	U	902	MGD	O11-C11	3.34	1.50	1.43
4	S	902	MGD	O11-C11	3.34	1.50	1.43
4	C	902	MGD	C14-N15	3.34	1.50	1.46
4	M	903	MGD	C6-N1	3.33	1.45	1.38
4	K	902	MGD	O11-C11	3.32	1.50	1.43
4	W	902	MGD	O11-C11	3.31	1.50	1.43
6	K	905	BTT	O5-C5	-3.30	1.29	1.36
4	K	903	MGD	C6-N1	3.29	1.45	1.38
4	I	903	MGD	O11-C23	3.29	1.48	1.43
4	W	902	MGD	PA-O3B	3.28	1.63	1.59
4	C	903	MGD	O11-C11	3.27	1.49	1.43
4	I	902	MGD	C14-N15	3.26	1.50	1.46
4	K	902	MGD	C14-N15	3.21	1.50	1.46
4	E	903	MGD	C6-N1	3.19	1.44	1.38
6	C	905	BTT	O5-C5	-3.19	1.29	1.36
4	I	903	MGD	PB-O3B	-3.18	1.56	1.59
4	S	903	MGD	PA-O3B	3.17	1.62	1.59
4	M	902	MGD	O11-C11	3.16	1.49	1.43
6	W	905	BTT	O5-C5	-3.14	1.30	1.36
4	C	902	MGD	O11-C11	3.12	1.49	1.43
4	I	903	MGD	O11-C11	3.11	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	903	MGD	C16-C21	3.10	1.44	1.38
4	O	902	MGD	O11-C11	3.10	1.49	1.43
4	C	903	MGD	O11-C23	3.09	1.48	1.43
4	Q	903	MGD	C6-N1	3.08	1.44	1.38
4	I	902	MGD	O11-C11	3.07	1.49	1.43
4	A	903	MGD	C6-N1	3.06	1.44	1.38
4	Q	902	MGD	C17-N18	3.06	1.44	1.38
4	G	902	MGD	O11-C11	3.05	1.49	1.43
6	O	905	BTT	O5-C5	-3.04	1.30	1.36
6	A	905	BTT	O5-C5	-3.02	1.30	1.36
4	O	903	MGD	C16-C21	3.02	1.43	1.38
4	M	902	MGD	C17-N18	3.01	1.44	1.38
4	O	903	MGD	C6-N1	3.01	1.44	1.38
4	I	903	MGD	C6-N1	3.00	1.44	1.38
4	U	902	MGD	C17-N18	3.00	1.44	1.38
6	Q	905	BTT	O5-C5	-2.99	1.30	1.36
4	W	903	MGD	C6-N1	2.99	1.44	1.38
4	G	903	MGD	C6-N1	2.98	1.44	1.38
4	S	902	MGD	C17-N18	2.98	1.44	1.38
4	A	903	MGD	C16-C21	2.98	1.43	1.38
4	W	903	MGD	C21-N20	2.97	1.40	1.36
4	C	903	MGD	C21-N20	2.95	1.40	1.36
4	G	903	MGD	C16-C21	2.95	1.43	1.38
4	O	903	MGD	C17-N18	2.94	1.44	1.38
4	O	902	MGD	C17-N18	2.94	1.44	1.38
4	C	902	MGD	C17-N18	2.94	1.44	1.38
4	A	903	MGD	C21-N20	2.93	1.40	1.36
4	K	902	MGD	C17-N18	2.91	1.44	1.38
6	E	905	BTT	O5-C5	-2.90	1.30	1.36
4	S	903	MGD	C16-C21	2.90	1.43	1.38
4	U	903	MGD	C16-C21	2.89	1.43	1.38
4	C	903	MGD	C6-N1	2.89	1.44	1.38
4	I	903	MGD	C16-C21	2.88	1.43	1.38
4	I	902	MGD	C17-N18	2.87	1.44	1.38
4	A	903	MGD	C17-N18	2.86	1.44	1.38
4	W	903	MGD	C17-N18	2.86	1.44	1.38
4	G	903	MGD	C17-N18	2.86	1.44	1.38
4	U	903	MGD	C8-N9	2.85	1.43	1.37
4	E	903	MGD	C17-N18	2.84	1.44	1.38
4	A	902	MGD	C17-N18	2.84	1.44	1.38
6	I	905	BTT	O5-C5	-2.84	1.30	1.36
4	C	903	MGD	C16-C21	2.83	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	903	MGD	C16-C21	2.82	1.43	1.38
4	M	903	MGD	C17-N18	2.81	1.44	1.38
4	E	903	MGD	C16-C21	2.80	1.43	1.38
4	C	903	MGD	C17-N18	2.80	1.44	1.38
6	M	905	BTT	O5-C5	-2.80	1.30	1.36
6	G	905	BTT	O5-C5	-2.79	1.30	1.36
4	S	903	MGD	O11-C23	2.78	1.47	1.43
4	E	903	MGD	PA-O3B	2.78	1.62	1.59
4	E	903	MGD	C21-N20	2.76	1.40	1.36
4	G	902	MGD	C17-N18	2.75	1.44	1.38
4	S	903	MGD	O11-C11	2.74	1.48	1.43
4	E	902	MGD	C17-N18	2.74	1.44	1.38
4	W	902	MGD	C17-N18	2.74	1.44	1.38
4	U	903	MGD	C17-N18	2.73	1.44	1.38
4	S	903	MGD	C6-N1	2.72	1.44	1.38
4	A	902	MGD	C6-N1	2.72	1.43	1.38
4	K	903	MGD	C16-C21	2.71	1.43	1.38
4	K	903	MGD	O4'-C1'	-2.70	1.35	1.42
4	Q	903	MGD	C17-N18	2.66	1.43	1.38
4	O	902	MGD	C21-N20	2.66	1.40	1.36
4	Q	903	MGD	C21-N20	2.64	1.40	1.36
4	W	903	MGD	C16-C21	2.63	1.43	1.38
4	S	903	MGD	C17-N18	2.62	1.43	1.38
4	I	903	MGD	C17-N18	2.61	1.43	1.38
4	W	903	MGD	O11-C11	2.61	1.48	1.43
4	C	903	MGD	C8-N9	2.59	1.43	1.37
4	W	903	MGD	C8-N9	2.58	1.43	1.37
4	U	903	MGD	C6-N1	2.57	1.43	1.38
4	A	902	MGD	O11-C11	2.56	1.48	1.43
4	G	903	MGD	C21-N20	2.56	1.40	1.36
4	W	903	MGD	C5'-C4'	-2.55	1.43	1.51
4	K	903	MGD	C21-N20	2.55	1.40	1.36
4	U	903	MGD	O17-C17	2.55	1.28	1.23
4	M	903	MGD	O11-C11	2.55	1.48	1.43
4	M	903	MGD	C8-N9	2.55	1.43	1.37
4	U	903	MGD	O11-C23	2.54	1.47	1.43
4	W	902	MGD	C21-N20	2.54	1.40	1.36
4	M	903	MGD	C21-N20	2.53	1.40	1.36
4	C	902	MGD	C6-N1	2.52	1.43	1.38
4	U	902	MGD	C6-N1	2.51	1.43	1.38
4	G	903	MGD	O17-C17	2.50	1.28	1.23
4	O	903	MGD	O4'-C1'	-2.49	1.36	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	902	MGD	C21-N20	2.48	1.40	1.36
4	I	902	MGD	C6-N1	2.46	1.43	1.38
4	Q	903	MGD	O17-C17	2.46	1.28	1.23
4	C	903	MGD	O17-C17	2.45	1.28	1.23
4	O	903	MGD	C21-N20	2.45	1.39	1.36
4	A	902	MGD	C21-N20	2.42	1.39	1.36
4	U	903	MGD	O11-C11	2.41	1.48	1.43
4	W	902	MGD	C6-N1	2.41	1.43	1.38
4	K	902	MGD	C21-N20	2.40	1.39	1.36
4	Q	903	MGD	C8-N9	2.39	1.42	1.37
4	A	903	MGD	O4'-C1'	-2.39	1.36	1.42
4	I	903	MGD	C8-N9	2.39	1.42	1.37
4	A	903	MGD	O4'-C4'	-2.37	1.39	1.45
4	K	903	MGD	C17-N18	2.36	1.43	1.38
4	W	903	MGD	C2'-C3'	2.36	1.59	1.53
4	C	902	MGD	C21-N20	2.36	1.39	1.36
4	M	903	MGD	C5'-C4'	-2.35	1.44	1.51
4	A	903	MGD	O11-C23	2.34	1.47	1.43
4	A	903	MGD	O11-C11	2.34	1.48	1.43
4	M	902	MGD	C6-N1	2.34	1.43	1.38
4	S	903	MGD	O17-C17	2.33	1.28	1.23
4	G	903	MGD	C8-N9	2.33	1.42	1.37
4	I	902	MGD	C21-N20	2.33	1.39	1.36
4	Q	903	MGD	O4'-C1'	-2.32	1.36	1.42
4	K	902	MGD	C6-N1	2.32	1.43	1.38
4	G	903	MGD	O11-C11	2.32	1.48	1.43
4	E	902	MGD	C21-N20	2.31	1.39	1.36
4	M	903	MGD	O11-C23	2.31	1.47	1.43
4	W	902	MGD	C8-N9	2.31	1.42	1.37
4	W	903	MGD	O17-C17	2.30	1.27	1.23
4	C	902	MGD	C8-N9	2.30	1.42	1.37
4	I	903	MGD	PA-O3B	2.30	1.62	1.59
4	M	902	MGD	C16-C21	2.30	1.42	1.38
4	Q	902	MGD	C21-N20	2.30	1.39	1.36
4	S	903	MGD	C8-N9	2.28	1.42	1.37
4	E	903	MGD	O11-C23	2.27	1.47	1.43
4	W	903	MGD	PA-O3B	2.26	1.61	1.59
4	K	903	MGD	C8-N9	2.26	1.42	1.37
4	G	902	MGD	C21-N20	2.26	1.39	1.36
4	G	902	MGD	C16-C21	2.25	1.42	1.38
4	S	903	MGD	PB-O3B	-2.24	1.57	1.59
4	G	903	MGD	O11-C23	2.24	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	902	MGD	C16-C21	2.24	1.42	1.38
4	K	903	MGD	O11-C23	2.24	1.47	1.43
4	O	903	MGD	O11-C11	2.24	1.47	1.43
4	Q	902	MGD	C6-N1	2.24	1.43	1.38
4	E	902	MGD	C16-C21	2.23	1.42	1.38
4	S	902	MGD	C6-N1	2.22	1.43	1.38
4	G	902	MGD	C6-N1	2.22	1.43	1.38
4	U	902	MGD	C21-N20	2.21	1.39	1.36
4	S	902	MGD	C10-C11	2.20	1.54	1.51
4	I	903	MGD	O17-C17	2.20	1.27	1.23
4	O	903	MGD	O17-C17	2.20	1.27	1.23
4	M	903	MGD	O17-C17	2.20	1.27	1.23
4	U	902	MGD	C8-N9	2.19	1.42	1.37
4	A	903	MGD	O17-C17	2.19	1.27	1.23
4	U	902	MGD	C16-C21	2.19	1.42	1.38
4	I	903	MGD	C21-N20	2.18	1.39	1.36
4	S	903	MGD	C5'-C4'	-2.18	1.45	1.51
4	I	902	MGD	C8-N9	2.17	1.42	1.37
4	G	903	MGD	C4-N3	2.17	1.39	1.34
4	Q	902	MGD	C8-N9	2.16	1.42	1.37
4	I	902	MGD	C16-C21	2.16	1.42	1.38
4	E	902	MGD	O6-C6	2.16	1.27	1.23
4	E	902	MGD	C6-N1	2.15	1.42	1.38
4	O	902	MGD	C6-N1	2.15	1.42	1.38
4	K	903	MGD	O11-C11	2.14	1.47	1.43
4	C	903	MGD	O6-C6	2.13	1.27	1.23
4	E	903	MGD	O17-C17	2.13	1.27	1.23
4	S	903	MGD	C2-N1	2.12	1.42	1.37
4	O	902	MGD	PA-O3B	2.12	1.61	1.59
4	Q	902	MGD	O6-C6	2.12	1.27	1.23
4	O	902	MGD	C4-N3	2.11	1.39	1.34
4	O	902	MGD	C8-N9	2.11	1.42	1.37
4	U	903	MGD	C21-N20	2.11	1.39	1.36
4	G	903	MGD	C2-N2	2.10	1.39	1.34
4	K	903	MGD	O4'-C4'	-2.10	1.40	1.45
4	C	902	MGD	C16-C21	2.10	1.42	1.38
4	S	902	MGD	C16-C21	2.09	1.42	1.38
4	S	902	MGD	C8-N9	2.08	1.42	1.37
4	O	902	MGD	O6-C6	2.08	1.27	1.23
4	G	903	MGD	C2'-C3'	2.08	1.59	1.53
4	M	902	MGD	O17-C17	2.07	1.27	1.23
4	U	902	MGD	O17-C17	2.07	1.27	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	903	MGD	O17-C17	2.07	1.27	1.23
4	O	902	MGD	C16-C21	2.06	1.42	1.38
4	O	903	MGD	C4-N3	2.05	1.38	1.34
4	W	902	MGD	C16-C21	2.04	1.42	1.38
4	W	903	MGD	O11-C23	2.03	1.46	1.43
4	Q	903	MGD	O11-C23	2.03	1.46	1.43
4	W	902	MGD	C2-N2	2.03	1.38	1.34
4	W	902	MGD	O4'-C1'	2.02	1.46	1.42
4	C	903	MGD	C2-N1	2.01	1.42	1.37
4	A	902	MGD	C4-N3	2.01	1.38	1.34
4	U	903	MGD	PB-O3B	-2.01	1.57	1.59

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	MGD	O2A-PA-O3B	-10.38	79.22	107.27
4	W	902	MGD	O2A-PA-O3B	-10.33	79.35	107.27
4	I	902	MGD	O2A-PA-O3B	-10.31	79.41	107.27
4	U	902	MGD	O2A-PA-O3B	-10.24	79.58	107.27
4	Q	902	MGD	O2A-PA-O3B	-10.24	79.60	107.27
4	K	902	MGD	O2A-PA-O3B	-10.21	79.68	107.27
4	G	902	MGD	O2A-PA-O3B	-10.20	79.70	107.27
4	M	902	MGD	O2A-PA-O3B	-10.03	80.16	107.27
4	C	902	MGD	O2A-PA-O3B	-10.02	80.18	107.27
4	E	903	MGD	O11-C23-C14	-10.02	102.28	108.96
4	E	902	MGD	O2A-PA-O3B	-9.99	80.26	107.27
4	O	903	MGD	O11-C23-C14	-9.94	102.34	108.96
4	S	902	MGD	O2A-PA-O3B	-9.92	80.45	107.27
4	G	903	MGD	O11-C23-C14	-9.89	102.37	108.96
4	O	902	MGD	O2A-PA-O3B	-9.76	80.89	107.27
4	A	903	MGD	O11-C23-C14	-9.50	102.63	108.96
4	Q	903	MGD	O11-C23-C14	-9.49	102.63	108.96
4	K	903	MGD	O11-C23-C14	-9.47	102.64	108.96
4	M	903	MGD	O11-C23-C14	-9.35	102.72	108.96
4	W	903	MGD	O11-C23-C14	-8.94	103.00	108.96
4	U	903	MGD	O11-C23-C14	-8.74	103.13	108.96
4	I	903	MGD	O11-C23-C14	-8.43	103.34	108.96
4	C	903	MGD	O11-C23-C14	-8.00	103.63	108.96
4	S	903	MGD	O11-C23-C14	-7.98	103.64	108.96
4	G	903	MGD	O4'-C4'-C5'	-7.53	85.22	109.33
4	Q	903	MGD	O4'-C4'-C5'	-7.32	85.90	109.33
4	M	903	MGD	O4'-C4'-C5'	-7.28	86.02	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	903	MGD	O4'-C4'-C5'	-7.19	86.31	109.33
4	W	903	MGD	O4'-C4'-C5'	-6.78	87.61	109.33
4	U	903	MGD	O4'-C4'-C5'	-6.76	87.67	109.33
4	C	903	MGD	O4'-C4'-C5'	-6.72	87.82	109.33
4	I	903	MGD	O4'-C4'-C5'	-6.71	87.84	109.33
4	K	903	MGD	O4'-C4'-C5'	-6.34	89.01	109.33
4	S	903	MGD	O4'-C4'-C5'	-6.27	89.26	109.33
4	A	903	MGD	O4'-C4'-C5'	-6.17	89.57	109.33
6	U	905	BTT	O5-C5-C6	-6.01	103.24	119.45
6	O	905	BTT	O5-C5-C6	-5.90	103.52	119.45
6	C	905	BTT	O5-C5-C6	-5.88	103.59	119.45
6	I	905	BTT	O5-C5-C6	-5.85	103.65	119.45
6	W	905	BTT	O5-C5-C6	-5.84	103.69	119.45
6	K	905	BTT	O5-C5-C6	-5.83	103.70	119.45
6	S	905	BTT	O5-C5-C6	-5.80	103.81	119.45
4	M	903	MGD	O11-C23-N22	-5.75	103.39	108.61
6	Q	905	BTT	O5-C5-C6	-5.65	104.19	119.45
6	M	905	BTT	O5-C5-C6	-5.65	104.21	119.45
6	A	905	BTT	O5-C5-C6	-5.63	104.26	119.45
4	E	903	MGD	O11-C23-N22	-5.60	103.52	108.61
6	G	905	BTT	O5-C5-C6	-5.58	104.40	119.45
6	E	905	BTT	O5-C5-C6	-5.56	104.46	119.45
4	E	903	MGD	O4'-C4'-C5'	-5.52	91.67	109.33
4	Q	902	MGD	O2A-PA-O3A	-5.50	82.64	107.57
4	A	902	MGD	O2A-PA-O3A	-5.29	83.57	107.57
4	S	902	MGD	O2A-PA-O3A	-5.28	83.61	107.57
4	Q	902	MGD	C23-C14-N15	5.26	113.03	107.87
4	W	902	MGD	C23-C14-N15	5.24	113.01	107.87
4	C	902	MGD	C23-C14-N15	5.20	112.98	107.87
4	K	902	MGD	C23-C14-N15	5.20	112.97	107.87
4	Q	903	MGD	O11-C23-N22	-5.19	103.89	108.61
4	C	902	MGD	O2A-PA-O3A	-5.18	84.09	107.57
4	Q	902	MGD	O2A-PA-O1A	-5.12	88.62	112.44
4	G	902	MGD	C23-C14-N15	5.09	112.86	107.87
4	M	902	MGD	C23-C14-N15	5.08	112.85	107.87
4	I	902	MGD	O2A-PA-O3A	-5.07	84.59	107.57
4	G	902	MGD	O2A-PA-O3A	-5.07	84.60	107.57
4	M	902	MGD	O2A-PA-O3A	-5.06	84.62	107.57
4	E	902	MGD	C23-C14-N15	5.06	112.84	107.87
4	O	902	MGD	C23-C14-N15	5.06	112.83	107.87
4	G	903	MGD	O11-C23-N22	-5.03	104.04	108.61
4	W	902	MGD	O2A-PA-O3A	-5.02	84.80	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	902	MGD	C23-C14-N15	5.01	112.79	107.87
4	U	903	MGD	O11-C23-N22	-5.01	104.06	108.61
4	O	903	MGD	O11-C23-N22	-5.00	104.07	108.61
4	A	902	MGD	C23-C14-N15	5.00	112.78	107.87
4	K	902	MGD	O2A-PA-O3A	-4.97	85.04	107.57
4	U	902	MGD	O2A-PA-O3A	-4.97	85.06	107.57
4	O	902	MGD	O2A-PA-O3A	-4.94	85.19	107.57
4	K	903	MGD	O11-C23-N22	-4.93	104.13	108.61
4	I	902	MGD	C23-C14-N15	4.93	112.71	107.87
4	S	903	MGD	O11-C23-N22	-4.92	104.14	108.61
4	A	903	MGD	O11-C23-N22	-4.90	104.16	108.61
4	E	902	MGD	O2A-PA-O3A	-4.89	85.39	107.57
4	S	902	MGD	C23-C14-N15	4.87	112.65	107.87
4	S	902	MGD	O2A-PA-O1A	-4.75	90.34	112.44
4	A	902	MGD	O2A-PA-O1A	-4.71	90.54	112.44
4	G	902	MGD	O2A-PA-O1A	-4.63	90.89	112.44
4	K	902	MGD	O2A-PA-O1A	-4.60	91.05	112.44
4	U	902	MGD	O2A-PA-O1A	-4.58	91.16	112.44
4	C	902	MGD	O2A-PA-O1A	-4.48	91.61	112.44
4	E	902	MGD	O2A-PA-O1A	-4.46	91.71	112.44
4	M	902	MGD	O2A-PA-O1A	-4.38	92.05	112.44
4	O	902	MGD	O2A-PA-O1A	-4.23	92.77	112.44
4	W	902	MGD	O2A-PA-O1A	-4.13	93.22	112.44
4	W	903	MGD	O11-C23-N22	-4.08	104.90	108.61
4	I	902	MGD	O2A-PA-O1A	-4.04	93.64	112.44
4	C	903	MGD	O11-C23-N22	-3.97	105.00	108.61
4	G	903	MGD	O5'-C5'-C4'	3.84	122.08	108.99
4	A	903	MGD	C2'-C1'-N9	3.78	123.76	113.25
4	O	903	MGD	O3B-PB-O1B	3.63	121.62	110.70
4	K	902	MGD	O3B-PA-O1A	3.60	121.55	110.70
4	Q	903	MGD	O5'-C5'-C4'	3.56	121.13	108.99
4	A	903	MGD	O4'-C1'-N9	-3.53	100.35	108.36
4	I	903	MGD	O11-C23-N22	-3.49	105.44	108.61
4	O	903	MGD	O4'-C1'-N9	-3.48	100.47	108.36
4	U	903	MGD	O5'-C5'-C4'	3.48	120.84	108.99
4	M	903	MGD	O5'-C5'-C4'	3.42	120.65	108.99
4	G	902	MGD	O3A-C10-C11	-3.39	100.21	108.58
4	G	903	MGD	O2B-PB-O3B	-3.39	98.11	107.27
4	O	903	MGD	O2B-PB-O5'	-3.33	92.47	107.57
4	A	902	MGD	O3A-C10-C11	-3.33	100.36	108.58
4	Q	903	MGD	O2B-PB-O3B	-3.30	98.36	107.27
4	W	903	MGD	O5'-C5'-C4'	3.21	119.93	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	903	MGD	O2B-PB-O5'	-3.19	93.12	107.57
4	G	903	MGD	O3B-PB-O1B	3.19	120.29	110.70
4	K	903	MGD	C4'-O4'-C1'	3.15	116.43	109.47
4	Q	902	MGD	O3A-C10-C11	-3.15	100.81	108.58
4	O	903	MGD	C2'-C1'-N9	3.13	121.97	113.25
4	K	903	MGD	O4'-C1'-N9	-3.13	101.26	108.36
4	K	903	MGD	C2'-C1'-N9	3.13	121.95	113.25
4	E	903	MGD	C2'-C1'-N9	3.12	121.92	113.25
4	K	903	MGD	O3B-PB-O1B	3.10	120.02	110.70
4	O	902	MGD	O3B-PA-O1A	3.09	119.99	110.70
4	A	903	MGD	O3B-PB-O1B	3.02	119.78	110.70
4	O	903	MGD	C4'-O4'-C1'	3.01	116.11	109.47
4	A	903	MGD	C4'-O4'-C1'	3.01	116.11	109.47
4	A	903	MGD	O2B-PB-O5'	-3.01	93.94	107.57
4	U	902	MGD	O3A-C10-C11	-3.00	101.17	108.58
4	Q	903	MGD	O3B-PB-O1B	2.99	119.69	110.70
4	G	902	MGD	O4'-C4'-C5'	-2.97	99.83	109.33
4	E	903	MGD	C4'-O4'-C1'	2.95	115.98	109.47
4	M	902	MGD	O3A-C10-C11	-2.94	101.31	108.58
6	W	905	BTT	O5-C5-C4	-2.90	110.69	118.42
4	C	902	MGD	O3B-PA-O1A	2.90	119.42	110.70
4	S	903	MGD	O4'-C4'-C3'	2.89	110.90	105.15
4	U	902	MGD	O3B-PA-O1A	2.88	119.38	110.70
4	G	903	MGD	C4'-O4'-C1'	2.88	115.81	109.47
4	Q	903	MGD	O4'-C1'-N9	-2.85	101.89	108.36
4	M	903	MGD	PB-O5'-C5'	-2.85	105.05	121.35
4	S	902	MGD	O3A-C10-C11	-2.84	101.56	108.58
4	K	903	MGD	O2B-PB-O5'	-2.84	94.70	107.57
4	C	902	MGD	O3A-C10-C11	-2.83	101.59	108.58
6	K	905	BTT	O5-C5-C4	-2.83	110.88	118.42
6	C	905	BTT	O5-C5-C4	-2.82	110.89	118.42
4	W	902	MGD	O3B-PA-O1A	2.81	119.17	110.70
6	O	905	BTT	O5-C5-C4	-2.81	110.92	118.42
4	M	902	MGD	O5'-C5'-C4'	-2.81	99.44	108.99
4	Q	903	MGD	C4'-O4'-C1'	2.81	115.66	109.47
6	Q	905	BTT	O5-C5-C4	-2.80	110.94	118.42
4	O	903	MGD	O2B-PB-O3B	-2.80	99.71	107.27
4	A	902	MGD	O3B-PA-O1A	2.77	119.03	110.70
4	G	902	MGD	O3B-PA-O1A	2.77	119.03	110.70
6	A	905	BTT	O5-C5-C4	-2.77	111.03	118.42
4	I	902	MGD	O4'-C4'-C5'	-2.77	100.47	109.33
4	I	902	MGD	O3B-PA-O1A	2.76	119.00	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	902	MGD	O3B-PA-O1A	2.75	118.98	110.70
4	Q	902	MGD	O3B-PA-O1A	2.75	118.96	110.70
6	U	905	BTT	O5-C5-C4	-2.74	111.10	118.42
6	G	905	BTT	O5-C5-C4	-2.73	111.14	118.42
4	U	902	MGD	O4'-C4'-C5'	-2.72	100.62	109.33
6	S	905	BTT	O5-C5-C4	-2.72	111.17	118.42
4	W	903	MGD	PB-O5'-C5'	-2.72	105.79	121.35
6	M	905	BTT	O5-C5-C4	-2.71	111.18	118.42
4	E	902	MGD	O3A-C10-C11	-2.71	101.89	108.58
4	O	903	MGD	O5'-PB-O1B	2.70	119.62	108.94
4	A	903	MGD	O5'-PB-O1B	2.70	119.62	108.94
6	E	905	BTT	O5-C5-C4	-2.69	111.25	118.42
4	E	902	MGD	O11-C23-C14	2.68	110.75	108.96
4	Q	903	MGD	C2'-C1'-N9	2.68	120.71	113.25
6	I	905	BTT	O5-C5-C4	-2.68	111.28	118.42
4	O	903	MGD	O5'-C5'-C4'	2.68	118.11	108.99
6	U	905	BTT	O1-C1-C2	2.67	125.56	118.42
4	M	902	MGD	O3B-PA-O1A	2.66	118.70	110.70
6	I	905	BTT	O1-C1-C2	2.66	125.52	118.42
6	S	905	BTT	O1-C1-C2	2.65	125.50	118.42
4	S	902	MGD	O4'-C4'-C5'	-2.64	100.88	109.33
4	Q	902	MGD	O11-C23-C14	2.63	110.72	108.96
6	C	905	BTT	O1-C1-C2	2.62	125.43	118.42
6	K	905	BTT	O1-C1-C2	2.62	125.43	118.42
4	I	902	MGD	O3A-C10-C11	-2.62	102.12	108.58
6	O	905	BTT	O1-C1-C2	2.61	125.41	118.42
4	K	903	MGD	O5'-PB-O1B	2.61	119.28	108.94
4	E	903	MGD	O4'-C1'-N9	-2.60	102.47	108.36
4	Q	902	MGD	O4'-C4'-C5'	-2.60	101.01	109.33
4	Q	903	MGD	O5'-PB-O1B	2.59	119.22	108.94
4	G	903	MGD	O2B-PB-O5'	-2.59	95.83	107.57
6	G	905	BTT	O1-C1-C2	2.58	125.31	118.42
6	A	905	BTT	O1-C1-C2	2.56	125.26	118.42
6	Q	905	BTT	O1-C1-C2	2.55	125.24	118.42
6	E	905	BTT	O1-C1-C2	2.55	125.22	118.42
4	C	903	MGD	O5'-C5'-C4'	2.54	117.65	108.99
6	M	905	BTT	O1-C1-C2	2.52	125.16	118.42
4	U	903	MGD	PB-O5'-C5'	-2.52	106.91	121.35
6	W	905	BTT	O1-C1-C2	2.51	125.12	118.42
4	G	903	MGD	C2'-C1'-N9	2.49	120.17	113.25
4	S	902	MGD	O5'-C5'-C4'	-2.45	100.65	108.99
4	W	903	MGD	O2B-PB-O3B	-2.45	100.66	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	903	MGD	O4'-C1'-N9	-2.44	102.82	108.36
4	S	902	MGD	O3B-PA-O1A	2.43	118.03	110.70
4	C	902	MGD	O4'-C4'-C5'	-2.43	101.55	109.33
4	E	903	MGD	O2B-PB-O5'	-2.43	96.56	107.57
4	O	902	MGD	O4'-C4'-C5'	-2.40	101.65	109.33
4	O	902	MGD	O5'-C5'-C4'	-2.40	100.83	108.99
4	K	902	MGD	O4'-C4'-C5'	-2.37	101.73	109.33
4	G	903	MGD	O5'-PB-O1B	2.36	118.31	108.94
4	W	902	MGD	O11-C23-C14	2.36	110.53	108.96
4	U	902	MGD	O5'-C5'-C4'	-2.35	100.99	108.99
4	I	903	MGD	O4'-C4'-C3'	2.34	109.81	105.15
4	I	902	MGD	O11-C23-C14	2.34	110.53	108.96
4	E	903	MGD	O3B-PB-O1B	2.34	117.74	110.70
4	A	902	MGD	O5'-C5'-C4'	-2.33	101.06	108.99
4	E	902	MGD	O4'-C4'-C5'	-2.31	101.94	109.33
4	O	902	MGD	O3A-C10-C11	-2.30	102.90	108.58
4	A	902	MGD	O11-C23-C14	2.30	110.50	108.96
4	E	902	MGD	O5'-C5'-C4'	-2.28	101.22	108.99
4	C	902	MGD	O5'-C5'-C4'	-2.27	101.25	108.99
4	M	902	MGD	O11-C23-C14	2.26	110.47	108.96
4	Q	902	MGD	O5'-C5'-C4'	-2.26	101.30	108.99
4	W	902	MGD	O5'-C5'-C4'	-2.22	101.42	108.99
4	W	903	MGD	O4'-C4'-C3'	2.20	109.51	105.15
4	M	902	MGD	O4'-C4'-C5'	-2.20	102.30	109.33
4	K	902	MGD	O3A-C10-C11	-2.19	103.19	108.58
4	M	903	MGD	C3'-C2'-C1'	2.11	105.46	101.46
4	C	902	MGD	O11-C23-C14	2.10	110.37	108.96
4	A	903	MGD	O2B-PB-O3B	-2.10	101.60	107.27
4	W	902	MGD	O4'-C4'-C5'	-2.09	102.64	109.33
4	G	902	MGD	O5'-C5'-C4'	-2.09	101.89	108.99
4	U	903	MGD	C3'-C2'-C1'	2.08	105.40	101.46
4	K	903	MGD	O3A-PA-O1A	-2.05	100.82	108.94
4	W	903	MGD	C3'-C2'-C1'	2.02	105.28	101.46
4	W	903	MGD	C2'-C1'-N9	2.01	118.86	113.25
4	I	903	MGD	C5'-C4'-C3'	-2.01	107.98	115.21
4	I	902	MGD	O5'-C5'-C4'	-2.01	102.16	108.99
4	I	903	MGD	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (155) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	MGD	C5'-O5'-PB-O1B
4	A	902	MGD	C5'-O5'-PB-O2B
4	A	902	MGD	C5'-O5'-PB-O3B
4	A	902	MGD	C10-O3A-PA-O2A
4	A	902	MGD	O3A-C10-C11-O11
4	A	902	MGD	O3A-C10-C11-C12
4	A	903	MGD	C5'-O5'-PB-O1B
4	A	903	MGD	C5'-O5'-PB-O2B
4	A	903	MGD	C5'-O5'-PB-O3B
4	A	903	MGD	C4'-C5'-O5'-PB
4	C	902	MGD	C5'-O5'-PB-O1B
4	C	902	MGD	C5'-O5'-PB-O2B
4	C	902	MGD	C5'-O5'-PB-O3B
4	C	902	MGD	C10-O3A-PA-O2A
4	C	902	MGD	O3A-C10-C11-O11
4	C	902	MGD	O3A-C10-C11-C12
4	C	903	MGD	C5'-O5'-PB-O1B
4	C	903	MGD	C5'-O5'-PB-O2B
4	C	903	MGD	C5'-O5'-PB-O3B
4	E	902	MGD	C5'-O5'-PB-O1B
4	E	902	MGD	C5'-O5'-PB-O2B
4	E	902	MGD	C5'-O5'-PB-O3B
4	E	902	MGD	C10-O3A-PA-O2A
4	E	902	MGD	O3A-C10-C11-O11
4	E	902	MGD	O3A-C10-C11-C12
4	E	903	MGD	C5'-O5'-PB-O1B
4	E	903	MGD	C5'-O5'-PB-O2B
4	E	903	MGD	C5'-O5'-PB-O3B
4	E	903	MGD	C4'-C5'-O5'-PB
4	G	902	MGD	C5'-O5'-PB-O1B
4	G	902	MGD	C5'-O5'-PB-O2B
4	G	902	MGD	C5'-O5'-PB-O3B
4	G	902	MGD	C10-O3A-PA-O2A
4	G	902	MGD	O3A-C10-C11-O11
4	G	902	MGD	O3A-C10-C11-C12
4	G	903	MGD	C5'-O5'-PB-O1B
4	G	903	MGD	C5'-O5'-PB-O2B
4	G	903	MGD	C4'-C5'-O5'-PB
4	I	902	MGD	C5'-O5'-PB-O1B
4	I	902	MGD	C5'-O5'-PB-O2B
4	I	902	MGD	C5'-O5'-PB-O3B
4	I	902	MGD	C10-O3A-PA-O2A
4	I	902	MGD	O3A-C10-C11-O11

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Mol	Chain	Res	Type	Atoms
4	I	902	MGD	O3A-C10-C11-C12
4	I	903	MGD	C5'-O5'-PB-O1B
4	I	903	MGD	C5'-O5'-PB-O2B
4	I	903	MGD	C5'-O5'-PB-O3B
4	K	902	MGD	PA-O3B-PB-O5'
4	K	902	MGD	C5'-O5'-PB-O1B
4	K	902	MGD	C5'-O5'-PB-O2B
4	K	902	MGD	C5'-O5'-PB-O3B
4	K	902	MGD	C10-O3A-PA-O2A
4	K	902	MGD	O3A-C10-C11-O11
4	K	902	MGD	O3A-C10-C11-C12
4	K	903	MGD	C5'-O5'-PB-O1B
4	K	903	MGD	C5'-O5'-PB-O2B
4	K	903	MGD	C5'-O5'-PB-O3B
4	K	903	MGD	C4'-C5'-O5'-PB
4	M	902	MGD	C5'-O5'-PB-O1B
4	M	902	MGD	C5'-O5'-PB-O2B
4	M	902	MGD	C5'-O5'-PB-O3B
4	M	902	MGD	C10-O3A-PA-O2A
4	M	902	MGD	O3A-C10-C11-O11
4	M	902	MGD	O3A-C10-C11-C12
4	M	903	MGD	C5'-O5'-PB-O1B
4	M	903	MGD	C5'-O5'-PB-O2B
4	M	903	MGD	C5'-O5'-PB-O3B
4	O	902	MGD	C5'-O5'-PB-O1B
4	O	902	MGD	C5'-O5'-PB-O2B
4	O	902	MGD	C5'-O5'-PB-O3B
4	O	902	MGD	C10-O3A-PA-O2A
4	O	902	MGD	O3A-C10-C11-C12
4	O	903	MGD	C5'-O5'-PB-O1B
4	O	903	MGD	C5'-O5'-PB-O2B
4	O	903	MGD	C4'-C5'-O5'-PB
4	Q	902	MGD	C5'-O5'-PB-O1B
4	Q	902	MGD	C5'-O5'-PB-O2B
4	Q	902	MGD	C5'-O5'-PB-O3B
4	Q	902	MGD	C10-O3A-PA-O2A
4	Q	902	MGD	O3A-C10-C11-O11
4	Q	902	MGD	O3A-C10-C11-C12
4	Q	903	MGD	C5'-O5'-PB-O1B
4	Q	903	MGD	C5'-O5'-PB-O2B
4	Q	903	MGD	C4'-C5'-O5'-PB
4	S	902	MGD	C5'-O5'-PB-O1B

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Mol	Chain	Res	Type	Atoms
4	S	902	MGD	C5'-O5'-PB-O2B
4	S	902	MGD	C5'-O5'-PB-O3B
4	S	902	MGD	C10-O3A-PA-O2A
4	S	902	MGD	O3A-C10-C11-O11
4	S	902	MGD	O3A-C10-C11-C12
4	S	903	MGD	C5'-O5'-PB-O1B
4	S	903	MGD	C5'-O5'-PB-O2B
4	S	903	MGD	C5'-O5'-PB-O3B
4	U	902	MGD	C5'-O5'-PB-O1B
4	U	902	MGD	C5'-O5'-PB-O2B
4	U	902	MGD	C5'-O5'-PB-O3B
4	U	902	MGD	C10-O3A-PA-O2A
4	U	902	MGD	O3A-C10-C11-O11
4	U	902	MGD	O3A-C10-C11-C12
4	U	903	MGD	C5'-O5'-PB-O1B
4	U	903	MGD	C5'-O5'-PB-O2B
4	U	903	MGD	C5'-O5'-PB-O3B
4	W	902	MGD	C5'-O5'-PB-O1B
4	W	902	MGD	C5'-O5'-PB-O2B
4	W	902	MGD	C5'-O5'-PB-O3B
4	W	902	MGD	C10-O3A-PA-O2A
4	W	902	MGD	O3A-C10-C11-O11
4	W	902	MGD	O3A-C10-C11-C12
4	W	903	MGD	C5'-O5'-PB-O1B
4	W	903	MGD	C5'-O5'-PB-O2B
4	W	903	MGD	C5'-O5'-PB-O3B
4	K	903	MGD	PA-O3B-PB-O1B
4	K	903	MGD	C3'-C4'-C5'-O5'
4	O	902	MGD	O3A-C10-C11-O11
4	A	903	MGD	C3'-C4'-C5'-O5'
4	O	903	MGD	C3'-C4'-C5'-O5'
4	O	903	MGD	PA-O3B-PB-O2B
4	A	902	MGD	C10-O3A-PA-O3B
4	C	902	MGD	C10-O3A-PA-O3B
4	E	902	MGD	C10-O3A-PA-O3B
4	G	902	MGD	C10-O3A-PA-O3B
4	I	902	MGD	C10-O3A-PA-O3B
4	K	902	MGD	C10-O3A-PA-O3B
4	M	902	MGD	C10-O3A-PA-O3B
4	O	902	MGD	C10-O3A-PA-O3B
4	Q	902	MGD	C10-O3A-PA-O3B
4	S	902	MGD	C10-O3A-PA-O3B

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Mol	Chain	Res	Type	Atoms
4	U	902	MGD	C10-O3A-PA-O3B
4	W	902	MGD	C10-O3A-PA-O3B
4	W	903	MGD	C4'-C5'-O5'-PB
4	E	903	MGD	PA-O3B-PB-O1B
4	E	903	MGD	C2'-C1'-N9-C8
4	A	903	MGD	O3A-C10-C11-O11
4	E	903	MGD	O3A-C10-C11-O11
4	G	903	MGD	O3A-C10-C11-O11
4	K	903	MGD	O3A-C10-C11-O11
4	O	903	MGD	O3A-C10-C11-O11
4	Q	903	MGD	O3A-C10-C11-O11
4	E	903	MGD	C2'-C1'-N9-C4
4	E	903	MGD	C3'-C4'-C5'-O5'
4	A	903	MGD	PA-O3B-PB-O1B
4	A	903	MGD	C2'-C1'-N9-C8
4	M	903	MGD	C4'-C5'-O5'-PB
4	A	903	MGD	PA-O3B-PB-O2B
4	K	902	MGD	PB-O3B-PA-O2A
4	M	903	MGD	O4'-C4'-C5'-O5'
4	Q	903	MGD	C3'-C4'-C5'-O5'
4	U	903	MGD	O4'-C4'-C5'-O5'
4	G	903	MGD	C3'-C4'-C5'-O5'
4	W	903	MGD	O4'-C4'-C5'-O5'
4	K	903	MGD	C2'-C1'-N9-C8
4	E	903	MGD	O3A-C10-C11-C12
4	K	903	MGD	PA-O3B-PB-O2B
4	O	903	MGD	PA-O3B-PB-O1B
4	W	902	MGD	PB-O3B-PA-O2A

There are no ring outliers.

70 monomers are involved in 229 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	U	905	BTT	1	0
6	G	905	BTT	1	0
7	N	304	SF4	1	0
7	N	302	SF4	1	0
4	M	903	MGD	8	0
4	S	902	MGD	7	0
7	F	303	SF4	3	0
7	J	303	SF4	2	0
7	X	303	SF4	2	0

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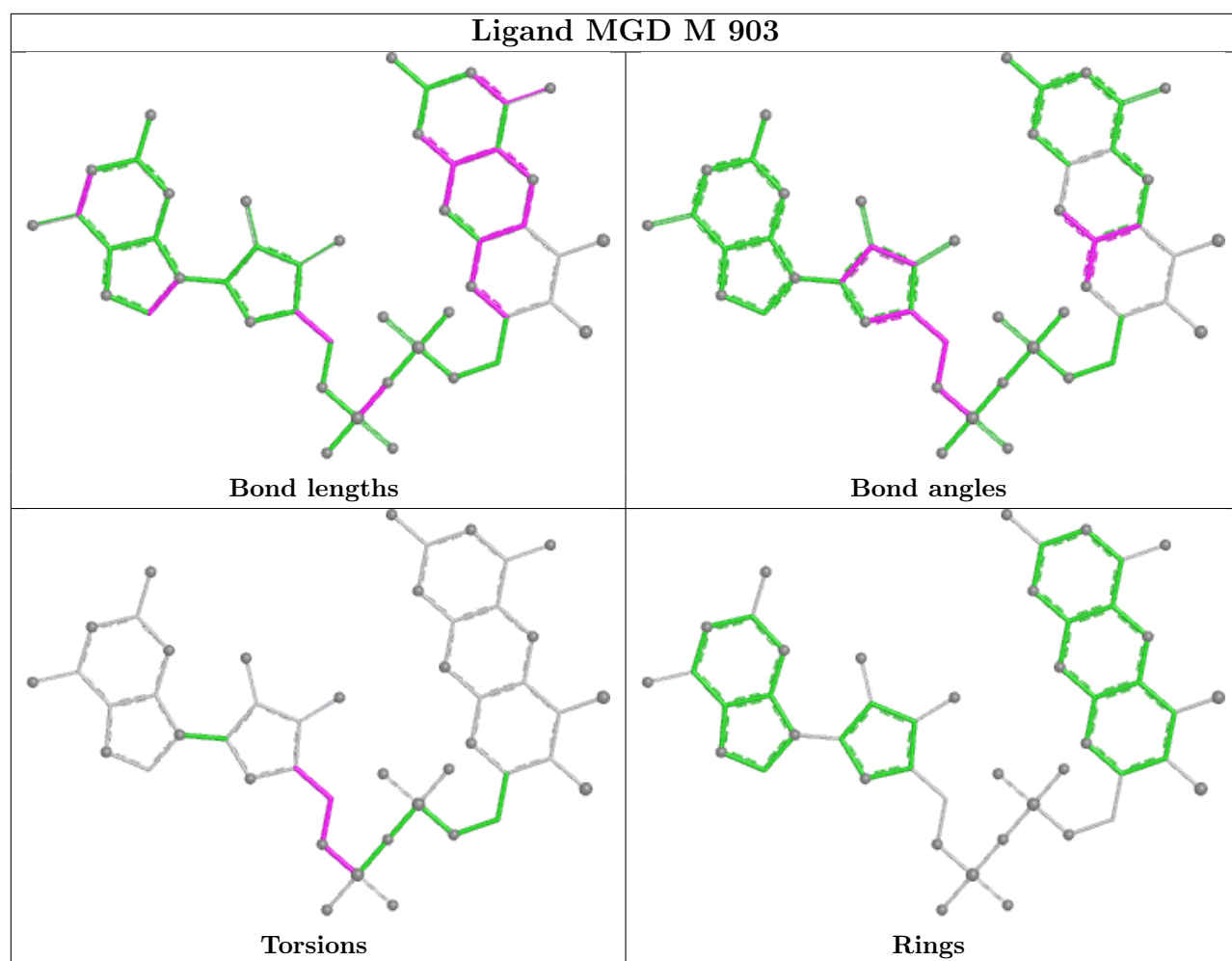
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	905	BTT	1	0
4	I	902	MGD	5	0
7	D	304	SF4	1	0
4	W	903	MGD	9	0
7	L	302	SF4	1	0
4	M	902	MGD	8	0
7	H	302	SF4	1	0
4	E	903	MGD	7	0
4	I	903	MGD	5	0
6	M	905	BTT	1	0
7	J	304	SF4	1	0
4	U	903	MGD	9	0
7	T	304	SF4	1	0
4	W	902	MGD	5	0
7	T	302	SF4	1	0
7	X	304	SF4	1	0
4	Q	902	MGD	5	0
4	G	902	MGD	6	0
6	O	905	BTT	1	0
4	O	902	MGD	6	0
7	V	304	SF4	1	0
7	R	302	SF4	1	0
4	G	903	MGD	10	0
7	J	302	SF4	1	0
4	Q	903	MGD	11	0
7	F	304	SF4	1	0
6	W	905	BTT	1	0
7	P	302	SF4	1	0
7	B	303	SF4	2	0
6	E	905	BTT	1	0
6	A	905	BTT	1	0
7	R	303	SF4	2	0
7	H	303	SF4	2	0
4	A	902	MGD	5	0
6	K	905	BTT	1	0
7	P	304	SF4	1	0
4	A	903	MGD	6	0
4	S	903	MGD	4	0
6	Q	905	BTT	1	0
7	B	304	SF4	1	0
7	H	304	SF4	1	0
6	C	905	BTT	1	0

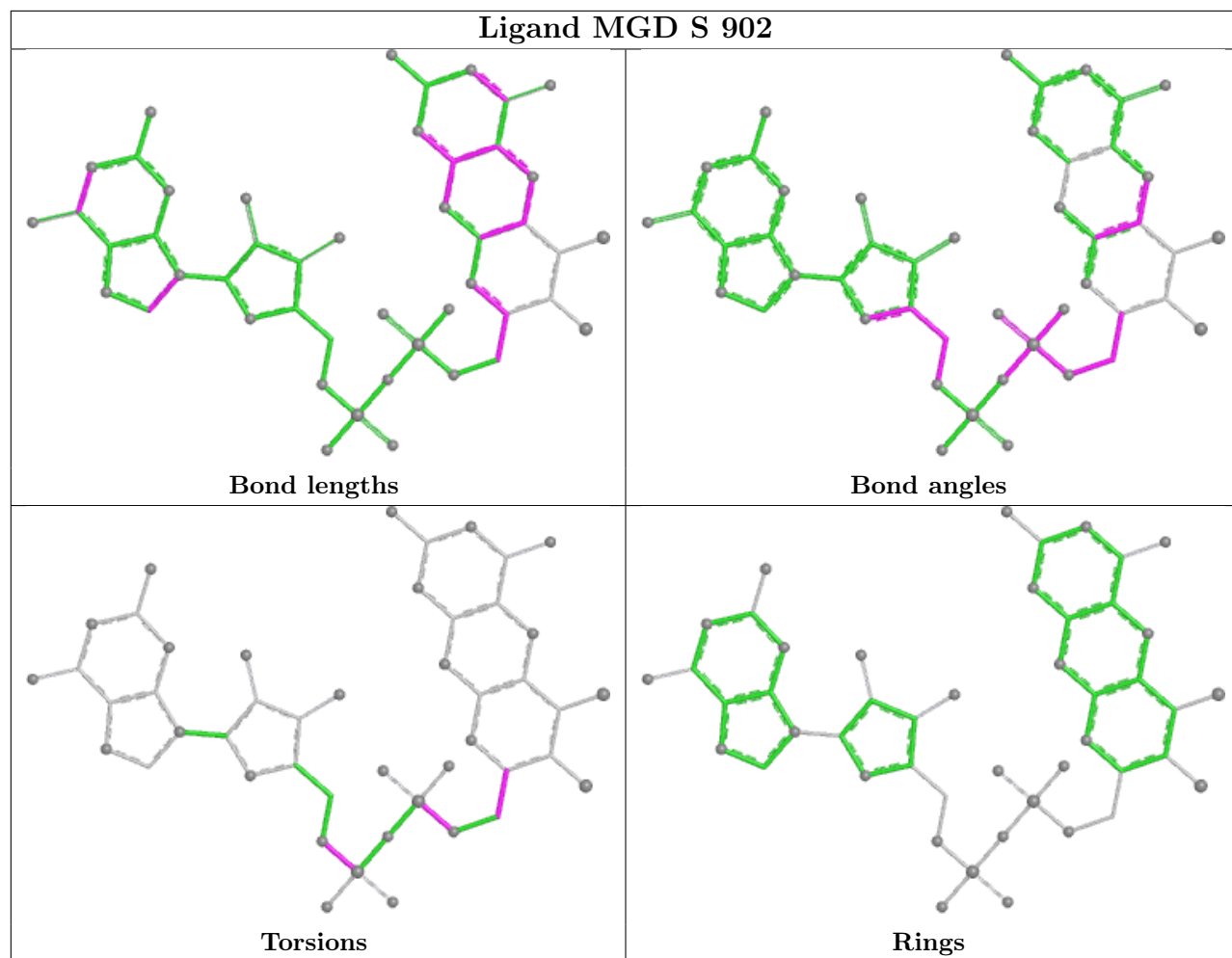
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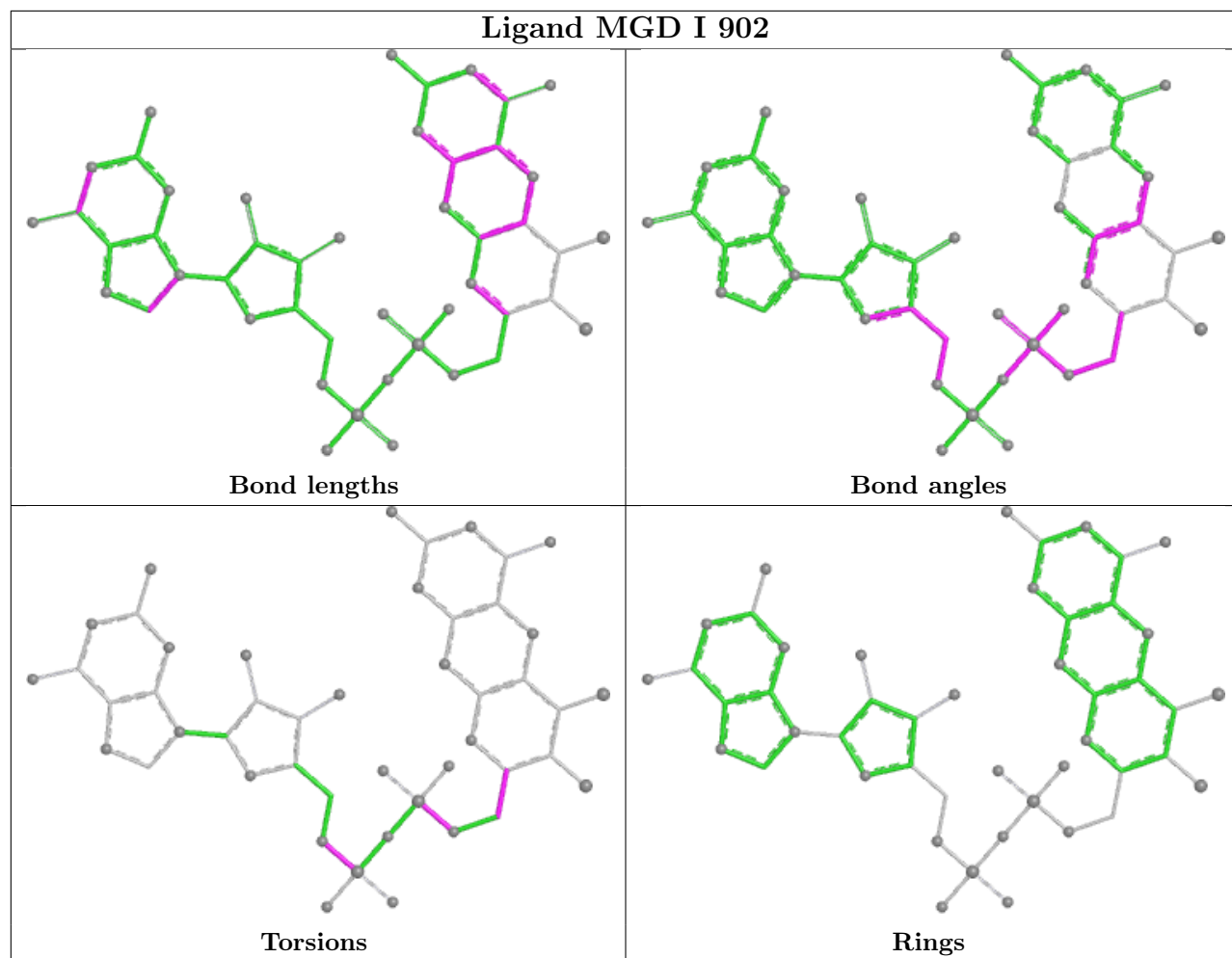
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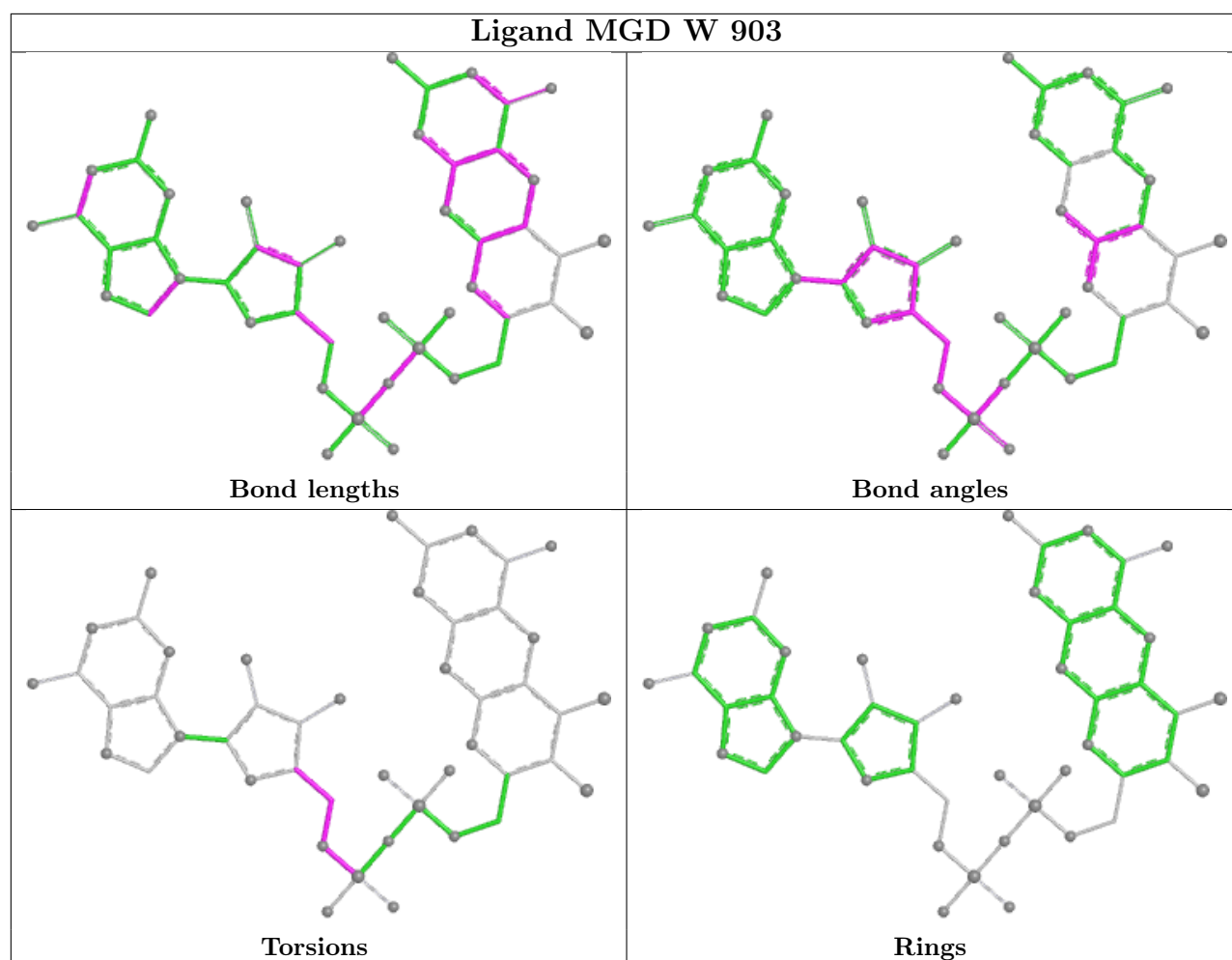
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	V	303	SF4	2	0
7	P	303	SF4	2	0
4	O	903	MGD	11	0
7	L	303	SF4	2	0
4	E	902	MGD	6	0
4	U	902	MGD	6	0
7	L	304	SF4	1	0
4	K	903	MGD	7	0
7	N	303	SF4	3	0
7	X	302	SF4	1	0
7	V	302	SF4	1	0
7	D	302	SF4	1	0
7	D	303	SF4	2	0
7	R	304	SF4	1	0
7	T	303	SF4	2	0
4	C	903	MGD	9	0
4	K	902	MGD	8	0
6	I	905	BTT	1	0
4	C	902	MGD	6	0

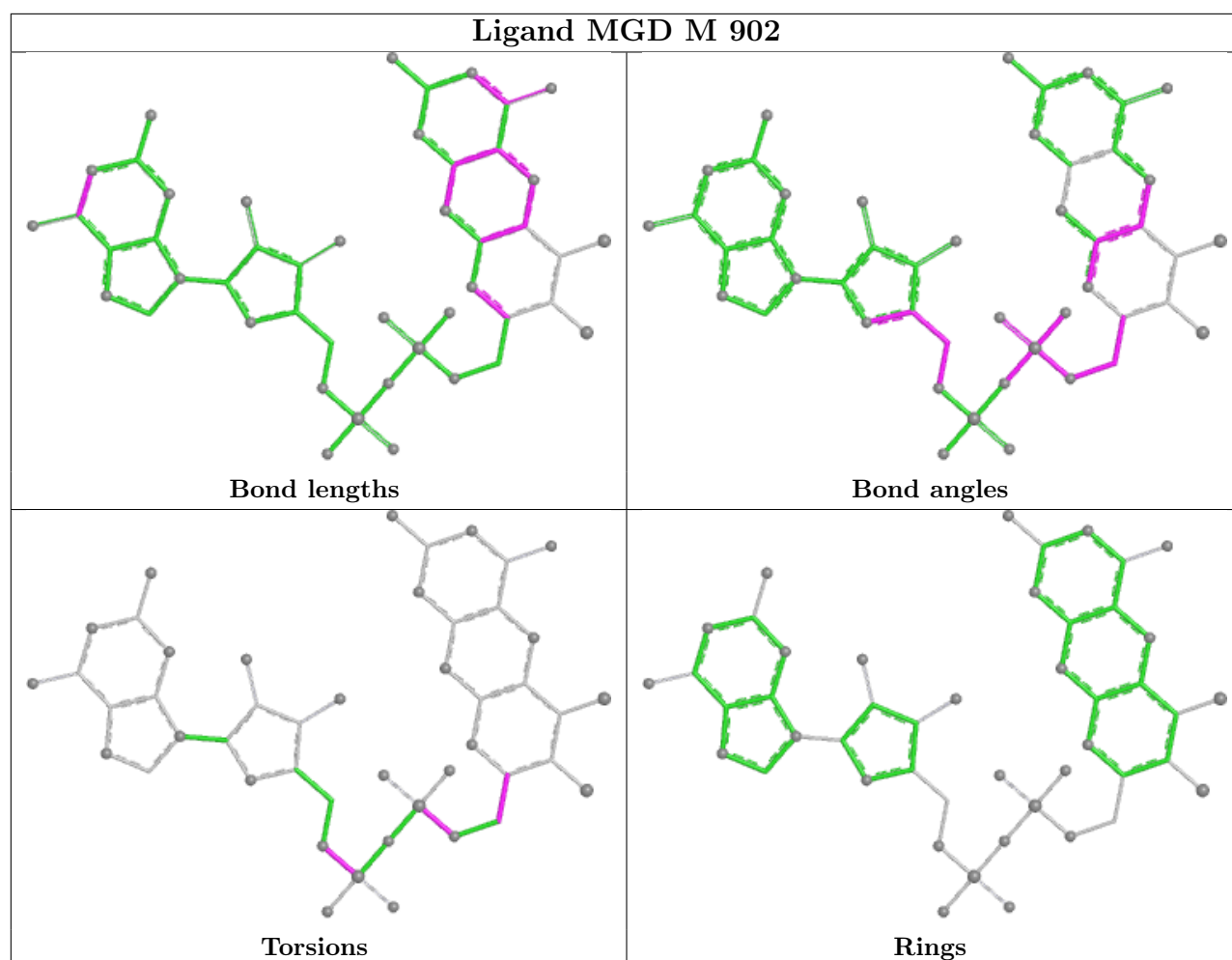
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

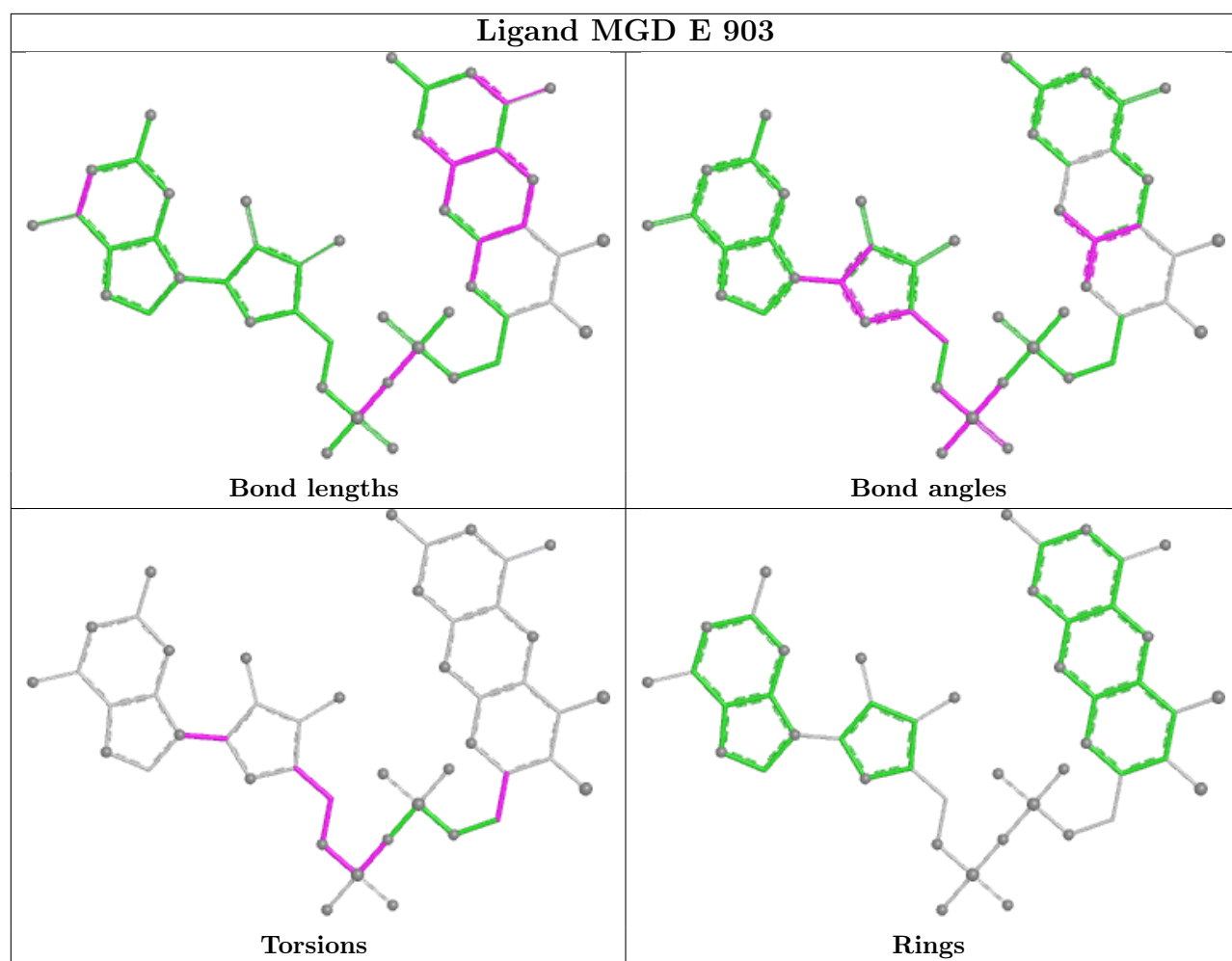


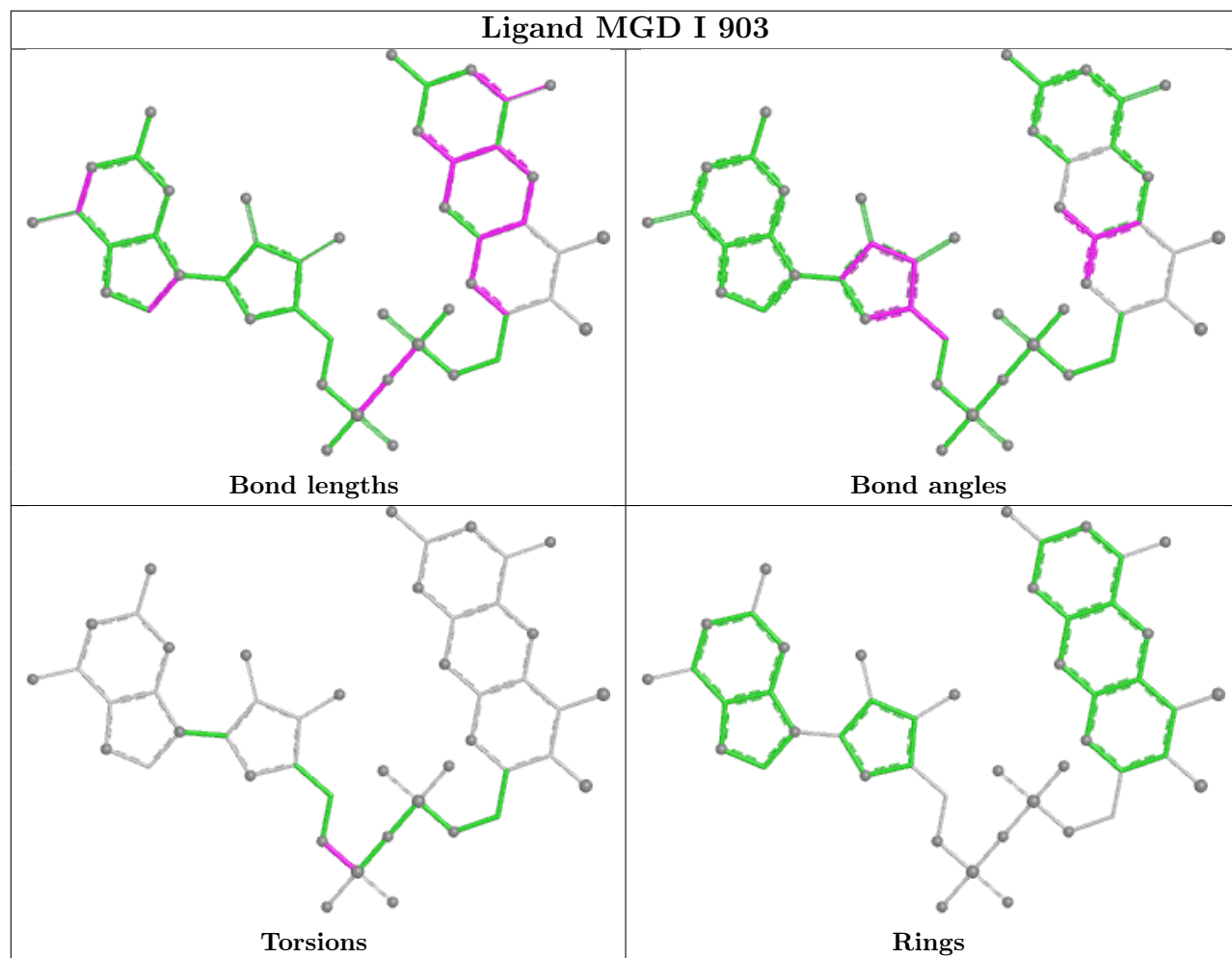


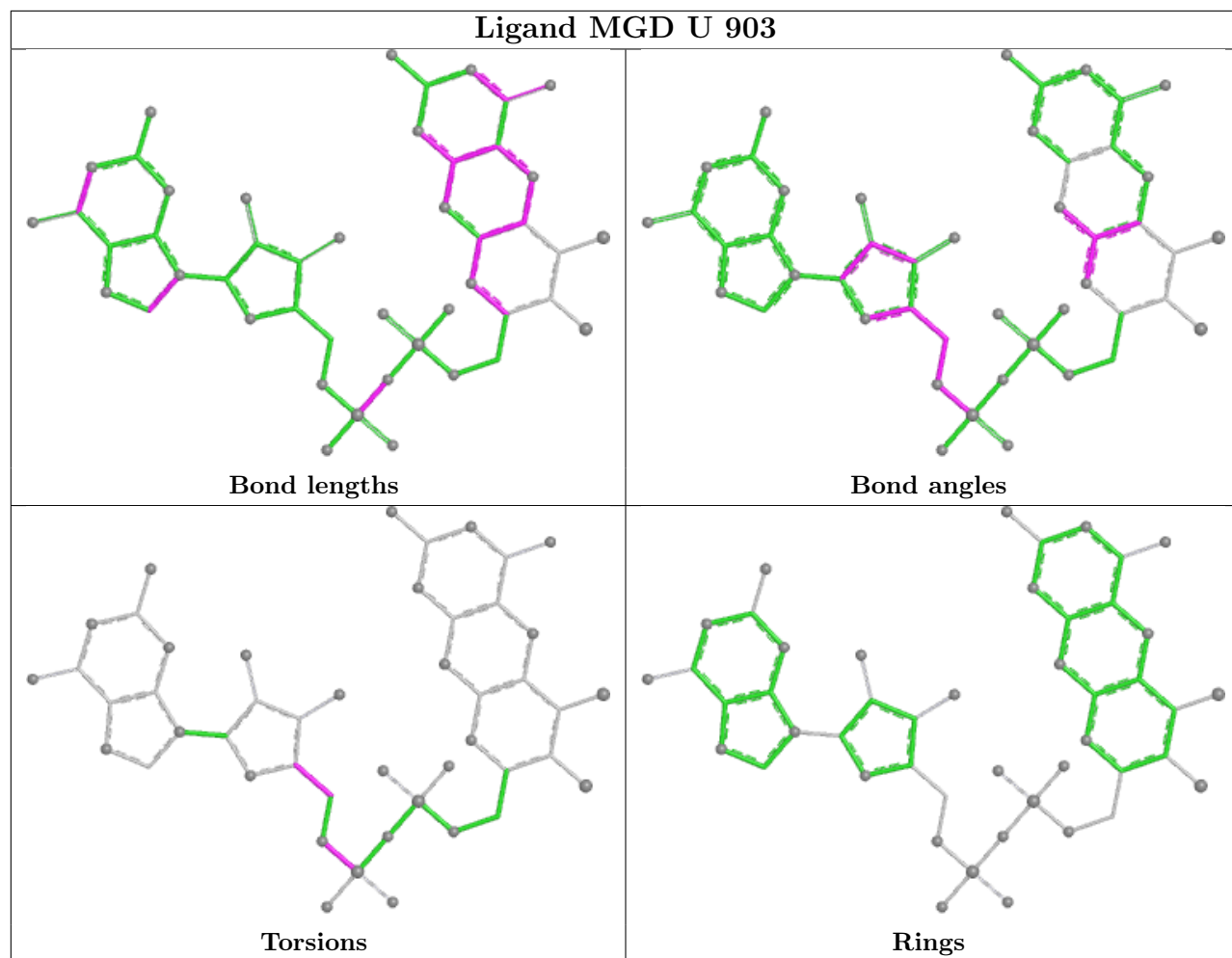


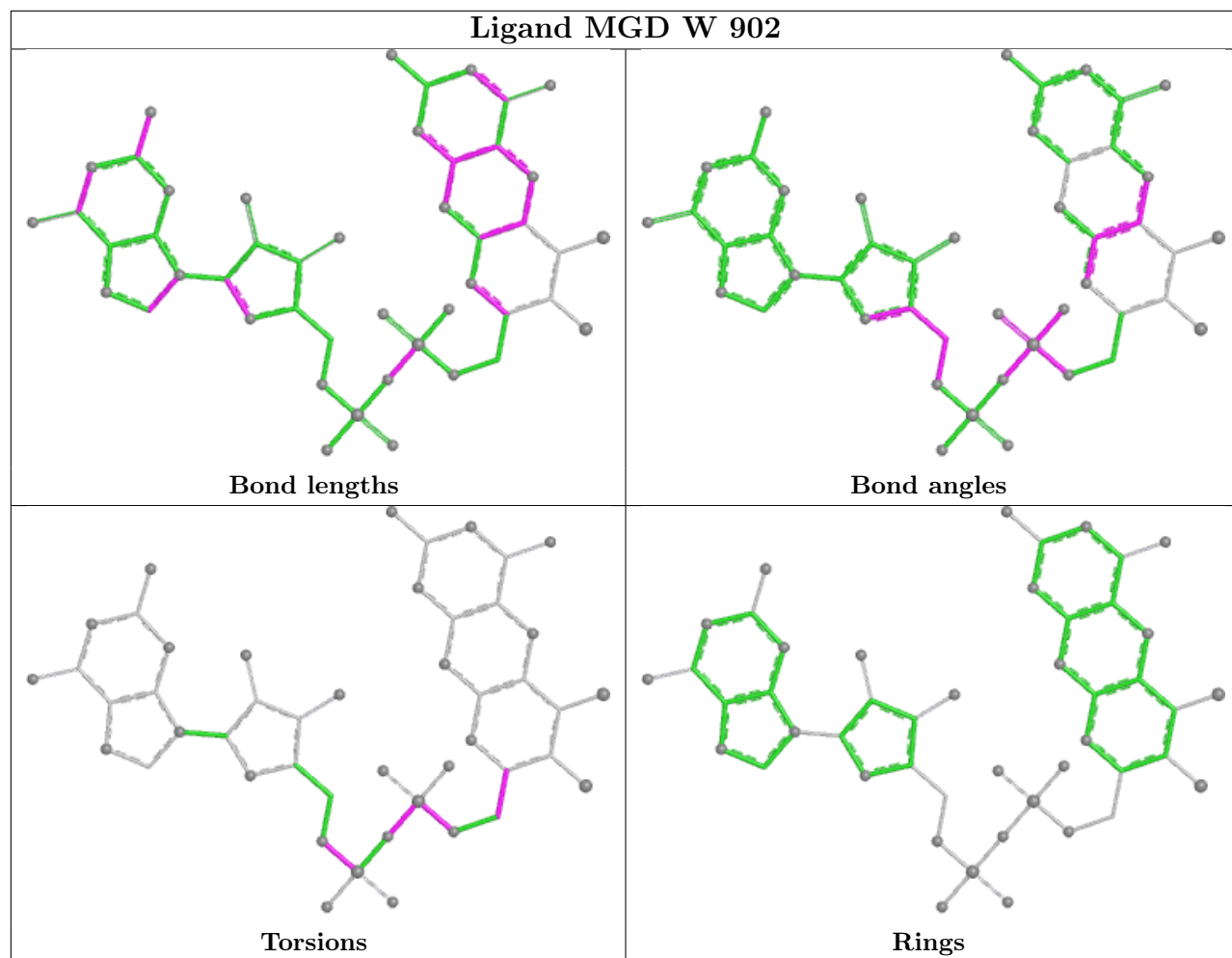


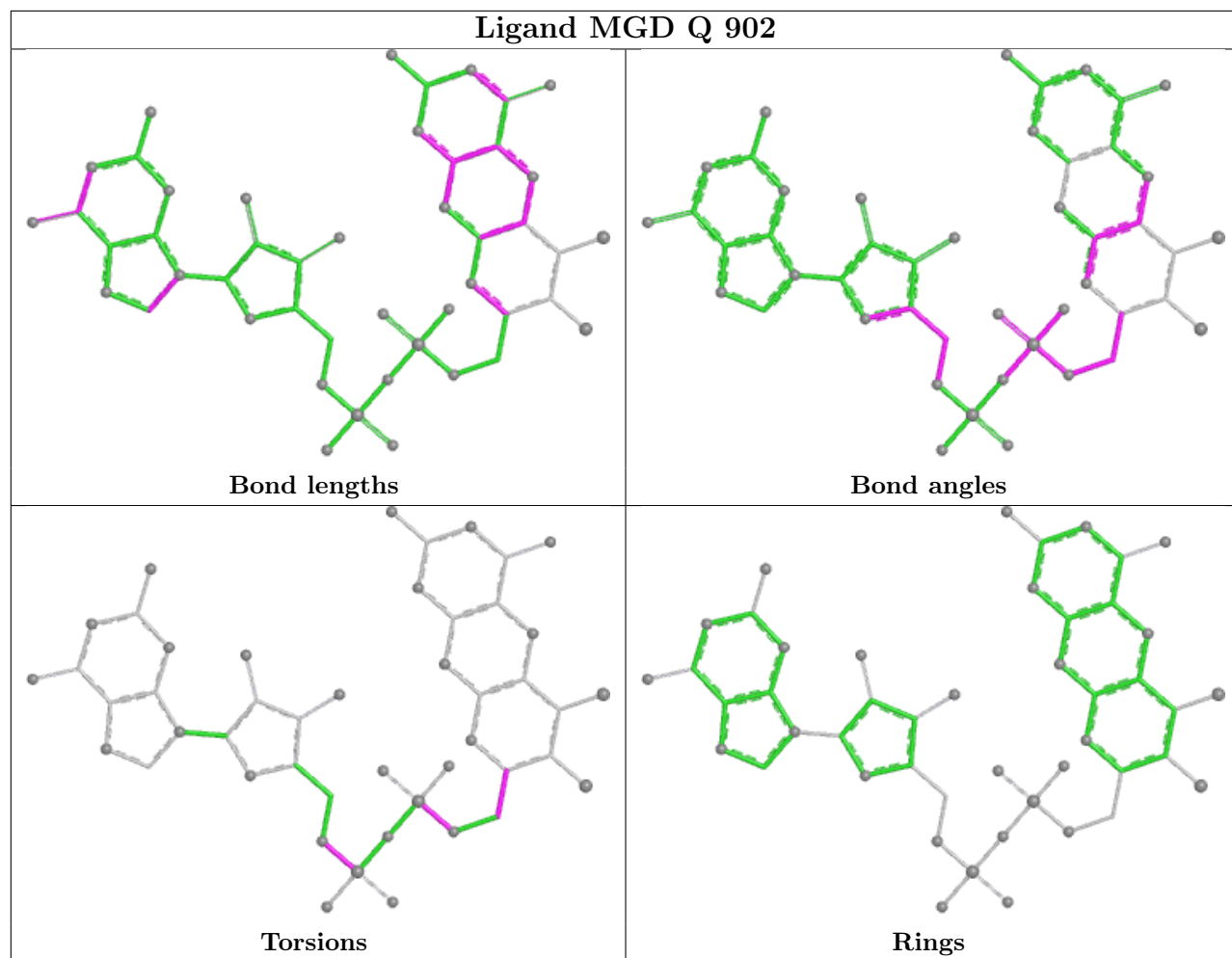


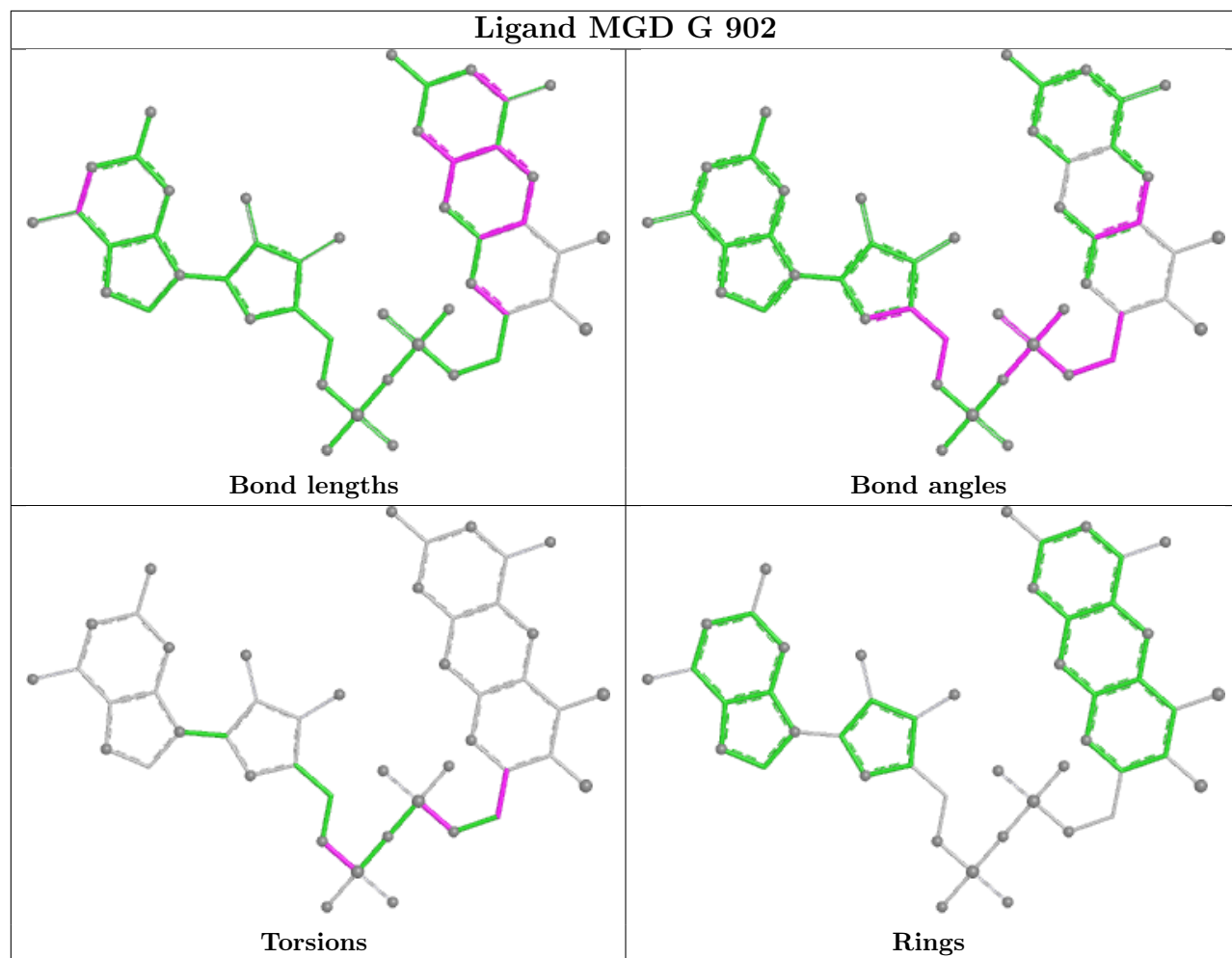


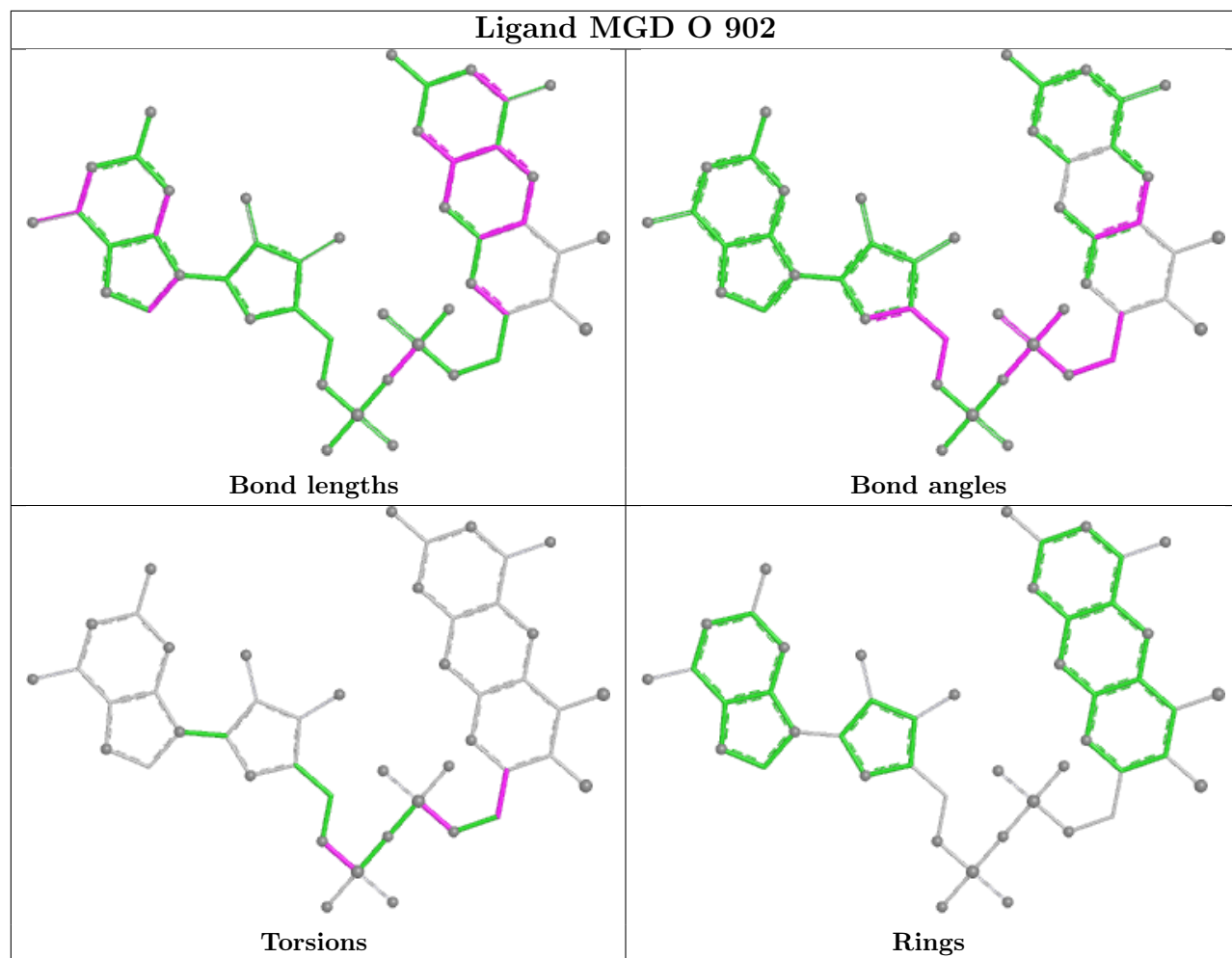


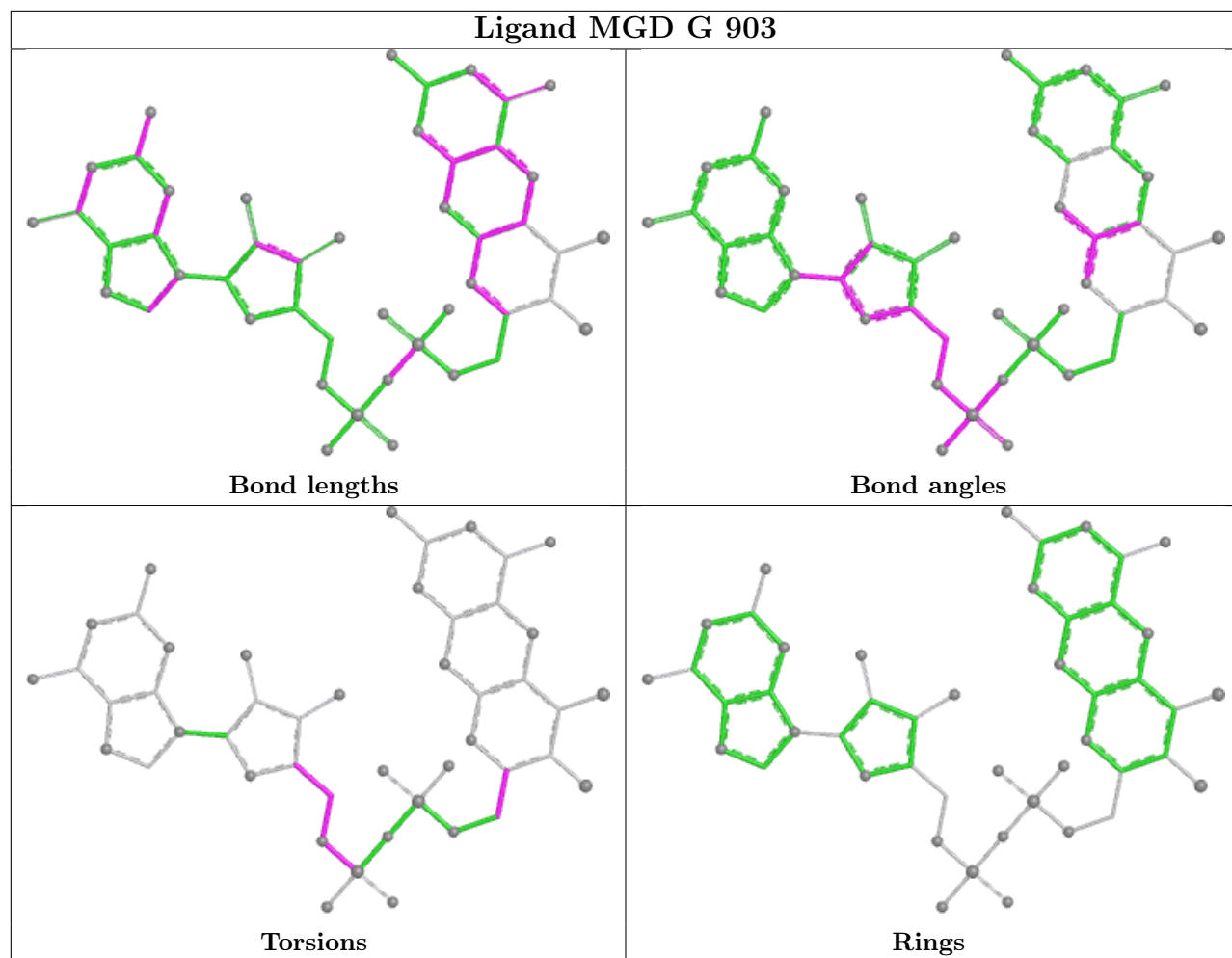


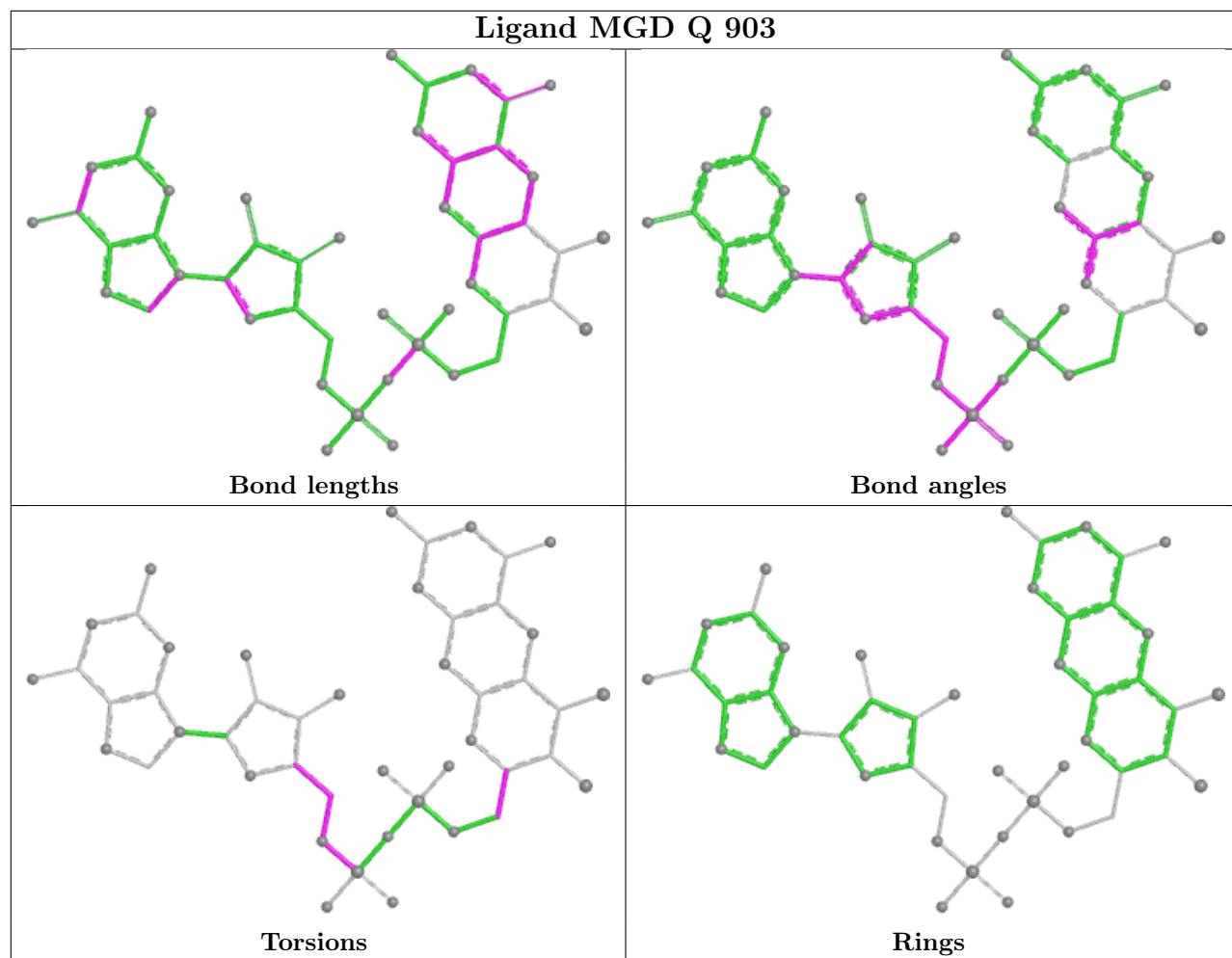


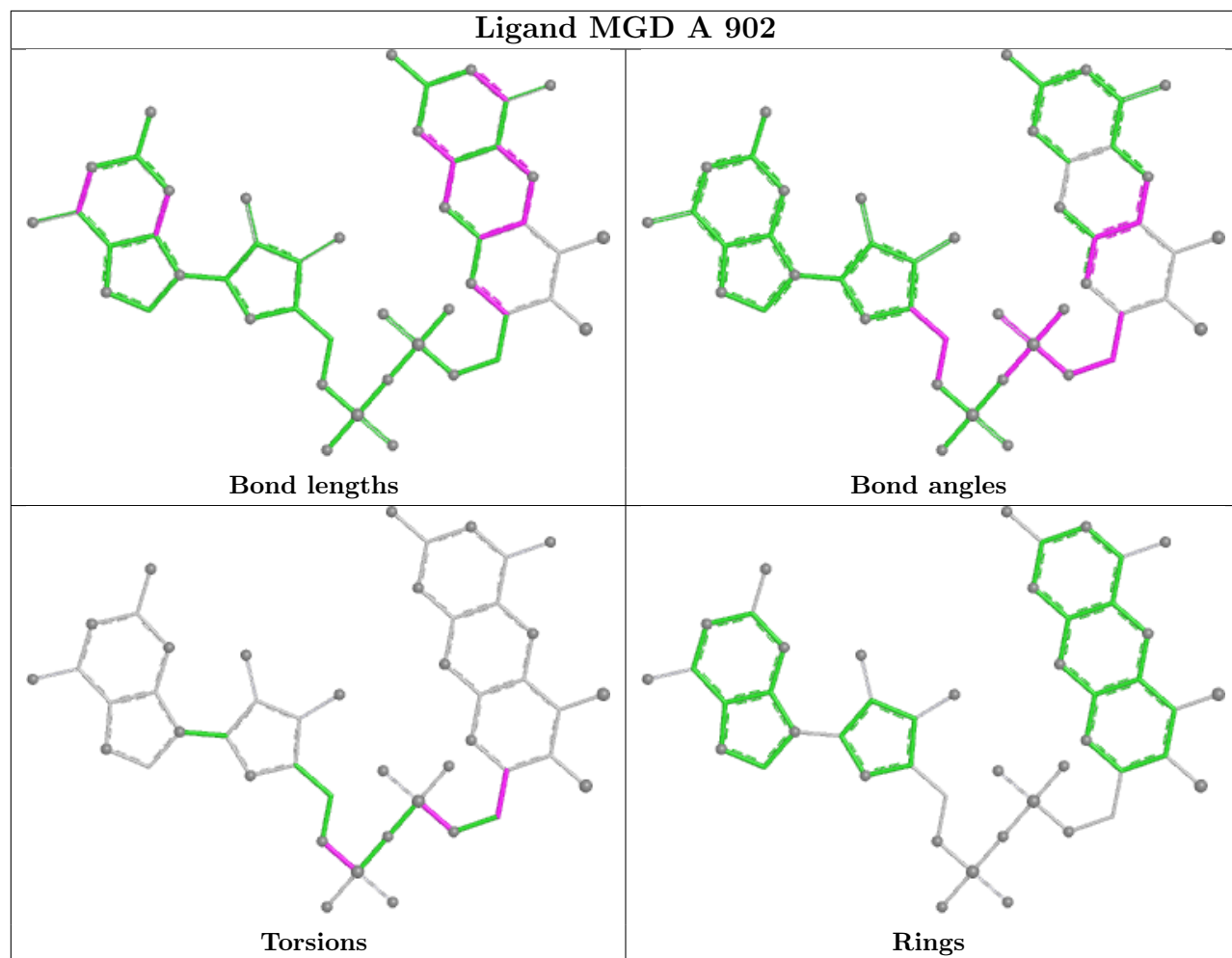


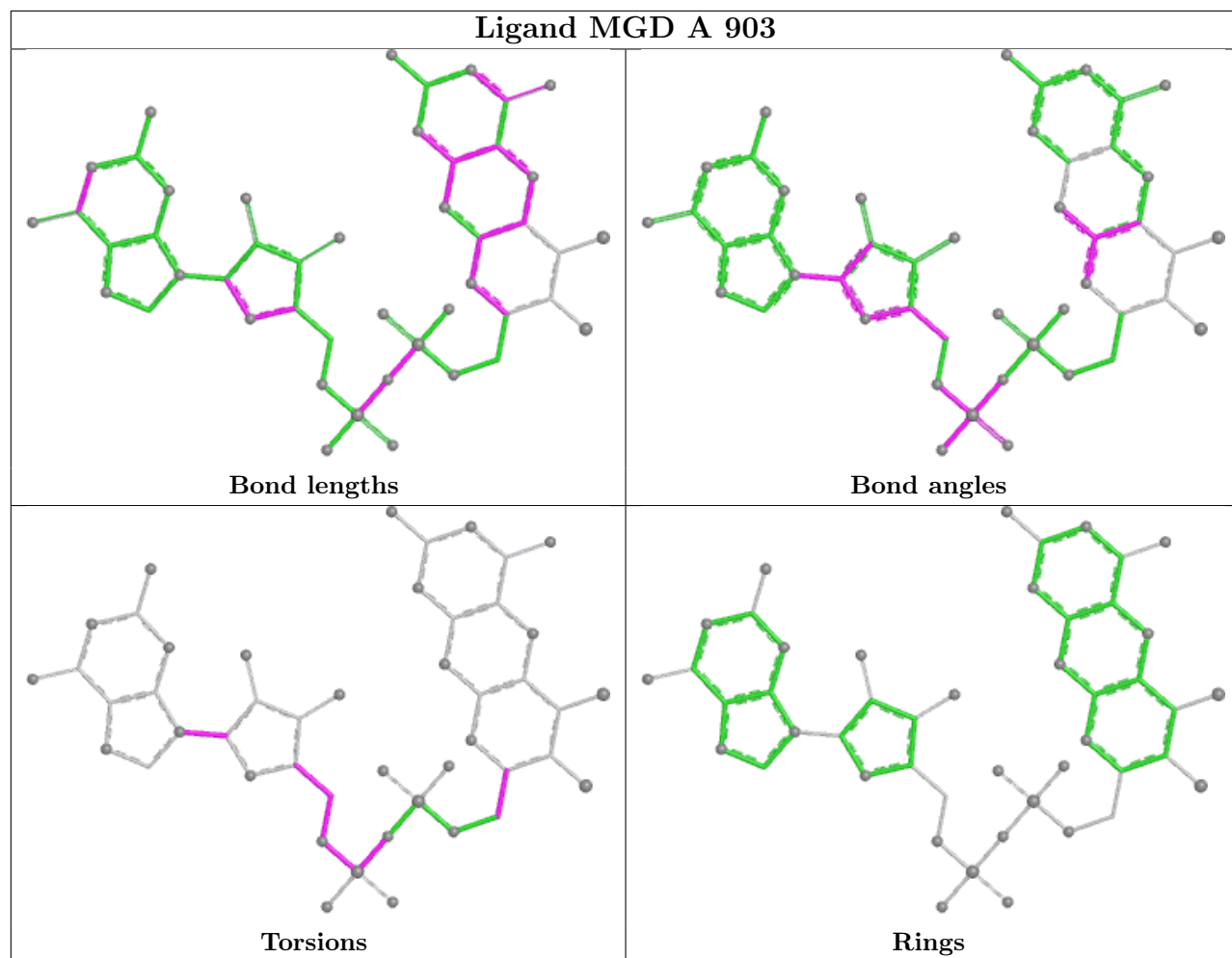


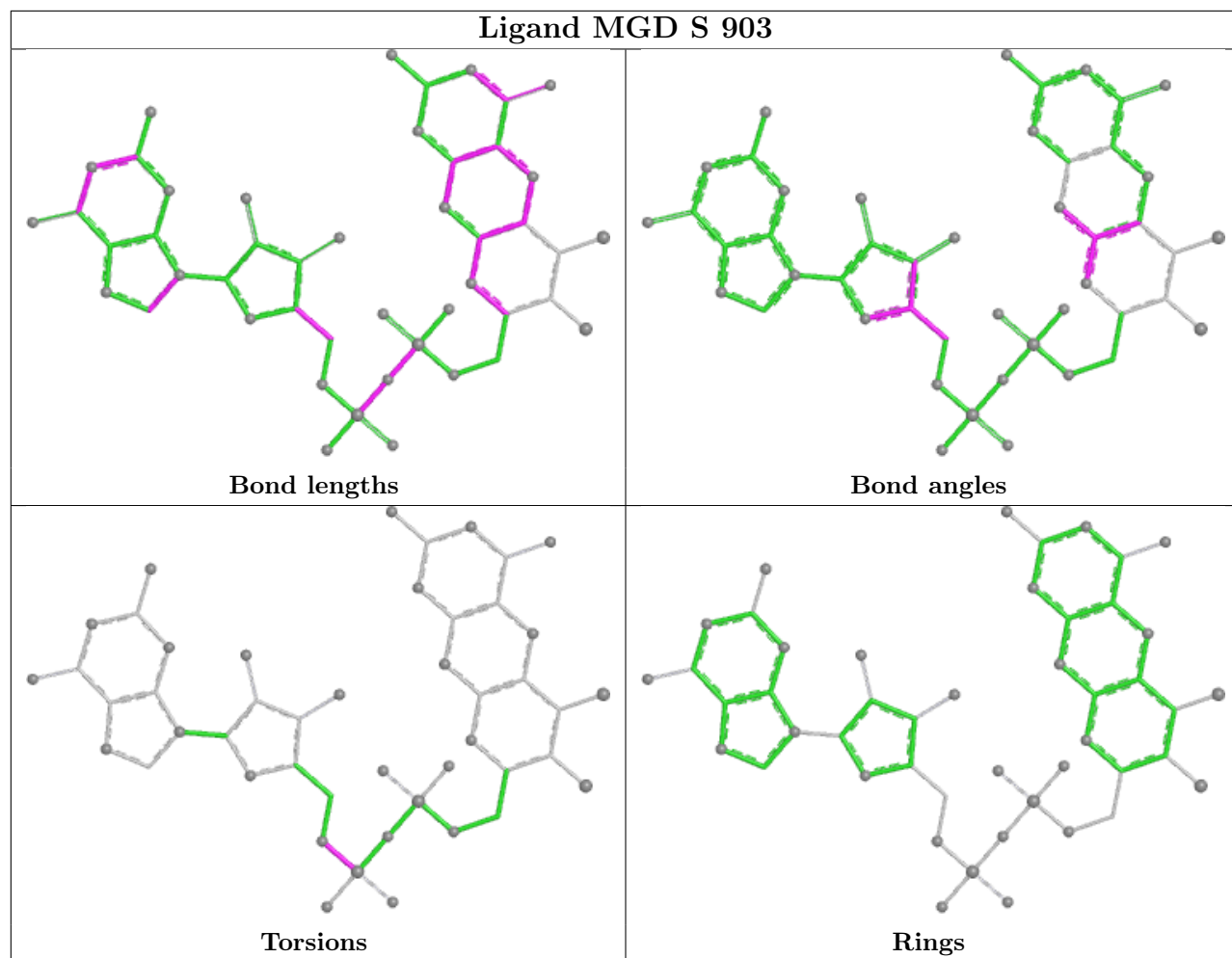


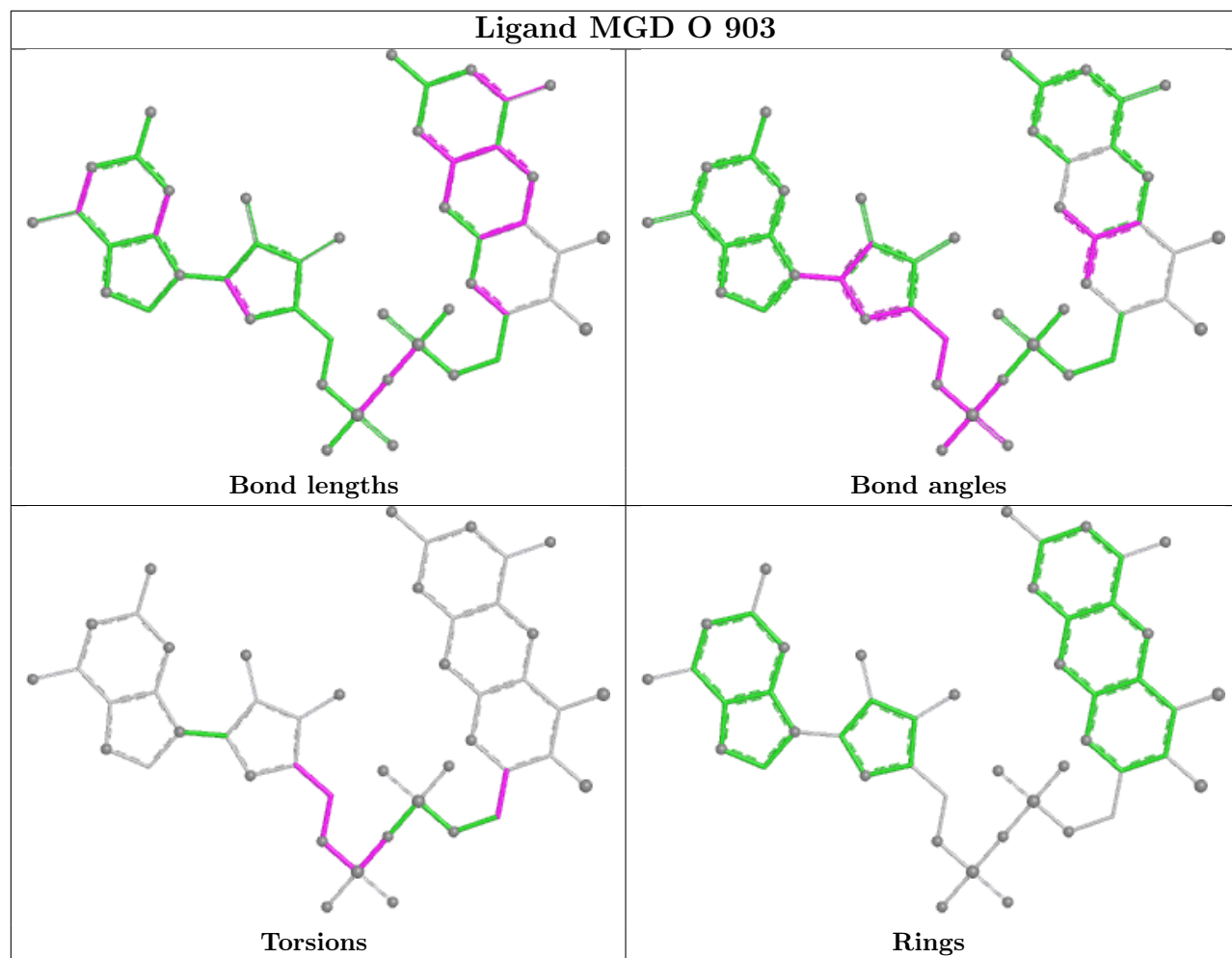


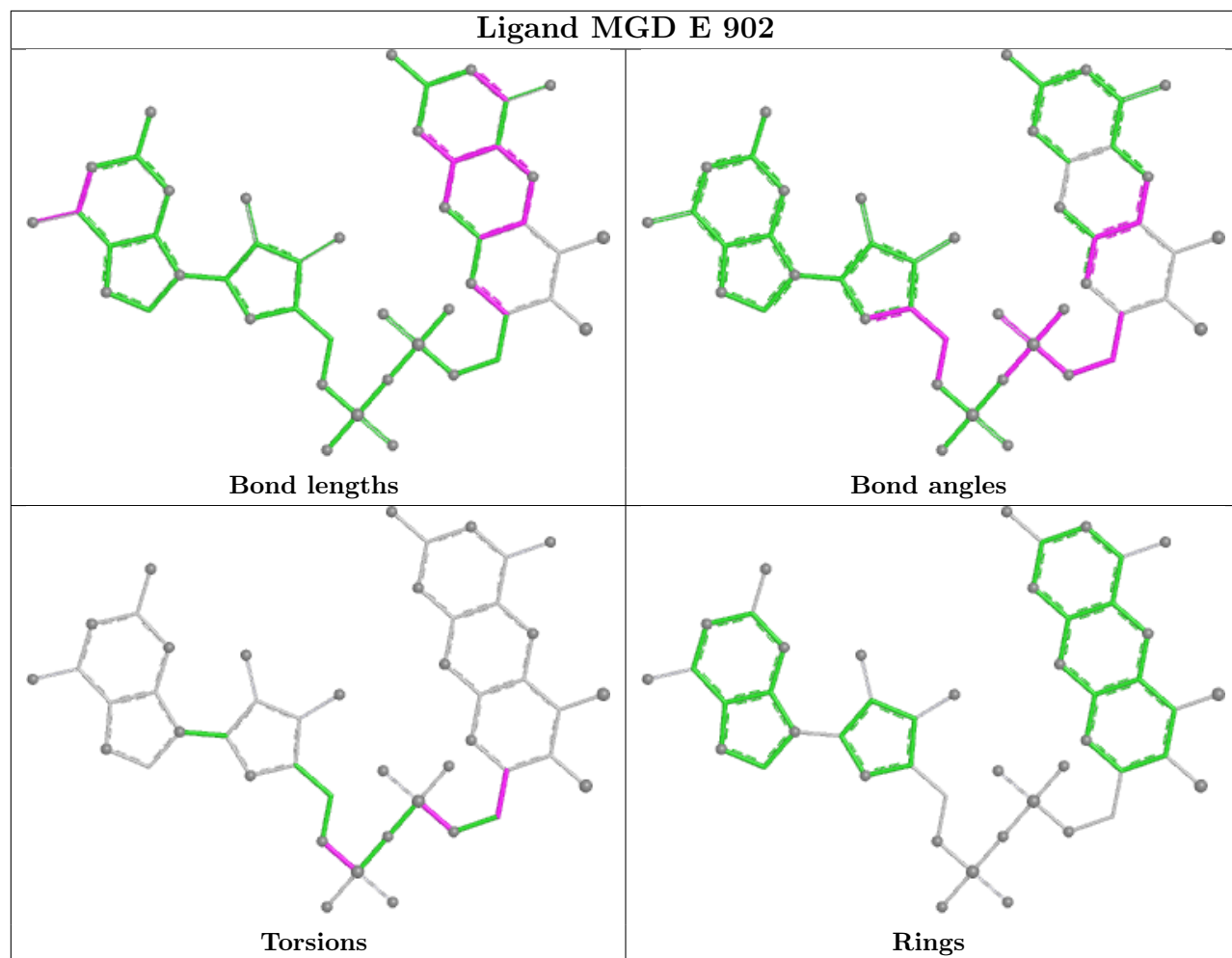


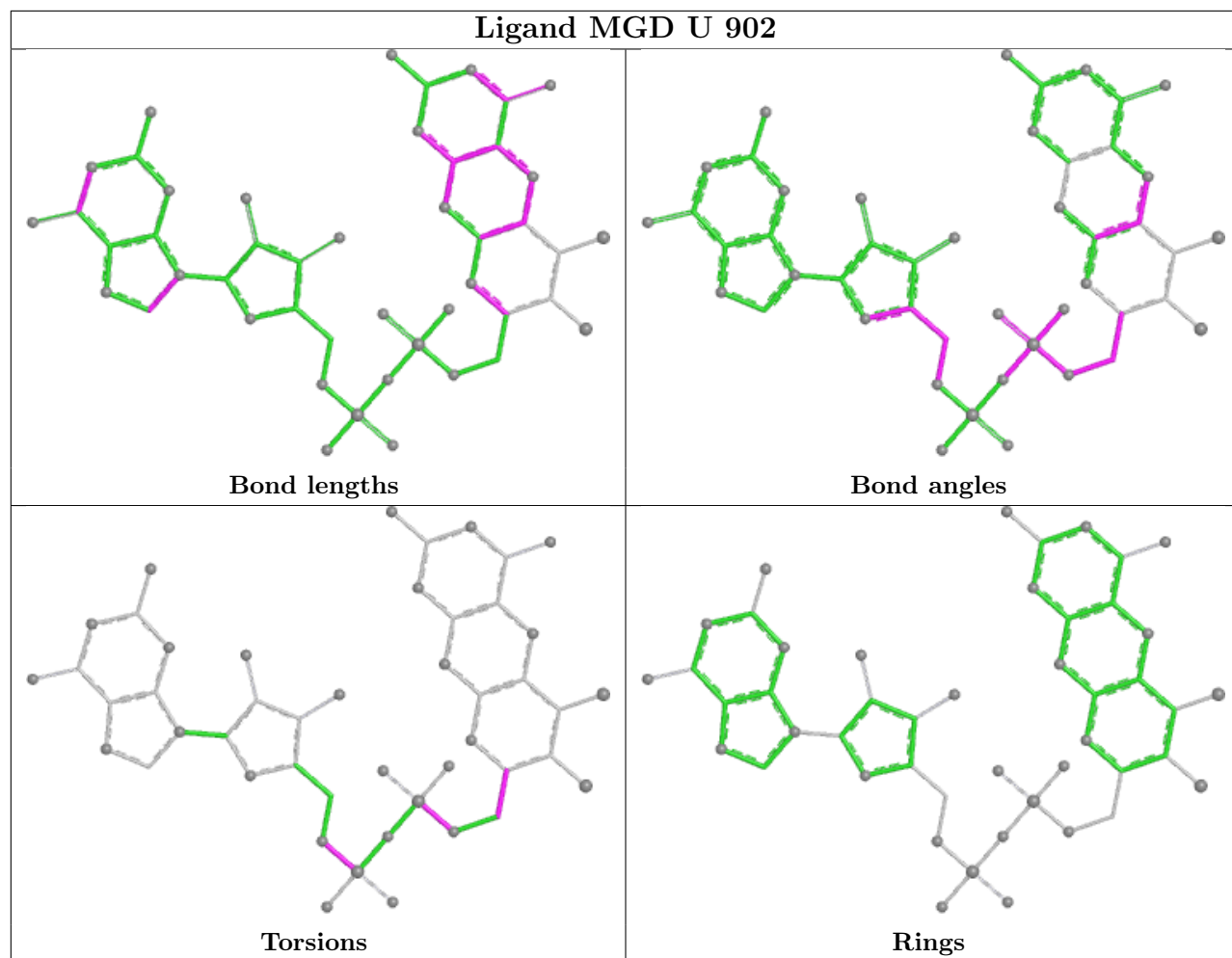


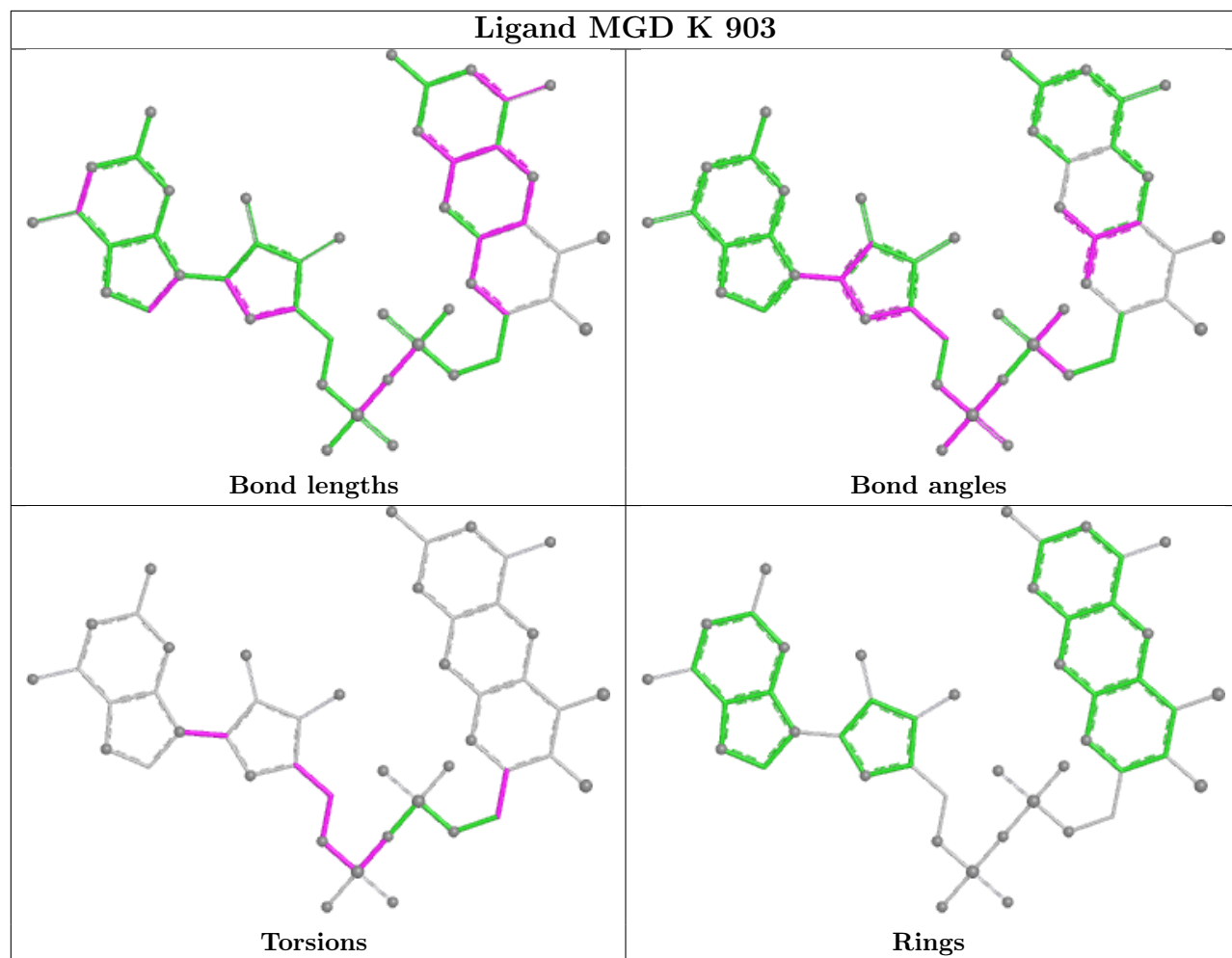


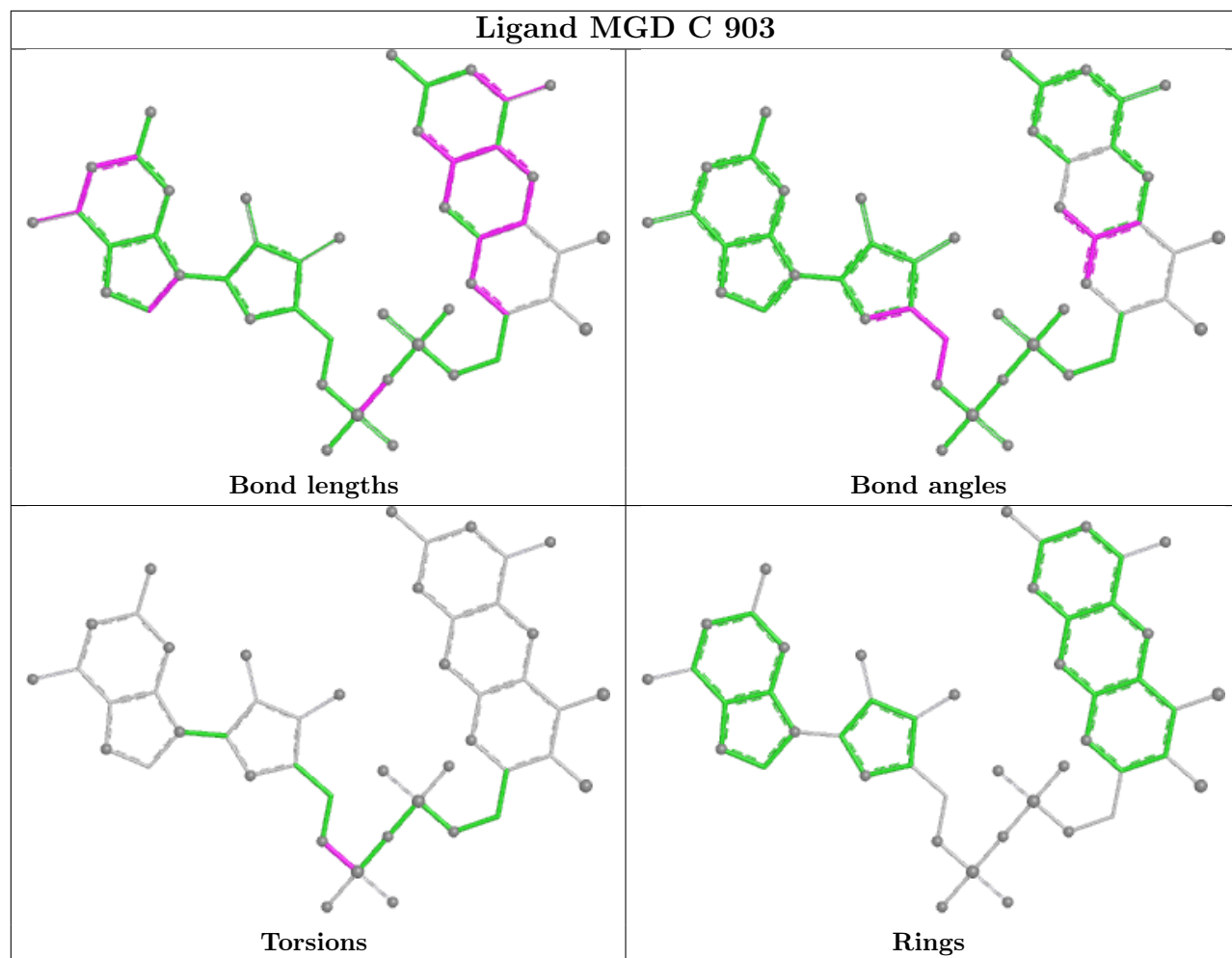


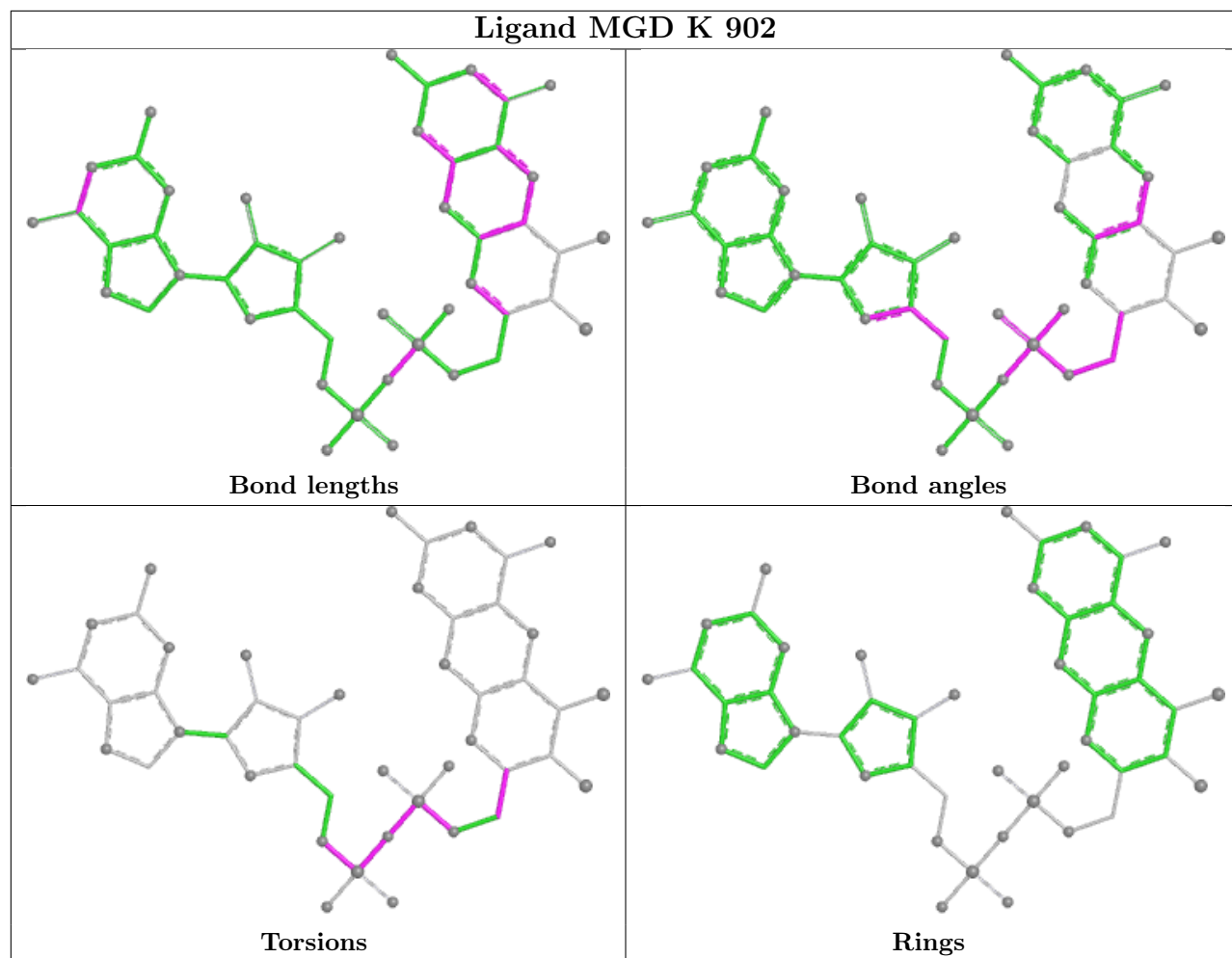


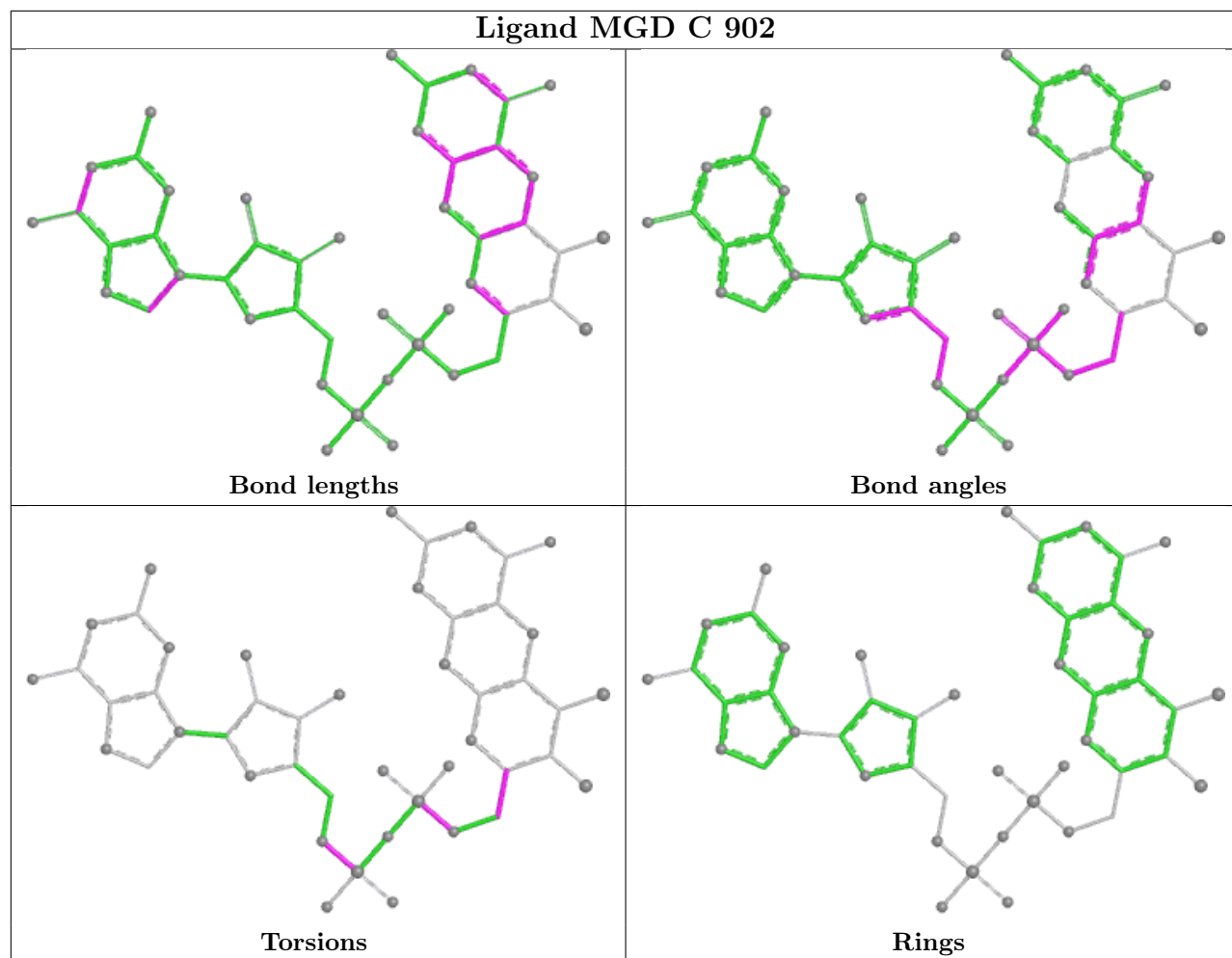












5.7 Other polymers [i](#)

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.