



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 09:08 am GMT

PDB ID : 4V4D  
Title : Crystal Structure of Pyrogallol-Phloroglucinol Transhydroxylase from *Pelobacter acidigallici* complexed with pyrogallol  
Authors : Messerschmidt, A.; Niessen, H.; Abt, D.; Einsle, O.; Schink, B.; Kroneck, P.M.H.  
Deposited on : 2004-06-02  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28972

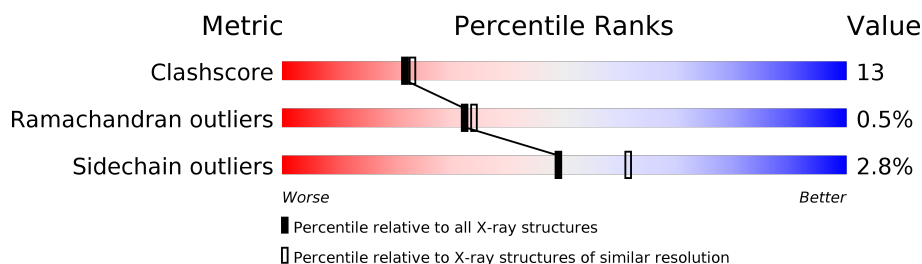
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)


















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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	875	
1	C	875	
1	E	875	
1	G	875	
1	I	875	
1	K	875	
1	M	875	

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Mol	Chain	Length	Quality of chain
1	O	875	
1	Q	875	
1	S	875	
1	U	875	
1	W	875	
2	B	274	
2	D	274	
2	F	274	
2	H	274	
2	J	274	
2	L	274	
2	N	274	
2	P	274	
2	R	274	
2	T	274	
2	V	274	
2	X	274	

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
6	PYG	A	905	-	X	-	-
6	PYG	C	905	-	X	-	-
6	PYG	E	905	-	X	-	-
6	PYG	G	905	-	X	-	-
6	PYG	I	905	-	X	-	-
6	PYG	K	905	-	X	-	-
6	PYG	M	905	-	X	-	-
6	PYG	O	905	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PYG	Q	905	-	X	-	-
6	PYG	S	905	-	X	-	-
6	PYG	U	905	-	X	-	-
6	PYG	W	905	-	X	-	-
7	SF4	B	303	-	-	X	-
7	SF4	D	303	-	-	X	-
7	SF4	F	303	-	-	X	-
7	SF4	H	303	-	-	X	-
7	SF4	J	302	-	-	X	-
7	SF4	L	303	-	-	X	-
7	SF4	N	302	-	-	X	-
7	SF4	N	303	-	-	X	-
7	SF4	P	303	-	-	X	-
7	SF4	R	303	-	-	X	-
7	SF4	T	303	-	-	X	-
7	SF4	V	303	-	-	X	-
7	SF4	X	303	-	-	X	-
7	SF4	X	304	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 121808 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 (three-letter code: CA) (formula: Ca).

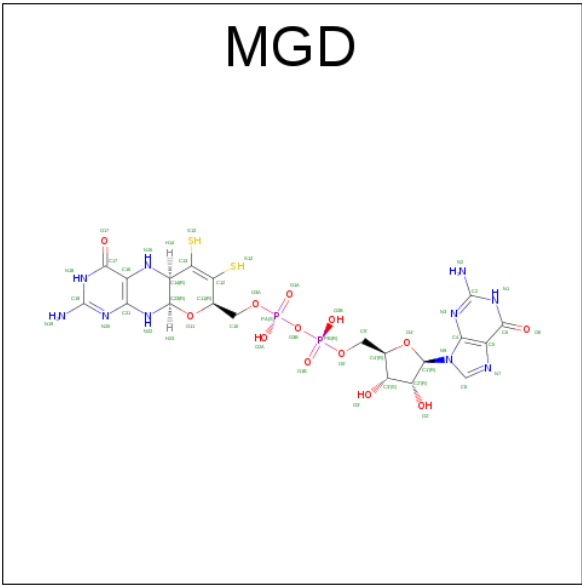
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		

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

- 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 (three-letter code: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



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

- Molecule 5 is MOLYBDENUM(IV) ION (three-letter code: 4MO) (formula: Mo).

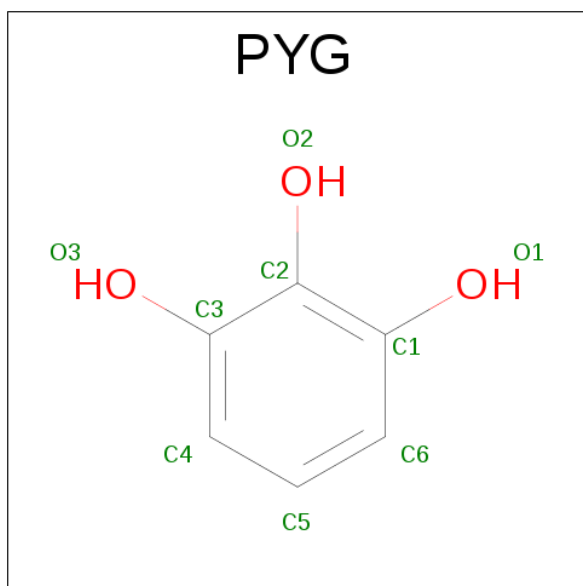
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mo	0	0
			1	1		
5	Q	1	Total	Mo	0	0
			1	1		
5	K	1	Total	Mo	0	0
			1	1		
5	E	1	Total	Mo	0	0
			1	1		
5	I	1	Total	Mo	0	0
			1	1		
5	C	1	Total	Mo	0	0
			1	1		
5	W	1	Total	Mo	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		
5	U	1	Total	Mo	0	0
			1	1		
5	O	1	Total	Mo	0	0
			1	1		
5	S	1	Total	Mo	0	0
			1	1		
5	M	1	Total	Mo	0	0
			1	1		

- Molecule 6 is BENZENE-1,2,3-TRIOL (three-letter code: PYG) (formula:  $C_6H_6O_3$ ).



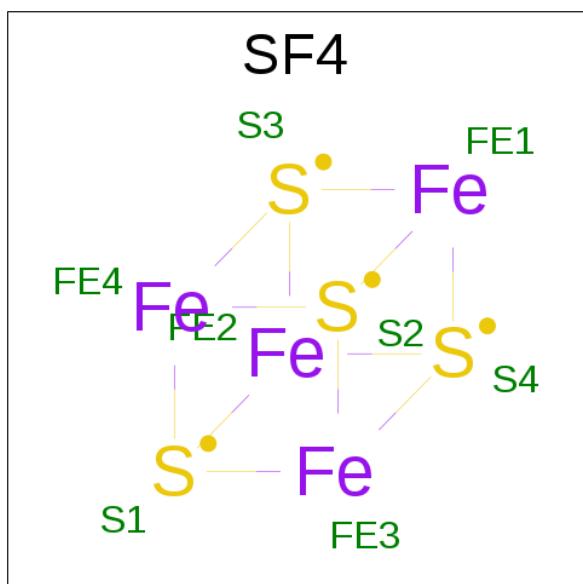
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	6	3		
6	C	1	Total	C	O	0	0
			9	6	3		
6	E	1	Total	C	O	0	0
			9	6	3		
6	G	1	Total	C	O	0	0
			9	6	3		
6	I	1	Total	C	O	0	0
			9	6	3		
6	K	1	Total	C	O	0	0
			9	6	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			9	6	3		
6	O	1	Total	C	O	0	0
			9	6	3		
6	Q	1	Total	C	O	0	0
			9	6	3		
6	S	1	Total	C	O	0	0
			9	6	3		
6	U	1	Total	C	O	0	0
			9	6	3		
6	W	1	Total	C	O	0	0
			9	6	3		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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		
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		
7	D	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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
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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	170	Total 170	O 170	0	0
8	C	681	Total 681	O 681	0	0
8	D	166	Total 166	O 166	0	0
8	E	684	Total 684	O 684	0	0
8	F	163	Total 163	O 163	0	0
8	G	683	Total 683	O 683	0	0
8	H	161	Total 161	O 161	0	0
8	I	671	Total 671	O 671	0	0

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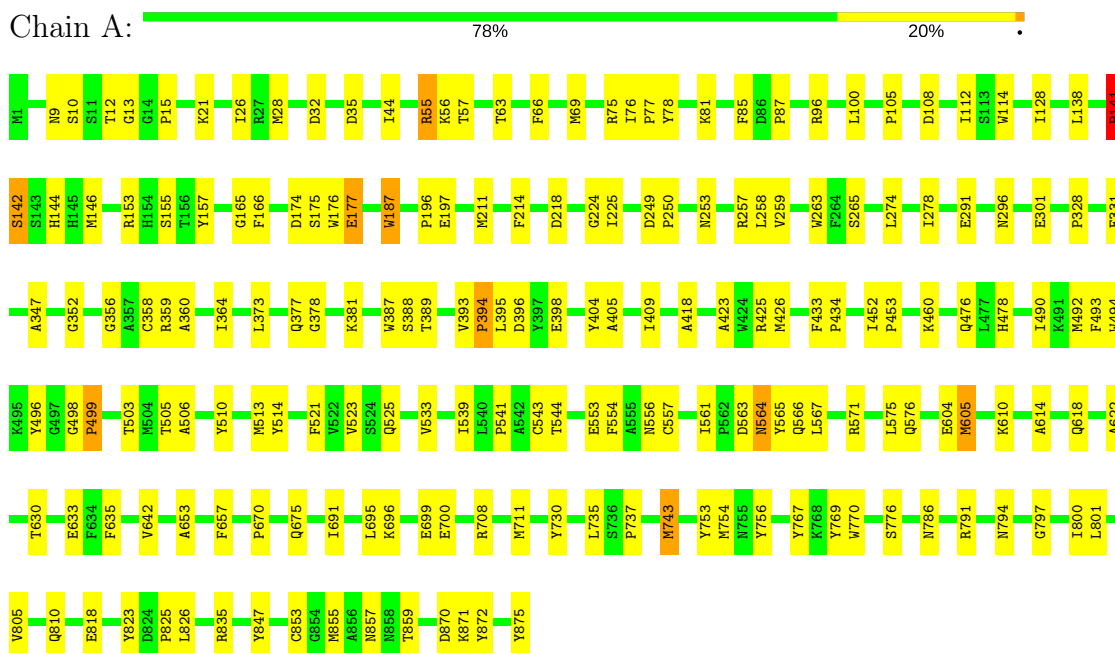
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	163	Total 163	O 163	0	0
8	K	681	Total 681	O 681	0	0
8	L	165	Total 165	O 165	0	0
8	M	684	Total 684	O 684	0	0
8	N	159	Total 159	O 159	0	0
8	O	672	Total 672	O 672	0	0
8	P	164	Total 164	O 164	0	0
8	Q	690	Total 690	O 690	0	0
8	R	161	Total 161	O 161	0	0
8	S	663	Total 663	O 663	0	0
8	T	163	Total 163	O 163	0	0
8	U	668	Total 668	O 668	0	0
8	V	157	Total 157	O 157	0	0
8	W	675	Total 675	O 675	0	0
8	X	164	Total 164	O 164	0	0

### 3 Residue-property plots

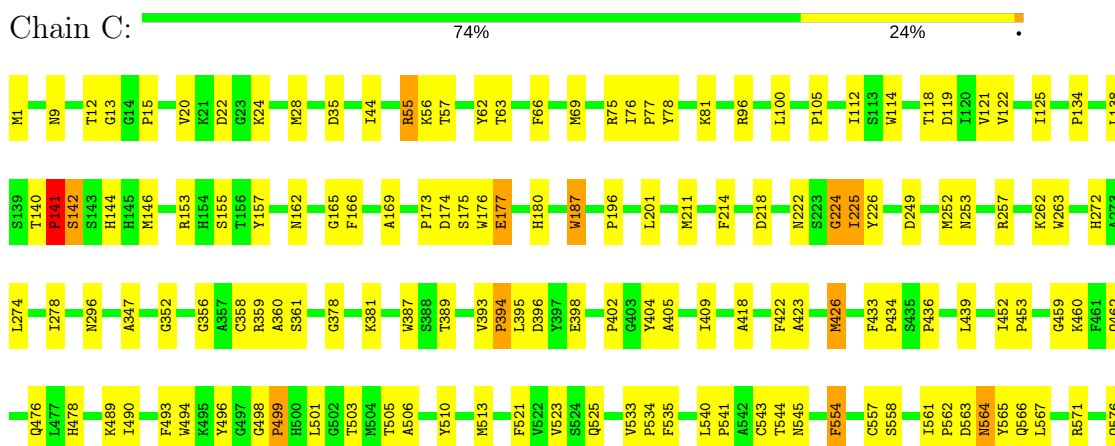
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

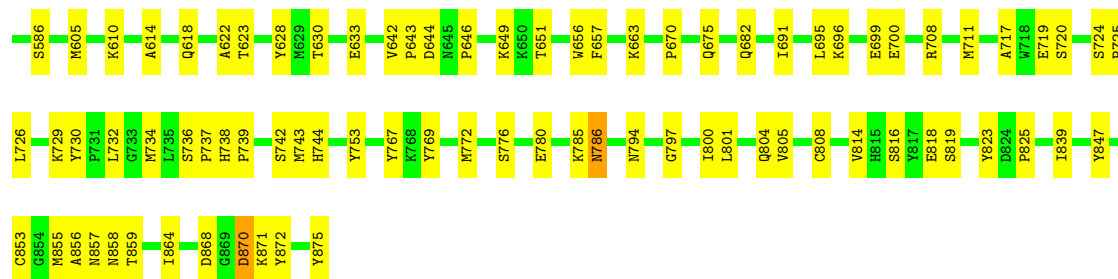
Note EDS was not executed.

- Molecule 1: Pyrogallol hydroxytransferase large subunit



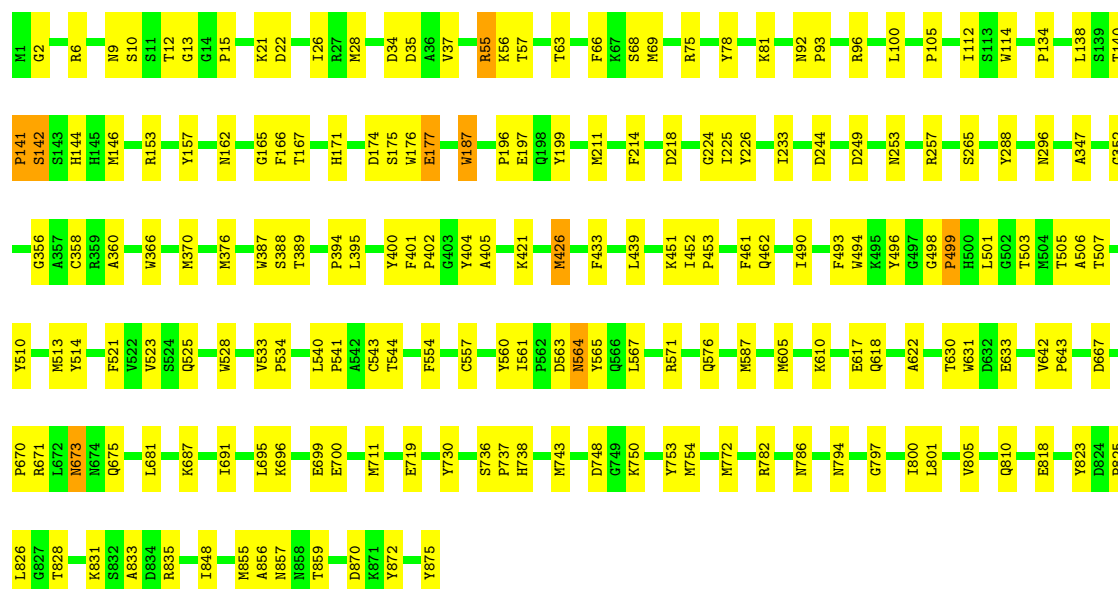
- Molecule 1: Pyrogallol hydroxytransferase large subunit





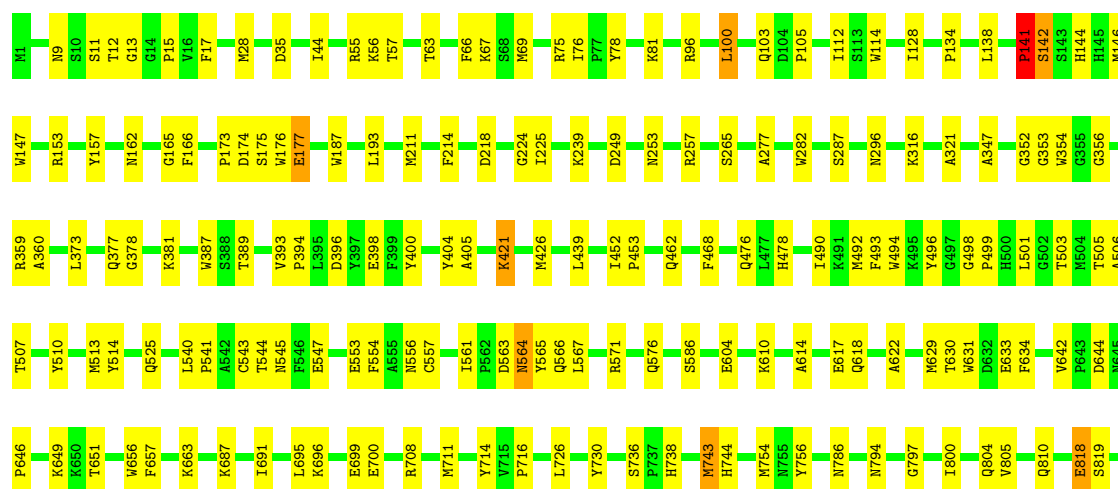
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain E: 79% 20%



• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain G: 79% 20%

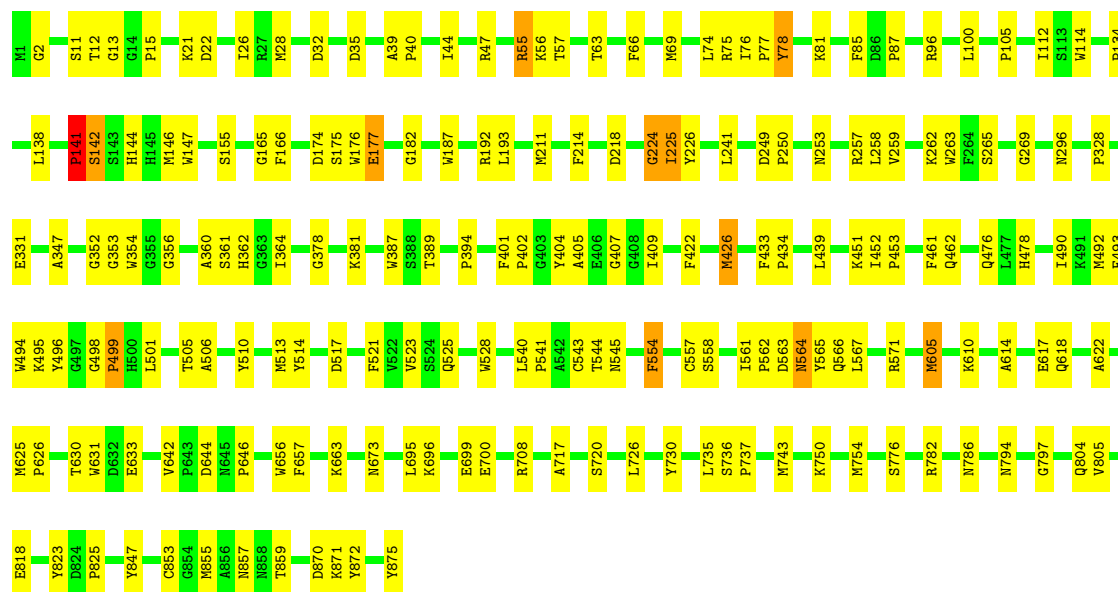






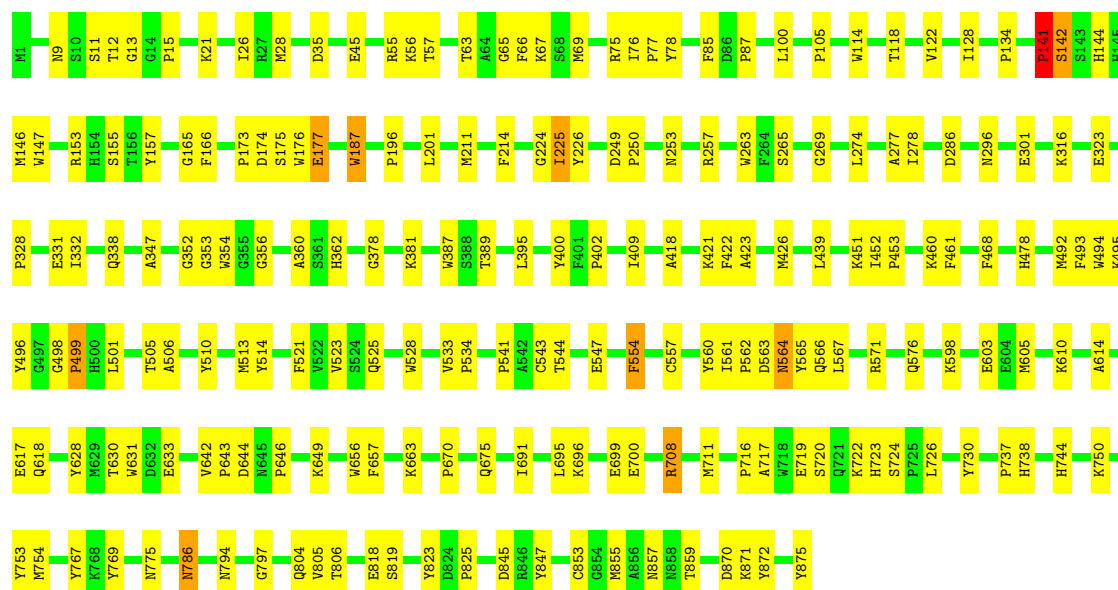
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain I: 78% 20% .



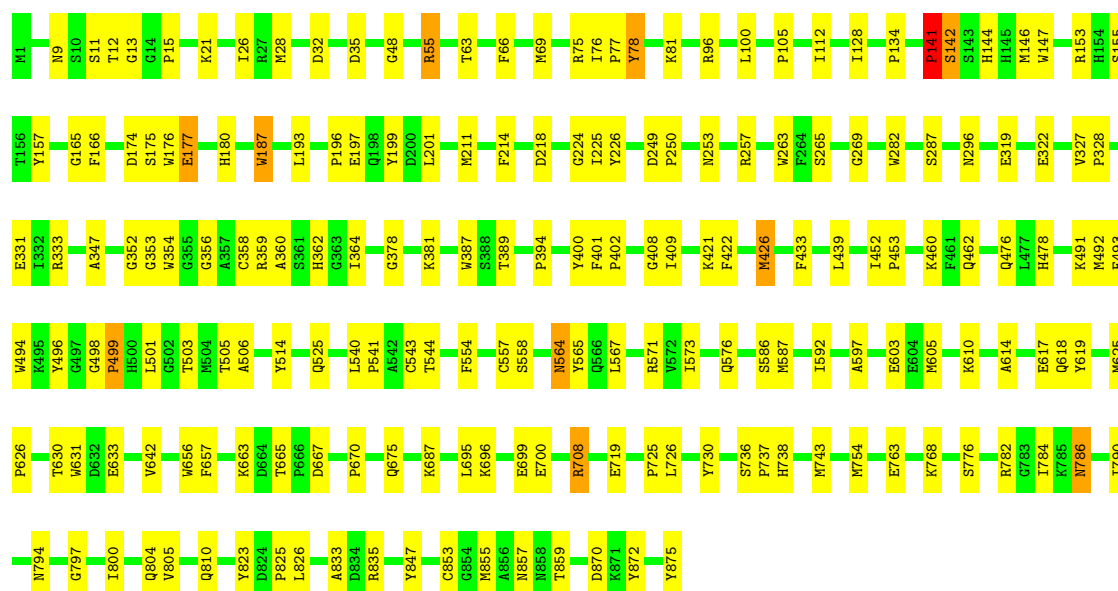
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain K: 77% 22% .

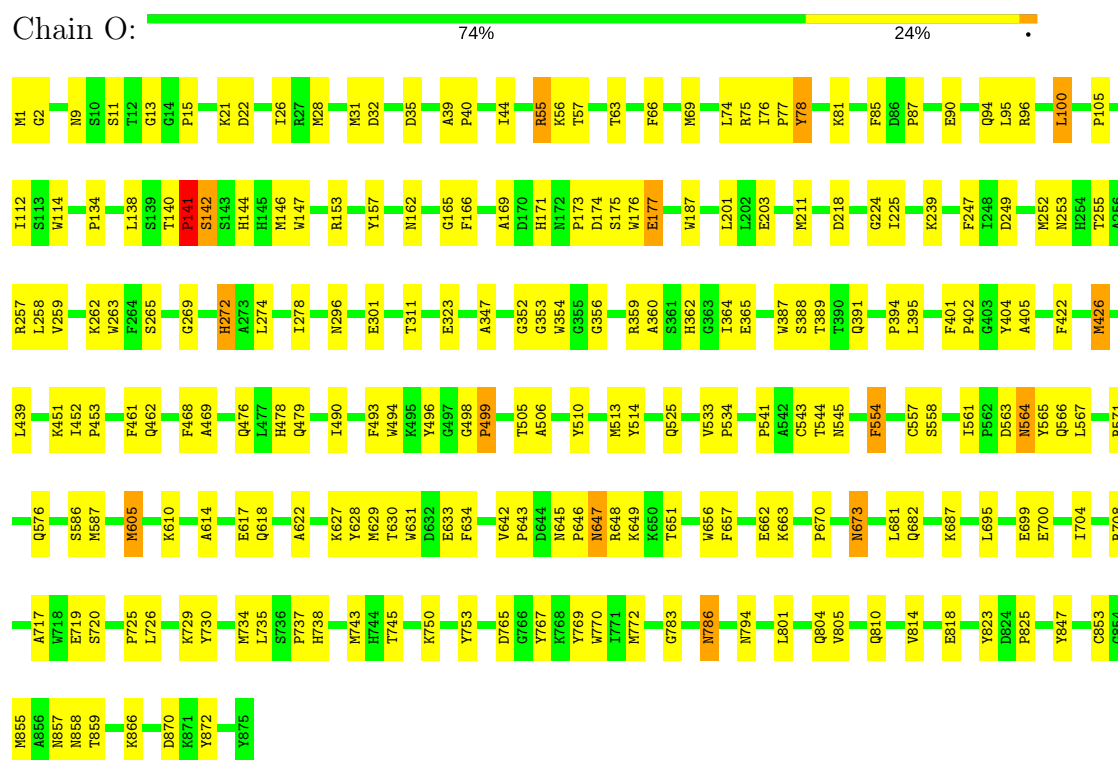


• Molecule 1: Pyrogallol hydroxytransferase large subunit

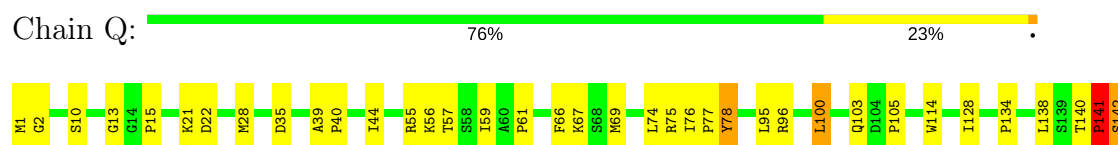
Chain M: 78% 21% .

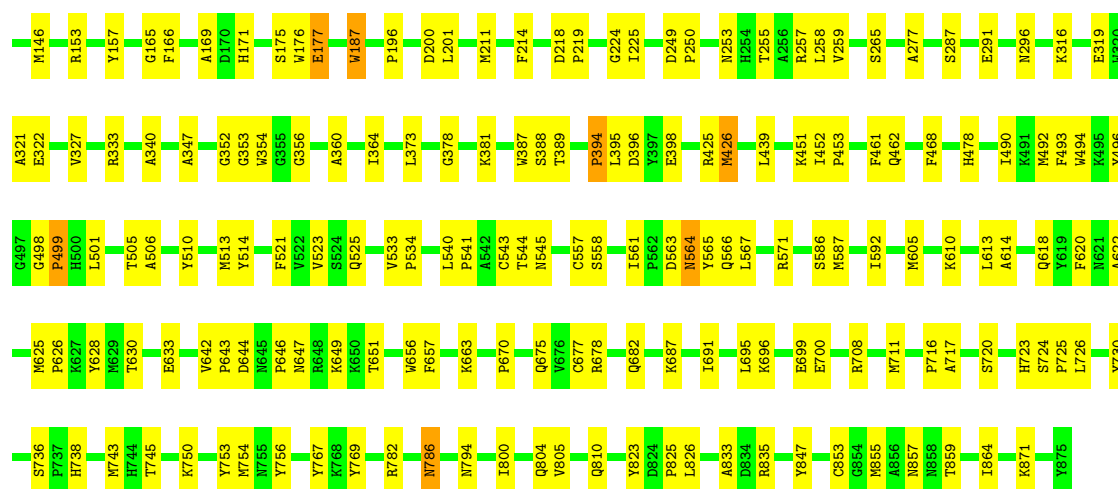


• Molecule 1: Pyrogallol hydroxytransferase large subunit



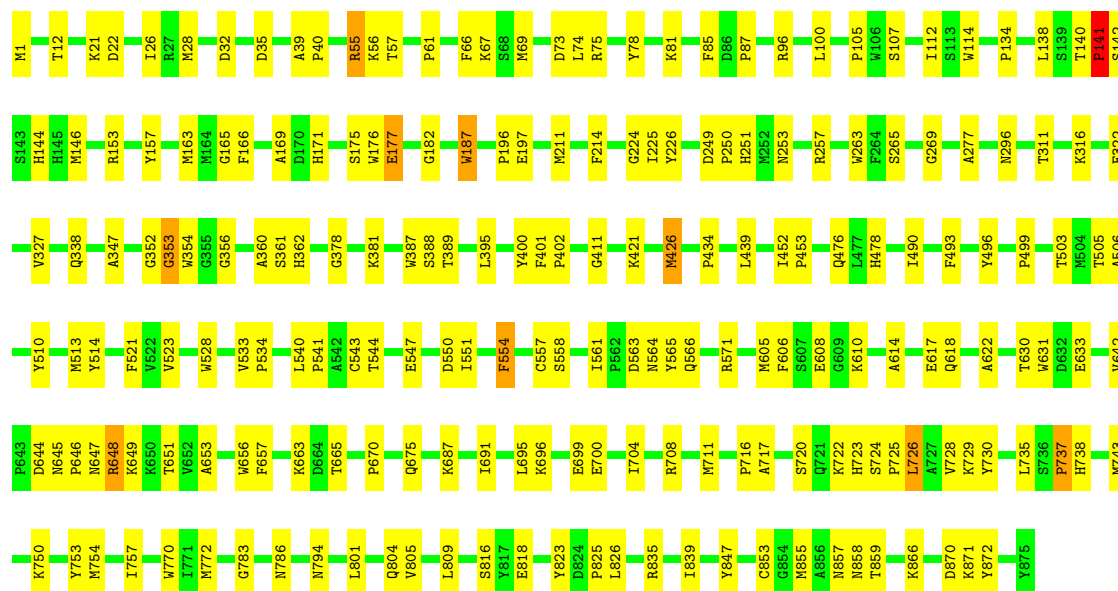
• Molecule 1: Pyrogallol hydroxytransferase large subunit





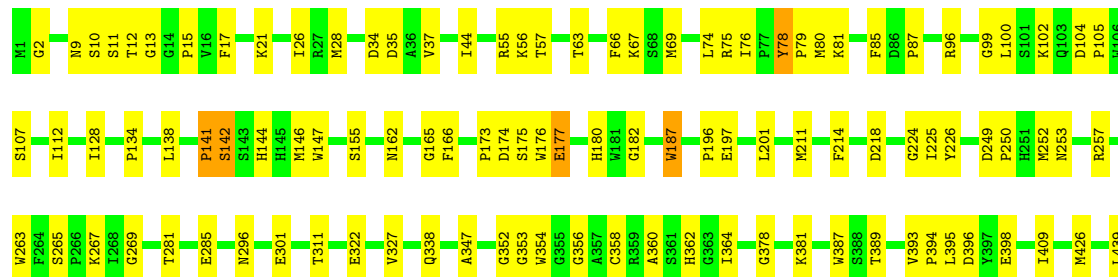
• Molecule 1: Pyrogallol hydroxytransferase large subunit

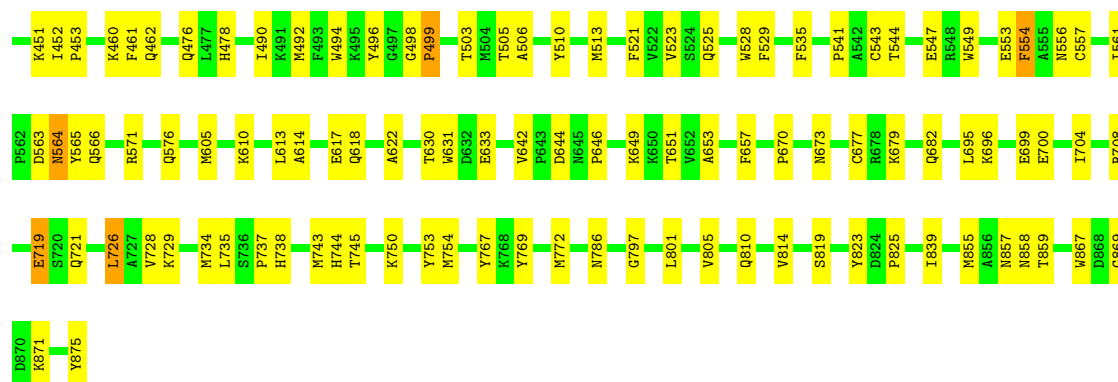
Chain S: 76% 23%



• Molecule 1: Pyrogallol hydroxytransferase large subunit

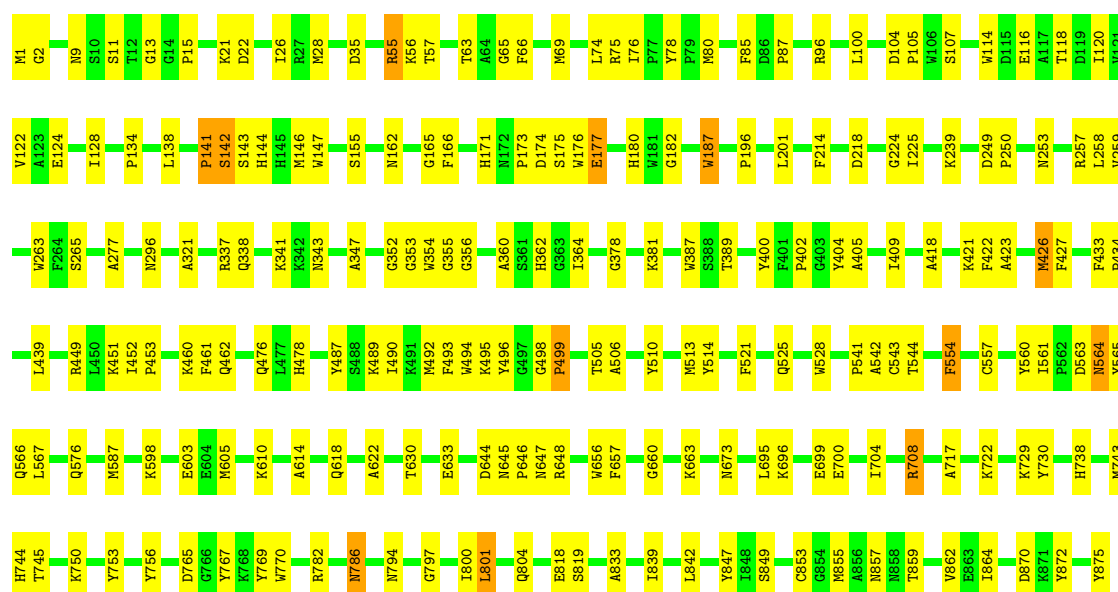
Chain U: 76% 23%





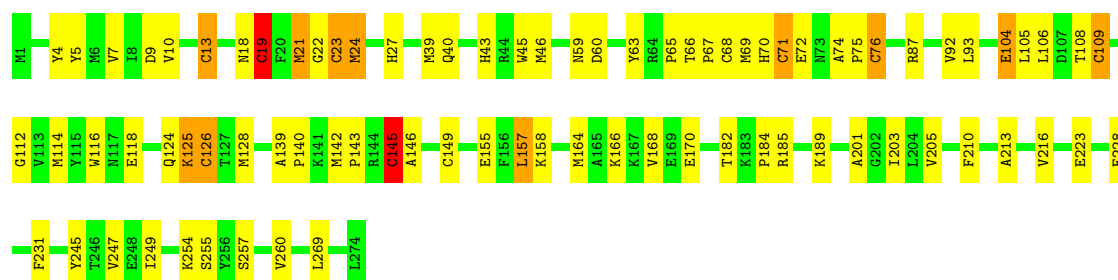
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain W: 76% 23% •



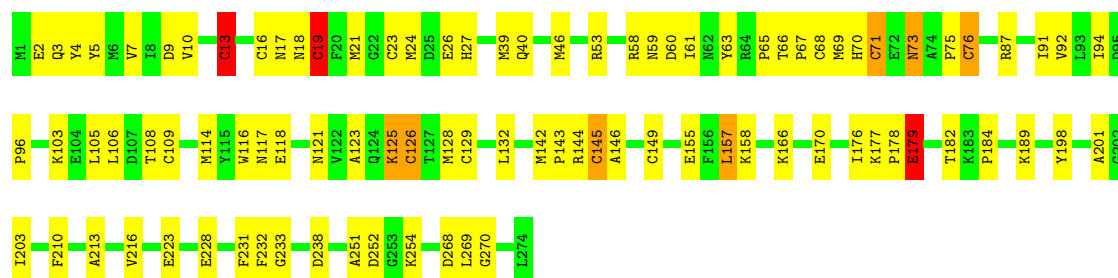
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain B: 70% 26% • •



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain D: 66% 30% • •



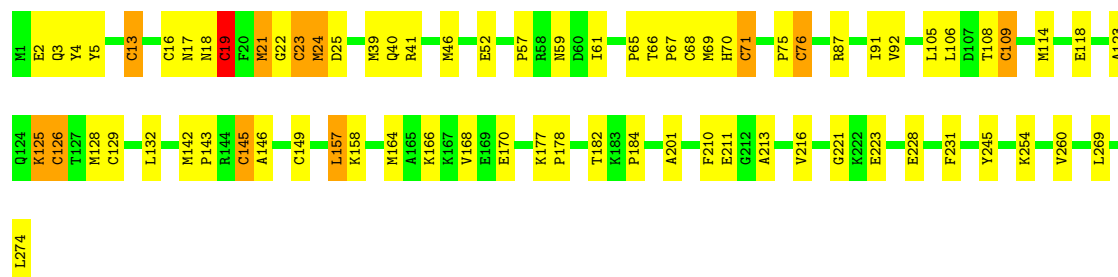
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain F: 70% 27%



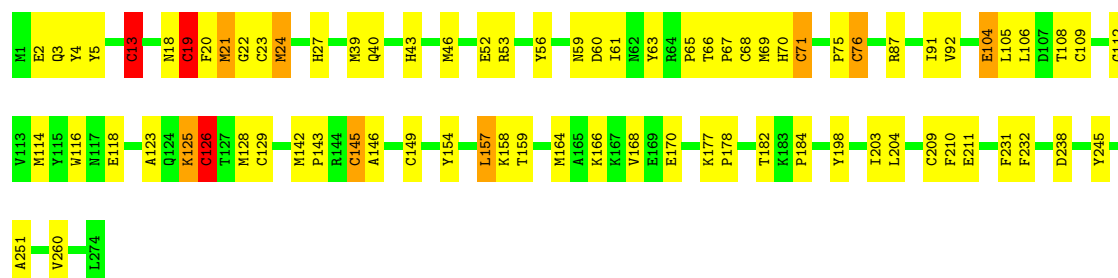
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain H: 73% 23%



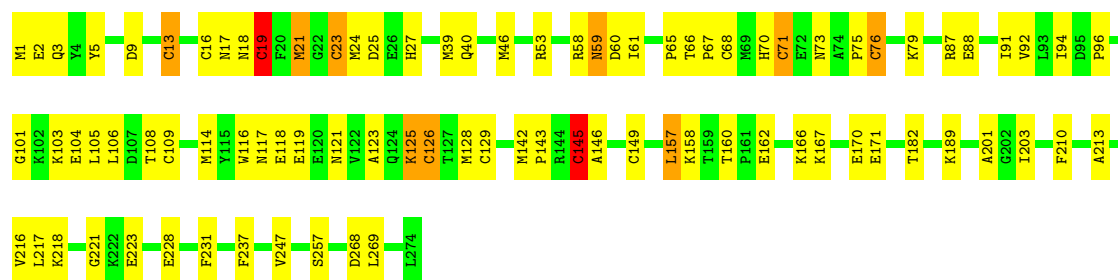
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain J: 71% 25%



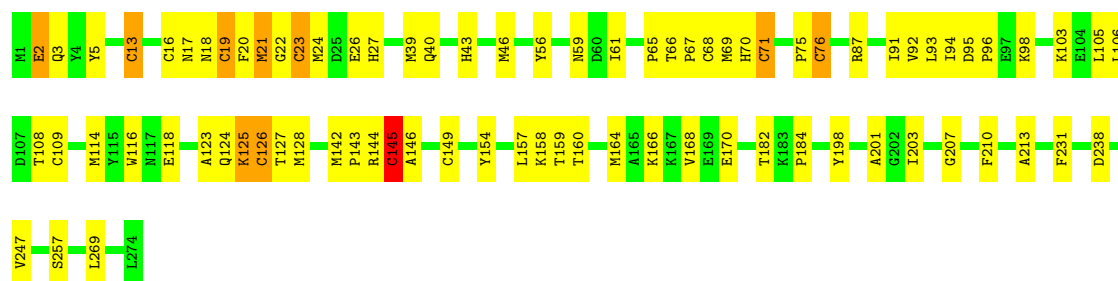
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain L: 68% 28%



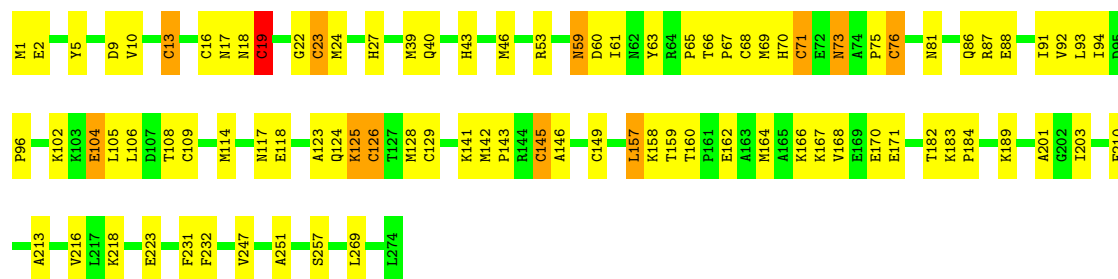
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain N: 70% 26%



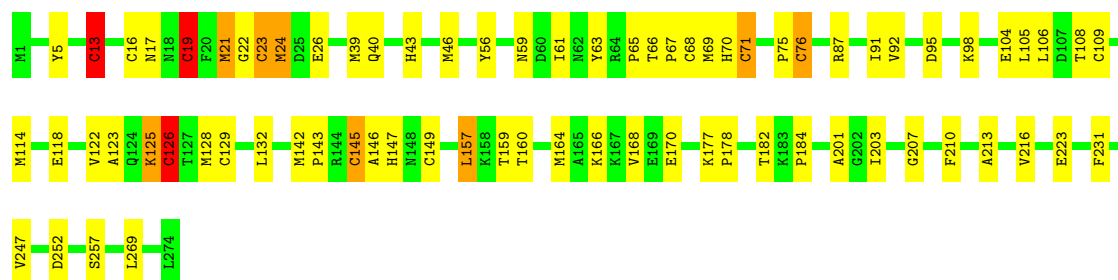
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain P: 67% 29%



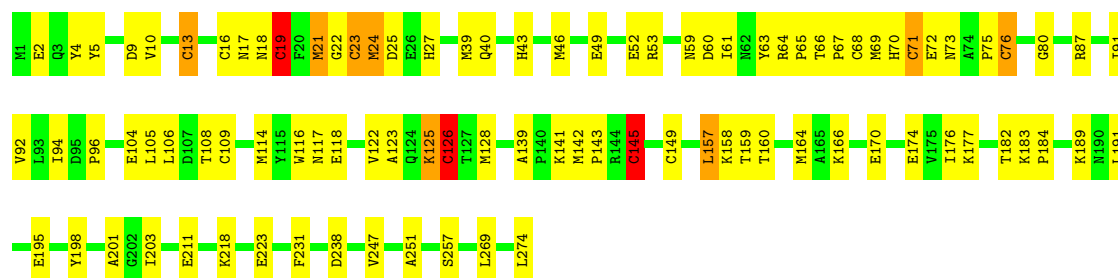
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain R: 73% 23%



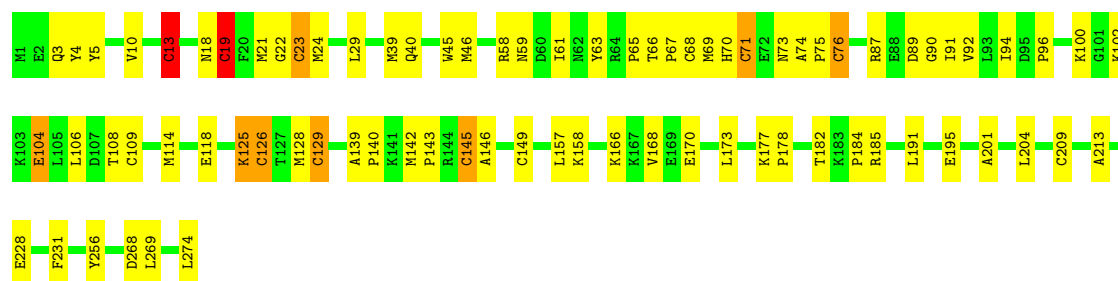
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain T: 66% 30%



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain V: 71% 26% . .



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain X: 59% 38% .



## 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, $\alpha$ , $\beta$ , $\gamma$	172.47Å 178.14Å 179.05Å 64.11° 64.45° 65.11°	Depositor
Resolution (Å)	24.99 – 2.20	Depositor
% Data completeness (in resolution range)	96.7 (24.99-2.20)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.178 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	121808	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.34	0/7219	0.63	3/9786 (0.0%)
1	C	0.33	0/7219	0.61	3/9786 (0.0%)
1	E	0.33	0/7219	0.62	2/9786 (0.0%)
1	G	0.34	0/7219	0.63	3/9786 (0.0%)
1	I	0.33	0/7219	0.62	3/9786 (0.0%)
1	K	0.34	0/7219	0.63	3/9786 (0.0%)
1	M	0.34	0/7219	0.63	3/9786 (0.0%)
1	O	0.34	0/7219	0.62	3/9786 (0.0%)
1	Q	0.34	0/7219	0.63	3/9786 (0.0%)
1	S	0.33	0/7219	0.62	4/9786 (0.0%)
1	U	0.33	0/7219	0.61	2/9786 (0.0%)
1	W	0.33	0/7219	0.61	2/9786 (0.0%)
2	B	0.50	5/2231 (0.2%)	0.68	4/3009 (0.1%)
2	D	0.42	2/2231 (0.1%)	0.63	2/3009 (0.1%)
2	F	0.50	4/2231 (0.2%)	0.67	2/3009 (0.1%)
2	H	0.48	4/2231 (0.2%)	0.68	2/3009 (0.1%)
2	J	0.46	3/2231 (0.1%)	0.66	2/3009 (0.1%)
2	L	0.47	4/2231 (0.2%)	0.68	2/3009 (0.1%)
2	N	0.49	4/2231 (0.2%)	0.67	2/3009 (0.1%)
2	P	0.47	3/2231 (0.1%)	0.65	3/3009 (0.1%)
2	R	0.51	4/2231 (0.2%)	0.67	3/3009 (0.1%)
2	T	0.46	4/2231 (0.2%)	0.65	2/3009 (0.1%)
2	V	0.43	3/2231 (0.1%)	0.64	1/3009 (0.0%)
2	X	0.41	2/2231 (0.1%)	0.62	2/3009 (0.1%)
All	All	0.37	42/113400 (0.0%)	0.63	61/153540 (0.0%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	126	CYS	CB-SG	-9.31	1.66	1.82
2	R	19	CYS	CB-SG	-8.27	1.68	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	19	CYS	CB-SG	-8.17	1.68	1.82
2	P	23	CYS	CB-SG	-8.13	1.68	1.82
2	J	19	CYS	CB-SG	-8.10	1.68	1.82
2	F	126	CYS	CB-SG	-7.92	1.68	1.82
2	B	19	CYS	CB-SG	-7.69	1.69	1.82
2	H	19	CYS	CB-SG	-7.66	1.69	1.82
2	R	23	CYS	CB-SG	-7.64	1.69	1.82
2	B	23	CYS	CB-SG	-7.55	1.69	1.82
2	F	23	CYS	CB-SG	-7.53	1.69	1.82
2	R	145	CYS	CB-SG	-7.52	1.69	1.82
2	L	19	CYS	CB-SG	-7.51	1.69	1.82
2	B	145	CYS	CB-SG	-7.51	1.69	1.82
2	P	19	CYS	CB-SG	-7.36	1.69	1.82
2	L	126	CYS	CB-SG	-7.32	1.69	1.82
2	D	19	CYS	CB-SG	-7.25	1.70	1.82
2	P	126	CYS	CB-SG	-7.21	1.70	1.82
2	F	19	CYS	CB-SG	-7.13	1.70	1.82
2	J	126	CYS	CB-SG	-7.09	1.70	1.82
2	H	126	CYS	CB-SG	-7.07	1.70	1.82
2	T	19	CYS	CB-SG	-6.88	1.70	1.82
2	B	126	CYS	CB-SG	-6.85	1.70	1.82
2	T	126	CYS	CB-SG	-6.74	1.70	1.82
2	D	126	CYS	CB-SG	-6.74	1.70	1.82
2	X	19	CYS	CB-SG	-6.72	1.70	1.82
2	V	23	CYS	CB-SG	-6.54	1.71	1.82
2	R	126	CYS	CB-SG	-6.53	1.71	1.82
2	F	145	CYS	CB-SG	-6.37	1.71	1.82
2	V	126	CYS	CB-SG	-6.29	1.71	1.82
2	V	19	CYS	CB-SG	-6.28	1.71	1.82
2	H	23	CYS	CB-SG	-6.25	1.71	1.82
2	T	23	CYS	CB-SG	-6.17	1.71	1.82
2	X	126	CYS	CB-SG	-6.08	1.72	1.82
2	N	23	CYS	CB-SG	-5.99	1.72	1.81
2	N	145	CYS	CB-SG	-5.96	1.72	1.81
2	L	145	CYS	CB-SG	-5.63	1.72	1.81
2	L	23	CYS	CB-SG	-5.61	1.72	1.81
2	T	145	CYS	CB-SG	-5.23	1.73	1.81
2	J	145	CYS	CB-SG	-5.04	1.73	1.81
2	B	109	CYS	CB-SG	-5.03	1.73	1.81
2	H	109	CYS	CB-SG	-5.02	1.73	1.81

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	352	GLY	N-CA-C	-8.63	91.53	113.10
1	A	352	GLY	N-CA-C	-8.48	91.90	113.10
1	C	352	GLY	N-CA-C	-8.23	92.51	113.10
1	O	352	GLY	N-CA-C	-8.19	92.63	113.10
1	M	352	GLY	N-CA-C	-8.13	92.77	113.10
1	Q	352	GLY	N-CA-C	-8.08	92.91	113.10
1	S	352	GLY	N-CA-C	-8.06	92.96	113.10
1	U	352	GLY	N-CA-C	-8.05	92.99	113.10
1	I	352	GLY	N-CA-C	-7.93	93.26	113.10
1	G	352	GLY	N-CA-C	-7.85	93.48	113.10
1	E	352	GLY	N-CA-C	-7.84	93.50	113.10
1	K	352	GLY	N-CA-C	-7.64	94.01	113.10
1	Q	224	GLY	N-CA-C	-6.77	96.17	113.10
1	A	224	GLY	N-CA-C	-6.59	96.62	113.10
1	E	224	GLY	N-CA-C	-6.51	96.82	113.10
1	G	224	GLY	N-CA-C	-6.32	97.30	113.10
2	L	19	CYS	CB-CA-C	-6.25	97.90	110.40
1	O	224	GLY	N-CA-C	-6.25	97.48	113.10
2	R	19	CYS	CB-CA-C	-6.20	98.00	110.40
2	N	19	CYS	CB-CA-C	-6.17	98.06	110.40
1	W	224	GLY	N-CA-C	-6.16	97.69	113.10
1	K	224	GLY	N-CA-C	-6.14	97.75	113.10
1	M	224	GLY	N-CA-C	-6.03	98.01	113.10
2	H	19	CYS	CB-CA-C	-5.86	98.69	110.40
2	T	13	CYS	CA-CB-SG	-5.84	103.48	114.00
1	U	224	GLY	N-CA-C	-5.82	98.55	113.10
2	J	19	CYS	CB-CA-C	-5.79	98.81	110.40
1	S	224	GLY	N-CA-C	-5.77	98.67	113.10
2	F	13	CYS	CA-CB-SG	-5.77	103.62	114.00
1	Q	141	PRO	N-CA-C	-5.76	97.12	112.10
2	B	19	CYS	CB-CA-C	-5.74	98.92	110.40
1	C	224	GLY	N-CA-C	-5.72	98.79	113.10
1	M	141	PRO	N-CA-C	-5.70	97.27	112.10
2	F	19	CYS	CB-CA-C	-5.67	99.06	110.40
1	I	224	GLY	N-CA-C	-5.67	98.93	113.10
2	T	19	CYS	CB-CA-C	-5.66	99.08	110.40
2	D	13	CYS	CA-CB-SG	-5.64	103.84	114.00
2	P	23	CYS	CB-CA-C	-5.63	99.14	110.40
1	G	141	PRO	N-CA-C	-5.62	97.49	112.10
2	J	13	CYS	CA-CB-SG	-5.61	103.90	114.00
2	P	13	CYS	CA-CB-SG	-5.58	103.95	114.00
2	N	13	CYS	CA-CB-SG	-5.54	104.02	114.00
2	X	19	CYS	CB-CA-C	-5.51	99.39	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	13	CYS	CA-CB-SG	-5.48	104.14	114.00
2	B	145	CYS	CB-CA-C	-5.41	99.59	110.40
2	P	19	CYS	CB-CA-C	-5.39	99.63	110.40
2	R	13	CYS	CA-CB-SG	-5.38	104.32	114.00
2	L	13	CYS	CA-CB-SG	-5.37	104.33	114.00
2	X	13	CYS	CA-CB-SG	-5.32	104.43	114.00
1	A	141	PRO	N-CA-C	-5.31	98.30	112.10
2	B	13	CYS	CA-CB-SG	-5.25	104.55	114.00
1	S	353	GLY	N-CA-C	-5.21	100.07	113.10
2	R	23	CYS	CB-CA-C	-5.16	100.08	110.40
1	O	141	PRO	N-CA-C	-5.16	98.70	112.10
1	I	141	PRO	N-CA-C	-5.13	98.77	112.10
2	D	19	CYS	CB-CA-C	-5.11	100.17	110.40
2	V	13	CYS	CA-CB-SG	-5.11	104.80	114.00
2	B	23	CYS	CB-CA-C	-5.11	100.18	110.40
1	K	141	PRO	N-CA-C	-5.08	98.90	112.10
1	S	141	PRO	N-CA-C	-5.08	98.90	112.10
1	C	141	PRO	N-CA-C	-5.03	99.03	112.10

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	154	0
1	C	6998	0	6632	186	0
1	E	6998	0	6632	155	0
1	G	6998	0	6632	150	0
1	I	6998	0	6632	158	0
1	K	6998	0	6632	156	0
1	M	6998	0	6632	170	0
1	O	6998	0	6632	194	0
1	Q	6998	0	6632	184	0
1	S	6998	0	6632	169	0
1	U	6998	0	6632	187	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	6998	0	6632	175	0
2	B	2182	0	2077	77	0
2	D	2182	0	2077	86	0
2	F	2182	0	2077	73	0
2	H	2182	0	2077	71	0
2	J	2182	0	2077	73	0
2	L	2182	0	2077	79	0
2	N	2182	0	2077	85	0
2	P	2182	0	2077	84	0
2	R	2182	0	2077	76	0
2	T	2182	0	2077	78	0
2	V	2182	0	2077	62	0
2	X	2182	0	2077	91	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	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
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	13	0
4	C	94	0	44	13	0
4	E	94	0	44	14	0
4	G	94	0	44	10	0
4	I	94	0	44	12	0
4	K	94	0	44	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	94	0	44	15	0
4	O	94	0	44	11	0
4	Q	94	0	44	10	0
4	S	94	0	44	10	0
4	U	94	0	44	13	0
4	W	94	0	44	12	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	9	0	5	1	0
6	C	9	0	5	0	0
6	E	9	0	5	1	0
6	G	9	0	5	0	0
6	I	9	0	5	1	0
6	K	9	0	5	0	0
6	M	9	0	5	1	0
6	O	9	0	5	1	0
6	Q	9	0	5	1	0
6	S	9	0	5	1	0
6	U	9	0	5	1	0
6	W	9	0	5	0	0
7	B	24	0	0	4	0
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	3	0
7	T	24	0	0	4	0
7	V	24	0	0	4	0
7	X	24	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	681	0	0	10	0
8	B	170	0	0	1	0
8	C	681	0	0	14	0
8	D	166	0	0	1	0
8	E	684	0	0	8	0
8	F	163	0	0	3	0
8	G	683	0	0	9	0
8	H	161	0	0	0	0
8	I	671	0	0	10	0
8	J	163	0	0	1	0
8	K	681	0	0	9	0
8	L	165	0	0	2	0
8	M	684	0	0	10	0
8	N	159	0	0	4	0
8	O	672	0	0	21	0
8	P	164	0	0	4	0
8	Q	690	0	0	14	0
8	R	161	0	0	1	0
8	S	663	0	0	15	0
8	T	163	0	0	2	0
8	U	668	0	0	12	0
8	V	157	0	0	1	0
8	W	675	0	0	20	0
8	X	164	0	0	7	0
All	All	121808	0	105096	2898	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (2898) 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:U:426:MET:HE1	1:U:618:GLN:HG2	1.24	1.15
1:K:426:MET:HE1	1:K:618:GLN:HG2	1.23	1.09
2:B:68:CYS:HB2	2:B:126:CYS:HB3	1.36	1.05
2:F:68:CYS:HB2	2:F:126:CYS:HB3	1.40	1.04
2:H:68:CYS:HB2	2:H:126:CYS:HB3	1.38	1.03
2:L:68:CYS:HB2	2:L:126:CYS:HB3	1.38	1.02
1:O:557:CYS:H	1:O:564:ASN:HD21	1.00	1.00
2:R:207:GLY:HA2	1:U:728:VAL:HG12	1.43	1.00
1:S:557:CYS:H	1:S:564:ASN:HD21	1.10	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:68:CYS:HB2	2:X:126:CYS:HB3	1.44	1.00
1:A:557:CYS:H	1:A:564:ASN:HD21	1.10	0.99
2:X:19:CYS:HB3	2:X:145:CYS:HB3	1.42	0.99
1:K:557:CYS:H	1:K:564:ASN:HD21	1.03	0.98
1:M:557:CYS:H	1:M:564:ASN:HD21	0.99	0.98
2:T:68:CYS:HB2	2:T:126:CYS:HB3	1.46	0.97
2:N:68:CYS:HB2	2:N:126:CYS:HB3	1.45	0.96
2:J:68:CYS:HB2	2:J:126:CYS:HB3	1.45	0.96
2:N:207:GLY:HA2	1:S:728:VAL:HG12	1.44	0.95
2:R:68:CYS:HB2	2:R:126:CYS:HB3	1.48	0.95
2:P:2:GLU:HG2	2:P:158:LYS:HG2	1.48	0.94
2:P:68:CYS:HB2	2:P:126:CYS:HB3	1.47	0.94
2:V:68:CYS:HB2	2:V:126:CYS:HB3	1.49	0.94
2:D:19:CYS:HB3	2:D:145:CYS:HB3	1.47	0.93
1:S:426:MET:HE3	1:S:426:MET:HA	1.49	0.93
1:G:557:CYS:H	1:G:564:ASN:HD21	1.14	0.93
1:G:146:MET:HE1	1:G:544:THR:HB	1.51	0.92
1:Q:557:CYS:H	1:Q:564:ASN:HD21	1.02	0.92
1:M:426:MET:HE3	1:M:426:MET:HA	1.50	0.92
2:F:70:HIS:HD2	2:F:92:VAL:H	1.16	0.92
1:C:557:CYS:H	1:C:564:ASN:HD21	1.09	0.92
1:E:557:CYS:H	1:E:564:ASN:HD21	1.09	0.92
1:W:557:CYS:H	1:W:564:ASN:HD21	1.12	0.91
2:T:70:HIS:HD2	2:T:92:VAL:H	1.18	0.91
1:A:426:MET:HE1	1:A:618:GLN:HG2	1.53	0.91
1:O:426:MET:HE3	1:O:426:MET:HA	1.53	0.91
1:I:557:CYS:H	1:I:564:ASN:HD21	0.91	0.90
1:Q:426:MET:HE1	1:Q:618:GLN:HG2	1.53	0.90
1:M:610:LYS:NZ	1:M:618:GLN:HE22	1.69	0.90
1:U:557:CYS:H	1:U:564:ASN:HD21	1.13	0.89
1:O:100:LEU:HD12	1:O:105:PRO:HG3	1.55	0.89
2:F:68:CYS:HB2	2:F:126:CYS:CB	2.02	0.89
1:C:360:ALA:HB1	1:C:859:THR:HG23	1.54	0.88
2:D:68:CYS:HB2	2:D:126:CYS:HB3	1.54	0.88
2:H:70:HIS:HD2	2:H:92:VAL:H	1.18	0.88
1:C:610:LYS:NZ	1:C:618:GLN:HE22	1.69	0.88
2:D:128:MET:HA	7:D:303:SF4:S1	2.14	0.87
2:L:40:GLN:HE22	2:L:118:GLU:H	1.15	0.87
2:N:70:HIS:HD2	2:N:92:VAL:H	1.21	0.87
2:B:70:HIS:HD2	2:B:92:VAL:H	1.22	0.87
1:G:360:ALA:HB1	1:G:859:THR:HG23	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:426:MET:HE3	1:Q:426:MET:HA	1.57	0.87
1:W:146:MET:HE3	1:W:544:THR:HB	1.57	0.86
1:G:66:PHE:CD1	1:G:69:MET:HE3	2.10	0.86
1:S:753:TYR:HB3	2:T:24:MET:HE3	1.57	0.86
2:T:68:CYS:HB2	2:T:126:CYS:CB	2.06	0.85
2:P:19:CYS:HB3	2:P:145:CYS:HB3	1.57	0.85
1:W:28:MET:HE1	1:W:66:PHE:HB3	1.58	0.85
1:O:610:LYS:NZ	1:O:618:GLN:HE22	1.75	0.85
1:G:426:MET:HE1	1:G:618:GLN:HG2	1.56	0.85
1:E:66:PHE:CD1	1:E:69:MET:HE3	2.11	0.85
2:X:128:MET:HA	7:X:303:SF4:S1	2.16	0.84
2:J:68:CYS:HB2	2:J:126:CYS:CB	2.07	0.84
2:R:68:CYS:HB2	2:R:126:CYS:CB	2.06	0.84
1:O:28:MET:HE1	1:O:66:PHE:HB3	1.57	0.84
1:W:610:LYS:NZ	1:W:618:GLN:HE22	1.76	0.84
2:B:68:CYS:HB2	2:B:126:CYS:CB	2.07	0.84
1:I:557:CYS:N	1:I:564:ASN:HD21	1.75	0.84
2:H:76:CYS:HB3	2:H:108:THR:OG1	1.76	0.84
1:W:66:PHE:CD1	1:W:69:MET:HE3	2.13	0.84
2:P:128:MET:HA	7:P:303:SF4:S1	2.18	0.83
1:M:695:LEU:O	1:M:699:GLU:HG2	1.78	0.83
2:P:70:HIS:HD2	2:P:92:VAL:H	1.25	0.83
2:V:46:MET:HE1	2:V:66:THR:N	1.93	0.83
2:H:68:CYS:HB2	2:H:126:CYS:CB	2.08	0.83
1:Q:426:MET:CE	1:Q:618:GLN:HG2	2.07	0.83
1:Q:66:PHE:CD1	1:Q:69:MET:HE3	2.13	0.83
1:S:360:ALA:HB1	1:S:859:THR:HG23	1.58	0.83
2:L:128:MET:HA	7:L:303:SF4:S1	2.17	0.83
2:V:128:MET:HA	7:V:303:SF4:S1	2.18	0.83
1:K:426:MET:CE	1:K:618:GLN:HG2	2.07	0.83
1:O:426:MET:CE	1:O:618:GLN:HG2	2.08	0.83
1:U:426:MET:CE	1:U:618:GLN:HG2	2.09	0.83
1:A:426:MET:CE	1:A:618:GLN:HG2	2.09	0.82
1:G:610:LYS:NZ	1:G:618:GLN:HE22	1.78	0.82
1:Q:100:LEU:HD21	1:Q:534:PRO:HB2	1.60	0.82
2:L:68:CYS:HB2	2:L:126:CYS:CB	2.08	0.82
1:A:426:MET:HA	1:A:426:MET:HE3	1.61	0.82
2:R:128:MET:HA	7:R:303:SF4:S1	2.19	0.82
2:D:143:PRO:HB3	7:D:303:SF4:S1	2.18	0.82
2:N:40:GLN:HE22	2:N:118:GLU:H	1.28	0.82
2:J:128:MET:HA	7:J:302:SF4:S1	2.19	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:19:CYS:HB3	2:V:145:CYS:HB3	1.60	0.81
2:J:70:HIS:HD2	2:J:92:VAL:H	1.26	0.81
1:I:146:MET:HE1	1:I:544:THR:HB	1.63	0.81
1:U:66:PHE:CD1	1:U:69:MET:HE3	2.17	0.80
1:Q:319:GLU:HG2	1:U:726:LEU:HD13	1.61	0.80
1:A:786:ASN:HD22	1:A:805:VAL:H	1.30	0.80
1:M:557:CYS:N	1:M:564:ASN:HD21	1.80	0.80
2:N:46:MET:HE3	2:N:66:THR:H	1.47	0.80
1:C:66:PHE:CD1	1:C:69:MET:HE3	2.16	0.80
2:R:70:HIS:HD2	2:R:92:VAL:H	1.29	0.80
2:L:70:HIS:HD2	2:L:92:VAL:H	1.29	0.80
1:C:141:PRO:HA	1:C:496:TYR:HB3	1.64	0.80
1:Q:28:MET:HE1	1:Q:67:LYS:N	1.96	0.80
2:H:68:CYS:CB	2:H:126:CYS:HB3	2.11	0.79
1:I:557:CYS:H	1:I:564:ASN:ND2	1.76	0.79
1:M:360:ALA:HB1	1:M:859:THR:HG23	1.64	0.79
1:E:610:LYS:NZ	1:E:618:GLN:HE22	1.79	0.79
1:M:786:ASN:ND2	1:M:804:GLN:HA	1.98	0.79
1:S:66:PHE:CD1	1:S:69:MET:HE3	2.17	0.79
1:Q:66:PHE:HD1	1:Q:69:MET:HE3	1.47	0.79
2:X:68:CYS:CB	2:X:126:CYS:HB3	2.13	0.79
2:F:46:MET:HE3	2:F:66:THR:H	1.47	0.79
1:O:786:ASN:ND2	1:O:805:VAL:H	1.81	0.79
1:U:695:LEU:O	1:U:699:GLU:HG2	1.82	0.79
1:A:28:MET:HE1	1:A:66:PHE:HB3	1.65	0.78
1:G:823:TYR:CZ	1:G:825:PRO:HG3	2.17	0.78
1:O:823:TYR:CZ	1:O:825:PRO:HG3	2.17	0.78
2:T:128:MET:HA	7:T:303:SF4:S1	2.23	0.78
2:F:40:GLN:HE22	2:F:118:GLU:H	1.31	0.78
1:C:823:TYR:CZ	1:C:825:PRO:HG3	2.19	0.78
2:V:68:CYS:CB	2:V:126:CYS:HB3	2.14	0.78
2:L:166:LYS:O	2:L:170:GLU:HG3	1.84	0.78
2:L:68:CYS:CB	2:L:126:CYS:HB3	2.14	0.78
2:N:128:MET:HA	7:N:303:SF4:S1	2.24	0.78
1:E:426:MET:CE	1:E:618:GLN:HG2	2.14	0.77
1:I:360:ALA:HB1	1:I:859:THR:HG23	1.64	0.77
1:O:356:GLY:H	4:O:903:MGD:H5'2	1.48	0.77
2:V:70:HIS:HD2	2:V:92:VAL:H	1.32	0.77
1:A:360:ALA:HB1	1:A:859:THR:HG23	1.65	0.77
1:E:165:GLY:HA3	1:E:166:PHE:HB3	1.64	0.77
1:K:165:GLY:HA3	1:K:166:PHE:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:LYS:NZ	1:A:618:GLN:HE22	1.81	0.77
2:T:19:CYS:HB3	2:T:145:CYS:HB3	1.64	0.77
1:E:360:ALA:HB1	1:E:859:THR:HG23	1.65	0.77
1:I:66:PHE:CD1	1:I:69:MET:HE3	2.20	0.77
1:O:557:CYS:N	1:O:564:ASN:HD21	1.81	0.77
2:V:68:CYS:HB2	2:V:126:CYS:CB	2.15	0.77
1:A:503:THR:HG21	4:A:902:MGD:O2A	1.84	0.77
1:K:610:LYS:NZ	1:K:618:GLN:HE22	1.83	0.77
1:O:66:PHE:CD1	1:O:69:MET:HE3	2.19	0.77
1:Q:165:GLY:HA3	1:Q:166:PHE:HB3	1.66	0.77
2:L:76:CYS:HB3	2:L:108:THR:OG1	1.85	0.77
1:W:561:ILE:HG22	1:W:564:ASN:HB3	1.66	0.77
1:K:66:PHE:CD1	1:K:69:MET:HE3	2.19	0.77
1:O:479:GLN:HG2	8:O:1175:HOH:O	1.83	0.76
2:P:68:CYS:HB2	2:P:126:CYS:CB	2.14	0.76
2:L:68:CYS:HB3	2:L:70:HIS:CE1	2.21	0.76
1:I:426:MET:HE1	1:I:618:GLN:HG2	1.67	0.76
1:Q:610:LYS:NZ	1:Q:618:GLN:HE22	1.83	0.76
1:S:695:LEU:O	1:S:699:GLU:HG2	1.86	0.76
2:T:68:CYS:CB	2:T:126:CYS:HB3	2.15	0.76
1:O:165:GLY:HA3	1:O:166:PHE:HB3	1.66	0.76
1:I:165:GLY:HA3	1:I:166:PHE:HB3	1.68	0.76
1:K:557:CYS:H	1:K:564:ASN:ND2	1.83	0.76
1:G:141:PRO:HA	1:G:496:TYR:HB3	1.68	0.76
2:H:128:MET:HA	7:H:303:SF4:S1	2.26	0.76
1:S:426:MET:CE	1:S:618:GLN:HG2	2.15	0.76
2:F:68:CYS:CB	2:F:126:CYS:HB3	2.16	0.75
2:T:2:GLU:HG2	2:T:158:LYS:HG2	1.68	0.75
1:A:141:PRO:HA	1:A:496:TYR:HB3	1.68	0.75
1:I:823:TYR:CZ	1:I:825:PRO:HG3	2.22	0.75
2:L:46:MET:HE1	2:L:66:THR:N	2.02	0.75
1:M:823:TYR:CZ	1:M:825:PRO:HG3	2.19	0.75
2:V:76:CYS:HB3	2:V:108:THR:OG1	1.85	0.75
1:C:426:MET:CE	1:C:618:GLN:HG2	2.17	0.75
2:D:68:CYS:CB	2:D:126:CYS:HB3	2.16	0.75
1:I:426:MET:CE	1:I:618:GLN:HG2	2.16	0.75
2:J:40:GLN:NE2	2:J:118:GLU:H	1.84	0.75
1:Q:100:LEU:HD13	1:Q:105:PRO:HG3	1.68	0.75
2:F:46:MET:HE3	2:F:66:THR:N	2.00	0.75
2:P:76:CYS:HB3	2:P:108:THR:OG1	1.85	0.75
1:U:66:PHE:HD1	1:U:69:MET:HE3	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:MET:HE3	1:C:426:MET:HA	1.68	0.75
1:W:426:MET:CE	1:W:618:GLN:HG2	2.17	0.75
1:W:645:ASN:ND2	1:W:648:ARG:HB3	2.01	0.75
1:K:211:MET:HE1	1:K:338:GLN:HG2	1.69	0.75
2:L:59:ASN:H	2:L:59:ASN:HD22	1.35	0.75
2:D:46:MET:HE1	2:D:66:THR:N	2.02	0.74
2:F:128:MET:HA	7:F:303:SF4:S1	2.27	0.74
1:G:165:GLY:HA3	1:G:166:PHE:HB3	1.69	0.74
1:K:823:TYR:CZ	1:K:825:PRO:HG3	2.21	0.74
1:M:786:ASN:HD21	1:M:804:GLN:HA	1.49	0.74
1:O:146:MET:HE1	1:O:544:THR:HB	1.67	0.74
2:P:68:CYS:CB	2:P:126:CYS:HB3	2.17	0.74
2:B:68:CYS:CB	2:B:126:CYS:HB3	2.14	0.74
2:H:142:MET:HE2	2:H:146:ALA:CB	2.17	0.74
2:R:76:CYS:HB3	2:R:108:THR:OG1	1.86	0.74
1:E:426:MET:HE1	1:E:618:GLN:HG2	1.70	0.74
2:R:68:CYS:HB3	2:R:70:HIS:CE1	2.23	0.74
1:M:146:MET:HE3	1:M:544:THR:HB	1.70	0.74
2:L:59:ASN:H	2:L:59:ASN:ND2	1.86	0.73
1:M:426:MET:CE	1:M:618:GLN:HG2	2.17	0.73
1:S:100:LEU:HD12	1:S:105:PRO:HG3	1.69	0.73
2:J:68:CYS:CB	2:J:126:CYS:HB3	2.18	0.73
1:K:28:MET:HE1	1:K:66:PHE:HB3	1.70	0.73
1:K:356:GLY:N	4:K:903:MGD:O2B	2.20	0.73
1:M:141:PRO:HA	1:M:496:TYR:HB3	1.70	0.73
1:O:426:MET:HE2	1:O:618:GLN:HG2	1.71	0.73
1:A:356:GLY:N	4:A:903:MGD:O2B	2.20	0.73
1:E:141:PRO:HA	1:E:496:TYR:HB3	1.68	0.73
1:M:165:GLY:HA3	1:M:166:PHE:HB3	1.70	0.73
2:R:68:CYS:CB	2:R:126:CYS:HB3	2.18	0.73
1:S:503:THR:HG21	4:S:902:MGD:O2A	1.88	0.73
1:A:823:TYR:CZ	1:A:825:PRO:HG3	2.23	0.73
1:S:610:LYS:NZ	1:S:618:GLN:HE22	1.87	0.73
1:O:753:TYR:HB3	2:P:24:MET:HE3	1.70	0.73
1:G:394:PRO:HG3	8:G:1319:HOH:O	1.88	0.73
1:G:695:LEU:O	1:G:699:GLU:HG2	1.89	0.73
1:G:503:THR:HG21	4:G:902:MGD:O2A	1.87	0.73
2:B:128:MET:HA	7:B:303:SF4:S1	2.29	0.72
1:S:823:TYR:CZ	1:S:825:PRO:HG3	2.23	0.72
1:U:28:MET:HE1	1:U:66:PHE:HB3	1.71	0.72
1:I:146:MET:CE	1:I:544:THR:HB	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:69:MET:HB3	2:J:184:PRO:HB3	1.71	0.72
1:K:360:ALA:HB1	1:K:859:THR:HG23	1.71	0.72
1:M:610:LYS:HZ3	1:M:618:GLN:HE22	1.37	0.72
1:W:753:TYR:HB3	2:X:24:MET:HE3	1.71	0.72
4:A:903:MGD:O2B	4:A:903:MGD:O2A	2.07	0.72
1:I:141:PRO:HA	1:I:496:TYR:HB3	1.71	0.72
1:K:141:PRO:HA	1:K:496:TYR:HB3	1.71	0.72
1:O:141:PRO:HA	1:O:496:TYR:HB3	1.72	0.72
1:U:610:LYS:NZ	1:U:618:GLN:HE22	1.86	0.72
2:H:46:MET:HE1	2:H:65:PRO:HA	1.71	0.72
2:N:68:CYS:CB	2:N:126:CYS:HB3	2.18	0.72
2:L:19:CYS:HB3	2:L:145:CYS:HB3	1.69	0.72
2:N:2:GLU:HG2	2:N:158:LYS:HG2	1.72	0.72
1:Q:695:LEU:O	1:Q:699:GLU:HG2	1.89	0.72
1:W:356:GLY:H	4:W:903:MGD:H5'2	1.55	0.72
1:A:66:PHE:CD1	1:A:69:MET:HE3	2.24	0.72
1:A:610:LYS:HZ2	1:A:618:GLN:HE22	1.36	0.72
1:Q:100:LEU:CD2	1:Q:534:PRO:HB2	2.20	0.72
1:G:100:LEU:HD12	1:G:105:PRO:HG3	1.70	0.72
1:I:610:LYS:NZ	1:I:618:GLN:HE22	1.88	0.72
2:X:143:PRO:HB3	7:X:303:SF4:S1	2.29	0.72
2:H:40:GLN:HE22	2:H:118:GLU:H	1.37	0.71
1:W:165:GLY:HA3	1:W:166:PHE:HB3	1.71	0.71
1:A:695:LEU:O	1:A:699:GLU:HG2	1.90	0.71
1:G:146:MET:CE	1:G:544:THR:HB	2.20	0.71
1:G:28:MET:HE1	1:G:66:PHE:HB3	1.72	0.71
1:I:695:LEU:O	1:I:699:GLU:HG2	1.90	0.71
1:S:356:GLY:H	4:S:903:MGD:H5'2	1.53	0.71
2:X:100:LYS:HG2	2:X:122:VAL:HB	1.72	0.71
2:B:68:CYS:HB3	2:B:70:HIS:CE1	2.25	0.71
1:W:426:MET:HE1	1:W:618:GLN:HG2	1.72	0.71
2:N:76:CYS:HB3	2:N:108:THR:OG1	1.90	0.71
1:M:100:LEU:HD12	1:M:105:PRO:HG3	1.72	0.71
2:P:40:GLN:HE22	2:P:118:GLU:H	1.37	0.71
1:Q:823:TYR:CZ	1:Q:825:PRO:HG3	2.25	0.71
1:U:165:GLY:HA3	1:U:166:PHE:HB3	1.70	0.71
1:C:356:GLY:H	4:C:903:MGD:H5'2	1.56	0.71
1:W:141:PRO:HA	1:W:496:TYR:HB3	1.72	0.71
1:A:753:TYR:HB3	2:B:24:MET:HE3	1.71	0.71
2:P:59:ASN:HD22	2:P:59:ASN:H	1.37	0.71
1:W:557:CYS:N	1:W:564:ASN:HD21	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:MET:HE1	1:C:618:GLN:HG2	1.73	0.71
1:C:695:LEU:O	1:C:699:GLU:HG2	1.89	0.71
2:D:76:CYS:HB3	2:D:108:THR:OG1	1.90	0.71
1:E:610:LYS:HZ2	1:E:618:GLN:HE22	1.36	0.71
1:Q:218:ASP:OD2	1:Q:253:ASN:HB2	1.90	0.71
1:U:823:TYR:CZ	1:U:825:PRO:HG3	2.26	0.71
2:J:71:CYS:HB2	2:J:182:THR:O	1.91	0.71
1:M:696:LYS:O	1:M:700:GLU:HG3	1.91	0.71
2:D:75:PRO:HD2	7:D:304:SF4:S4	2.31	0.70
1:K:695:LEU:O	1:K:699:GLU:HG2	1.90	0.70
2:N:21:MET:CE	2:N:21:MET:HA	2.22	0.70
2:V:143:PRO:HB3	7:V:303:SF4:S1	2.31	0.70
2:X:87:ARG:HG3	2:X:91:ILE:O	1.92	0.70
2:F:46:MET:HE1	2:F:65:PRO:HA	1.73	0.70
2:H:70:HIS:CD2	2:H:92:VAL:H	2.07	0.70
2:N:68:CYS:HB2	2:N:126:CYS:CB	2.19	0.70
2:R:143:PRO:HB3	7:R:303:SF4:S1	2.31	0.70
1:W:360:ALA:HB1	1:W:859:THR:HG23	1.74	0.70
2:F:142:MET:HE2	2:F:146:ALA:CB	2.21	0.70
1:C:557:CYS:N	1:C:564:ASN:HD21	1.88	0.70
2:N:46:MET:HE3	2:N:66:THR:N	2.07	0.70
2:D:71:CYS:HB2	2:D:182:THR:O	1.91	0.70
2:H:46:MET:HE3	2:H:66:THR:H	1.57	0.70
1:C:155:SER:OG	1:C:409:ILE:HG12	1.91	0.70
2:X:68:CYS:HB3	2:X:70:HIS:CE1	2.27	0.70
1:C:28:MET:HE1	1:C:66:PHE:HB3	1.74	0.70
1:E:28:MET:HE1	1:E:66:PHE:HB3	1.74	0.70
1:E:66:PHE:HD1	1:E:69:MET:HE3	1.57	0.70
1:E:695:LEU:O	1:E:699:GLU:HG2	1.90	0.70
1:K:66:PHE:HD1	1:K:69:MET:HE3	1.57	0.70
1:S:558:SER:H	1:S:564:ASN:ND2	1.90	0.70
1:I:28:MET:HE1	1:I:66:PHE:HB3	1.73	0.69
1:O:360:ALA:HB1	1:O:859:THR:HG23	1.73	0.69
2:F:40:GLN:NE2	2:F:118:GLU:H	1.90	0.69
1:U:696:LYS:O	1:U:700:GLU:HG3	1.92	0.69
1:I:786:ASN:ND2	1:I:804:GLN:HA	2.07	0.69
2:L:5:TYR:HB2	2:L:157:LEU:CD1	2.23	0.69
2:X:2:GLU:HG2	2:X:158:LYS:HG2	1.72	0.69
2:F:68:CYS:HB3	2:F:70:HIS:CE1	2.28	0.69
2:J:40:GLN:HE22	2:J:118:GLU:H	1.40	0.69
1:G:44:ILE:HD11	1:G:394:PRO:HG2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:356:GLY:N	4:I:903:MGD:O1B	2.26	0.69
1:I:44:ILE:HD11	1:I:394:PRO:HG2	1.73	0.69
2:J:23:CYS:HB3	2:J:39:MET:HE3	1.74	0.69
2:H:21:MET:CE	2:H:21:MET:HA	2.22	0.69
2:X:69:MET:HB3	2:X:184:PRO:HB3	1.74	0.69
1:Q:800:ILE:HD12	1:Q:800:ILE:N	2.08	0.69
2:T:68:CYS:HB3	2:T:70:HIS:CE1	2.27	0.69
1:K:753:TYR:HB3	2:L:24:MET:HE3	1.73	0.69
1:S:557:CYS:N	1:S:564:ASN:HD21	1.86	0.69
1:C:610:LYS:HZ2	1:C:618:GLN:HE22	1.38	0.69
2:D:73:ASN:HB3	2:D:182:THR:HA	1.73	0.69
2:R:40:GLN:HE22	2:R:118:GLU:H	1.39	0.68
1:G:378:GLY:O	1:G:381:LYS:HG2	1.93	0.68
1:M:35:ASP:OD1	1:M:55:ARG:HD3	1.93	0.68
1:Q:211:MET:HE1	2:R:231:PHE:HZ	1.58	0.68
2:D:40:GLN:NE2	2:D:117:ASN:HA	2.08	0.68
1:A:66:PHE:HZ	1:A:146:MET:HE1	1.59	0.68
1:C:165:GLY:HA3	1:C:166:PHE:HB3	1.75	0.68
1:Q:141:PRO:HA	1:Q:496:TYR:HB3	1.76	0.68
1:U:141:PRO:HA	1:U:496:TYR:HB3	1.74	0.68
1:E:510:TYR:O	1:E:513:MET:HG2	1.94	0.68
1:G:426:MET:CE	1:G:618:GLN:HG2	2.24	0.68
2:H:143:PRO:HB3	7:H:303:SF4:S1	2.34	0.68
1:S:165:GLY:HA3	1:S:166:PHE:HB3	1.75	0.68
2:X:46:MET:HE1	2:X:65:PRO:HA	1.73	0.68
2:X:68:CYS:HB2	2:X:126:CYS:CB	2.22	0.68
2:H:142:MET:HE2	2:H:146:ALA:HB1	1.75	0.68
2:J:21:MET:HA	2:J:21:MET:CE	2.22	0.68
2:T:76:CYS:HB3	2:T:108:THR:OG1	1.94	0.68
1:W:610:LYS:HZ2	1:W:618:GLN:HE22	1.41	0.68
1:A:218:ASP:OD2	1:A:253:ASN:HB2	1.95	0.67
1:G:162:ASN:HA	8:G:1362:HOH:O	1.92	0.67
1:I:75:ARG:HH21	1:I:543:CYS:HA	1.58	0.67
1:I:610:LYS:HZ2	1:I:618:GLN:HE22	1.40	0.67
1:O:610:LYS:HZ3	1:O:618:GLN:HE22	1.40	0.67
1:C:753:TYR:HB3	2:D:24:MET:HE3	1.77	0.67
1:Q:134:PRO:HB2	1:Q:439:LEU:HD11	1.75	0.67
1:Q:146:MET:HE1	1:Q:544:THR:HB	1.76	0.67
2:H:68:CYS:HB3	2:H:70:HIS:CE1	2.30	0.67
2:L:21:MET:HE2	2:L:21:MET:HA	1.76	0.67
1:W:75:ARG:HH21	1:W:543:CYS:HA	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:71:CYS:HB2	2:L:182:THR:O	1.94	0.67
2:H:2:GLU:HG2	2:H:158:LYS:HG2	1.76	0.67
1:M:610:LYS:HZ1	1:M:618:GLN:HE22	1.41	0.67
2:X:95:ASP:HB3	2:X:98:LYS:HB2	1.75	0.67
2:F:142:MET:HE2	2:F:146:ALA:HB1	1.77	0.67
1:O:695:LEU:O	1:O:699:GLU:HG2	1.95	0.67
1:E:561:ILE:HG22	1:E:564:ASN:HB3	1.76	0.67
2:N:71:CYS:HB2	2:N:182:THR:O	1.94	0.67
1:U:142:SER:OG	4:U:902:MGD:O1A	2.11	0.67
1:W:494:TRP:HE1	1:W:525:GLN:HE21	1.43	0.67
2:F:69:MET:HB3	2:F:184:PRO:HB3	1.78	0.66
2:T:201:ALA:HB2	2:T:269:LEU:HB2	1.77	0.66
1:U:134:PRO:HB2	1:U:439:LEU:HD11	1.76	0.66
1:W:426:MET:HE3	1:W:622:ALA:HB2	1.77	0.66
1:E:823:TYR:CZ	1:E:825:PRO:HG3	2.30	0.66
1:U:182:GLY:HA3	1:U:364:ILE:HG23	1.76	0.66
1:U:617:GLU:HG3	1:U:631:TRP:CG	2.29	0.66
2:L:75:PRO:HD2	7:L:304:SF4:S4	2.35	0.66
1:E:100:LEU:HD12	1:E:105:PRO:HG3	1.75	0.66
1:W:74:LEU:HD12	1:W:750:LYS:HA	1.76	0.66
1:C:146:MET:HE1	1:C:544:THR:HB	1.77	0.66
1:M:28:MET:HE1	1:M:66:PHE:HB3	1.76	0.66
1:C:460:LYS:HE3	8:C:1230:HOH:O	1.96	0.66
4:K:903:MGD:O2A	4:K:903:MGD:O2B	2.12	0.66
2:L:1:MET:HG3	2:L:88:GLU:HB3	1.76	0.66
2:V:68:CYS:HB3	2:V:70:HIS:CE1	2.30	0.66
2:B:46:MET:HE1	2:B:65:PRO:CA	2.25	0.66
1:S:66:PHE:HD1	1:S:69:MET:HE3	1.60	0.66
1:M:166:PHE:N	1:M:439:LEU:HD12	2.11	0.66
1:M:218:ASP:OD2	1:M:253:ASN:HB2	1.96	0.66
1:O:426:MET:HE1	1:O:618:GLN:HG2	1.77	0.66
1:Q:28:MET:HE1	1:Q:67:LYS:H	1.60	0.66
1:I:426:MET:HA	1:I:426:MET:HE3	1.75	0.66
2:T:46:MET:HE1	2:T:66:THR:N	2.11	0.66
1:G:114:TRP:CZ2	1:G:541:PRO:HD2	2.30	0.65
2:P:143:PRO:HB3	7:P:303:SF4:S1	2.35	0.65
2:J:76:CYS:HB3	2:J:108:THR:OG1	1.96	0.65
1:C:75:ARG:HH21	1:C:543:CYS:HA	1.61	0.65
1:I:426:MET:HE3	1:I:622:ALA:HB2	1.78	0.65
1:I:66:PHE:HA	1:I:69:MET:CE	2.26	0.65
2:P:46:MET:HE1	2:P:66:THR:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:71:CYS:HB2	2:H:182:THR:O	1.96	0.65
1:K:630:THR:OG1	1:K:633:GLU:HG3	1.96	0.65
2:T:40:GLN:HE22	2:T:118:GLU:H	1.45	0.65
1:S:311:THR:HG21	8:S:1497:HOH:O	1.96	0.65
2:N:46:MET:HE1	2:N:65:PRO:HA	1.79	0.65
1:U:356:GLY:H	4:U:903:MGD:H5'2	1.61	0.65
1:C:146:MET:CE	1:C:544:THR:HB	2.26	0.65
1:I:214:PHE:HA	1:I:347:ALA:HB3	1.78	0.65
2:N:68:CYS:HB3	2:N:70:HIS:CE1	2.32	0.65
1:Q:360:ALA:HB1	1:Q:859:THR:HG23	1.79	0.65
1:U:801:LEU:HD11	1:U:839:ILE:HD11	1.78	0.65
1:E:356:GLY:H	4:E:903:MGD:H5'2	1.60	0.65
2:B:76:CYS:HB3	2:B:108:THR:OG1	1.95	0.65
1:Q:610:LYS:HZ2	1:Q:618:GLN:HE22	1.44	0.65
1:M:356:GLY:H	4:M:903:MGD:H5'2	1.62	0.65
1:O:649:LYS:HE3	1:O:651:THR:HG22	1.79	0.65
1:C:561:ILE:HG22	1:C:564:ASN:HB3	1.80	0.64
1:Q:166:PHE:N	1:Q:439:LEU:HD12	2.12	0.64
1:U:460:LYS:HE3	8:U:1232:HOH:O	1.97	0.64
2:F:114:MET:HE2	2:F:123:ALA:HB1	1.80	0.64
1:G:561:ILE:HG22	1:G:564:ASN:HB3	1.78	0.64
1:Q:649:LYS:HE3	1:Q:651:THR:CG2	2.27	0.64
1:S:81:LYS:HB2	1:S:112:ILE:HD13	1.79	0.64
1:G:610:LYS:HZ3	1:G:618:GLN:HE22	1.44	0.64
2:P:59:ASN:ND2	2:P:59:ASN:H	1.95	0.64
2:L:143:PRO:HB3	7:L:303:SF4:S1	2.38	0.64
1:M:76:ILE:HG22	1:M:541:PRO:HG3	1.80	0.64
2:T:143:PRO:HB3	7:T:303:SF4:S1	2.37	0.64
1:C:426:MET:HE1	1:C:618:GLN:O	1.98	0.64
2:D:68:CYS:HB2	2:D:126:CYS:CB	2.27	0.64
1:U:211:MET:HE1	1:U:338:GLN:HG2	1.79	0.64
1:W:426:MET:HA	1:W:426:MET:HE3	1.78	0.64
2:X:19:CYS:CB	2:X:145:CYS:HB3	2.22	0.64
1:A:66:PHE:HD1	1:A:69:MET:HE3	1.61	0.64
2:H:46:MET:HE3	2:H:66:THR:N	2.12	0.64
2:J:5:TYR:HB2	2:J:157:LEU:CD1	2.28	0.64
1:S:28:MET:HE1	1:S:66:PHE:HB3	1.77	0.64
2:T:21:MET:HE2	2:T:21:MET:HA	1.80	0.64
1:C:257:ARG:HD3	2:D:61:ILE:HG21	1.79	0.64
1:A:165:GLY:HA3	1:A:166:PHE:HB3	1.78	0.64
1:C:738:HIS:HE2	4:C:902:MGD:H15	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:MET:HE1	1:M:754:MET:HE3	1.80	0.64
1:M:426:MET:HE1	1:M:618:GLN:HG2	1.77	0.64
2:N:23:CYS:HB3	2:N:39:MET:HE3	1.79	0.64
1:S:426:MET:HE1	1:S:618:GLN:HG2	1.77	0.64
2:B:40:GLN:NE2	2:B:118:GLU:H	1.96	0.63
1:C:610:LYS:HZ3	1:C:618:GLN:HE22	1.44	0.63
1:M:211:MET:HE1	2:N:231:PHE:HZ	1.64	0.63
1:O:719:GLU:HG2	1:O:859:THR:O	1.98	0.63
2:B:5:TYR:HB2	2:B:157:LEU:CD1	2.28	0.63
1:C:772:MET:HB2	1:C:801:LEU:HD13	1.81	0.63
1:M:66:PHE:CD1	1:M:69:MET:HE3	2.32	0.63
1:C:696:LYS:O	1:C:700:GLU:HG3	1.99	0.63
2:F:5:TYR:HB2	2:F:157:LEU:CD1	2.28	0.63
1:I:134:PRO:HB2	1:I:439:LEU:HD11	1.80	0.63
1:W:786:ASN:HD21	1:W:804:GLN:HA	1.63	0.63
2:B:46:MET:HE3	2:B:66:THR:H	1.63	0.63
2:F:201:ALA:HB2	2:F:269:LEU:HB2	1.81	0.63
1:I:630:THR:OG1	1:I:633:GLU:HG3	1.97	0.63
1:S:478:HIS:HD2	8:S:1203:HOH:O	1.82	0.63
1:S:561:ILE:HG22	1:S:564:ASN:HB3	1.80	0.63
2:V:69:MET:HB3	2:V:184:PRO:HB3	1.79	0.63
2:X:70:HIS:HD2	2:X:92:VAL:H	1.46	0.63
2:N:75:PRO:HD2	7:N:304:SF4:S4	2.39	0.63
1:O:394:PRO:HG3	8:O:1321:HOH:O	1.97	0.63
2:R:125:LYS:HD2	2:R:126:CYS:O	1.98	0.63
1:M:725:PRO:HA	1:S:704:ILE:HG13	1.79	0.63
1:M:32:ASP:HB2	8:M:1657:HOH:O	1.99	0.63
1:G:610:LYS:HB3	1:G:614:ALA:HB3	1.80	0.63
1:I:66:PHE:HA	1:I:69:MET:HE3	1.80	0.63
1:M:66:PHE:HD1	1:M:69:MET:HE3	1.64	0.63
1:U:146:MET:CE	1:U:544:THR:HB	2.28	0.63
1:G:870:ASP:HB3	1:G:872:TYR:CE1	2.34	0.63
1:G:218:ASP:OD2	1:G:253:ASN:HB2	1.99	0.62
1:W:426:MET:HE1	1:W:618:GLN:O	1.99	0.62
2:F:76:CYS:HB3	2:F:108:THR:OG1	1.99	0.62
1:G:553:GLU:HG2	1:G:556:ASN:HB2	1.81	0.62
1:K:786:ASN:ND2	1:K:805:VAL:H	1.97	0.62
1:E:218:ASP:OD2	1:E:253:ASN:HB2	1.98	0.62
1:U:76:ILE:HG22	1:U:541:PRO:HG3	1.81	0.62
1:M:823:TYR:CE2	1:M:825:PRO:HG3	2.34	0.62
1:W:560:TYR:HB2	8:W:1673:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:68:CYS:HB3	2:J:70:HIS:CE1	2.34	0.62
1:W:28:MET:HE1	1:W:66:PHE:CB	2.27	0.62
2:J:143:PRO:HB3	7:J:302:SF4:S1	2.40	0.62
1:M:197:GLU:OE2	1:M:667:ASP:HB2	1.99	0.62
1:O:469:ALA:HA	8:O:1517:HOH:O	1.99	0.62
2:T:23:CYS:HB3	2:T:39:MET:HE3	1.82	0.62
1:U:35:ASP:OD1	1:U:55:ARG:HD3	1.99	0.62
2:B:46:MET:HE1	2:B:65:PRO:HA	1.79	0.62
1:E:560:TYR:HB2	8:E:1683:HOH:O	1.98	0.62
2:J:46:MET:CE	2:J:66:THR:H	2.13	0.62
1:K:610:LYS:HZ2	1:K:618:GLN:HE22	1.48	0.62
1:K:823:TYR:CE2	1:K:825:PRO:HG3	2.35	0.62
2:B:21:MET:HE2	2:B:21:MET:HA	1.82	0.62
1:K:557:CYS:N	1:K:564:ASN:HD21	1.87	0.62
1:Q:557:CYS:N	1:Q:564:ASN:HD21	1.85	0.62
1:E:394:PRO:HG3	8:E:1321:HOH:O	1.98	0.61
2:N:207:GLY:HA2	1:S:728:VAL:CG1	2.26	0.61
2:P:114:MET:HE3	2:P:123:ALA:HB1	1.80	0.61
1:Q:35:ASP:OD1	1:Q:55:ARG:HD3	2.00	0.61
1:C:726:LEU:HD23	8:C:1193:HOH:O	2.00	0.61
1:K:871:LYS:HG2	8:K:1230:HOH:O	1.99	0.61
1:S:75:ARG:HH21	1:S:543:CYS:HA	1.64	0.61
2:X:40:GLN:NE2	2:X:117:ASN:HA	2.15	0.61
1:O:90:GLU:HB2	8:O:1242:HOH:O	2.00	0.61
1:Q:753:TYR:HB3	2:R:24:MET:HE3	1.82	0.61
2:R:95:ASP:HB3	2:R:98:LYS:HB2	1.80	0.61
1:C:66:PHE:HA	1:C:69:MET:CE	2.30	0.61
2:D:40:GLN:HE22	2:D:118:GLU:H	1.48	0.61
1:I:394:PRO:HG3	8:I:1315:HOH:O	2.00	0.61
1:O:146:MET:CE	1:O:544:THR:HB	2.30	0.61
2:J:114:MET:HA	2:J:125:LYS:HB3	1.81	0.61
1:K:301:GLU:CD	1:K:301:GLU:H	2.04	0.61
1:M:75:ARG:NH2	1:M:543:CYS:HA	2.14	0.61
2:N:207:GLY:CA	1:S:728:VAL:HG12	2.24	0.61
1:W:695:LEU:O	1:W:699:GLU:HG2	1.99	0.61
2:H:114:MET:HE2	2:H:123:ALA:HB1	1.82	0.61
1:G:211:MET:HE1	2:H:231:PHE:HZ	1.66	0.61
1:M:557:CYS:H	1:M:564:ASN:ND2	1.84	0.61
1:U:21:LYS:HB3	1:U:26:ILE:HD11	1.82	0.61
1:K:146:MET:CE	1:K:544:THR:HB	2.31	0.61
1:E:673:ASN:H	1:E:673:ASN:HD22	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:LEU:HD23	2:D:114:MET:HE3	1.83	0.61
1:E:114:TRP:CZ2	1:E:541:PRO:HD2	2.36	0.61
2:F:46:MET:HE1	2:F:65:PRO:CA	2.31	0.61
2:F:75:PRO:HD2	7:F:304:SF4:S4	2.41	0.61
2:P:69:MET:HB3	2:P:184:PRO:HB3	1.82	0.61
2:X:23:CYS:HB3	2:X:39:MET:HE3	1.82	0.61
2:N:143:PRO:HB3	7:N:303:SF4:S1	2.41	0.60
1:A:100:LEU:HD12	1:A:105:PRO:HG3	1.83	0.60
2:N:142:MET:HE2	2:N:146:ALA:CB	2.30	0.60
1:Q:696:LYS:O	1:Q:700:GLU:HG3	2.01	0.60
1:Q:823:TYR:CE2	1:Q:825:PRO:HG3	2.36	0.60
1:C:696:LYS:HD3	8:C:1677:HOH:O	2.01	0.60
2:H:125:LYS:HD2	2:H:126:CYS:O	2.02	0.60
1:O:311:THR:HG21	8:O:1499:HOH:O	2.00	0.60
1:Q:649:LYS:HE3	1:Q:651:THR:HG22	1.82	0.60
1:S:35:ASP:OD1	1:S:55:ARG:HD3	2.00	0.60
2:T:71:CYS:HB2	2:T:182:THR:O	2.01	0.60
2:B:143:PRO:HB3	7:B:303:SF4:S1	2.42	0.60
1:O:142:SER:HB3	4:O:902:MGD:O1A	2.01	0.60
1:O:738:HIS:HE2	4:O:902:MGD:H15	1.48	0.60
1:U:503:THR:HG21	4:U:902:MGD:O2A	2.01	0.60
1:E:630:THR:OG1	1:E:633:GLU:HG3	2.00	0.60
1:G:571:ARG:HB2	1:G:642:VAL:HB	1.84	0.60
1:I:478:HIS:HD2	8:I:1200:HOH:O	1.84	0.60
2:L:119:GLU:HB2	8:L:941:HOH:O	2.00	0.60
1:O:44:ILE:HD11	1:O:394:PRO:HG2	1.83	0.60
1:O:35:ASP:OD1	1:O:55:ARG:HD3	2.01	0.60
1:C:700:GLU:HG2	8:C:1568:HOH:O	2.01	0.60
1:G:610:LYS:HZ1	1:G:618:GLN:HE22	1.50	0.60
2:J:46:MET:HE1	2:J:65:PRO:CA	2.31	0.60
2:P:46:MET:CE	2:P:66:THR:N	2.64	0.60
2:R:46:MET:HE1	2:R:65:PRO:CA	2.32	0.60
1:Q:333:ARG:NH1	1:U:729:LYS:HE3	2.17	0.60
2:X:1:MET:HG3	2:X:88:GLU:HB3	1.84	0.60
1:E:426:MET:HA	1:E:426:MET:HE3	1.83	0.60
1:O:21:LYS:HB3	1:O:26:ILE:HD11	1.83	0.60
1:O:75:ARG:HH21	1:O:543:CYS:HA	1.64	0.60
2:X:40:GLN:HE22	2:X:118:GLU:H	1.49	0.60
1:A:460:LYS:HE3	8:A:1230:HOH:O	2.02	0.60
2:B:106:LEU:HD23	2:B:114:MET:HG3	1.82	0.60
1:E:426:MET:HE3	1:E:622:ALA:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:356:GLY:H	4:K:903:MGD:H5'2	1.67	0.60
1:Q:708:ARG:HD2	8:Q:1043:HOH:O	2.02	0.60
1:U:44:ILE:HD11	1:U:394:PRO:HG2	1.83	0.60
1:M:826:LEU:HD21	1:M:835:ARG:HD3	1.84	0.60
2:R:87:ARG:HG3	2:R:91:ILE:O	2.01	0.60
2:D:70:HIS:HD2	2:D:92:VAL:H	1.50	0.60
1:I:75:ARG:NH2	1:I:543:CYS:HA	2.17	0.60
1:W:786:ASN:ND2	1:W:804:GLN:HA	2.16	0.60
1:C:753:TYR:HB3	2:D:24:MET:CE	2.31	0.59
1:G:146:MET:HE2	1:G:545:ASN:H	1.67	0.59
2:P:75:PRO:HD2	7:P:304:SF4:S4	2.42	0.59
2:P:46:MET:HE1	2:P:65:PRO:CA	2.32	0.59
2:X:75:PRO:HD2	7:X:304:SF4:S4	2.42	0.59
1:G:494:TRP:HE1	1:G:525:GLN:HE21	1.50	0.59
2:L:40:GLN:HE22	2:L:118:GLU:N	1.95	0.59
1:O:253:ASN:O	1:O:257:ARG:HG3	2.02	0.59
2:R:21:MET:HE2	2:R:21:MET:HA	1.82	0.59
2:R:56:TYR:HA	2:R:59:ASN:ND2	2.16	0.59
1:W:138:LEU:HB2	1:W:490:ILE:HD12	1.85	0.59
2:F:143:PRO:HB3	7:F:303:SF4:S1	2.41	0.59
1:O:610:LYS:HZ2	1:O:618:GLN:HE22	1.49	0.59
1:O:66:PHE:HA	1:O:69:MET:HE2	1.83	0.59
1:O:783:GLY:O	1:O:866:LYS:HD2	2.02	0.59
1:S:528:TRP:CD2	1:S:750:LYS:HD3	2.37	0.59
1:U:738:HIS:HE2	4:U:902:MGD:H15	1.51	0.59
1:U:753:TYR:HB3	2:V:24:MET:CE	2.31	0.59
2:V:201:ALA:HB2	2:V:269:LEU:HB2	1.84	0.59
1:A:69:MET:HE1	1:A:754:MET:HE3	1.84	0.59
1:E:823:TYR:CE2	1:E:825:PRO:HG3	2.38	0.59
1:O:823:TYR:CE2	1:O:825:PRO:HG3	2.37	0.59
1:Q:171:HIS:HB2	8:Q:1675:HOH:O	2.01	0.59
1:W:146:MET:HE3	1:W:544:THR:CB	2.30	0.59
2:D:106:LEU:HD11	2:D:116:TRP:HB2	1.84	0.59
2:H:46:MET:HE1	2:H:65:PRO:CA	2.32	0.59
1:K:28:MET:HE3	1:K:63:THR:O	2.02	0.59
1:S:738:HIS:HE2	4:S:902:MGD:H15	1.48	0.59
2:T:114:MET:HE3	2:T:123:ALA:HB1	1.84	0.59
2:X:181:GLY:O	2:X:183:LYS:HE2	2.03	0.59
1:E:557:CYS:N	1:E:564:ASN:HD21	1.89	0.59
2:F:71:CYS:HB2	2:F:182:THR:O	2.03	0.59
1:G:214:PHE:HA	1:G:347:ALA:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:426:MET:HA	1:I:426:MET:CE	2.31	0.59
1:M:166:PHE:H	1:M:439:LEU:HD12	1.67	0.59
1:O:426:MET:HE1	1:O:618:GLN:O	2.03	0.59
1:Q:800:ILE:HD11	1:Q:833:ALA:HB1	1.85	0.59
1:W:708:ARG:HD2	8:W:1044:HOH:O	2.02	0.59
2:T:70:HIS:CD2	2:T:92:VAL:H	2.09	0.59
1:U:2:GLY:O	1:U:21:LYS:HE3	2.03	0.59
1:A:557:CYS:N	1:A:564:ASN:HD21	1.93	0.59
1:C:563:ASP:O	1:C:566:GLN:HG2	2.03	0.59
2:F:70:HIS:CD2	2:F:92:VAL:H	2.08	0.59
1:Q:319:GLU:HG2	1:U:726:LEU:CD1	2.30	0.59
1:C:177:GLU:OE2	1:C:177:GLU:HA	2.03	0.59
1:E:786:ASN:HD22	1:E:805:VAL:H	1.49	0.59
2:H:201:ALA:HB2	2:H:269:LEU:HB2	1.85	0.59
2:L:201:ALA:HB2	2:L:269:LEU:HB2	1.83	0.59
2:P:125:LYS:HD2	2:P:126:CYS:O	2.01	0.59
2:P:46:MET:CE	2:P:66:THR:H	2.15	0.59
1:G:81:LYS:HB2	1:G:112:ILE:HD13	1.85	0.59
1:G:730:TYR:CE1	1:G:794:ASN:HA	2.38	0.59
2:L:46:MET:CE	2:L:66:THR:N	2.65	0.59
1:O:563:ASP:O	1:O:566:GLN:HG2	2.03	0.59
1:Q:630:THR:OG1	1:Q:633:GLU:HG3	2.03	0.59
1:Q:786:ASN:ND2	1:Q:804:GLN:HA	2.17	0.59
1:S:146:MET:HG2	4:S:902:MGD:N7	2.18	0.59
1:W:696:LYS:O	1:W:700:GLU:HG3	2.03	0.59
2:B:46:MET:HE3	2:B:66:THR:N	2.18	0.58
2:D:68:CYS:HB3	2:D:70:HIS:CE1	2.38	0.58
1:E:138:LEU:HB2	1:E:490:ILE:HD12	1.83	0.58
1:G:66:PHE:HA	1:G:69:MET:CE	2.33	0.58
1:O:146:MET:HG2	4:O:902:MGD:N7	2.18	0.58
2:R:104:GLU:H	2:R:104:GLU:CD	2.06	0.58
1:U:146:MET:HE1	1:U:544:THR:HB	1.84	0.58
1:U:311:THR:HG21	8:U:1502:HOH:O	2.03	0.58
2:F:166:LYS:O	2:F:170:GLU:HG3	2.03	0.58
2:H:106:LEU:HD22	2:H:114:MET:HB3	1.85	0.58
1:O:610:LYS:HB3	1:O:614:ALA:HB3	1.84	0.58
1:S:214:PHE:HA	1:S:347:ALA:HB3	1.85	0.58
1:A:557:CYS:H	1:A:564:ASN:ND2	1.92	0.58
2:J:211:GLU:HB2	2:J:231:PHE:HA	1.84	0.58
2:R:56:TYR:HA	2:R:59:ASN:HD22	1.68	0.58
2:V:142:MET:HE2	2:V:146:ALA:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:146:MET:HE1	1:K:544:THR:HB	1.83	0.58
1:O:753:TYR:HB3	2:P:24:MET:CE	2.34	0.58
1:U:825:PRO:HD2	8:U:1337:HOH:O	2.03	0.58
1:W:855:MET:HB2	1:W:857:ASN:OD1	2.03	0.58
2:N:46:MET:HE1	2:N:65:PRO:CA	2.33	0.58
2:P:105:LEU:HB3	2:P:114:MET:CE	2.34	0.58
2:V:71:CYS:HB2	2:V:182:THR:O	2.03	0.58
1:W:118:THR:O	1:W:122:VAL:HG23	2.03	0.58
1:A:394:PRO:HG3	8:A:1318:HOH:O	2.04	0.58
1:G:174:ASP:OD1	1:G:175:SER:N	2.35	0.58
2:L:218:LYS:HG2	2:L:223:GLU:HA	1.86	0.58
2:N:87:ARG:HD3	2:N:93:LEU:HD12	1.85	0.58
2:T:125:LYS:HD2	2:T:126:CYS:O	2.03	0.58
1:U:561:ILE:HG22	1:U:564:ASN:HB3	1.84	0.58
2:F:13:CYS:HB3	2:F:63:TYR:HB2	1.86	0.58
2:N:114:MET:HE2	2:N:123:ALA:HB1	1.84	0.58
2:B:71:CYS:HB2	2:B:182:THR:O	2.03	0.58
1:E:211:MET:HE3	1:E:244:ASP:HB2	1.86	0.58
1:O:28:MET:HE1	1:O:66:PHE:CB	2.32	0.58
1:Q:855:MET:HB2	1:Q:857:ASN:OD1	2.03	0.58
2:X:46:MET:HE3	2:X:66:THR:H	1.69	0.58
2:L:2:GLU:HG2	2:L:158:LYS:HG2	1.86	0.58
1:Q:738:HIS:HE2	4:Q:902:MGD:H15	1.52	0.58
2:R:5:TYR:HB2	2:R:157:LEU:HD13	1.86	0.58
1:Q:786:ASN:ND2	1:Q:805:VAL:H	2.02	0.58
2:R:70:HIS:CD2	2:R:92:VAL:H	2.16	0.58
1:M:319:GLU:HG2	1:S:726:LEU:CD1	2.34	0.58
2:X:106:LEU:HD11	2:X:116:TRP:HB2	1.85	0.58
1:A:56:LYS:HG2	1:A:57:THR:O	2.04	0.57
1:C:142:SER:HB3	4:C:902:MGD:O1A	2.04	0.57
1:I:253:ASN:O	1:I:257:ARG:HG3	2.04	0.57
1:Q:291:GLU:CD	1:Q:291:GLU:H	2.07	0.57
2:R:46:MET:HE1	2:R:65:PRO:HA	1.86	0.57
2:D:18:ASN:HB2	7:D:302:SF4:S1	2.45	0.57
2:J:46:MET:HE1	2:J:65:PRO:HA	1.86	0.57
2:P:105:LEU:HB3	2:P:114:MET:HE1	1.87	0.57
1:G:66:PHE:HD1	1:G:69:MET:HE3	1.62	0.57
2:N:87:ARG:HG3	2:N:91:ILE:O	2.05	0.57
1:O:75:ARG:NH2	1:O:543:CYS:HA	2.19	0.57
2:P:23:CYS:HB3	2:P:39:MET:HE3	1.85	0.57
1:S:630:THR:OG1	1:S:633:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:46:MET:HE1	2:J:66:THR:N	2.19	0.57
1:M:134:PRO:HB2	1:M:439:LEU:HD11	1.85	0.57
1:M:75:ARG:HH21	1:M:543:CYS:HA	1.69	0.57
1:O:479:GLN:N	8:O:1175:HOH:O	2.37	0.57
1:U:21:LYS:CB	1:U:26:ILE:HD11	2.34	0.57
1:U:360:ALA:HB1	1:U:859:THR:HG23	1.86	0.57
2:X:114:MET:HA	2:X:125:LYS:HB3	1.85	0.57
1:C:394:PRO:HG3	8:C:1321:HOH:O	2.03	0.57
2:D:59:ASN:H	2:D:59:ASN:ND2	2.01	0.57
1:I:138:LEU:HB2	1:I:490:ILE:HD12	1.86	0.57
1:M:66:PHE:HA	1:M:69:MET:HE2	1.86	0.57
2:P:18:ASN:HB2	7:P:302:SF4:S1	2.44	0.57
1:S:476:GLN:OE1	1:S:708:ARG:NH2	2.38	0.57
1:W:400:TYR:CE1	1:W:421:LYS:HD2	2.38	0.57
1:E:66:PHE:HA	1:E:69:MET:CE	2.34	0.57
2:H:75:PRO:HD2	7:H:304:SF4:S4	2.45	0.57
1:M:494:TRP:HE1	1:M:525:GLN:HE21	1.51	0.57
1:U:66:PHE:HZ	1:U:146:MET:HE1	1.69	0.57
1:Q:319:GLU:CG	1:U:726:LEU:HD13	2.34	0.57
1:W:557:CYS:H	1:W:564:ASN:ND2	1.94	0.57
1:C:418:ALA:HB1	1:C:423:ALA:HB2	1.87	0.57
1:O:81:LYS:HB2	1:O:112:ILE:HD13	1.86	0.57
1:A:378:GLY:O	1:A:381:LYS:HG2	2.05	0.57
1:C:138:LEU:HB2	1:C:490:ILE:HD12	1.86	0.57
1:E:66:PHE:HA	1:E:69:MET:HE2	1.85	0.57
1:I:175:SER:HB2	1:I:176:TRP:CE3	2.39	0.57
1:K:85:PHE:CE2	1:K:87:PRO:HG3	2.39	0.57
1:U:510:TYR:O	1:U:513:MET:HG2	2.04	0.57
1:W:142:SER:HB3	4:W:902:MGD:H5'2	1.87	0.57
1:I:426:MET:HE1	1:I:618:GLN:O	2.05	0.57
1:O:617:GLU:HG3	1:O:631:TRP:CG	2.40	0.57
1:O:647:ASN:HB2	8:O:1442:HOH:O	2.04	0.57
1:Q:494:TRP:HE1	1:Q:525:GLN:HE21	1.52	0.57
1:S:783:GLY:O	1:S:866:LYS:HD2	2.05	0.57
1:U:104:ASP:OD2	1:U:107:SER:HB3	2.05	0.57
2:B:114:MET:HA	2:B:125:LYS:HB3	1.86	0.57
1:C:9:ASN:HA	1:C:576:GLN:HA	1.85	0.57
2:J:75:PRO:HD2	7:J:303:SF4:S4	2.44	0.57
1:K:201:LEU:HD13	1:K:387:TRP:HB2	1.87	0.57
1:O:66:PHE:HD1	1:O:69:MET:HE3	1.65	0.57
1:Q:75:ARG:HH21	1:Q:543:CYS:HA	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:142:MET:HE2	2:R:146:ALA:C	2.24	0.57
1:C:644:ASP:C	1:C:646:PRO:HD3	2.25	0.56
2:D:26:GLU:HB2	2:D:144:ARG:HH11	1.70	0.56
2:F:5:TYR:HB2	2:F:157:LEU:HD11	1.86	0.56
1:G:211:MET:HE1	2:H:231:PHE:CZ	2.40	0.56
2:J:19:CYS:O	2:J:22:GLY:N	2.38	0.56
1:K:45:GLU:HG3	8:K:1516:HOH:O	2.04	0.56
1:K:460:LYS:HE3	8:K:1229:HOH:O	2.05	0.56
1:M:11:SER:HA	1:M:147:TRP:HB2	1.86	0.56
1:M:797:GLY:HA2	1:M:875:TYR:CE2	2.40	0.56
1:U:85:PHE:CE2	1:U:87:PRO:HG3	2.40	0.56
2:B:205:VAL:HG13	2:B:254:LYS:NZ	2.20	0.56
2:F:21:MET:HA	2:F:21:MET:CE	2.34	0.56
1:G:557:CYS:N	1:G:564:ASN:HD21	1.94	0.56
1:M:319:GLU:HG2	1:S:726:LEU:HD13	1.88	0.56
1:M:426:MET:HE1	1:M:618:GLN:O	2.03	0.56
2:P:106:LEU:HD23	2:P:114:MET:HE3	1.87	0.56
2:X:105:LEU:HB3	2:X:114:MET:HE1	1.87	0.56
2:X:157:LEU:N	2:X:157:LEU:HD12	2.20	0.56
1:G:35:ASP:OD1	1:G:55:ARG:HD3	2.06	0.56
2:T:18:ASN:HB2	7:T:302:SF4:S1	2.46	0.56
2:V:87:ARG:HG3	2:V:91:ILE:O	2.05	0.56
1:O:100:LEU:CD1	1:O:105:PRO:HG3	2.32	0.56
1:O:211:MET:HE1	2:P:231:PHE:HZ	1.70	0.56
2:R:129:CYS:HB3	2:R:132:LEU:HD12	1.87	0.56
2:R:166:LYS:HG2	2:R:170:GLU:OE2	2.05	0.56
1:A:730:TYR:CE1	1:A:794:ASN:HA	2.41	0.56
1:E:100:LEU:CD1	1:E:105:PRO:HG3	2.36	0.56
2:H:87:ARG:HG3	2:H:91:ILE:O	2.04	0.56
1:I:644:ASP:O	1:I:646:PRO:HD3	2.04	0.56
1:K:561:ILE:HG22	1:K:564:ASN:HB3	1.88	0.56
1:K:786:ASN:ND2	1:K:804:GLN:HA	2.20	0.56
1:M:128:ILE:CD1	1:M:492:MET:HB2	2.35	0.56
1:M:738:HIS:HE2	4:M:902:MGD:H15	1.53	0.56
2:N:201:ALA:HB2	2:N:269:LEU:HB2	1.85	0.56
2:T:10:VAL:HG13	2:T:63:TYR:O	2.05	0.56
1:U:553:GLU:HG2	1:U:556:ASN:HB2	1.88	0.56
2:X:46:MET:HE3	2:X:66:THR:N	2.20	0.56
1:C:387:TRP:CE2	1:C:389:THR:HA	2.40	0.56
2:D:40:GLN:HE21	2:D:117:ASN:HA	1.70	0.56
1:K:387:TRP:CE2	1:K:389:THR:HA	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:69:MET:HB3	2:N:184:PRO:HB3	1.86	0.56
1:Q:153:ARG:O	1:Q:157:TYR:HB3	2.05	0.56
1:A:387:TRP:CE2	1:A:389:THR:HA	2.40	0.56
2:H:142:MET:CE	2:H:146:ALA:HB1	2.35	0.56
1:S:617:GLU:HG3	1:S:631:TRP:CG	2.41	0.56
2:D:7:VAL:HB	2:D:155:GLU:HB3	1.86	0.56
1:I:823:TYR:CE2	1:I:825:PRO:HG3	2.40	0.56
2:N:5:TYR:HB2	2:N:157:LEU:CD1	2.36	0.56
2:P:19:CYS:CB	2:P:145:CYS:HB3	2.32	0.56
2:T:142:MET:HE1	8:T:430:HOH:O	2.06	0.56
1:W:660:GLY:HA2	8:W:1205:HOH:O	2.05	0.56
2:X:46:MET:HE1	2:X:65:PRO:CA	2.36	0.56
1:A:696:LYS:O	1:A:700:GLU:HG3	2.05	0.56
1:A:823:TYR:CE2	1:A:825:PRO:HG3	2.40	0.56
1:E:146:MET:CE	1:E:544:THR:HB	2.35	0.56
1:E:66:PHE:HZ	1:E:146:MET:CE	2.19	0.56
2:H:70:HIS:HD2	2:H:92:VAL:N	1.97	0.56
2:J:21:MET:HE2	2:J:21:MET:HA	1.85	0.56
2:P:46:MET:HE1	2:P:65:PRO:HA	1.88	0.56
1:Q:541:PRO:HB2	1:Q:586:SER:HA	1.87	0.56
1:Q:66:PHE:HA	1:Q:69:MET:HE2	1.88	0.56
1:M:333:ARG:NH1	1:S:729:LYS:HE3	2.20	0.56
2:X:59:ASN:H	2:X:59:ASN:ND2	2.04	0.56
1:C:478:HIS:HD2	8:C:1204:HOH:O	1.89	0.56
1:C:870:ASP:HB3	1:C:872:TYR:CE1	2.41	0.56
1:O:645:ASN:ND2	1:O:648:ARG:HB3	2.20	0.56
1:E:142:SER:OG	4:E:902:MGD:O1A	2.24	0.56
1:I:249:ASP:CG	4:I:903:MGD:H1'	2.27	0.56
2:J:87:ARG:HG3	2:J:91:ILE:O	2.06	0.56
1:M:478:HIS:HD2	8:M:1203:HOH:O	1.88	0.56
2:R:46:MET:CE	2:R:66:THR:H	2.18	0.56
2:B:69:MET:HB3	2:B:184:PRO:HB3	1.88	0.55
2:F:87:ARG:HG3	2:F:91:ILE:O	2.05	0.55
1:G:177:GLU:HA	1:G:177:GLU:OE2	2.06	0.55
1:I:565:TYR:C	1:I:567:LEU:H	2.09	0.55
1:M:400:TYR:CE1	1:M:421:LYS:HD2	2.41	0.55
1:O:476:GLN:OE1	1:O:708:ARG:NH2	2.39	0.55
1:S:146:MET:CE	1:S:544:THR:HB	2.36	0.55
1:W:75:ARG:NH2	1:W:543:CYS:HA	2.20	0.55
1:C:66:PHE:HZ	1:C:146:MET:CE	2.20	0.55
1:I:74:LEU:HD12	1:I:750:LYS:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:114:MET:HE3	2:J:123:ALA:HB1	1.87	0.55
1:M:211:MET:CE	2:N:231:PHE:CZ	2.89	0.55
1:W:647:ASN:HB2	8:W:1445:HOH:O	2.05	0.55
2:D:69:MET:HB3	2:D:184:PRO:HB3	1.88	0.55
1:K:100:LEU:CD1	1:K:105:PRO:HG3	2.36	0.55
1:K:478:HIS:HD2	8:K:1202:HOH:O	1.88	0.55
1:M:146:MET:HE3	1:M:544:THR:CB	2.35	0.55
1:O:649:LYS:HE2	8:O:1459:HOH:O	2.07	0.55
2:P:68:CYS:HB3	2:P:70:HIS:CE1	2.42	0.55
1:U:253:ASN:O	1:U:257:ARG:HG3	2.07	0.55
1:U:786:ASN:HD22	1:U:805:VAL:H	1.54	0.55
2:V:23:CYS:HB3	2:V:39:MET:HE3	1.88	0.55
2:V:75:PRO:HD2	7:V:304:SF4:S4	2.46	0.55
1:W:356:GLY:H	4:W:903:MGD:C5'	2.19	0.55
1:G:617:GLU:HG3	1:G:631:TRP:CG	2.41	0.55
1:I:44:ILE:HD11	1:I:394:PRO:CG	2.37	0.55
1:M:708:ARG:HD2	8:M:1044:HOH:O	2.04	0.55
1:A:175:SER:HB2	1:A:176:TRP:CE3	2.41	0.55
1:E:426:MET:HE1	1:E:618:GLN:O	2.06	0.55
2:H:40:GLN:NE2	2:H:118:GLU:H	2.02	0.55
1:M:426:MET:HA	1:M:426:MET:CE	2.32	0.55
1:O:765:ASP:HB2	8:O:1165:HOH:O	2.05	0.55
1:U:128:ILE:CD1	1:U:492:MET:HB2	2.36	0.55
1:A:249:ASP:CG	4:A:903:MGD:H1'	2.27	0.55
2:H:69:MET:HB3	2:H:184:PRO:HB3	1.87	0.55
2:P:70:HIS:CD2	2:P:92:VAL:H	2.15	0.55
1:A:85:PHE:CE2	1:A:87:PRO:HG3	2.42	0.55
1:C:494:TRP:HE1	1:C:525:GLN:HE21	1.54	0.55
1:E:800:ILE:HD12	1:E:800:ILE:N	2.22	0.55
2:H:46:MET:CE	2:H:66:THR:H	2.19	0.55
1:I:15:PRO:HD3	1:I:554:PHE:CD1	2.41	0.55
1:I:55:ARG:HD2	8:I:1633:HOH:O	2.05	0.55
2:J:70:HIS:CD2	2:J:92:VAL:H	2.16	0.55
2:L:105:LEU:HB3	2:L:114:MET:CE	2.37	0.55
1:M:187:TRP:CH2	1:M:196:PRO:HB3	2.41	0.55
1:O:138:LEU:HB2	1:O:490:ILE:HD12	1.89	0.55
1:O:673:ASN:HD22	1:O:673:ASN:H	1.53	0.55
2:D:3:GLN:O	2:D:158:LYS:HA	2.07	0.55
1:I:142:SER:HB3	4:I:902:MGD:O1A	2.06	0.55
1:Q:146:MET:HG2	4:Q:902:MGD:N7	2.22	0.55
1:Q:426:MET:HA	1:Q:426:MET:CE	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:35:ASP:OD1	1:W:55:ARG:HD3	2.07	0.55
2:D:59:ASN:H	2:D:59:ASN:HD22	1.54	0.55
1:E:197:GLU:OE2	1:E:667:ASP:HB2	2.07	0.55
1:E:730:TYR:CZ	1:E:794:ASN:HA	2.42	0.55
2:J:164:MET:O	2:J:168:VAL:HG23	2.06	0.55
2:J:46:MET:CE	2:J:66:THR:N	2.69	0.55
1:O:32:ASP:OD1	1:O:56:LYS:HD2	2.07	0.55
1:Q:114:TRP:CZ2	1:Q:541:PRO:HD2	2.41	0.55
2:R:19:CYS:O	2:R:22:GLY:N	2.40	0.55
1:A:81:LYS:HB2	1:A:112:ILE:HD13	1.88	0.55
2:H:166:LYS:O	2:H:170:GLU:HG3	2.07	0.55
1:I:96:ARG:HD2	1:I:514:TYR:O	2.07	0.55
1:K:708:ARG:HD2	8:K:1042:HOH:O	2.07	0.55
2:N:166:LYS:O	2:N:170:GLU:HG3	2.06	0.55
2:P:71:CYS:HB2	2:P:182:THR:O	2.05	0.55
1:Q:166:PHE:H	1:Q:439:LEU:HD12	1.71	0.55
2:V:46:MET:HE1	2:V:65:PRO:C	2.27	0.55
2:X:105:LEU:HB3	2:X:114:MET:CE	2.37	0.55
1:E:426:MET:HA	1:E:426:MET:CE	2.37	0.54
1:E:66:PHE:HZ	1:E:146:MET:HE1	1.71	0.54
2:H:19:CYS:HB3	2:H:145:CYS:HB3	1.89	0.54
1:M:800:ILE:HD12	1:M:800:ILE:N	2.22	0.54
2:R:75:PRO:HD2	7:R:304:SF4:S4	2.47	0.54
2:R:46:MET:CE	2:R:66:THR:N	2.70	0.54
1:A:826:LEU:HD21	1:A:835:ARG:HD3	1.88	0.54
1:C:66:PHE:HZ	1:C:146:MET:HE1	1.72	0.54
2:L:40:GLN:NE2	2:L:117:ASN:HA	2.22	0.54
1:M:214:PHE:HA	1:M:347:ALA:HB3	1.89	0.54
1:O:301:GLU:H	1:O:301:GLU:CD	2.11	0.54
1:Q:177:GLU:OE2	1:Q:177:GLU:HA	2.07	0.54
1:U:66:PHE:HZ	1:U:146:MET:CE	2.20	0.54
1:A:142:SER:OG	4:A:902:MGD:O1A	2.12	0.54
1:C:76:ILE:HG22	1:C:541:PRO:HG3	1.88	0.54
1:E:870:ASP:HB3	1:E:872:TYR:CE1	2.42	0.54
1:I:142:SER:CB	4:I:902:MGD:O1A	2.55	0.54
2:L:46:MET:CE	2:L:66:THR:H	2.20	0.54
2:T:106:LEU:HD11	2:T:116:TRP:HB2	1.89	0.54
2:V:46:MET:CE	2:V:66:THR:N	2.67	0.54
1:W:277:ALA:HB2	1:W:321:ALA:HB2	1.88	0.54
1:C:15:PRO:HD3	1:C:554:PHE:CD1	2.42	0.54
1:C:823:TYR:CE2	1:C:825:PRO:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:MET:CE	2:F:146:ALA:HB1	2.36	0.54
1:G:541:PRO:HB2	1:G:586:SER:HA	1.90	0.54
2:H:3:GLN:O	2:H:158:LYS:HA	2.08	0.54
1:I:114:TRP:CZ2	1:I:541:PRO:HD2	2.41	0.54
2:L:167:LYS:HZ3	2:L:171:GLU:CD	2.11	0.54
1:M:21:LYS:HB3	1:M:26:ILE:HD11	1.90	0.54
1:O:563:ASP:HA	1:O:565:TYR:CE1	2.42	0.54
1:S:610:LYS:HZ2	1:S:618:GLN:HE22	1.55	0.54
2:T:52:GLU:HG3	2:T:61:ILE:HD12	1.89	0.54
1:W:11:SER:HA	1:W:147:TRP:HB2	1.88	0.54
1:I:563:ASP:O	1:I:566:GLN:HG2	2.08	0.54
2:J:104:GLU:CD	2:J:104:GLU:H	2.09	0.54
2:R:157:LEU:H	2:R:157:LEU:HD12	1.72	0.54
1:S:647:ASN:O	1:S:648:ARG:O	2.25	0.54
1:A:211:MET:HE1	2:B:231:PHE:HZ	1.72	0.54
1:C:100:LEU:HD12	1:C:105:PRO:HG3	1.90	0.54
2:H:19:CYS:O	2:H:22:GLY:N	2.40	0.54
1:K:610:LYS:HB3	1:K:614:ALA:HB3	1.90	0.54
1:M:353:GLY:O	1:M:354:TRP:HB2	2.08	0.54
1:O:561:ILE:HG22	1:O:564:ASN:HB3	1.88	0.54
1:Q:214:PHE:HA	1:Q:347:ALA:HB3	1.90	0.54
1:Q:55:ARG:HD2	8:Q:1631:HOH:O	2.07	0.54
2:R:23:CYS:HB3	2:R:39:MET:HE3	1.89	0.54
2:R:40:GLN:NE2	2:R:118:GLU:H	2.04	0.54
1:U:142:SER:CB	4:U:902:MGD:O1A	2.56	0.54
1:W:563:ASP:O	1:W:566:GLN:HG2	2.07	0.54
2:X:76:CYS:HB3	2:X:108:THR:OG1	2.07	0.54
1:M:541:PRO:HB2	1:M:586:SER:HA	1.89	0.54
1:Q:142:SER:CB	4:Q:902:MGD:O1A	2.56	0.54
1:U:753:TYR:HB3	2:V:24:MET:HE3	1.88	0.54
1:W:499:PRO:HG3	4:W:902:MGD:O5'	2.08	0.54
2:X:125:LYS:HD2	2:X:126:CYS:O	2.08	0.54
1:A:76:ILE:HG22	1:A:541:PRO:HG3	1.89	0.54
2:F:2:GLU:HG2	2:F:158:LYS:HG2	1.90	0.54
1:M:617:GLU:HG3	1:M:631:TRP:CG	2.43	0.54
1:M:211:MET:HE1	2:N:231:PHE:CZ	2.43	0.54
2:P:201:ALA:HB2	2:P:269:LEU:HB2	1.88	0.54
1:Q:142:SER:HB3	4:Q:902:MGD:O1A	2.07	0.54
1:S:729:LYS:HD2	8:S:1133:HOH:O	2.08	0.54
1:W:214:PHE:HA	1:W:347:ALA:HB3	1.90	0.54
2:B:75:PRO:HD2	7:B:304:SF4:S4	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:SER:HB2	1:G:176:TRP:CE3	2.42	0.54
2:H:59:ASN:H	2:H:59:ASN:ND2	2.06	0.54
2:L:21:MET:CE	2:L:21:MET:HA	2.38	0.54
2:N:43:HIS:ND1	8:N:403:HOH:O	2.33	0.54
1:O:142:SER:CB	4:O:902:MGD:O1A	2.55	0.54
1:O:257:ARG:HD3	2:P:61:ILE:HG21	1.90	0.54
1:A:100:LEU:CD1	1:A:105:PRO:HG3	2.38	0.53
1:C:142:SER:CB	4:C:902:MGD:O1A	2.56	0.53
2:D:198:TYR:HB3	2:D:238:ASP:HA	1.90	0.53
1:E:673:ASN:ND2	1:E:673:ASN:H	2.06	0.53
1:E:826:LEU:HD21	1:E:835:ARG:HD3	1.90	0.53
1:G:476:GLN:OE1	1:G:708:ARG:NH2	2.40	0.53
2:R:247:VAL:O	2:R:257:SER:HA	2.07	0.53
2:T:87:ARG:HG3	2:T:91:ILE:O	2.07	0.53
1:W:563:ASP:HA	1:W:565:TYR:CE1	2.43	0.53
1:W:610:LYS:HZ3	1:W:618:GLN:HE22	1.56	0.53
2:B:59:ASN:H	2:B:59:ASN:ND2	2.06	0.53
1:C:253:ASN:O	1:C:257:ARG:HG3	2.09	0.53
1:E:15:PRO:HD3	1:E:554:PHE:CD1	2.43	0.53
1:G:604:GLU:HB3	8:G:1121:HOH:O	2.08	0.53
1:I:12:THR:O	1:I:226:TYR:HA	2.08	0.53
2:N:5:TYR:CD2	2:N:164:MET:HG2	2.43	0.53
1:O:494:TRP:HE1	1:O:525:GLN:HE21	1.56	0.53
1:Q:44:ILE:HD11	1:Q:394:PRO:HG2	1.90	0.53
1:S:610:LYS:HZ3	1:S:618:GLN:HE22	1.56	0.53
1:U:610:LYS:HZ1	1:U:618:GLN:HE22	1.54	0.53
1:W:847:TYR:CZ	1:W:853:CYS:HB3	2.44	0.53
1:A:630:THR:OG1	1:A:633:GLU:HG3	2.09	0.53
2:D:23:CYS:HB3	2:D:39:MET:CE	2.38	0.53
1:E:557:CYS:H	1:E:564:ASN:ND2	1.91	0.53
1:G:15:PRO:HD3	1:G:554:PHE:CD1	2.43	0.53
1:G:66:PHE:HA	1:G:69:MET:HE3	1.91	0.53
1:M:141:PRO:CA	1:M:496:TYR:HB3	2.38	0.53
2:T:40:GLN:NE2	2:T:117:ASN:HA	2.23	0.53
2:T:159:THR:OG1	2:T:160:THR:N	2.42	0.53
2:T:218:LYS:HG2	2:T:223:GLU:HA	1.91	0.53
2:T:75:PRO:HD2	7:T:304:SF4:S4	2.49	0.53
1:G:426:MET:HE3	1:G:622:ALA:HB2	1.89	0.53
1:G:296:ASN:HB3	1:G:657:PHE:CZ	2.43	0.53
2:H:211:GLU:HB2	2:H:231:PHE:HA	1.90	0.53
1:M:476:GLN:OE1	1:M:708:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:106:LEU:CD2	2:N:114:MET:HB3	2.38	0.53
2:P:106:LEU:HD23	2:P:114:MET:CE	2.38	0.53
2:R:5:TYR:O	2:R:157:LEU:HD12	2.08	0.53
1:S:426:MET:HE2	1:S:618:GLN:HG2	1.89	0.53
1:U:563:ASP:O	1:U:566:GLN:HG2	2.08	0.53
2:X:218:LYS:HA	2:X:222:LYS:O	2.08	0.53
1:A:561:ILE:HG22	1:A:564:ASN:HB3	1.91	0.53
1:C:719:GLU:HG2	1:C:859:THR:O	2.09	0.53
1:I:66:PHE:HZ	1:I:146:MET:CE	2.22	0.53
1:K:426:MET:O	1:K:426:MET:HE2	2.09	0.53
1:K:767:TYR:HB3	1:K:769:TYR:CE1	2.43	0.53
2:N:21:MET:HE1	2:N:24:MET:HE3	1.90	0.53
1:O:140:THR:HB	1:O:169:ALA:HB3	1.91	0.53
2:P:216:VAL:HG13	2:P:223:GLU:HG3	1.90	0.53
2:T:46:MET:HE1	2:T:66:THR:H	1.73	0.53
1:W:134:PRO:HD2	8:W:1360:HOH:O	2.09	0.53
1:W:561:ILE:CG2	1:W:564:ASN:HB3	2.37	0.53
1:W:797:GLY:HA2	1:W:875:TYR:CE2	2.43	0.53
2:D:2:GLU:HG2	2:D:158:LYS:HG2	1.90	0.53
1:E:730:TYR:CE1	1:E:794:ASN:HA	2.44	0.53
2:R:142:MET:HE2	2:R:146:ALA:CB	2.38	0.53
1:E:175:SER:HB2	1:E:176:TRP:CE3	2.43	0.53
1:G:146:MET:HG2	4:G:902:MGD:N7	2.24	0.53
2:N:40:GLN:NE2	2:N:118:GLU:H	2.00	0.53
1:Q:69:MET:HE1	1:Q:754:MET:HE3	1.91	0.53
2:R:68:CYS:HB2	2:R:126:CYS:HB2	1.89	0.53
1:A:478:HIS:HD2	8:A:1203:HOH:O	1.92	0.53
1:A:670:PRO:HG2	1:A:675:GLN:CD	2.29	0.53
2:B:210:PHE:HD2	2:B:213:ALA:HB2	1.73	0.53
1:C:66:PHE:HA	1:C:69:MET:HE3	1.90	0.53
1:C:786:ASN:ND2	1:C:804:GLN:HA	2.24	0.53
2:D:142:MET:CE	2:D:146:ALA:HB1	2.39	0.53
1:E:528:TRP:CG	1:E:750:LYS:HD3	2.43	0.53
2:L:23:CYS:HB3	2:L:39:MET:HE3	1.91	0.53
1:O:629:MET:HE1	1:O:634:PHE:HA	1.91	0.53
1:S:253:ASN:O	1:S:257:ARG:HG3	2.09	0.53
2:V:18:ASN:HB2	7:V:302:SF4:S1	2.48	0.53
1:W:418:ALA:HB1	1:W:423:ALA:HB2	1.89	0.53
1:W:722:LYS:HG2	8:W:1565:HOH:O	2.09	0.53
2:X:73:ASN:HB3	2:X:182:THR:HA	1.90	0.53
1:C:610:LYS:HB3	1:C:614:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:70:HIS:HD2	2:F:92:VAL:N	1.98	0.53
1:I:328:PRO:HB2	1:I:331:GLU:HG3	1.90	0.53
1:I:142:SER:OG	4:I:902:MGD:O1A	2.25	0.53
2:L:114:MET:HE3	2:L:123:ALA:HB1	1.91	0.53
2:L:114:MET:HA	2:L:125:LYS:HB3	1.91	0.53
1:M:142:SER:OG	4:M:902:MGD:O1A	2.21	0.53
1:O:499:PRO:HG3	4:O:902:MGD:O5'	2.09	0.53
1:Q:211:MET:HE1	2:R:231:PHE:CZ	2.42	0.53
1:U:478:HIS:HD2	8:U:1205:HOH:O	1.91	0.53
2:V:114:MET:HA	2:V:125:LYS:HB3	1.89	0.53
1:G:356:GLY:HA2	1:G:359:ARG:NH1	2.24	0.53
1:G:400:TYR:CE1	1:G:421:LYS:HD2	2.44	0.53
1:K:786:ASN:HD21	1:K:804:GLN:HA	1.73	0.53
2:P:87:ARG:HG3	2:P:91:ILE:O	2.09	0.53
1:Q:296:ASN:HB3	1:Q:657:PHE:CZ	2.44	0.53
1:U:44:ILE:HD11	1:U:394:PRO:CG	2.38	0.53
1:W:56:LYS:HE2	8:W:1468:HOH:O	2.09	0.53
2:X:99:ALA:HA	2:X:102:LYS:HD2	1.90	0.53
2:B:106:LEU:HA	2:B:114:MET:HG3	1.90	0.52
1:K:66:PHE:HZ	1:K:146:MET:CE	2.22	0.52
2:X:129:CYS:HB3	2:X:131:HIS:CE1	2.44	0.52
1:A:214:PHE:HA	1:A:347:ALA:HB3	1.91	0.52
1:A:691:ILE:HD11	1:A:711:MET:HE3	1.91	0.52
1:E:146:MET:HG2	4:E:902:MGD:N7	2.24	0.52
1:I:528:TRP:CG	1:I:750:LYS:HD3	2.43	0.52
2:J:5:TYR:HB2	2:J:157:LEU:HD12	1.91	0.52
1:Q:96:ARG:HD2	1:Q:514:TYR:O	2.09	0.52
2:R:43:HIS:ND1	8:R:902:HOH:O	2.34	0.52
1:W:239:LYS:HE2	8:W:1600:HOH:O	2.09	0.52
1:A:426:MET:HA	1:A:426:MET:CE	2.37	0.52
1:A:249:ASP:OD1	4:A:903:MGD:H1'	2.09	0.52
1:G:452:ILE:HB	1:G:453:PRO:HD3	1.91	0.52
2:H:23:CYS:HB3	2:H:39:MET:HE3	1.89	0.52
2:J:203:ILE:N	2:J:203:ILE:HD12	2.24	0.52
1:K:66:PHE:HZ	1:K:146:MET:HE1	1.74	0.52
2:L:162:GLU:H	2:L:162:GLU:CD	2.12	0.52
1:M:571:ARG:HB2	1:M:642:VAL:HB	1.91	0.52
1:Q:394:PRO:HG3	8:Q:1315:HOH:O	2.09	0.52
1:S:114:TRP:CZ2	1:S:541:PRO:HD2	2.43	0.52
1:W:800:ILE:HD12	1:W:800:ILE:N	2.25	0.52
2:X:218:LYS:O	2:X:246:THR:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASN:O	1:A:257:ARG:HG3	2.09	0.52
2:D:105:LEU:C	2:D:114:MET:HE2	2.30	0.52
1:I:730:TYR:CE1	1:I:794:ASN:HA	2.45	0.52
1:K:656:TRP:CD2	1:K:663:LYS:HA	2.44	0.52
2:N:56:TYR:HA	2:N:59:ASN:HD22	1.74	0.52
1:Q:533:VAL:HB	1:Q:534:PRO:HD3	1.91	0.52
2:X:4:TYR:CE2	2:X:158:LYS:HD2	2.44	0.52
1:E:565:TYR:C	1:E:567:LEU:H	2.13	0.52
2:F:203:ILE:N	2:F:203:ILE:HD12	2.24	0.52
1:K:253:ASN:O	1:K:257:ARG:HG3	2.10	0.52
1:U:563:ASP:HA	1:U:565:TYR:CE1	2.44	0.52
1:U:610:LYS:HB3	1:U:614:ALA:HB3	1.90	0.52
2:X:40:GLN:HB3	2:X:43:HIS:CE1	2.44	0.52
1:C:426:MET:HE3	1:C:622:ALA:HB2	1.91	0.52
1:I:617:GLU:HG3	1:I:631:TRP:CG	2.45	0.52
1:I:786:ASN:HD21	1:I:804:GLN:HA	1.71	0.52
1:K:28:MET:CE	1:K:66:PHE:HB3	2.38	0.52
1:O:704:ILE:HG23	8:O:1642:HOH:O	2.09	0.52
1:Q:691:ILE:HD11	1:Q:711:MET:HE3	1.90	0.52
1:S:505:THR:O	1:S:506:ALA:C	2.47	0.52
2:T:166:LYS:HG2	2:T:170:GLU:OE2	2.09	0.52
1:U:823:TYR:CE2	1:U:825:PRO:HG3	2.44	0.52
2:X:164:MET:O	2:X:168:VAL:HG23	2.10	0.52
2:B:21:MET:CE	2:B:21:MET:HA	2.39	0.52
1:E:75:ARG:HH21	1:E:543:CYS:HA	1.74	0.52
1:I:13:GLY:HA3	1:I:63:THR:OG1	2.10	0.52
1:M:211:MET:CE	2:N:231:PHE:HZ	2.23	0.52
1:O:478:HIS:HD2	8:O:1204:HOH:O	1.93	0.52
2:P:104:GLU:H	2:P:104:GLU:CD	2.13	0.52
1:Q:452:ILE:HB	1:Q:453:PRO:HD3	1.92	0.52
1:S:153:ARG:O	1:S:157:TYR:HB3	2.09	0.52
2:T:5:TYR:HB2	2:T:157:LEU:HD12	1.92	0.52
1:U:452:ILE:N	1:U:453:PRO:CD	2.72	0.52
1:U:649:LYS:HE3	1:U:651:THR:CG2	2.40	0.52
1:A:144:HIS:HB2	4:A:902:MGD:O1B	2.10	0.52
2:B:104:GLU:H	2:B:104:GLU:CD	2.10	0.52
2:B:166:LYS:HG2	2:B:170:GLU:OE2	2.09	0.52
2:B:70:HIS:CD2	2:B:92:VAL:H	2.13	0.52
1:C:153:ARG:O	1:C:157:TYR:HB3	2.09	0.52
1:E:153:ARG:O	1:E:157:TYR:HB3	2.10	0.52
1:E:738:HIS:HE2	4:E:902:MGD:H15	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:MET:HE1	2:F:231:PHE:CZ	2.44	0.52
1:I:47:ARG:HD2	1:I:241:LEU:HD22	1.90	0.52
2:L:18:ASN:HB2	7:L:302:SF4:S1	2.50	0.52
1:O:353:GLY:O	1:O:354:TRP:HB2	2.10	0.52
1:Q:565:TYR:C	1:Q:567:LEU:H	2.12	0.52
1:Q:871:LYS:HG2	8:Q:1226:HOH:O	2.10	0.52
1:U:187:TRP:CH2	1:U:196:PRO:HB3	2.45	0.52
2:X:204:LEU:HD23	2:X:209:CYS:HA	1.90	0.52
2:X:5:TYR:HB2	2:X:157:LEU:HD13	1.91	0.52
1:K:617:GLU:HG3	1:K:631:TRP:CG	2.45	0.52
1:K:75:ARG:NH2	1:K:543:CYS:HA	2.25	0.52
1:M:452:ILE:HB	1:M:453:PRO:HD3	1.91	0.52
1:O:55:ARG:HD2	8:O:1634:HOH:O	2.09	0.52
1:O:74:LEU:HD12	1:O:750:LYS:HA	1.91	0.52
2:P:19:CYS:HB2	2:P:46:MET:HG2	1.91	0.52
1:Q:2:GLY:O	1:Q:21:LYS:HE3	2.09	0.52
1:Q:767:TYR:HB3	1:Q:769:TYR:CE1	2.44	0.52
1:Q:786:ASN:HD22	1:Q:805:VAL:H	1.57	0.52
1:W:56:LYS:HG2	1:W:57:THR:O	2.09	0.52
2:F:39:MET:HE2	2:F:45:TRP:CD2	2.45	0.52
2:L:142:MET:HE1	8:L:929:HOH:O	2.09	0.52
1:M:610:LYS:HB3	1:M:614:ALA:HB3	1.91	0.52
1:M:9:ASN:HA	1:M:576:GLN:HA	1.91	0.52
1:O:541:PRO:HB2	1:O:586:SER:HA	1.92	0.52
1:O:628:TYR:CE2	1:O:643:PRO:HG2	2.45	0.52
1:Q:561:ILE:HG22	1:Q:564:ASN:HB3	1.92	0.52
1:U:395:LEU:HD12	1:U:566:GLN:HA	1.92	0.52
1:W:478:HIS:HD2	8:W:1206:HOH:O	1.93	0.52
1:W:738:HIS:HE2	4:W:902:MGD:H15	1.58	0.52
1:A:700:GLU:HG2	8:A:1564:HOH:O	2.09	0.51
2:D:53:ARG:HB2	2:D:60:ASP:OD1	2.10	0.51
1:I:211:MET:HE1	2:J:231:PHE:HZ	1.74	0.51
1:M:503:THR:HG21	4:M:902:MGD:O2A	2.10	0.51
2:T:46:MET:CE	2:T:66:THR:H	2.23	0.51
1:U:138:LEU:HB2	1:U:490:ILE:HD12	1.92	0.51
1:U:99:GLY:HA2	1:U:102:LYS:HE2	1.91	0.51
1:W:870:ASP:HB3	1:W:872:TYR:CE1	2.45	0.51
2:F:56:TYR:HA	2:F:59:ASN:HD22	1.75	0.51
1:G:505:THR:O	1:G:506:ALA:C	2.49	0.51
2:L:160:THR:HB	2:L:162:GLU:OE1	2.10	0.51
1:Q:356:GLY:H	4:Q:903:MGD:H5'2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:452:ILE:N	1:Q:453:PRO:CD	2.73	0.51
2:R:142:MET:CE	2:R:146:ALA:HB1	2.41	0.51
1:S:75:ARG:HH22	1:S:547:GLU:CD	2.13	0.51
1:U:729:LYS:HD2	8:U:1135:HOH:O	2.10	0.51
1:W:128:ILE:CD1	1:W:492:MET:HB2	2.40	0.51
2:X:18:ASN:HB2	7:X:302:SF4:S1	2.51	0.51
2:B:203:ILE:N	2:B:203:ILE:HD12	2.25	0.51
1:C:262:LYS:HG2	2:D:232:PHE:CE1	2.46	0.51
2:F:1:MET:SD	2:F:88:GLU:HB3	2.50	0.51
1:G:563:ASP:O	1:G:566:GLN:HG2	2.10	0.51
1:I:387:TRP:CE2	1:I:389:THR:HA	2.45	0.51
2:J:70:HIS:HD2	2:J:92:VAL:N	2.02	0.51
2:L:103:LYS:HE2	2:L:116:TRP:NE1	2.25	0.51
1:O:1:MET:H2	1:O:22:ASP:CG	2.13	0.51
1:O:571:ARG:HB2	1:O:642:VAL:HB	1.91	0.51
1:S:187:TRP:CH2	1:S:196:PRO:HB3	2.45	0.51
1:S:1:MET:H3	1:S:22:ASP:CG	2.13	0.51
1:C:75:ARG:NH2	1:C:543:CYS:HA	2.25	0.51
2:D:23:CYS:HB3	2:D:39:MET:HE3	1.93	0.51
1:E:533:VAL:HB	1:E:534:PRO:HD3	1.92	0.51
2:L:216:VAL:HG13	2:L:223:GLU:HG3	1.92	0.51
1:O:323:GLU:HB2	8:O:1568:HOH:O	2.11	0.51
1:O:356:GLY:H	4:O:903:MGD:C5'	2.21	0.51
1:S:696:LYS:O	1:S:700:GLU:HG3	2.10	0.51
1:S:722:LYS:HG2	8:S:1557:HOH:O	2.09	0.51
1:W:656:TRP:CD2	1:W:663:LYS:HA	2.46	0.51
1:A:21:LYS:HB3	1:A:26:ILE:HD11	1.93	0.51
1:A:75:ARG:NH2	1:A:543:CYS:HA	2.25	0.51
1:A:870:ASP:HB3	1:A:872:TYR:CE1	2.46	0.51
1:I:730:TYR:CZ	1:I:794:ASN:HA	2.46	0.51
1:M:28:MET:HE3	1:M:63:THR:O	2.11	0.51
1:O:558:SER:H	1:O:564:ASN:ND2	2.07	0.51
1:Q:146:MET:CE	1:Q:544:THR:HB	2.41	0.51
2:R:59:ASN:ND2	2:R:59:ASN:H	2.08	0.51
1:S:211:MET:HE1	1:S:338:GLN:HG2	1.92	0.51
1:S:141:PRO:HA	1:S:496:TYR:HB3	1.92	0.51
1:W:794:ASN:HD22	1:W:862:VAL:HG12	1.75	0.51
1:A:291:GLU:H	1:A:291:GLU:CD	2.14	0.51
1:G:128:ILE:CD1	1:G:492:MET:HB2	2.40	0.51
1:M:100:LEU:CD1	1:M:105:PRO:HG3	2.39	0.51
1:M:165:GLY:CA	1:M:166:PHE:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:13:GLY:HA3	1:M:63:THR:OG1	2.10	0.51
2:N:21:MET:HE3	2:N:21:MET:HA	1.91	0.51
1:O:15:PRO:HD3	1:O:554:PHE:CD1	2.46	0.51
2:T:104:GLU:H	2:T:104:GLU:CD	2.14	0.51
1:A:737:PRO:CG	4:A:903:MGD:H2'	2.41	0.51
2:D:10:VAL:HG13	2:D:63:TYR:O	2.11	0.51
1:K:395:LEU:HD12	1:K:566:GLN:HA	1.93	0.51
1:K:402:PRO:HG2	1:K:422:PHE:CE1	2.45	0.51
2:L:119:GLU:O	2:L:119:GLU:HG2	2.09	0.51
1:O:165:GLY:CA	1:O:166:PHE:HB3	2.36	0.51
2:X:19:CYS:O	2:X:22:GLY:N	2.44	0.51
1:G:630:THR:OG1	1:G:633:GLU:HG3	2.09	0.51
2:N:56:TYR:HA	2:N:59:ASN:ND2	2.26	0.51
1:C:144:HIS:HB2	4:C:902:MGD:O1B	2.11	0.51
1:K:155:SER:OG	1:K:409:ILE:HG12	2.11	0.51
1:K:76:ILE:HG22	1:K:541:PRO:HG3	1.93	0.51
1:M:197:GLU:OE2	1:M:665:THR:OG1	2.15	0.51
1:O:56:LYS:HE2	8:O:1466:HOH:O	2.11	0.51
1:O:66:PHE:HA	1:O:69:MET:CE	2.41	0.51
1:O:211:MET:HE1	2:P:231:PHE:CZ	2.46	0.51
1:Q:296:ASN:O	1:Q:687:LYS:HB3	2.11	0.51
1:U:165:GLY:CA	1:U:166:PHE:HB3	2.40	0.51
1:U:426:MET:HE3	1:U:622:ALA:HB2	1.92	0.51
1:A:146:MET:HE1	1:A:544:THR:HB	1.93	0.51
1:C:510:TYR:O	1:C:513:MET:HG2	2.11	0.51
1:E:21:LYS:CB	1:E:26:ILE:HD11	2.41	0.51
2:F:68:CYS:HB2	2:F:126:CYS:HB2	1.90	0.51
1:G:146:MET:HE3	1:G:545:ASN:OD1	2.11	0.51
2:H:21:MET:HE3	2:H:21:MET:HA	1.93	0.51
1:I:175:SER:HB2	1:I:176:TRP:CZ3	2.46	0.51
1:I:495:LYS:HD3	8:I:1105:HOH:O	2.11	0.51
2:J:18:ASN:HB2	7:J:301:SF4:S1	2.51	0.51
1:M:201:LEU:HD13	1:M:387:TRP:HB2	1.93	0.51
2:R:21:MET:CE	2:R:21:MET:HA	2.40	0.51
1:U:265:SER:O	1:U:810:GLN:NE2	2.43	0.51
1:W:66:PHE:HD1	1:W:69:MET:HE3	1.74	0.51
1:A:66:PHE:HA	1:A:69:MET:CE	2.41	0.50
1:C:118:THR:O	1:C:122:VAL:HG23	2.11	0.50
1:C:628:TYR:CE2	1:C:643:PRO:HG2	2.46	0.50
1:E:800:ILE:CD1	1:E:833:ALA:HB1	2.42	0.50
1:G:855:MET:HB2	1:G:857:ASN:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:174:ASP:OD1	1:I:175:SER:N	2.40	0.50
1:I:361:SER:OG	1:I:717:ALA:HB1	2.11	0.50
2:L:53:ARG:HB2	2:L:60:ASP:OD1	2.11	0.50
1:M:142:SER:CB	4:M:902:MGD:O1A	2.59	0.50
2:N:19:CYS:O	2:N:22:GLY:N	2.44	0.50
2:N:70:HIS:CD2	2:N:92:VAL:H	2.13	0.50
1:Q:557:CYS:H	1:Q:564:ASN:ND2	1.87	0.50
1:S:100:LEU:CD1	1:S:105:PRO:HG3	2.39	0.50
1:S:855:MET:HB2	1:S:857:ASN:OD1	2.10	0.50
1:W:76:ILE:HG22	1:W:541:PRO:HG3	1.92	0.50
1:A:505:THR:O	1:A:506:ALA:C	2.50	0.50
1:C:786:ASN:HD21	1:C:804:GLN:HA	1.76	0.50
1:E:134:PRO:HB2	1:E:439:LEU:HD11	1.93	0.50
1:G:426:MET:HA	1:G:426:MET:HE3	1.92	0.50
1:K:176:TRP:O	1:K:177:GLU:C	2.50	0.50
2:L:70:HIS:CD2	2:L:92:VAL:H	2.19	0.50
1:Q:142:SER:OG	4:Q:902:MGD:O1A	2.27	0.50
1:S:12:THR:O	1:S:226:TYR:HA	2.11	0.50
1:U:100:LEU:CD1	1:U:105:PRO:HG3	2.40	0.50
2:V:4:TYR:CE2	2:V:158:LYS:HD2	2.46	0.50
1:W:165:GLY:HA3	1:W:166:PHE:CB	2.37	0.50
2:X:73:ASN:O	2:X:75:PRO:HD3	2.11	0.50
1:C:558:SER:H	1:C:564:ASN:ND2	2.08	0.50
2:D:19:CYS:HB2	2:D:46:MET:HG2	1.92	0.50
1:E:21:LYS:HB3	1:E:26:ILE:HD11	1.93	0.50
1:I:35:ASP:OD1	1:I:55:ARG:HD3	2.12	0.50
1:K:165:GLY:CA	1:K:166:PHE:HB3	2.40	0.50
1:K:400:TYR:CE1	1:K:421:LYS:HD2	2.47	0.50
1:K:610:LYS:HZ3	1:K:618:GLN:HE22	1.59	0.50
1:K:730:TYR:CE1	1:K:794:ASN:HA	2.46	0.50
1:M:356:GLY:HA2	1:M:359:ARG:NH1	2.27	0.50
1:M:558:SER:H	1:M:564:ASN:ND2	2.09	0.50
1:S:610:LYS:HB3	1:S:614:ALA:HB3	1.93	0.50
2:T:49:GLU:HG3	2:T:64:ARG:NH2	2.26	0.50
1:U:218:ASP:OD2	1:U:253:ASN:HB2	2.11	0.50
1:W:387:TRP:CE2	1:W:389:THR:HA	2.47	0.50
1:A:855:MET:HB2	1:A:857:ASN:OD1	2.11	0.50
2:H:213:ALA:O	2:H:228:GLU:HA	2.11	0.50
1:I:76:ILE:HG22	1:I:541:PRO:HG3	1.92	0.50
2:L:40:GLN:NE2	2:L:118:GLU:H	1.95	0.50
1:M:825:PRO:HD2	8:M:1334:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:46:MET:CE	2:N:66:THR:H	2.19	0.50
2:T:71:CYS:HA	2:T:184:PRO:HA	1.92	0.50
2:B:40:GLN:HE22	2:B:118:GLU:H	1.59	0.50
1:E:494:TRP:HE1	1:E:525:GLN:HE21	1.59	0.50
1:G:696:LYS:O	1:G:700:GLU:HG3	2.12	0.50
1:G:9:ASN:HA	1:G:576:GLN:HA	1.94	0.50
2:J:46:MET:HE3	2:J:66:THR:H	1.76	0.50
2:J:56:TYR:HA	2:J:59:ASN:HD22	1.76	0.50
1:K:378:GLY:O	1:K:381:LYS:HG2	2.11	0.50
1:M:333:ARG:CZ	1:S:729:LYS:HE3	2.42	0.50
2:T:19:CYS:O	2:T:22:GLY:N	2.43	0.50
2:T:46:MET:CE	2:T:66:THR:N	2.74	0.50
1:U:557:CYS:N	1:U:564:ASN:HD21	1.95	0.50
1:U:56:LYS:HG2	1:U:57:THR:O	2.11	0.50
1:W:730:TYR:CE1	1:W:794:ASN:HA	2.46	0.50
1:A:377:GLN:O	1:A:381:LYS:HE2	2.12	0.50
1:A:66:PHE:HA	1:A:69:MET:HE2	1.94	0.50
1:C:780:GLU:HB2	8:C:1183:HOH:O	2.10	0.50
1:E:400:TYR:CE1	1:E:421:LYS:HD2	2.46	0.50
1:E:855:MET:HB2	1:E:857:ASN:OD1	2.12	0.50
1:O:174:ASP:OD1	1:O:175:SER:N	2.40	0.50
1:O:1:MET:N	1:O:22:ASP:OD1	2.42	0.50
1:O:452:ILE:HB	1:O:453:PRO:HD3	1.94	0.50
2:P:5:TYR:HB2	2:P:157:LEU:HD12	1.92	0.50
1:Q:501:LEU:HD13	1:Q:823:TYR:CD2	2.47	0.50
2:R:105:LEU:HB3	2:R:114:MET:HE1	1.92	0.50
1:S:387:TRP:CE2	1:S:389:THR:HA	2.45	0.50
2:T:68:CYS:HB2	2:T:126:CYS:HB2	1.90	0.50
1:Q:725:PRO:HA	1:U:704:ILE:HG13	1.94	0.50
1:U:855:MET:HB2	1:U:857:ASN:OD1	2.11	0.50
2:V:125:LYS:HD2	2:V:126:CYS:O	2.12	0.50
2:B:19:CYS:O	2:B:22:GLY:N	2.45	0.50
2:D:94:ILE:O	2:D:96:PRO:HD3	2.12	0.50
2:F:56:TYR:HA	2:F:59:ASN:ND2	2.27	0.50
1:G:797:GLY:HA2	1:G:875:TYR:CE2	2.47	0.50
1:I:146:MET:HE2	1:I:545:ASN:H	1.76	0.50
1:K:142:SER:HB3	4:K:902:MGD:O1A	2.12	0.50
1:M:177:GLU:OE2	1:M:177:GLU:HA	2.12	0.50
1:M:501:LEU:HD13	1:M:823:TYR:CD2	2.46	0.50
1:M:855:MET:HB2	1:M:857:ASN:OD1	2.12	0.50
1:O:772:MET:HB2	1:O:801:LEU:HD13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:214:PHE:HA	1:U:347:ALA:HB3	1.93	0.50
1:C:142:SER:OG	4:C:902:MGD:O1A	2.29	0.50
1:I:21:LYS:HB3	1:I:26:ILE:HD11	1.94	0.50
1:I:85:PHE:CE2	1:I:87:PRO:HG3	2.46	0.50
1:K:118:THR:O	1:K:122:VAL:HG23	2.12	0.50
1:K:177:GLU:HA	1:K:177:GLU:OE2	2.11	0.50
1:M:81:LYS:HB2	1:M:112:ILE:HD13	1.94	0.50
1:M:426:MET:HE2	1:M:618:GLN:HG2	1.92	0.50
1:S:361:SER:OG	1:S:717:ALA:HB1	2.11	0.50
1:S:146:MET:HE1	1:S:544:THR:HB	1.92	0.50
1:S:786:ASN:ND2	1:S:804:GLN:HA	2.26	0.50
1:S:772:MET:HB2	1:S:801:LEU:HD13	1.92	0.50
2:V:19:CYS:HB2	2:V:46:MET:HG2	1.93	0.50
1:W:426:MET:HE2	1:W:618:GLN:HG2	1.91	0.50
2:X:77:VAL:HG22	2:X:84:VAL:HG12	1.93	0.50
2:B:106:LEU:HD11	2:B:116:TRP:HB2	1.94	0.50
1:C:816:SER:OG	1:C:839:ILE:HG13	2.11	0.50
1:O:141:PRO:CA	1:O:496:TYR:HB3	2.41	0.50
1:O:855:MET:HB2	1:O:857:ASN:OD1	2.11	0.50
1:Q:478:HIS:HD2	8:Q:1199:HOH:O	1.95	0.50
2:R:71:CYS:HB2	2:R:182:THR:O	2.11	0.50
1:S:197:GLU:HG3	1:S:653:ALA:HB1	1.93	0.50
1:S:757:ILE:HD11	8:S:1651:HOH:O	2.10	0.50
2:T:211:GLU:HB2	2:T:231:PHE:HA	1.93	0.50
1:U:176:TRP:O	1:U:177:GLU:C	2.50	0.50
1:A:146:MET:HG2	4:A:902:MGD:N7	2.26	0.49
1:A:356:GLY:H	4:A:903:MGD:H5'2	1.77	0.49
1:C:12:THR:O	1:C:226:TYR:HA	2.12	0.49
1:E:387:TRP:CE2	1:E:389:THR:HA	2.47	0.49
1:I:528:TRP:CD2	1:I:750:LYS:HD3	2.46	0.49
1:K:571:ARG:HB2	1:K:642:VAL:HB	1.94	0.49
2:L:104:GLU:H	2:L:104:GLU:CD	2.15	0.49
1:O:717:ALA:HB3	1:O:720:SER:HB3	1.93	0.49
2:R:46:MET:HE3	2:R:66:THR:H	1.76	0.49
2:T:105:LEU:HD12	8:T:496:HOH:O	2.11	0.49
2:T:59:ASN:H	2:T:59:ASN:HD22	1.60	0.49
1:U:670:PRO:HB3	1:U:682:GLN:HB2	1.94	0.49
1:C:505:THR:O	1:C:506:ALA:C	2.50	0.49
2:D:114:MET:HA	2:D:125:LYS:HB3	1.95	0.49
2:F:46:MET:CE	2:F:66:THR:N	2.73	0.49
1:G:146:MET:HE1	1:G:544:THR:CB	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:478:HIS:HD2	8:G:1204:HOH:O	1.95	0.49
1:G:800:ILE:N	1:G:800:ILE:HD12	2.27	0.49
1:G:786:ASN:ND2	1:G:805:VAL:H	2.09	0.49
1:K:153:ARG:O	1:K:157:TYR:HB3	2.12	0.49
1:O:730:TYR:CE1	1:O:794:ASN:HA	2.47	0.49
1:S:647:ASN:O	1:S:648:ARG:HG2	2.12	0.49
1:U:673:ASN:HD22	1:U:673:ASN:H	1.59	0.49
1:U:74:LEU:HD12	1:U:750:LYS:HA	1.94	0.49
2:V:104:GLU:H	2:V:104:GLU:CD	2.13	0.49
1:W:66:PHE:HA	1:W:69:MET:CE	2.42	0.49
1:A:177:GLU:HA	1:A:177:GLU:OE2	2.12	0.49
1:C:786:ASN:ND2	1:C:805:VAL:H	2.10	0.49
2:D:166:LYS:O	2:D:170:GLU:HG3	2.12	0.49
1:E:503:THR:HG21	4:E:902:MGD:O2A	2.12	0.49
1:G:239:LYS:HE2	8:G:1599:HOH:O	2.12	0.49
1:O:263:TRP:CZ2	1:O:265:SER:HB2	2.46	0.49
1:Q:175:SER:HB2	1:Q:176:TRP:CE3	2.48	0.49
1:S:870:ASP:HB3	1:S:872:TYR:CE1	2.47	0.49
1:A:153:ARG:O	1:A:157:TYR:HB3	2.12	0.49
1:C:166:PHE:N	1:C:439:LEU:HD12	2.27	0.49
1:C:141:PRO:CA	1:C:496:TYR:HB3	2.38	0.49
1:C:563:ASP:HA	1:C:565:TYR:CE1	2.47	0.49
2:H:4:TYR:CE2	2:H:158:LYS:HD2	2.46	0.49
2:H:46:MET:CE	2:H:66:THR:N	2.74	0.49
1:I:494:TRP:HE1	1:I:525:GLN:HE21	1.60	0.49
1:I:561:ILE:HG22	1:I:564:ASN:HB3	1.94	0.49
1:K:174:ASP:OD1	1:K:175:SER:N	2.45	0.49
1:K:257:ARG:HD3	2:L:61:ILE:HG21	1.93	0.49
1:K:870:ASP:HB3	1:K:872:TYR:CE1	2.47	0.49
1:Q:1:MET:H3	1:Q:22:ASP:CG	2.16	0.49
1:Q:322:GLU:HG3	1:Q:327:VAL:O	2.13	0.49
1:Q:510:TYR:O	1:Q:513:MET:HG2	2.13	0.49
1:Q:56:LYS:HG2	1:Q:57:THR:O	2.13	0.49
1:U:96:ARG:HD3	1:U:535:PHE:O	2.11	0.49
1:W:451:LYS:HG3	1:W:461:PHE:CE2	2.47	0.49
1:A:146:MET:CE	1:A:544:THR:HB	2.42	0.49
1:C:452:ILE:HB	1:C:453:PRO:HD3	1.95	0.49
1:C:871:LYS:HG2	8:C:1231:HOH:O	2.13	0.49
1:E:75:ARG:NH2	1:E:543:CYS:HA	2.28	0.49
2:F:177:LYS:N	2:F:178:PRO:HD3	2.28	0.49
1:G:377:GLN:O	1:G:381:LYS:HE2	2.12	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:J:68:CYS:HB2	2:J:126:CYS:HB2	1.94	0.49
1:O:451:LYS:HG3	1:O:461:PHE:CE2	2.47	0.49
1:Q:66:PHE:HZ	1:Q:146:MET:CE	2.24	0.49
1:U:387:TRP:CE2	1:U:389:THR:HA	2.47	0.49
1:A:737:PRO:HG3	4:A:903:MGD:H2'	1.94	0.49
1:C:174:ASP:OD1	1:C:175:SER:N	2.43	0.49
2:D:106:LEU:HD23	2:D:114:MET:HG3	1.95	0.49
2:D:4:TYR:CE2	2:D:158:LYS:HD2	2.48	0.49
1:E:610:LYS:HZ3	1:E:618:GLN:HE22	1.60	0.49
2:H:21:MET:HE2	2:H:21:MET:HA	1.92	0.49
1:I:356:GLY:H	4:I:903:MGD:H5'2	1.77	0.49
1:M:296:ASN:O	1:M:687:LYS:HB3	2.12	0.49
1:O:628:TYR:HE2	1:O:643:PRO:HG2	1.77	0.49
1:S:533:VAL:HB	1:S:534:PRO:HD3	1.93	0.49
1:S:786:ASN:HD22	1:S:805:VAL:H	1.60	0.49
2:T:139:ALA:O	2:T:141:LYS:HG3	2.12	0.49
2:T:23:CYS:O	2:T:27:HIS:N	2.42	0.49
1:W:104:ASP:OD2	1:W:107:SER:HB3	2.13	0.49
1:W:28:MET:HE2	8:X:480:HOH:O	2.13	0.49
1:E:528:TRP:CD2	1:E:750:LYS:HD3	2.48	0.49
2:F:5:TYR:HB2	2:F:157:LEU:HD12	1.94	0.49
1:I:717:ALA:HB3	1:I:720:SER:HB3	1.95	0.49
1:M:870:ASP:HB3	1:M:872:TYR:CE1	2.47	0.49
1:O:700:GLU:HB3	8:O:1199:HOH:O	2.13	0.49
2:R:23:CYS:O	2:R:26:GLU:N	2.45	0.49
2:R:46:MET:HE3	2:R:66:THR:N	2.27	0.49
2:T:5:TYR:HB2	2:T:157:LEU:CD1	2.43	0.49
1:W:15:PRO:HD3	1:W:554:PHE:CD1	2.47	0.49
1:C:801:LEU:HD11	1:C:839:ILE:HD11	1.95	0.49
2:F:59:ASN:ND2	2:F:59:ASN:H	2.11	0.49
1:G:786:ASN:HD22	1:G:805:VAL:H	1.61	0.49
2:L:46:MET:HE1	2:L:65:PRO:C	2.33	0.49
2:L:87:ARG:HG3	2:L:91:ILE:O	2.13	0.49
1:Q:800:ILE:CD1	1:Q:800:ILE:N	2.76	0.49
1:S:510:TYR:O	1:S:513:MET:HG2	2.12	0.49
1:S:85:PHE:CE2	1:S:87:PRO:HG3	2.48	0.49
1:U:141:PRO:CA	1:U:496:TYR:HB3	2.41	0.49
1:W:218:ASP:OD2	1:W:253:ASN:HB2	2.12	0.49
2:X:198:TYR:HB3	2:X:238:ASP:HA	1.94	0.49
1:A:32:ASP:HB2	8:A:1657:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:738:HIS:HE2	4:G:902:MGD:H15	1.61	0.49
1:K:510:TYR:O	1:K:513:MET:HG2	2.12	0.49
1:M:175:SER:HB2	1:M:176:TRP:CE3	2.48	0.49
1:M:197:GLU:HG3	1:M:199:TYR:CD1	2.48	0.49
1:M:797:GLY:HA2	1:M:875:TYR:CZ	2.48	0.49
2:N:105:LEU:HB3	2:N:114:MET:HE3	1.95	0.49
2:N:87:ARG:HD3	2:N:93:LEU:CD1	2.43	0.49
1:O:729:LYS:HD2	8:O:1131:HOH:O	2.13	0.49
1:Q:425:ARG:HD3	1:Q:622:ALA:O	2.13	0.49
1:S:138:LEU:HB2	1:S:490:ILE:HD12	1.95	0.49
1:S:554:PHE:HB3	8:S:1028:HOH:O	2.12	0.49
1:U:505:THR:O	1:U:506:ALA:C	2.51	0.49
1:U:13:GLY:HA3	1:U:63:THR:OG1	2.13	0.49
2:V:59:ASN:ND2	2:V:59:ASN:H	2.11	0.49
2:X:71:CYS:HA	2:X:184:PRO:HA	1.93	0.49
1:A:791:ARG:NH2	8:A:1580:HOH:O	2.46	0.49
2:B:201:ALA:HB2	2:B:269:LEU:HB2	1.95	0.49
1:G:56:LYS:HG2	1:G:57:THR:O	2.13	0.49
1:G:629:MET:HE1	1:G:634:PHE:HA	1.94	0.49
1:K:211:MET:HE2	2:L:231:PHE:CZ	2.48	0.49
1:K:426:MET:HA	1:K:426:MET:HE3	1.94	0.49
2:L:105:LEU:HB3	2:L:114:MET:HE2	1.93	0.49
2:P:46:MET:HE1	2:P:66:THR:H	1.77	0.49
1:Q:253:ASN:O	1:Q:257:ARG:HG3	2.12	0.49
1:Q:756:TYR:HB2	2:R:24:MET:HE1	1.95	0.49
1:U:630:THR:OG1	1:U:633:GLU:HG3	2.13	0.49
1:U:76:ILE:CG2	1:U:541:PRO:HG3	2.41	0.49
2:X:157:LEU:H	2:X:157:LEU:HD12	1.78	0.49
2:X:180:LEU:HB2	8:X:520:HOH:O	2.12	0.49
1:C:649:LYS:HE2	1:C:651:THR:HG22	1.95	0.48
2:D:121:ASN:CG	1:S:608:GLU:O	2.51	0.48
1:G:257:ARG:HD3	2:H:61:ILE:HG21	1.95	0.48
1:K:847:TYR:CZ	1:K:853:CYS:HB3	2.48	0.48
1:K:737:PRO:HG2	4:K:903:MGD:H2'	1.95	0.48
2:R:203:ILE:HD12	2:R:203:ILE:N	2.28	0.48
1:S:28:MET:CE	1:S:66:PHE:HB3	2.43	0.48
2:V:96:PRO:O	2:V:100:LYS:HG3	2.13	0.48
1:C:100:LEU:CD1	1:C:105:PRO:HG3	2.43	0.48
1:C:114:TRP:CZ2	1:C:541:PRO:HD2	2.48	0.48
1:C:20:VAL:HG13	1:C:24:LYS:O	2.13	0.48
1:E:56:LYS:HG2	1:E:57:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:356:GLY:H	4:G:903:MGD:H5'2	1.78	0.48
2:H:142:MET:HE2	2:H:146:ALA:HB3	1.95	0.48
1:I:797:GLY:HA2	1:I:875:TYR:CE2	2.48	0.48
1:K:797:GLY:HA2	1:K:875:TYR:CE2	2.48	0.48
2:N:106:LEU:HD23	2:N:114:MET:HB3	1.95	0.48
1:O:56:LYS:HG2	1:O:57:THR:O	2.13	0.48
1:U:78:TYR:O	1:U:80:MET:HG3	2.13	0.48
1:A:75:ARG:HH21	1:A:543:CYS:HA	1.78	0.48
1:E:452:ILE:N	1:E:453:PRO:CD	2.76	0.48
1:G:510:TYR:O	1:G:513:MET:HG2	2.13	0.48
2:J:105:LEU:HB3	2:J:114:MET:HE1	1.95	0.48
2:N:142:MET:HE2	2:N:146:ALA:HB1	1.95	0.48
1:Q:250:PRO:HD3	4:Q:903:MGD:C2	2.43	0.48
1:S:656:TRP:CD2	1:S:663:LYS:HA	2.48	0.48
2:V:94:ILE:O	2:V:96:PRO:HD3	2.14	0.48
1:W:610:LYS:HB3	1:W:614:ALA:HB3	1.94	0.48
1:W:765:ASP:HB2	8:W:1167:HOH:O	2.13	0.48
2:B:18:ASN:HB2	7:B:302:SF4:S1	2.54	0.48
1:C:1:MET:H3	1:C:22:ASP:CG	2.16	0.48
2:J:106:LEU:HD11	2:J:116:TRP:HB2	1.94	0.48
2:J:53:ARG:HB2	2:J:60:ASP:OD1	2.13	0.48
2:J:59:ASN:H	2:J:59:ASN:ND2	2.11	0.48
1:M:730:TYR:CZ	1:M:794:ASN:HA	2.48	0.48
1:O:505:THR:O	1:O:506:ALA:C	2.52	0.48
1:U:165:GLY:HA3	1:U:166:PHE:CB	2.37	0.48
1:U:610:LYS:HZ3	1:U:618:GLN:HE22	1.57	0.48
1:W:645:ASN:HD21	1:W:648:ARG:HB3	1.75	0.48
2:X:252:ASP:C	2:X:254:LYS:H	2.17	0.48
1:A:871:LYS:HE2	8:A:1231:HOH:O	2.12	0.48
1:C:214:PHE:HA	1:C:347:ALA:HB3	1.94	0.48
1:C:44:ILE:HD11	1:C:394:PRO:HG2	1.95	0.48
1:E:400:TYR:CZ	1:E:421:LYS:HD2	2.48	0.48
1:E:142:SER:CB	4:E:902:MGD:O1A	2.61	0.48
1:G:176:TRP:O	1:G:177:GLU:C	2.51	0.48
1:G:13:GLY:HA3	1:G:63:THR:OG1	2.12	0.48
2:H:166:LYS:HG2	2:H:170:GLU:OE2	2.13	0.48
1:K:9:ASN:HA	1:K:576:GLN:HA	1.96	0.48
1:M:250:PRO:HD3	4:M:903:MGD:C2	2.43	0.48
1:O:786:ASN:ND2	1:O:804:GLN:HA	2.28	0.48
1:Q:505:THR:O	1:Q:506:ALA:C	2.52	0.48
1:U:28:MET:HE1	1:U:66:PHE:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:78:TYR:C	1:U:541:PRO:HG2	2.34	0.48
2:V:142:MET:HE2	2:V:146:ALA:CB	2.43	0.48
1:W:176:TRP:O	1:W:177:GLU:C	2.52	0.48
1:A:296:ASN:HB3	1:A:657:PHE:CZ	2.49	0.48
2:F:114:MET:HG2	2:F:125:LYS:HG2	1.94	0.48
1:I:155:SER:OG	1:I:409:ILE:HG12	2.14	0.48
1:I:402:PRO:HG2	1:I:422:PHE:CE1	2.49	0.48
1:I:476:GLN:OE1	1:I:708:ARG:NH2	2.47	0.48
1:K:187:TRP:CH2	1:K:196:PRO:HB3	2.48	0.48
1:O:2:GLY:N	1:O:22:ASP:OD1	2.47	0.48
2:P:141:LYS:HA	8:P:500:HOH:O	2.14	0.48
1:Q:451:LYS:HG3	1:Q:461:PHE:CE2	2.48	0.48
1:U:66:PHE:HA	1:U:69:MET:HE2	1.95	0.48
2:V:90:GLY:HA3	2:V:185:ARG:CZ	2.44	0.48
1:A:494:TRP:HE1	1:A:525:GLN:HE21	1.61	0.48
1:E:34:ASP:HB3	1:E:37:VAL:HG22	1.94	0.48
1:E:561:ILE:CG2	1:E:564:ASN:HB3	2.43	0.48
1:G:165:GLY:CA	1:G:166:PHE:HB3	2.41	0.48
2:H:177:LYS:N	2:H:178:PRO:HD3	2.29	0.48
1:I:263:TRP:CZ2	1:I:265:SER:HB2	2.49	0.48
1:K:100:LEU:HD12	1:K:105:PRO:HG3	1.95	0.48
1:M:452:ILE:N	1:M:453:PRO:CD	2.76	0.48
1:O:725:PRO:HD2	8:O:1193:HOH:O	2.12	0.48
1:Q:786:ASN:HD21	1:Q:804:GLN:HA	1.78	0.48
1:U:394:PRO:HG3	8:U:1323:HOH:O	2.13	0.48
1:U:797:GLY:HA2	1:U:875:TYR:CE2	2.48	0.48
1:W:1:MET:H2	1:W:22:ASP:CG	2.17	0.48
1:W:452:ILE:N	1:W:453:PRO:CD	2.77	0.48
2:X:250:ASP:HB2	8:X:433:HOH:O	2.14	0.48
2:X:43:HIS:ND1	8:X:406:HOH:O	2.35	0.48
1:A:610:LYS:HB3	1:A:614:ALA:HB3	1.95	0.48
1:A:767:TYR:HB3	1:A:769:TYR:CE1	2.49	0.48
2:F:46:MET:CE	2:F:66:THR:H	2.21	0.48
1:G:730:TYR:CZ	1:G:794:ASN:HA	2.49	0.48
1:I:218:ASP:OD2	1:I:253:ASN:HB2	2.14	0.48
2:L:58:ARG:HD2	2:L:268:ASP:OD1	2.14	0.48
2:P:73:ASN:OD1	2:P:183:LYS:HE3	2.13	0.48
1:W:177:GLU:OE2	1:W:177:GLU:HA	2.14	0.48
1:A:730:TYR:CZ	1:A:794:ASN:HA	2.49	0.48
1:A:756:TYR:HB2	2:B:24:MET:HE1	1.95	0.48
1:C:436:PRO:HG3	8:C:1445:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:GLY:HA3	1:E:166:PHE:CB	2.35	0.48
2:F:166:LYS:HG2	2:F:170:GLU:OE2	2.14	0.48
1:I:224:GLY:O	1:I:225:ILE:HB	2.14	0.48
1:M:144:HIS:HB2	4:M:902:MGD:O1B	2.13	0.48
2:P:53:ARG:HB2	2:P:60:ASP:OD1	2.14	0.48
1:S:55:ARG:HD2	8:S:1627:HOH:O	2.14	0.48
1:S:691:ILE:HD11	1:S:711:MET:HE3	1.95	0.48
1:S:730:TYR:CE1	1:S:794:ASN:HA	2.48	0.48
1:U:571:ARG:HB2	1:U:642:VAL:HB	1.94	0.48
1:W:263:TRP:CZ2	1:W:265:SER:HB2	2.49	0.48
1:A:847:TYR:CZ	1:A:853:CYS:HB3	2.49	0.48
1:E:772:MET:HB2	1:E:801:LEU:HD13	1.96	0.48
2:F:256:TYR:HB2	2:F:274:LEU:HD21	1.95	0.48
1:G:141:PRO:CA	1:G:496:TYR:HB3	2.40	0.48
2:J:40:GLN:HB3	2:J:43:HIS:CE1	2.49	0.48
1:K:362:HIS:HB3	1:K:717:ALA:HB2	1.95	0.48
2:N:247:VAL:O	2:N:257:SER:HA	2.14	0.48
1:O:140:THR:OG1	1:O:171:HIS:HE1	1.97	0.48
1:O:94:GLN:HE21	1:O:95:LEU:HG	1.78	0.48
1:Q:114:TRP:CZ2	1:Q:587:MET:HG2	2.49	0.48
1:S:165:GLY:CA	1:S:166:PHE:HB3	2.44	0.48
1:U:871:LYS:HE2	8:U:1233:HOH:O	2.14	0.48
1:U:146:MET:HG2	4:U:902:MGD:N7	2.29	0.48
2:V:19:CYS:O	2:V:22:GLY:N	2.47	0.48
1:A:96:ARG:HD2	1:A:514:TYR:O	2.14	0.47
1:C:35:ASP:OD1	1:C:55:ARG:HD3	2.14	0.47
1:C:571:ARG:HB2	1:C:642:VAL:HB	1.95	0.47
2:D:19:CYS:CB	2:D:145:CYS:HB3	2.34	0.47
1:K:146:MET:HG2	4:K:902:MGD:N7	2.29	0.47
2:N:142:MET:CE	2:N:146:ALA:HB1	2.43	0.47
1:O:252:MET:HE3	8:P:468:HOH:O	2.14	0.47
1:Q:75:ARG:NH2	1:Q:543:CYS:HA	2.29	0.47
2:R:46:MET:HE1	2:R:66:THR:N	2.29	0.47
1:S:563:ASP:HA	1:S:565:TYR:CE1	2.49	0.47
2:T:21:MET:CA	2:T:21:MET:CE	2.92	0.47
1:U:12:THR:O	1:U:226:TYR:HA	2.14	0.47
1:W:505:THR:O	1:W:506:ALA:C	2.52	0.47
2:X:59:ASN:HD22	2:X:59:ASN:H	1.62	0.47
1:A:197:GLU:HG3	1:A:653:ALA:HB1	1.96	0.47
1:C:459:GLY:O	1:C:489:LYS:HE2	2.13	0.47
1:C:395:LEU:HD12	1:C:566:GLN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:797:GLY:HA2	1:C:875:TYR:CD2	2.49	0.47
2:D:114:MET:HB3	2:D:125:LYS:HB3	1.96	0.47
2:D:216:VAL:HG13	2:D:223:GLU:HG3	1.95	0.47
1:G:12:THR:HB	1:G:743:MET:HG3	1.96	0.47
1:I:165:GLY:CA	1:I:166:PHE:HB3	2.41	0.47
1:I:258:LEU:HG	1:I:259:VAL:HG13	1.95	0.47
1:I:558:SER:H	1:I:564:ASN:ND2	2.12	0.47
1:K:296:ASN:HB3	1:K:657:PHE:CZ	2.49	0.47
1:K:744:HIS:HA	1:K:819:SER:CB	2.44	0.47
1:M:15:PRO:HD3	1:M:554:PHE:CD1	2.49	0.47
1:M:505:THR:O	1:M:506:ALA:C	2.52	0.47
2:N:59:ASN:H	2:N:59:ASN:ND2	2.12	0.47
1:O:258:LEU:HG	1:O:259:VAL:HG13	1.95	0.47
1:O:825:PRO:HD2	8:O:1334:HOH:O	2.13	0.47
2:P:114:MET:HA	2:P:125:LYS:HB3	1.95	0.47
2:P:164:MET:O	2:P:168:VAL:HG23	2.13	0.47
1:Q:800:ILE:CD1	1:Q:833:ALA:HB1	2.42	0.47
2:R:210:PHE:HD2	2:R:213:ALA:HB2	1.79	0.47
1:S:649:LYS:HE2	8:S:1458:HOH:O	2.13	0.47
2:T:69:MET:HB3	2:T:184:PRO:HB3	1.96	0.47
1:U:521:PHE:CE2	1:U:523:VAL:CG2	2.97	0.47
1:W:100:LEU:HD12	1:W:105:PRO:HG3	1.96	0.47
1:W:253:ASN:O	1:W:257:ARG:HG3	2.13	0.47
1:A:786:ASN:ND2	1:A:805:VAL:H	2.06	0.47
1:E:144:HIS:HB2	4:E:902:MGD:O1B	2.13	0.47
1:G:144:HIS:HB2	4:G:902:MGD:O1B	2.15	0.47
1:M:322:GLU:HG3	1:M:327:VAL:O	2.14	0.47
1:U:772:MET:HB2	1:U:801:LEU:HD13	1.96	0.47
1:W:78:TYR:O	1:W:80:MET:HG3	2.14	0.47
2:X:201:ALA:HB2	2:X:269:LEU:HB2	1.95	0.47
1:C:66:PHE:HA	1:C:69:MET:HE2	1.95	0.47
2:D:46:MET:CE	2:D:66:THR:N	2.74	0.47
1:E:2:GLY:N	1:E:22:ASP:OD1	2.46	0.47
2:F:94:ILE:O	2:F:96:PRO:HD3	2.15	0.47
1:I:696:LYS:O	1:I:700:GLU:HG3	2.14	0.47
1:K:494:TRP:HE1	1:K:525:GLN:HE21	1.62	0.47
1:M:55:ARG:HD2	8:M:1639:HOH:O	2.14	0.47
1:O:177:GLU:HA	1:O:177:GLU:OE2	2.14	0.47
1:O:847:TYR:CZ	1:O:853:CYS:HB3	2.49	0.47
1:O:85:PHE:CE2	1:O:87:PRO:HG3	2.49	0.47
2:P:86:GLN:NE2	8:P:475:HOH:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:265:SER:O	1:Q:810:GLN:NE2	2.46	0.47
2:T:59:ASN:H	2:T:59:ASN:ND2	2.12	0.47
1:U:9:ASN:HA	1:U:576:GLN:HA	1.96	0.47
1:W:15:PRO:HD3	1:W:554:PHE:CE1	2.48	0.47
2:X:97:GLU:OE2	2:X:100:LYS:HE2	2.14	0.47
1:A:301:GLU:CD	1:A:301:GLU:H	2.17	0.47
1:A:575:LEU:HD22	1:A:635:PHE:HA	1.97	0.47
1:A:797:GLY:HA2	1:A:875:TYR:CE2	2.49	0.47
1:C:797:GLY:HA2	1:C:875:TYR:CE2	2.49	0.47
1:E:138:LEU:HD12	1:E:167:THR:O	2.14	0.47
1:E:211:MET:CE	2:F:231:PHE:CZ	2.97	0.47
2:F:19:CYS:HB2	2:F:46:MET:HG2	1.96	0.47
1:G:69:MET:HE1	1:G:754:MET:HE3	1.95	0.47
1:K:65:GLY:HA3	2:L:21:MET:HG3	1.97	0.47
1:M:155:SER:OG	1:M:409:ILE:HG12	2.14	0.47
1:M:401:PHE:CD1	1:M:573:ILE:HD13	2.50	0.47
1:M:296:ASN:HB3	1:M:657:PHE:CZ	2.49	0.47
1:M:670:PRO:HG2	1:M:675:GLN:CD	2.35	0.47
2:N:2:GLU:HB3	2:N:158:LYS:HE2	1.96	0.47
2:N:46:MET:CE	2:N:66:THR:N	2.76	0.47
1:O:387:TRP:CE2	1:O:389:THR:HA	2.49	0.47
1:Q:201:LEU:HD13	1:Q:387:TRP:HB2	1.96	0.47
2:R:142:MET:HE2	2:R:147:HIS:N	2.28	0.47
1:U:100:LEU:HD12	1:U:105:PRO:HG3	1.97	0.47
1:U:744:HIS:HA	1:U:819:SER:CB	2.45	0.47
1:W:174:ASP:OD1	1:W:175:SER:N	2.40	0.47
1:A:426:MET:HE1	1:A:618:GLN:O	2.14	0.47
2:D:5:TYR:HB2	2:D:157:LEU:CD1	2.44	0.47
2:F:138:TRP:HB3	8:F:503:HOH:O	2.14	0.47
1:I:501:LEU:HD13	1:I:823:TYR:CD2	2.48	0.47
1:I:871:LYS:HE2	8:I:1228:HOH:O	2.14	0.47
2:N:18:ASN:HB2	7:N:302:SF4:S1	2.55	0.47
1:Q:501:LEU:HD13	1:Q:823:TYR:CG	2.49	0.47
1:S:296:ASN:HB3	1:S:657:PHE:CZ	2.49	0.47
1:S:823:TYR:CE2	1:S:825:PRO:HG3	2.49	0.47
1:S:144:HIS:HB2	4:S:902:MGD:O1B	2.14	0.47
1:U:737:PRO:HG3	4:U:903:MGD:H2'	1.95	0.47
2:X:203:ILE:HD12	2:X:203:ILE:N	2.29	0.47
1:A:356:GLY:HA2	1:A:359:ARG:NH1	2.30	0.47
1:C:426:MET:HE2	1:C:618:GLN:HG2	1.96	0.47
1:E:9:ASN:HA	1:E:576:GLN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:LYS:HE2	8:G:1466:HOH:O	2.14	0.47
1:I:81:LYS:HB2	1:I:112:ILE:HD13	1.95	0.47
1:I:165:GLY:HA3	1:I:166:PHE:CB	2.37	0.47
1:I:700:GLU:HG2	8:I:1563:HOH:O	2.14	0.47
2:L:5:TYR:HB2	2:L:157:LEU:HD12	1.96	0.47
1:M:610:LYS:NZ	1:M:618:GLN:NE2	2.50	0.47
1:S:177:GLU:HA	1:S:177:GLU:OE2	2.15	0.47
1:S:645:ASN:HB3	8:S:1038:HOH:O	2.14	0.47
1:U:105:PRO:HB2	1:U:529:PHE:HE2	1.80	0.47
1:W:630:THR:OG1	1:W:633:GLU:HG3	2.14	0.47
1:C:656:TRP:CD2	1:C:663:LYS:HA	2.50	0.47
1:E:696:LYS:O	1:E:700:GLU:HG3	2.15	0.47
1:K:75:ARG:HH21	1:K:543:CYS:HA	1.79	0.47
1:K:775:ASN:HA	1:K:806:THR:O	2.15	0.47
1:K:67:LYS:NZ	2:L:25:ASP:O	2.48	0.47
2:N:94:ILE:O	2:N:96:PRO:HD3	2.15	0.47
1:S:66:PHE:HZ	1:S:146:MET:CE	2.28	0.47
1:U:11:SER:HA	1:U:147:TRP:HB2	1.97	0.47
1:U:75:ARG:HH21	1:U:543:CYS:HA	1.80	0.47
1:U:744:HIS:HA	1:U:819:SER:HB3	1.96	0.47
1:U:767:TYR:HB3	1:U:769:TYR:CE1	2.50	0.47
1:W:100:LEU:CD1	1:W:105:PRO:HG3	2.44	0.47
2:B:205:VAL:HG13	2:B:254:LYS:HZ2	1.79	0.47
1:C:96:ARG:HD3	1:C:535:PHE:O	2.15	0.47
1:C:476:GLN:OE1	1:C:708:ARG:NH2	2.48	0.47
1:E:670:PRO:HG2	1:E:675:GLN:CD	2.35	0.47
2:J:52:GLU:HG3	2:J:61:ILE:HD12	1.97	0.47
2:L:103:LYS:HG2	2:L:116:TRP:CD2	2.50	0.47
2:L:21:MET:CE	2:L:21:MET:CA	2.93	0.47
1:M:630:THR:OG1	1:M:633:GLU:HG3	2.14	0.47
2:N:127:THR:HG22	8:N:519:HOH:O	2.15	0.47
1:O:657:PHE:CE1	1:O:681:LEU:HG	2.49	0.47
1:Q:141:PRO:HA	1:Q:496:TYR:O	2.15	0.47
1:U:177:GLU:HA	1:U:177:GLU:OE2	2.14	0.47
1:U:28:MET:CE	1:U:67:LYS:H	2.28	0.47
1:U:857:ASN:HB3	4:U:902:MGD:N19	2.30	0.47
1:W:528:TRP:CG	1:W:750:LYS:HD3	2.50	0.47
1:W:756:TYR:OH	2:X:41:ARG:HD3	2.15	0.47
2:B:46:MET:CE	2:B:66:THR:N	2.78	0.47
2:D:166:LYS:HG2	2:D:170:GLU:OE2	2.15	0.47
1:G:540:LEU:HA	1:G:541:PRO:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:PHE:HA	1:G:69:MET:HE2	1.97	0.47
1:I:610:LYS:HB3	1:I:614:ALA:HB3	1.96	0.47
1:K:56:LYS:HG2	1:K:57:THR:O	2.15	0.47
1:K:628:TYR:CE2	1:K:643:PRO:HG2	2.49	0.47
2:L:16:CYS:O	2:L:17:ASN:HB2	2.15	0.47
1:M:142:SER:HB3	4:M:902:MGD:O1A	2.14	0.47
2:N:5:TYR:HB2	2:N:157:LEU:HD12	1.97	0.47
1:O:365:GLU:OE1	1:O:365:GLU:HA	2.14	0.47
1:O:96:ARG:HD2	1:O:514:TYR:O	2.15	0.47
1:Q:66:PHE:HZ	1:Q:146:MET:HE1	1.79	0.47
8:Q:1676:HOH:O	1:S:871:LYS:HG2	2.15	0.47
1:U:175:SER:HB2	1:U:176:TRP:CE3	2.50	0.47
2:X:19:CYS:HB2	2:X:46:MET:HG2	1.97	0.47
1:A:175:SER:HB2	1:A:176:TRP:CZ3	2.50	0.47
1:C:162:ASN:HA	8:C:1363:HOH:O	2.14	0.47
1:C:717:ALA:HB3	1:C:720:SER:HB3	1.97	0.47
2:F:162:GLU:CD	2:F:162:GLU:H	2.19	0.47
1:G:100:LEU:CD1	1:G:105:PRO:HG3	2.43	0.47
1:G:11:SER:HA	1:G:147:TRP:HB2	1.97	0.47
2:H:157:LEU:N	2:H:157:LEU:HD12	2.29	0.47
1:I:182:GLY:HA3	1:I:364:ILE:HG23	1.97	0.47
1:I:571:ARG:HB2	1:I:642:VAL:HB	1.97	0.47
2:J:13:CYS:HB3	2:J:63:TYR:HB2	1.97	0.47
2:N:23:CYS:O	2:N:26:GLU:N	2.48	0.47
2:P:203:ILE:N	2:P:203:ILE:HD12	2.30	0.47
1:Q:387:TRP:CE2	1:Q:389:THR:HA	2.50	0.47
2:R:157:LEU:HD12	2:R:157:LEU:N	2.30	0.47
1:S:696:LYS:HD3	8:S:1659:HOH:O	2.15	0.47
1:S:737:PRO:HG3	4:S:903:MGD:H2'	1.97	0.47
1:U:296:ASN:HB3	1:U:657:PHE:CZ	2.50	0.47
1:U:476:GLN:OE1	1:U:708:ARG:NH2	2.48	0.47
2:D:142:MET:HE2	2:D:146:ALA:HB1	1.96	0.46
1:E:166:PHE:N	1:E:439:LEU:HD12	2.30	0.46
2:F:112:GLY:HA2	8:F:520:HOH:O	2.15	0.46
2:F:142:MET:HE2	2:F:146:ALA:HB3	1.96	0.46
1:G:691:ILE:HD11	1:G:711:MET:HE3	1.97	0.46
1:I:176:TRP:O	1:I:177:GLU:C	2.53	0.46
1:I:66:PHE:HA	1:I:69:MET:HE2	1.97	0.46
1:K:452:ILE:HB	1:K:453:PRO:HD3	1.97	0.46
1:M:282:TRP:HA	1:M:287:SER:OG	2.16	0.46
2:P:87:ARG:HD3	2:P:93:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:94:ILE:O	2:P:96:PRO:HD3	2.15	0.46
1:E:296:ASN:O	1:E:687:LYS:HB3	2.16	0.46
2:L:46:MET:HE1	2:L:65:PRO:CA	2.45	0.46
1:O:146:MET:HE3	1:O:545:ASN:OD1	2.16	0.46
1:O:426:MET:CE	1:O:426:MET:HA	2.37	0.46
1:O:498:GLY:N	1:O:499:PRO:HD3	2.30	0.46
2:T:21:MET:CE	2:T:21:MET:HA	2.43	0.46
1:U:166:PHE:N	1:U:439:LEU:HD12	2.30	0.46
1:U:269:GLY:HA2	1:U:362:HIS:CE1	2.50	0.46
1:U:322:GLU:HG3	1:U:327:VAL:O	2.16	0.46
1:A:114:TRP:CZ2	1:A:541:PRO:HD2	2.49	0.46
1:E:187:TRP:CH2	1:E:196:PRO:HB3	2.50	0.46
2:J:125:LYS:HD2	2:J:126:CYS:O	2.14	0.46
2:J:2:GLU:HG2	2:J:158:LYS:HG2	1.98	0.46
1:K:249:ASP:CG	4:K:903:MGD:H1'	2.36	0.46
1:O:656:TRP:CD2	1:O:663:LYS:HA	2.50	0.46
2:P:102:LYS:HB3	2:P:104:GLU:OE2	2.15	0.46
1:Q:670:PRO:HB3	1:Q:682:GLN:HB2	1.97	0.46
1:S:140:THR:HB	1:S:169:ALA:HB3	1.98	0.46
1:S:400:TYR:CE1	1:S:421:LYS:HD2	2.50	0.46
2:V:177:LYS:N	2:V:178:PRO:HD3	2.31	0.46
2:V:256:TYR:HB2	2:V:274:LEU:HD21	1.97	0.46
1:A:128:ILE:CD1	1:A:492:MET:HB2	2.45	0.46
1:A:563:ASP:O	1:A:566:GLN:HG2	2.16	0.46
2:B:10:VAL:HG13	2:B:63:TYR:O	2.15	0.46
2:B:213:ALA:O	2:B:228:GLU:HA	2.16	0.46
1:C:173:PRO:HG3	1:C:180:HIS:CG	2.50	0.46
1:C:503:THR:HG21	4:C:902:MGD:O2A	2.15	0.46
1:E:96:ARG:HD2	1:E:514:TYR:O	2.15	0.46
1:E:737:PRO:CG	4:E:903:MGD:H2'	2.45	0.46
2:H:5:TYR:CD2	2:H:164:MET:HG2	2.50	0.46
2:L:101:GLY:HA2	2:L:121:ASN:ND2	2.30	0.46
2:L:247:VAL:O	2:L:257:SER:HA	2.15	0.46
1:M:15:PRO:HD2	8:M:1003:HOH:O	2.15	0.46
1:M:77:PRO:HB2	1:M:78:TYR:CD2	2.50	0.46
1:M:211:MET:HE3	2:N:231:PHE:CZ	2.50	0.46
1:O:735:LEU:HD23	1:O:735:LEU:H	1.80	0.46
1:O:9:ASN:HA	1:O:576:GLN:HA	1.97	0.46
2:P:162:GLU:H	2:P:162:GLU:CD	2.18	0.46
1:Q:146:MET:HE2	1:Q:545:ASN:H	1.80	0.46
2:T:72:GLU:HB2	2:T:183:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:387:TRP:CZ2	1:U:389:THR:HA	2.51	0.46
2:B:112:GLY:HA2	8:B:521:HOH:O	2.14	0.46
2:B:249:ILE:O	2:B:255:SER:HA	2.15	0.46
1:C:81:LYS:HB2	1:C:112:ILE:HD13	1.97	0.46
2:D:94:ILE:HG13	2:D:125:LYS:HE3	1.98	0.46
1:E:521:PHE:CE2	1:E:523:VAL:HG22	2.50	0.46
1:E:691:ILE:HD11	1:E:711:MET:CE	2.45	0.46
1:I:353:GLY:O	1:I:354:TRP:HB2	2.16	0.46
1:I:656:TRP:CD2	1:I:663:LYS:HA	2.51	0.46
1:I:776:SER:HA	1:I:805:VAL:HG13	1.98	0.46
2:J:210:PHE:CE2	2:J:251:ALA:HB1	2.51	0.46
1:U:257:ARG:HD3	2:V:61:ILE:HG21	1.96	0.46
2:X:142:MET:CE	2:X:146:ALA:HB1	2.45	0.46
1:A:35:ASP:OD1	1:A:55:ARG:HD3	2.16	0.46
1:A:141:PRO:CA	1:A:496:TYR:HB3	2.43	0.46
1:E:671:ARG:HD2	8:E:1098:HOH:O	2.16	0.46
1:I:452:ILE:N	1:I:453:PRO:CD	2.79	0.46
1:I:451:LYS:HG3	1:I:461:PHE:CE2	2.50	0.46
1:I:510:TYR:O	1:I:513:MET:HG2	2.16	0.46
1:K:855:MET:HB2	1:K:857:ASN:OD1	2.16	0.46
2:L:9:ASP:HA	2:L:189:LYS:HB3	1.97	0.46
1:O:662:GLU:OE1	1:O:662:GLU:N	2.49	0.46
2:P:16:CYS:O	2:P:17:ASN:HB2	2.16	0.46
1:Q:396:ASP:OD2	1:Q:398:GLU:HB2	2.16	0.46
1:Q:69:MET:CE	1:Q:754:MET:HE3	2.45	0.46
2:R:129:CYS:CB	2:R:132:LEU:HD12	2.45	0.46
1:S:452:ILE:HB	1:S:453:PRO:HD3	1.97	0.46
1:S:528:TRP:CG	1:S:750:LYS:HD3	2.51	0.46
1:U:81:LYS:HB2	1:U:112:ILE:HD13	1.98	0.46
2:V:40:GLN:HE22	2:V:118:GLU:H	1.61	0.46
1:W:499:PRO:CB	1:W:745:THR:HG21	2.46	0.46
2:X:16:CYS:O	2:X:17:ASN:HB2	2.15	0.46
1:C:176:TRP:O	1:C:177:GLU:C	2.54	0.46
1:C:736:SER:OG	4:C:902:MGD:N19	2.42	0.46
2:D:58:ARG:HD2	2:D:268:ASP:OD1	2.16	0.46
2:D:26:GLU:HB2	2:D:144:ARG:NH1	2.31	0.46
2:D:9:ASP:HA	2:D:189:LYS:HB3	1.98	0.46
1:E:165:GLY:CA	1:E:166:PHE:HB3	2.39	0.46
1:G:387:TRP:CE2	1:G:389:THR:HA	2.51	0.46
1:G:44:ILE:HD11	1:G:394:PRO:CG	2.42	0.46
1:G:498:GLY:N	1:G:499:PRO:HD3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:23:CYS:O	2:J:27:HIS:N	2.35	0.46
2:N:20:PHE:CZ	2:N:24:MET:HE1	2.51	0.46
2:R:40:GLN:HB3	2:R:43:HIS:CE1	2.51	0.46
2:T:191:LEU:HG	2:T:195:GLU:HG3	1.98	0.46
1:A:265:SER:O	1:A:810:GLN:NE2	2.49	0.46
2:B:216:VAL:HG13	2:B:223:GLU:HG3	1.96	0.46
2:D:87:ARG:HG3	2:D:91:ILE:O	2.15	0.46
1:E:81:LYS:HB2	1:E:112:ILE:HD13	1.97	0.46
1:E:214:PHE:HA	1:E:347:ALA:HB3	1.98	0.46
1:E:452:ILE:HB	1:E:453:PRO:HD3	1.96	0.46
1:E:6:ARG:HD2	8:E:1012:HOH:O	2.16	0.46
1:G:452:ILE:N	1:G:453:PRO:CD	2.79	0.46
2:N:103:LYS:HG2	2:N:116:TRP:CD2	2.50	0.46
1:Q:258:LEU:HG	1:Q:259:VAL:HG13	1.98	0.46
1:Q:395:LEU:HD12	1:Q:566:GLN:HA	1.97	0.46
1:Q:610:LYS:HZ3	1:Q:618:GLN:HE22	1.58	0.46
2:R:201:ALA:HB2	2:R:269:LEU:HB2	1.98	0.46
1:A:395:LEU:HD13	1:A:571:ARG:HG3	1.98	0.46
2:B:72:GLU:HG2	2:B:185:ARG:NH2	2.30	0.46
2:B:87:ARG:HD3	2:B:93:LEU:HD12	1.97	0.46
1:C:730:TYR:CE1	1:C:794:ASN:HA	2.51	0.46
2:D:142:MET:HE2	2:D:146:ALA:CB	2.45	0.46
1:E:12:THR:O	1:E:226:TYR:HA	2.15	0.46
1:E:177:GLU:OE2	1:E:177:GLU:HA	2.14	0.46
1:E:498:GLY:N	1:E:499:PRO:HD3	2.31	0.46
1:I:296:ASN:HB3	1:I:657:PHE:CZ	2.51	0.46
1:K:11:SER:HA	1:K:147:TRP:HB2	1.96	0.46
1:K:418:ALA:HB1	1:K:423:ALA:HB2	1.97	0.46
1:K:563:ASP:HA	1:K:565:TYR:CE1	2.51	0.46
1:M:730:TYR:CE1	1:M:794:ASN:HA	2.50	0.46
2:N:198:TYR:HB3	2:N:238:ASP:HA	1.98	0.46
1:Q:364:ILE:HD13	1:Q:708:ARG:HG3	1.98	0.46
2:T:9:ASP:HA	2:T:189:LYS:HB3	1.98	0.46
1:U:250:PRO:HD3	4:U:903:MGD:C2	2.46	0.46
1:W:116:GLU:O	1:W:120:ILE:HG13	2.16	0.46
1:W:165:GLY:CA	1:W:166:PHE:HB3	2.41	0.46
2:X:255:SER:HB2	8:X:538:HOH:O	2.14	0.46
1:A:138:LEU:HB2	1:A:490:ILE:HD12	1.98	0.46
1:A:174:ASP:OD1	1:A:175:SER:N	2.43	0.46
1:A:28:MET:HE1	1:A:66:PHE:CB	2.43	0.46
2:D:179:GLU:CD	2:D:179:GLU:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:SER:HB3	4:E:902:MGD:O1A	2.15	0.46
2:H:23:CYS:HB3	2:H:39:MET:CE	2.45	0.46
1:I:177:GLU:HA	1:I:177:GLU:OE2	2.16	0.46
1:I:498:GLY:N	1:I:499:PRO:HD3	2.31	0.46
1:K:173:PRO:HA	1:K:468:PHE:CE1	2.50	0.46
1:K:211:MET:HE3	8:K:1447:HOH:O	2.16	0.46
1:K:452:ILE:N	1:K:453:PRO:CD	2.79	0.46
1:K:69:MET:HE1	1:K:754:MET:HE3	1.97	0.46
1:M:656:TRP:CD2	1:M:663:LYS:HA	2.51	0.46
1:M:66:PHE:HZ	1:M:146:MET:HE1	1.82	0.46
1:O:786:ASN:HD21	1:O:805:VAL:H	1.62	0.46
1:Q:128:ILE:CD1	1:Q:492:MET:HB2	2.46	0.46
1:Q:353:GLY:O	1:Q:354:TRP:HB2	2.15	0.46
1:S:452:ILE:N	1:S:453:PRO:CD	2.79	0.46
1:W:378:GLY:O	1:W:381:LYS:HG2	2.16	0.46
1:A:452:ILE:N	1:A:453:PRO:CD	2.80	0.45
1:C:561:ILE:N	1:C:562:PRO:HD3	2.32	0.45
1:C:361:SER:N	1:C:856:ALA:HB1	2.31	0.45
2:D:201:ALA:HB2	2:D:269:LEU:HB2	1.97	0.45
1:E:15:PRO:HD3	1:E:554:PHE:CE1	2.51	0.45
1:G:67:LYS:NZ	2:H:25:ASP:O	2.48	0.45
1:I:404:TYR:CD1	1:I:405:ALA:N	2.84	0.45
1:K:141:PRO:CA	1:K:496:TYR:HB3	2.45	0.45
1:O:66:PHE:HZ	1:O:146:MET:HE1	1.81	0.45
1:O:247:PHE:CZ	1:O:255:THR:HG22	2.51	0.45
1:O:395:LEU:HD12	1:O:566:GLN:HA	1.97	0.45
1:O:649:LYS:HE3	1:O:651:THR:CG2	2.45	0.45
2:R:216:VAL:HG13	2:R:223:GLU:HG3	1.99	0.45
1:W:673:ASN:HD22	1:W:673:ASN:H	1.64	0.45
2:B:46:MET:CE	2:B:66:THR:H	2.29	0.45
1:C:134:PRO:HB2	1:C:439:LEU:HD11	1.98	0.45
1:C:140:THR:HB	1:C:169:ALA:HB3	1.98	0.45
1:C:146:MET:HG2	4:C:902:MGD:N7	2.31	0.45
1:C:644:ASP:OD1	1:C:646:PRO:HG3	2.16	0.45
2:D:176:ILE:HG22	2:D:177:LYS:HG3	1.99	0.45
2:F:21:MET:HE2	2:F:21:MET:HA	1.98	0.45
1:I:517:ASP:HB3	8:I:1201:HOH:O	2.15	0.45
1:K:722:LYS:HG2	8:K:1560:HOH:O	2.16	0.45
1:M:174:ASP:OD1	1:M:175:SER:N	2.48	0.45
2:N:166:LYS:HE2	2:N:170:GLU:OE2	2.16	0.45
2:N:21:MET:HE2	2:N:21:MET:HA	1.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:40:GLN:NE2	2:P:117:ASN:HA	2.31	0.45
1:S:708:ARG:HD2	8:S:1045:HOH:O	2.14	0.45
2:T:19:CYS:HB2	2:T:46:MET:HG2	1.98	0.45
2:T:46:MET:HE1	2:T:65:PRO:CA	2.46	0.45
1:U:141:PRO:HA	1:U:496:TYR:O	2.16	0.45
1:U:144:HIS:HB2	4:U:902:MGD:O1B	2.16	0.45
1:U:34:ASP:HB3	1:U:37:VAL:HG22	1.99	0.45
1:W:744:HIS:HA	1:W:819:SER:CB	2.47	0.45
1:A:66:PHE:HZ	1:A:146:MET:CE	2.25	0.45
1:C:734:MET:HB2	1:C:814:VAL:HG23	1.98	0.45
2:D:177:LYS:N	2:D:178:PRO:HD3	2.31	0.45
2:H:245:TYR:HB2	2:H:260:VAL:CG1	2.47	0.45
1:I:521:PHE:CE2	1:I:523:VAL:HG22	2.52	0.45
1:K:144:HIS:HB2	4:K:902:MGD:O1B	2.17	0.45
2:L:106:LEU:HD11	2:L:116:TRP:HB2	1.96	0.45
1:M:387:TRP:CE2	1:M:389:THR:HA	2.51	0.45
1:Q:736:SER:O	4:Q:902:MGD:N18	2.49	0.45
2:R:142:MET:HE3	2:R:146:ALA:HB1	1.98	0.45
1:S:134:PRO:HB2	1:S:439:LEU:HD11	1.99	0.45
1:S:558:SER:H	1:S:564:ASN:HD22	1.58	0.45
2:V:23:CYS:HB3	2:V:39:MET:CE	2.45	0.45
2:V:5:TYR:HB2	2:V:157:LEU:CD1	2.46	0.45
2:X:70:HIS:CD2	2:X:92:VAL:H	2.31	0.45
2:B:19:CYS:HB2	2:B:46:MET:HG2	1.97	0.45
1:C:165:GLY:CA	1:C:166:PHE:HB3	2.43	0.45
1:C:263:TRP:HZ3	2:D:59:ASN:HD21	1.64	0.45
1:E:141:PRO:CA	1:E:496:TYR:HB3	2.42	0.45
1:I:11:SER:HA	1:I:147:TRP:HB2	1.97	0.45
1:K:263:TRP:CZ2	1:K:265:SER:HB2	2.51	0.45
1:K:353:GLY:O	1:K:354:TRP:HB2	2.16	0.45
1:K:142:SER:CB	4:K:902:MGD:O1A	2.65	0.45
2:L:213:ALA:O	2:L:228:GLU:HA	2.17	0.45
1:M:847:TYR:CZ	1:M:853:CYS:HB3	2.52	0.45
2:N:203:ILE:N	2:N:203:ILE:HD12	2.30	0.45
1:O:134:PRO:HB2	1:O:439:LEU:HD11	1.97	0.45
2:R:69:MET:HB3	2:R:184:PRO:HB3	1.98	0.45
1:U:142:SER:HB3	4:U:902:MGD:O1A	2.16	0.45
1:A:176:TRP:O	1:A:177:GLU:C	2.55	0.45
1:C:378:GLY:O	1:C:381:LYS:HG2	2.17	0.45
1:C:452:ILE:N	1:C:453:PRO:CD	2.79	0.45
1:C:767:TYR:HB3	1:C:769:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:TYR:CZ	1:C:853:CYS:HB3	2.52	0.45
2:D:114:MET:HE3	2:D:123:ALA:HB1	1.99	0.45
1:E:451:LYS:HG3	1:E:461:PHE:CE2	2.52	0.45
2:F:247:VAL:O	2:F:257:SER:HA	2.17	0.45
2:F:39:MET:HE2	2:F:45:TRP:CE2	2.51	0.45
1:G:173:PRO:HA	1:G:468:PHE:CE1	2.52	0.45
1:G:353:GLY:O	1:G:354:TRP:HB2	2.16	0.45
1:G:823:TYR:CE2	1:G:825:PRO:HG3	2.52	0.45
1:I:146:MET:HE3	1:I:545:ASN:OD1	2.16	0.45
2:J:142:MET:CE	2:J:146:ALA:HB1	2.47	0.45
1:K:738:HIS:HE2	4:K:902:MGD:H15	1.64	0.45
1:M:719:GLU:O	1:M:859:THR:HB	2.16	0.45
1:M:776:SER:HA	1:M:805:VAL:HG13	1.98	0.45
1:Q:146:MET:CE	1:Q:545:ASN:OD1	2.65	0.45
1:Q:782:ARG:HH11	1:Q:782:ARG:HG3	1.82	0.45
1:S:322:GLU:HG3	1:S:327:VAL:O	2.15	0.45
1:S:69:MET:HE1	1:S:754:MET:HE3	1.99	0.45
1:S:786:ASN:ND2	1:S:805:VAL:H	2.15	0.45
2:T:114:MET:HA	2:T:125:LYS:HB3	1.99	0.45
2:T:198:TYR:HB3	2:T:238:ASP:HA	1.99	0.45
1:U:677:CYS:O	1:U:679:LYS:HG3	2.17	0.45
2:X:143:PRO:HD3	2:X:156:PHE:CE2	2.52	0.45
2:X:177:LYS:N	2:X:178:PRO:HD3	2.31	0.45
2:B:7:VAL:HB	2:B:155:GLU:HB3	1.99	0.45
1:G:356:GLY:N	4:G:903:MGD:O1B	2.49	0.45
1:G:96:ARG:HD2	1:G:514:TYR:O	2.17	0.45
2:H:164:MET:O	2:H:168:VAL:HG23	2.16	0.45
2:H:16:CYS:O	2:H:17:ASN:HB2	2.16	0.45
2:L:94:ILE:O	2:L:96:PRO:HD3	2.16	0.45
1:M:501:LEU:HD13	1:M:823:TYR:CG	2.52	0.45
1:O:165:GLY:HA3	1:O:166:PHE:CB	2.34	0.45
1:O:66:PHE:HZ	1:O:146:MET:CE	2.30	0.45
2:P:142:MET:HE1	2:P:146:ALA:C	2.37	0.45
1:Q:15:PRO:HD2	8:Q:1003:HOH:O	2.15	0.45
1:Q:571:ARG:HB2	1:Q:642:VAL:HB	1.99	0.45
2:R:159:THR:OG1	2:R:160:THR:N	2.50	0.45
1:S:826:LEU:HD21	1:S:835:ARG:HD3	1.98	0.45
2:T:16:CYS:O	2:T:17:ASN:HB2	2.17	0.45
1:U:494:TRP:HE1	1:U:525:GLN:HE21	1.64	0.45
2:X:69:MET:HB2	7:X:304:SF4:S2	2.57	0.45
1:C:402:PRO:CD	1:C:623:THR:HG22	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:THR:OG1	1:E:171:HIS:HE1	2.00	0.45
1:E:797:GLY:HA2	1:E:875:TYR:CE2	2.51	0.45
2:H:129:CYS:HB3	2:H:132:LEU:HD12	1.99	0.45
1:K:165:GLY:HA3	1:K:166:PHE:CB	2.35	0.45
2:N:23:CYS:O	2:N:27:HIS:N	2.47	0.45
1:S:770:TRP:HB3	1:S:801:LEU:HD23	1.98	0.45
1:U:249:ASP:CG	4:U:903:MGD:H1'	2.37	0.45
1:W:146:MET:HG2	4:W:902:MGD:N7	2.31	0.45
1:W:782:ARG:HD3	1:W:864:ILE:O	2.17	0.45
2:F:179:GLU:OE1	2:F:179:GLU:N	2.44	0.45
2:H:18:ASN:HB2	7:H:302:SF4:S1	2.56	0.45
1:I:32:ASP:HB2	8:I:1650:HOH:O	2.15	0.45
2:N:5:TYR:HB2	2:N:157:LEU:HD11	1.98	0.45
1:O:402:PRO:HG2	1:O:422:PHE:CE1	2.51	0.45
1:S:66:PHE:HA	1:S:69:MET:HE2	1.98	0.45
2:T:5:TYR:CD2	2:T:164:MET:HG2	2.52	0.45
1:U:734:MET:HB2	1:U:814:VAL:HG23	1.99	0.45
1:W:201:LEU:HD13	1:W:387:TRP:HB2	1.99	0.45
1:A:510:TYR:O	1:A:513:MET:HG2	2.17	0.45
2:B:5:TYR:CD2	2:B:164:MET:HG2	2.52	0.45
1:C:501:LEU:HD13	1:C:823:TYR:CD2	2.52	0.45
2:D:23:CYS:O	2:D:27:HIS:N	2.44	0.45
1:E:197:GLU:HG3	1:E:199:TYR:CD1	2.51	0.45
2:H:21:MET:HE1	2:H:24:MET:CE	2.47	0.45
1:K:134:PRO:HB2	1:K:439:LEU:HD11	1.99	0.45
1:K:15:PRO:HD3	1:K:554:PHE:CD1	2.52	0.45
1:K:560:TYR:HB2	8:K:1677:HOH:O	2.16	0.45
2:L:19:CYS:HA	2:L:145:CYS:HA	1.99	0.45
1:M:48:GLY:HA3	2:R:252:ASP:O	2.17	0.45
1:Q:141:PRO:CA	1:Q:496:TYR:HB3	2.43	0.45
1:Q:74:LEU:HD12	1:Q:750:LYS:HA	1.99	0.45
1:U:211:MET:HE2	2:V:231:PHE:CZ	2.52	0.45
1:W:343:ASN:ND2	8:W:1430:HOH:O	2.50	0.45
1:W:510:TYR:O	1:W:513:MET:HG2	2.16	0.45
1:W:644:ASP:O	1:W:646:PRO:HD3	2.17	0.45
1:C:521:PHE:CE2	1:C:523:VAL:CG2	3.00	0.45
1:E:848:ILE:HG12	1:E:856:ALA:HB2	1.99	0.45
2:F:40:GLN:HB3	2:F:43:HIS:CE1	2.52	0.45
1:K:696:LYS:O	1:K:700:GLU:HG3	2.17	0.45
1:M:153:ARG:O	1:M:157:TYR:HB3	2.17	0.45
1:M:394:PRO:HG3	8:M:1320:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:265:SER:O	1:O:810:GLN:NE2	2.50	0.45
1:O:76:ILE:HG22	1:O:541:PRO:HG3	1.98	0.45
1:Q:257:ARG:HD3	2:R:61:ILE:HG21	1.98	0.45
1:S:277:ALA:HA	1:S:316:LYS:O	2.16	0.45
1:S:571:ARG:HB2	1:S:642:VAL:HB	1.99	0.45
1:S:847:TYR:CZ	1:S:853:CYS:HB3	2.52	0.45
1:U:174:ASP:OD1	1:U:175:SER:N	2.47	0.45
1:U:735:LEU:HD23	1:U:735:LEU:H	1.81	0.45
1:W:85:PHE:CE2	1:W:87:PRO:HG3	2.52	0.45
2:X:122:VAL:HG22	2:X:123:ALA:N	2.31	0.45
1:A:9:ASN:HA	1:A:576:GLN:HA	1.98	0.44
2:B:142:MET:CE	2:B:146:ALA:HB1	2.46	0.44
1:C:134:PRO:HD2	8:C:1359:HOH:O	2.17	0.44
1:C:786:ASN:HA	1:C:786:ASN:HD22	1.57	0.44
1:G:69:MET:CE	1:G:754:MET:HE3	2.47	0.44
1:I:77:PRO:HB2	1:I:78:TYR:CD2	2.52	0.44
1:K:277:ALA:HA	1:K:316:LYS:O	2.17	0.44
1:K:744:HIS:HA	1:K:819:SER:HB3	1.99	0.44
1:M:146:MET:HG2	4:M:902:MGD:N7	2.32	0.44
1:O:786:ASN:ND2	1:O:805:VAL:N	2.59	0.44
1:Q:378:GLY:O	1:Q:381:LYS:HG2	2.17	0.44
1:S:716:PRO:HB3	1:S:723:HIS:CD2	2.52	0.44
1:W:449:ARG:HD2	8:W:1037:HOH:O	2.17	0.44
2:X:40:GLN:NE2	8:X:443:HOH:O	2.49	0.44
1:A:498:GLY:N	1:A:499:PRO:HD3	2.32	0.44
2:B:40:GLN:HB3	2:B:43:HIS:CE1	2.53	0.44
1:C:211:MET:CE	2:D:231:PHE:CZ	2.99	0.44
1:C:296:ASN:HB3	1:C:657:PHE:CZ	2.52	0.44
1:G:249:ASP:CG	4:G:903:MGD:H1'	2.36	0.44
1:I:269:GLY:HA2	1:I:362:HIS:CE1	2.52	0.44
2:J:166:LYS:O	2:J:170:GLU:HG3	2.17	0.44
1:K:691:ILE:HD11	1:K:711:MET:CE	2.47	0.44
1:M:141:PRO:HA	1:M:496:TYR:O	2.17	0.44
1:M:253:ASN:O	1:M:257:ARG:HG3	2.17	0.44
1:O:114:TRP:CZ2	1:O:541:PRO:HD2	2.52	0.44
1:Q:277:ALA:HA	1:Q:316:LYS:O	2.17	0.44
1:Q:558:SER:H	1:Q:564:ASN:ND2	2.15	0.44
1:Q:847:TYR:CZ	1:Q:853:CYS:HB3	2.52	0.44
1:Q:211:MET:CE	2:R:231:PHE:CZ	3.00	0.44
2:T:203:ILE:HD12	2:T:203:ILE:N	2.31	0.44
1:U:644:ASP:C	1:U:646:PRO:HD3	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:40:GLN:NE2	2:V:118:GLU:H	2.16	0.44
1:W:187:TRP:CH2	1:W:196:PRO:HB3	2.52	0.44
1:W:794:ASN:HD21	1:W:842:LEU:HB3	1.82	0.44
2:X:23:CYS:HB3	2:X:39:MET:CE	2.46	0.44
2:X:249:ILE:HG22	2:X:250:ASP:N	2.32	0.44
1:A:15:PRO:HD2	8:A:1003:HOH:O	2.17	0.44
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.76	0.44
2:D:103:LYS:HG2	2:D:116:TRP:CD2	2.53	0.44
1:E:253:ASN:O	1:E:257:ARG:HG3	2.17	0.44
1:G:153:ARG:O	1:G:157:TYR:HB3	2.18	0.44
2:J:112:GLY:HA2	8:J:518:HOH:O	2.17	0.44
1:M:328:PRO:HB2	1:M:331:GLU:HG3	1.98	0.44
2:N:23:CYS:HB3	2:N:39:MET:CE	2.47	0.44
1:Q:249:ASP:CG	4:Q:903:MGD:H1'	2.37	0.44
1:W:134:PRO:HB2	1:W:439:LEU:HD11	1.99	0.44
1:A:708:ARG:HD2	8:A:1044:HOH:O	2.16	0.44
1:A:250:PRO:HD3	4:A:903:MGD:C2	2.48	0.44
2:B:142:MET:CE	2:B:146:ALA:CB	2.95	0.44
1:C:218:ASP:OD2	1:C:253:ASN:HB2	2.16	0.44
1:C:249:ASP:CG	4:C:903:MGD:H1'	2.38	0.44
1:C:252:MET:HB3	1:C:808:CYS:HB3	1.99	0.44
1:C:785:LYS:NZ	8:C:1622:HOH:O	2.48	0.44
2:D:129:CYS:CB	2:D:132:LEU:HD12	2.48	0.44
2:F:106:LEU:HD11	2:F:116:TRP:HB2	1.99	0.44
2:F:64:ARG:NH1	8:F:419:HOH:O	2.48	0.44
1:G:610:LYS:HZ3	1:G:618:GLN:NE2	2.14	0.44
1:I:433:PHE:HA	1:I:434:PRO:HD3	1.83	0.44
2:J:56:TYR:HA	2:J:59:ASN:ND2	2.32	0.44
1:K:737:PRO:CG	4:K:903:MGD:H2'	2.47	0.44
2:N:210:PHE:HD2	2:N:213:ALA:HB2	1.82	0.44
2:N:21:MET:HE1	2:N:24:MET:CE	2.48	0.44
1:O:426:MET:HE3	1:O:622:ALA:HB2	1.98	0.44
2:P:247:VAL:O	2:P:257:SER:HA	2.17	0.44
1:S:801:LEU:HD11	1:S:839:ILE:HD11	1.99	0.44
1:U:263:TRP:CZ2	1:U:265:SER:HB2	2.51	0.44
1:U:452:ILE:HB	1:U:453:PRO:HD3	2.00	0.44
1:W:114:TRP:CZ2	1:W:541:PRO:HD2	2.52	0.44
1:A:521:PHE:CE2	1:A:523:VAL:HG22	2.53	0.44
2:H:105:LEU:HB3	2:H:114:MET:CE	2.47	0.44
2:H:114:MET:HA	2:H:125:LYS:HB3	2.00	0.44
1:M:76:ILE:HA	1:M:77:PRO:HD3	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:656:TRP:CD2	1:Q:663:LYS:HA	2.52	0.44
1:Q:716:PRO:HB3	1:Q:723:HIS:CG	2.53	0.44
1:Q:730:TYR:CE1	1:Q:794:ASN:HA	2.52	0.44
2:R:177:LYS:N	2:R:178:PRO:HD3	2.32	0.44
1:S:540:LEU:HA	1:S:541:PRO:HD3	1.78	0.44
2:X:210:PHE:CE2	2:X:251:ALA:HB1	2.53	0.44
1:A:797:GLY:HA2	1:A:875:TYR:CZ	2.53	0.44
2:B:247:VAL:O	2:B:257:SER:HA	2.17	0.44
1:C:162:ASN:HD22	1:C:166:PHE:HE2	1.64	0.44
1:C:222:ASN:HA	4:C:903:MGD:H22	1.83	0.44
1:C:670:PRO:HB3	1:C:682:GLN:HB2	1.98	0.44
1:C:785:LYS:NZ	1:C:785:LYS:HB2	2.32	0.44
2:D:19:CYS:HA	2:D:145:CYS:HA	1.99	0.44
2:D:252:ASP:C	2:D:254:LYS:H	2.20	0.44
1:E:505:THR:O	1:E:506:ALA:C	2.55	0.44
2:F:139:ALA:HB3	2:F:140:PRO:HD3	2.00	0.44
1:G:175:SER:HB2	1:G:176:TRP:CZ3	2.52	0.44
1:G:501:LEU:HA	1:G:507:THR:HB	2.00	0.44
1:G:786:ASN:ND2	1:G:804:GLN:HA	2.32	0.44
1:G:142:SER:OG	4:G:902:MGD:O1A	2.25	0.44
1:I:673:ASN:H	1:I:673:ASN:HD22	1.65	0.44
1:K:533:VAL:HB	1:K:534:PRO:HD3	1.99	0.44
1:M:587:MET:HG3	1:M:592:ILE:CG1	2.48	0.44
1:O:146:MET:CE	1:O:545:ASN:OD1	2.66	0.44
1:O:144:HIS:NE2	6:O:905:PYG:O1	2.48	0.44
1:S:730:TYR:CZ	1:S:794:ASN:HA	2.52	0.44
1:U:28:MET:HE1	1:U:67:LYS:N	2.33	0.44
2:V:102:LYS:HB3	2:V:104:GLU:OE2	2.17	0.44
1:W:296:ASN:HB3	1:W:657:PHE:CZ	2.52	0.44
1:W:730:TYR:CZ	1:W:794:ASN:HA	2.52	0.44
2:B:4:TYR:CE2	2:B:158:LYS:HD2	2.53	0.44
1:C:165:GLY:HA3	1:C:166:PHE:CB	2.39	0.44
1:C:533:VAL:HB	1:C:534:PRO:HD3	1.99	0.44
1:E:265:SER:O	1:E:810:GLN:NE2	2.51	0.44
1:E:501:LEU:HB2	8:E:1360:HOH:O	2.18	0.44
1:E:857:ASN:HB3	4:E:902:MGD:N19	2.33	0.44
2:L:21:MET:CA	2:L:21:MET:HE2	2.44	0.44
2:L:75:PRO:O	2:L:79:LYS:HG3	2.17	0.44
1:M:176:TRP:O	1:M:177:GLU:C	2.56	0.44
1:M:96:ARG:HD2	1:M:514:TYR:O	2.17	0.44
1:O:673:ASN:ND2	1:O:673:ASN:H	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:70:HIS:HD2	2:P:92:VAL:N	2.04	0.44
1:Q:717:ALA:HB3	1:Q:720:SER:HB3	2.00	0.44
2:R:21:MET:CE	2:R:21:MET:CA	2.95	0.44
2:T:251:ALA:HB3	2:T:274:LEU:HD12	2.00	0.44
1:W:124:GLU:HG3	1:W:521:PHE:CD2	2.53	0.44
1:W:337:ARG:O	1:W:341:LYS:HG2	2.18	0.44
2:X:23:CYS:O	2:X:27:HIS:N	2.40	0.44
1:A:187:TRP:CH2	1:A:196:PRO:HB3	2.52	0.44
1:A:69:MET:CE	1:A:754:MET:HE3	2.47	0.44
1:C:201:LEU:HD13	1:C:387:TRP:HB2	1.98	0.44
1:I:855:MET:HB2	1:I:857:ASN:OD1	2.18	0.44
1:K:505:THR:O	1:K:506:ALA:C	2.56	0.44
1:K:13:GLY:HA3	1:K:63:THR:OG1	2.17	0.44
1:K:649:LYS:HG3	1:K:649:LYS:O	2.16	0.44
2:L:142:MET:HE1	2:L:146:ALA:HB1	1.99	0.44
1:M:784:ILE:HD13	1:M:790:ILE:HG21	2.00	0.44
1:O:404:TYR:CD1	1:O:405:ALA:N	2.85	0.44
1:O:499:PRO:CB	1:O:745:THR:HG21	2.48	0.44
1:O:857:ASN:HB3	4:O:902:MGD:N19	2.33	0.44
2:P:159:THR:HG23	2:P:160:THR:N	2.33	0.44
2:P:23:CYS:HB3	2:P:39:MET:CE	2.48	0.44
2:R:5:TYR:CD2	2:R:164:MET:HG2	2.52	0.44
2:T:174:GLU:OE1	2:T:191:LEU:HB3	2.18	0.44
1:U:74:LEU:HA	1:U:74:LEU:HD23	1.85	0.44
1:U:528:TRP:CD2	1:U:750:LYS:HD3	2.53	0.44
2:V:3:GLN:O	2:V:158:LYS:HA	2.18	0.44
1:W:353:GLY:O	1:W:354:TRP:HB2	2.18	0.44
2:X:94:ILE:O	2:X:96:PRO:HD3	2.16	0.44
1:A:55:ARG:HD2	8:A:1636:HOH:O	2.17	0.44
1:C:121:VAL:O	1:C:125:ILE:HG13	2.17	0.44
1:C:498:GLY:N	1:C:499:PRO:HD3	2.33	0.44
2:D:166:LYS:HE2	2:D:170:GLU:OE2	2.18	0.44
1:G:138:LEU:HB2	1:G:490:ILE:HD12	2.00	0.44
1:G:561:ILE:CG2	1:G:564:ASN:HB3	2.44	0.44
1:I:141:PRO:CA	1:I:496:TYR:HB3	2.44	0.44
1:I:870:ASP:HB3	1:I:872:TYR:CE1	2.52	0.44
1:K:644:ASP:C	1:K:646:PRO:HD3	2.38	0.44
1:M:433:PHE:N	1:M:433:PHE:CD1	2.86	0.44
1:M:565:TYR:C	1:M:567:LEU:H	2.20	0.44
1:O:533:VAL:HB	1:O:534:PRO:HD3	2.00	0.44
1:Q:498:GLY:N	1:Q:499:PRO:HD3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:19:CYS:HB2	2:R:46:MET:HG2	2.00	0.44
1:S:353:GLY:O	1:S:354:TRP:HB2	2.18	0.44
1:S:717:ALA:HB3	1:S:720:SER:HB3	2.00	0.44
2:V:13:CYS:HB3	2:V:63:TYR:HB2	2.00	0.44
2:V:166:LYS:O	2:V:170:GLU:HG3	2.17	0.44
1:W:565:TYR:C	1:W:567:LEU:H	2.21	0.44
1:A:426:MET:HE2	1:A:618:GLN:HG2	1.97	0.43
1:A:800:ILE:N	1:A:800:ILE:HD12	2.33	0.43
2:B:23:CYS:O	2:B:27:HIS:N	2.47	0.43
1:C:855:MET:HB2	1:C:857:ASN:OD1	2.18	0.43
1:E:401:PHE:HA	1:E:402:PRO:HD3	1.78	0.43
1:E:782:ARG:HG3	1:E:782:ARG:HH11	1.83	0.43
1:G:282:TRP:HA	1:G:287:SER:OG	2.18	0.43
1:G:644:ASP:C	1:G:646:PRO:HD3	2.37	0.43
1:K:451:LYS:HG3	1:K:461:PHE:CE2	2.53	0.43
1:K:521:PHE:CE2	1:K:523:VAL:CG2	3.01	0.43
1:K:598:LYS:HA	1:K:603:GLU:HB2	1.98	0.43
2:L:203:ILE:N	2:L:203:ILE:HD12	2.33	0.43
2:L:217:LEU:HB2	2:L:237:PHE:CD1	2.53	0.43
1:M:408:GLY:HA2	1:M:619:TYR:HE1	1.81	0.43
1:M:249:ASP:CG	4:M:903:MGD:H1'	2.38	0.43
2:N:164:MET:O	2:N:168:VAL:HG23	2.18	0.43
1:Q:187:TRP:CH2	1:Q:196:PRO:HB3	2.53	0.43
2:R:106:LEU:HD22	2:R:114:MET:HB3	2.00	0.43
1:U:356:GLY:H	4:U:903:MGD:C5'	2.30	0.43
2:X:142:MET:HE2	2:X:146:ALA:HB1	2.00	0.43
1:A:44:ILE:HD11	1:A:394:PRO:HG2	1.99	0.43
1:A:776:SER:HA	1:A:805:VAL:HG13	2.00	0.43
1:E:174:ASP:OD1	1:E:175:SER:N	2.46	0.43
1:G:103:GLN:N	1:G:103:GLN:CD	2.72	0.43
1:G:15:PRO:HD2	8:G:1003:HOH:O	2.16	0.43
1:G:134:PRO:HB2	1:G:439:LEU:HD11	1.99	0.43
1:I:401:PHE:HA	1:I:402:PRO:HD3	1.77	0.43
1:I:565:TYR:C	1:I:567:LEU:N	2.71	0.43
2:J:21:MET:HE1	2:J:24:MET:HE3	1.99	0.43
1:K:730:TYR:CZ	1:K:794:ASN:HA	2.52	0.43
1:M:15:PRO:HD3	1:M:554:PHE:CE1	2.53	0.43
2:N:105:LEU:HB3	2:N:114:MET:CE	2.48	0.43
2:P:142:MET:CE	2:P:146:ALA:HB1	2.48	0.43
1:Q:563:ASP:HA	1:Q:565:TYR:CE1	2.53	0.43
1:S:521:PHE:CE2	1:S:523:VAL:CG2	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:94:ILE:O	2:T:96:PRO:HD3	2.17	0.43
1:U:75:ARG:HH22	1:U:547:GLU:CD	2.20	0.43
2:X:83:ALA:HB1	2:X:99:ALA:HB2	2.00	0.43
1:A:155:SER:OG	1:A:409:ILE:HG12	2.18	0.43
1:A:165:GLY:CA	1:A:166:PHE:HB3	2.48	0.43
2:B:19:CYS:HA	2:B:145:CYS:HA	2.00	0.43
2:B:46:MET:HE1	2:B:65:PRO:CB	2.48	0.43
2:D:203:ILE:N	2:D:203:ILE:HD12	2.33	0.43
2:D:46:MET:HE1	2:D:65:PRO:C	2.38	0.43
1:I:166:PHE:N	1:I:439:LEU:HD12	2.34	0.43
2:L:3:GLN:O	2:L:158:LYS:HA	2.19	0.43
2:P:73:ASN:ND2	2:P:182:THR:HA	2.33	0.43
1:Q:176:TRP:O	1:Q:177:GLU:C	2.56	0.43
2:R:68:CYS:HB3	2:R:70:HIS:ND1	2.33	0.43
1:S:32:ASP:HB2	8:S:1642:HOH:O	2.17	0.43
1:S:550:ASP:OD1	1:S:551:ILE:N	2.42	0.43
8:Q:1676:HOH:O	1:S:871:LYS:HE2	2.17	0.43
2:T:122:VAL:HG22	2:T:123:ALA:N	2.32	0.43
2:T:247:VAL:O	2:T:257:SER:HA	2.18	0.43
2:T:76:CYS:O	2:T:80:GLY:N	2.51	0.43
2:V:106:LEU:HD22	2:V:114:MET:HG3	2.00	0.43
2:V:58:ARG:HD2	2:V:268:ASP:OD1	2.17	0.43
1:W:673:ASN:H	1:W:673:ASN:ND2	2.15	0.43
1:W:800:ILE:CD1	1:W:833:ALA:HB1	2.48	0.43
1:A:503:THR:CG2	4:A:902:MGD:O2A	2.61	0.43
2:F:4:TYR:CE2	2:F:158:LYS:HD2	2.54	0.43
1:G:393:VAL:HA	1:G:394:PRO:HD3	1.82	0.43
1:I:505:THR:O	1:I:506:ALA:C	2.56	0.43
2:J:146:ALA:HA	2:J:154:TYR:CD1	2.53	0.43
1:K:214:PHE:HA	1:K:347:ALA:HB3	1.99	0.43
1:M:356:GLY:H	4:M:903:MGD:C5'	2.30	0.43
1:Q:644:ASP:OD1	1:Q:646:PRO:HG3	2.18	0.43
1:S:716:PRO:HB3	1:S:723:HIS:CG	2.52	0.43
2:T:4:TYR:CE2	2:T:158:LYS:HD2	2.52	0.43
1:U:528:TRP:CG	1:U:750:LYS:HD3	2.54	0.43
1:W:449:ARG:NH1	8:W:1037:HOH:O	2.50	0.43
2:X:167:LYS:HZ2	2:X:173:LEU:HD11	1.84	0.43
1:A:13:GLY:HA3	1:A:63:THR:OG1	2.19	0.43
1:A:476:GLN:OE1	1:A:708:ARG:NH2	2.50	0.43
2:B:245:TYR:HB2	2:B:260:VAL:CG1	2.48	0.43
1:G:75:ARG:NH2	1:G:543:CYS:HA	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:265:SER:O	1:M:810:GLN:NE2	2.50	0.43
1:O:176:TRP:O	1:O:177:GLU:C	2.57	0.43
1:O:364:ILE:HD13	1:O:708:ARG:HG3	2.01	0.43
2:P:40:GLN:HB3	2:P:43:HIS:CE1	2.52	0.43
1:Q:499:PRO:CB	1:Q:745:THR:HG21	2.48	0.43
1:S:75:ARG:NH2	1:S:543:CYS:HA	2.30	0.43
1:S:61:PRO:HB3	8:S:1651:HOH:O	2.18	0.43
1:S:644:ASP:O	1:S:646:PRO:HD3	2.17	0.43
2:X:174:GLU:HB3	8:X:454:HOH:O	2.18	0.43
1:A:393:VAL:HA	1:A:394:PRO:HD3	1.79	0.43
1:C:732:LEU:CD1	1:C:864:ILE:HG12	2.47	0.43
2:D:129:CYS:HB3	2:D:132:LEU:HD12	2.00	0.43
1:E:786:ASN:ND2	1:E:805:VAL:H	2.14	0.43
1:G:265:SER:O	1:G:810:GLN:NE2	2.52	0.43
1:G:826:LEU:HD21	1:G:835:ARG:HD3	1.99	0.43
1:I:211:MET:HE1	2:J:231:PHE:CZ	2.53	0.43
1:K:114:TRP:CZ2	1:K:541:PRO:HD2	2.53	0.43
1:K:21:LYS:HB3	1:K:26:ILE:HD11	2.00	0.43
2:L:162:GLU:CD	2:L:162:GLU:N	2.72	0.43
2:N:16:CYS:O	2:N:17:ASN:HB2	2.18	0.43
1:O:39:ALA:HA	1:O:40:PRO:HD3	1.92	0.43
1:S:395:LEU:HD12	1:S:566:GLN:HA	2.01	0.43
1:U:269:GLY:HA2	1:U:362:HIS:CG	2.52	0.43
1:U:649:LYS:O	1:U:649:LYS:HG3	2.18	0.43
1:U:786:ASN:ND2	1:U:805:VAL:H	2.14	0.43
1:W:65:GLY:HA3	2:X:21:MET:HG3	1.99	0.43
1:A:175:SER:OG	6:A:905:PYG:C1	2.66	0.43
2:B:60:ASP:OD1	2:B:60:ASP:C	2.57	0.43
1:C:28:MET:CE	1:C:66:PHE:HB3	2.46	0.43
1:E:395:LEU:HD13	1:E:571:ARG:HG3	2.01	0.43
1:E:800:ILE:CD1	1:E:800:ILE:N	2.81	0.43
1:G:797:GLY:HA2	1:G:875:TYR:CZ	2.53	0.43
2:H:59:ASN:HD22	2:H:59:ASN:H	1.66	0.43
1:I:673:ASN:H	1:I:673:ASN:ND2	2.17	0.43
2:J:142:MET:HE2	2:J:146:ALA:CB	2.49	0.43
1:K:12:THR:O	1:K:226:TYR:HA	2.18	0.43
1:K:387:TRP:CZ2	1:K:389:THR:HA	2.54	0.43
1:K:501:LEU:HD13	1:K:823:TYR:CD2	2.54	0.43
1:M:737:PRO:CG	4:M:903:MGD:H2'	2.48	0.43
2:N:5:TYR:CE2	2:N:164:MET:HG2	2.54	0.43
1:O:610:LYS:HZ3	1:O:618:GLN:NE2	2.13	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:627:LYS:HD3	8:O:1215:HOH:O	2.18	0.43
1:O:737:PRO:CG	4:O:903:MGD:H2'	2.49	0.43
1:S:140:THR:OG1	1:S:171:HIS:HE1	2.01	0.43
1:U:549:TRP:HB3	1:U:613:LEU:HD13	2.01	0.43
1:U:197:GLU:HG3	1:U:653:ALA:HB1	1.99	0.43
1:U:267:LYS:HB3	1:U:721:GLN:NE2	2.34	0.43
2:V:5:TYR:HB2	2:V:157:LEU:HD11	2.01	0.43
1:W:66:PHE:HZ	1:W:146:MET:HE1	1.83	0.43
1:W:364:ILE:HD13	1:W:708:ARG:HG3	2.01	0.43
1:A:10:SER:HA	1:A:15:PRO:HA	2.01	0.43
1:A:364:ILE:HD13	1:A:708:ARG:HG3	2.00	0.43
1:C:15:PRO:HD3	1:C:554:PHE:CE1	2.54	0.43
2:D:213:ALA:O	2:D:228:GLU:HA	2.19	0.43
1:E:249:ASP:CG	4:E:903:MGD:H1'	2.38	0.43
2:H:210:PHE:HD2	2:H:213:ALA:HB2	1.84	0.43
1:I:176:TRP:CD1	1:I:193:LEU:HB2	2.54	0.43
2:J:5:TYR:HB2	2:J:157:LEU:HD11	2.01	0.43
1:K:249:ASP:OD1	4:K:903:MGD:H1'	2.18	0.43
1:M:12:THR:O	1:M:226:TYR:HA	2.19	0.43
1:M:69:MET:CE	1:M:754:MET:HE3	2.48	0.43
2:N:124:GLN:O	2:N:125:LYS:HB3	2.19	0.43
1:O:15:PRO:HD2	8:O:1003:HOH:O	2.17	0.43
2:P:210:PHE:CE2	2:P:251:ALA:HB1	2.54	0.43
1:Q:146:MET:HE3	1:Q:545:ASN:OD1	2.18	0.43
2:R:142:MET:CE	2:R:146:ALA:CB	2.97	0.43
1:S:21:LYS:HB3	1:S:26:ILE:HD11	2.01	0.43
1:U:378:GLY:O	1:U:381:LYS:HG2	2.19	0.43
1:W:498:GLY:N	1:W:499:PRO:HD3	2.33	0.43
1:W:767:TYR:HB3	1:W:769:TYR:CE1	2.54	0.43
1:A:274:LEU:O	1:A:278:ILE:HG13	2.19	0.43
1:A:433:PHE:HA	1:A:434:PRO:HD3	1.83	0.43
1:C:630:THR:OG1	1:C:633:GLU:HG3	2.18	0.43
2:F:125:LYS:HD2	2:F:126:CYS:O	2.19	0.43
2:F:210:PHE:HD2	2:F:213:ALA:HB2	1.83	0.43
1:G:75:ARG:HH21	1:G:543:CYS:HA	1.84	0.43
1:I:563:ASP:HA	1:I:565:TYR:CE1	2.54	0.43
1:O:146:MET:HE2	1:O:545:ASN:H	1.84	0.43
1:O:296:ASN:O	1:O:687:LYS:HB3	2.19	0.43
1:O:142:SER:HB3	4:O:902:MGD:H5'2	2.01	0.43
1:Q:468:PHE:HB2	8:Q:1671:HOH:O	2.17	0.43
1:Q:175:SER:OG	6:Q:905:PYG:C1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:545:HOH:O	1:S:729:LYS:HE2	2.19	0.43
1:S:144:HIS:NE2	6:S:905:PYG:O1	2.48	0.43
1:U:155:SER:OG	1:U:409:ILE:HG12	2.19	0.43
1:U:561:ILE:CG2	1:U:564:ASN:HB3	2.49	0.43
1:U:211:MET:CE	2:V:231:PHE:CZ	3.02	0.43
1:W:2:GLY:N	1:W:22:ASP:OD1	2.52	0.43
1:W:362:HIS:HB3	1:W:717:ALA:HB2	2.00	0.43
1:W:66:PHE:HA	1:W:69:MET:HE2	2.00	0.43
2:X:273:LYS:O	2:X:274:LEU:HD23	2.19	0.43
1:A:571:ARG:HB2	1:A:642:VAL:HB	2.01	0.43
2:D:125:LYS:HD2	2:D:126:CYS:O	2.19	0.43
2:F:166:LYS:HE2	2:F:170:GLU:OE2	2.18	0.43
1:G:75:ARG:HH22	1:G:547:GLU:CD	2.21	0.43
1:G:818:GLU:O	1:G:819:SER:HB2	2.19	0.43
1:I:144:HIS:HB2	4:I:902:MGD:O1B	2.19	0.43
1:I:825:PRO:HD2	8:I:1329:HOH:O	2.18	0.43
1:K:100:LEU:HD13	1:K:105:PRO:HG3	2.01	0.43
1:K:670:PRO:HG2	1:K:675:GLN:CD	2.39	0.43
1:O:175:SER:HB2	1:O:176:TRP:CE3	2.54	0.43
1:Q:138:LEU:HB2	1:Q:490:ILE:HD12	2.01	0.43
1:Q:540:LEU:HA	1:Q:541:PRO:HD3	1.78	0.43
1:S:141:PRO:HA	1:S:496:TYR:O	2.18	0.43
1:S:249:ASP:CG	4:S:903:MGD:H1'	2.39	0.43
2:T:176:ILE:HG22	2:T:177:LYS:HG3	2.01	0.43
1:U:281:THR:O	1:U:285:GLU:HG3	2.19	0.43
1:W:175:SER:HB2	1:W:176:TRP:CE3	2.54	0.43
2:B:46:MET:HE1	2:B:65:PRO:HB3	2.00	0.42
1:C:800:ILE:HD12	1:C:800:ILE:N	2.33	0.42
1:G:649:LYS:HE3	1:G:651:THR:CG2	2.49	0.42
1:I:15:PRO:HD3	1:I:554:PHE:CE1	2.54	0.42
1:I:175:SER:OG	6:I:905:PYG:C1	2.65	0.42
2:J:3:GLN:O	2:J:158:LYS:HA	2.18	0.42
2:J:20:PHE:CZ	2:J:24:MET:HE1	2.54	0.42
2:J:21:MET:HE1	2:J:24:MET:CE	2.49	0.42
2:N:114:MET:HA	2:N:125:LYS:HB3	2.01	0.42
2:R:16:CYS:O	2:R:17:ASN:HB2	2.19	0.42
1:S:251:HIS:HA	1:S:809:LEU:HD23	2.00	0.42
2:T:21:MET:HE2	2:T:21:MET:CA	2.47	0.42
1:U:451:LYS:HG3	1:U:461:PHE:CE2	2.54	0.42
1:W:182:GLY:HA3	1:W:364:ILE:HG23	2.01	0.42
1:W:433:PHE:HA	1:W:434:PRO:HD3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:MET:HE2	2:B:146:ALA:CB	2.49	0.42
2:D:70:HIS:CD2	2:D:92:VAL:H	2.31	0.42
1:E:176:TRP:O	1:E:177:GLU:C	2.57	0.42
1:E:366:TRP:O	1:E:370:MET:HG2	2.19	0.42
1:E:175:SER:OG	6:E:905:PYG:C1	2.67	0.42
2:F:95:ASP:HB3	2:F:98:LYS:HB2	2.01	0.42
1:I:2:GLY:O	1:I:21:LYS:HE3	2.19	0.42
1:I:708:ARG:HD2	8:I:1043:HOH:O	2.18	0.42
1:K:495:LYS:HD2	1:K:514:TYR:OH	2.19	0.42
1:O:173:PRO:HA	1:O:468:PHE:CE1	2.55	0.42
2:P:159:THR:OG1	2:P:160:THR:N	2.52	0.42
1:Q:219:PRO:HD2	1:Q:255:THR:OG1	2.19	0.42
1:Q:521:PHE:CE2	1:Q:523:VAL:HG22	2.54	0.42
1:Q:610:LYS:HB3	1:Q:614:ALA:HB3	2.00	0.42
1:Q:66:PHE:HA	1:Q:69:MET:CE	2.48	0.42
1:Q:677:CYS:C	1:Q:678:ARG:HG2	2.39	0.42
1:Q:77:PRO:HB2	1:Q:78:TYR:CE2	2.53	0.42
1:S:176:TRP:O	1:S:177:GLU:C	2.57	0.42
1:U:79:PRO:HB2	1:U:112:ILE:O	2.19	0.42
1:U:28:MET:HE1	1:U:67:LYS:H	1.84	0.42
1:U:69:MET:HE1	1:U:754:MET:HE3	2.00	0.42
1:U:144:HIS:NE2	6:U:905:PYG:O1	2.48	0.42
2:V:87:ARG:HB2	2:V:89:ASP:OD2	2.19	0.42
2:X:81:ASN:OD1	2:X:81:ASN:O	2.37	0.42
2:B:5:TYR:HB2	2:B:157:LEU:HD13	2.02	0.42
1:C:166:PHE:H	1:C:439:LEU:HD12	1.84	0.42
1:C:28:MET:HE3	1:C:63:THR:O	2.19	0.42
1:E:736:SER:OG	4:E:902:MGD:N19	2.48	0.42
1:G:756:TYR:CZ	2:H:41:ARG:HB3	2.54	0.42
2:L:23:CYS:O	2:L:27:HIS:N	2.45	0.42
1:M:737:PRO:HG3	4:M:903:MGD:H2'	2.01	0.42
1:O:272:HIS:ND1	1:O:272:HIS:N	2.68	0.42
2:P:5:TYR:CE2	2:P:164:MET:HG2	2.54	0.42
1:S:269:GLY:HA2	1:S:362:HIS:CE1	2.55	0.42
2:V:10:VAL:HG13	2:V:63:TYR:O	2.20	0.42
1:W:402:PRO:HG2	1:W:422:PHE:CE1	2.54	0.42
2:X:244:GLU:HG3	2:X:261:VAL:HG22	2.00	0.42
1:A:258:LEU:HG	1:A:259:VAL:HG13	2.00	0.42
1:A:533:VAL:HG12	1:A:539:ILE:HD13	2.02	0.42
1:E:404:TYR:CD1	1:E:405:ALA:N	2.87	0.42
1:E:433:PHE:CD1	1:E:433:PHE:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:736:SER:O	4:I:902:MGD:N18	2.52	0.42
2:J:4:TYR:CE2	2:J:158:LYS:HD2	2.55	0.42
1:K:691:ILE:HD11	1:K:711:MET:HE3	2.00	0.42
1:M:540:LEU:HA	1:M:541:PRO:HD3	1.81	0.42
1:M:800:ILE:CD1	1:M:833:ALA:HB1	2.49	0.42
1:O:44:ILE:HG23	1:O:203:GLU:HG3	2.01	0.42
2:P:5:TYR:CD2	2:P:164:MET:HG2	2.54	0.42
1:S:411:GLY:HA3	1:S:434:PRO:HB3	2.01	0.42
1:S:561:ILE:CG2	1:S:564:ASN:HB3	2.47	0.42
2:B:105:LEU:HB3	2:B:114:MET:HE1	2.01	0.42
2:B:142:MET:HE3	2:B:146:ALA:HB1	2.01	0.42
2:B:5:TYR:O	2:B:157:LEU:HD12	2.20	0.42
1:E:563:ASP:HA	1:E:565:TYR:CE1	2.54	0.42
1:G:396:ASP:OD2	1:G:398:GLU:HB2	2.20	0.42
1:G:744:HIS:HA	1:G:819:SER:HB3	2.02	0.42
1:I:735:LEU:HD23	1:I:735:LEU:H	1.85	0.42
1:K:720:SER:O	1:K:724:SER:HB3	2.18	0.42
2:N:3:GLN:O	2:N:158:LYS:HA	2.20	0.42
1:O:15:PRO:HB2	1:O:31:MET:SD	2.59	0.42
1:O:387:TRP:CZ2	1:O:389:THR:HA	2.55	0.42
1:O:452:ILE:N	1:O:453:PRO:CD	2.81	0.42
1:S:700:GLU:HG2	8:S:1563:HOH:O	2.19	0.42
1:S:737:PRO:CG	4:S:903:MGD:H2'	2.50	0.42
1:S:816:SER:OG	1:S:839:ILE:HG13	2.18	0.42
1:U:10:SER:HA	1:U:15:PRO:HA	2.01	0.42
1:U:162:ASN:HD22	1:U:166:PHE:HE2	1.67	0.42
2:V:168:VAL:HG13	2:V:173:LEU:HB2	2.01	0.42
1:W:142:SER:CB	4:W:902:MGD:O1A	2.67	0.42
1:W:839:ILE:HA	1:W:839:ILE:HD13	1.92	0.42
1:A:418:ALA:HB1	1:A:423:ALA:HB2	2.00	0.42
1:A:452:ILE:HB	1:A:453:PRO:HD3	2.01	0.42
2:B:9:ASP:HA	2:B:189:LYS:HB3	2.00	0.42
1:C:146:MET:HE3	1:C:545:ASN:OD1	2.20	0.42
1:C:211:MET:HE1	2:D:231:PHE:HZ	1.85	0.42
1:E:610:LYS:NZ	1:E:618:GLN:NE2	2.57	0.42
1:G:249:ASP:OD2	4:G:903:MGD:H1'	2.19	0.42
1:G:277:ALA:HB2	1:G:321:ALA:HB2	2.01	0.42
1:G:387:TRP:CZ2	1:G:389:THR:HA	2.55	0.42
1:G:426:MET:HA	1:G:426:MET:CE	2.50	0.42
1:I:378:GLY:O	1:I:381:LYS:HG2	2.20	0.42
1:I:540:LEU:HA	1:I:541:PRO:HD3	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:782:ARG:HH11	1:I:782:ARG:HG3	1.85	0.42
2:J:166:LYS:HG2	2:J:170:GLU:OE2	2.20	0.42
2:J:71:CYS:HA	2:J:184:PRO:HA	2.01	0.42
2:L:23:CYS:HB3	2:L:39:MET:CE	2.49	0.42
1:M:610:LYS:HZ3	1:M:618:GLN:NE2	2.10	0.42
1:O:13:GLY:HA3	1:O:63:THR:OG1	2.19	0.42
2:P:10:VAL:HG13	2:P:63:TYR:O	2.19	0.42
1:S:651:THR:HB	1:S:665:THR:HG22	2.01	0.42
1:S:735:LEU:HD23	1:S:735:LEU:H	1.84	0.42
1:U:797:GLY:HA2	1:U:875:TYR:CD2	2.54	0.42
2:B:164:MET:O	2:B:168:VAL:HG23	2.19	0.42
1:C:395:LEU:HD13	1:C:571:ARG:HG2	2.02	0.42
1:I:250:PRO:HD3	4:I:903:MGD:C2	2.50	0.42
1:I:521:PHE:CE2	1:I:523:VAL:CG2	3.02	0.42
1:I:56:LYS:HG2	1:I:57:THR:O	2.19	0.42
2:J:177:LYS:N	2:J:178:PRO:HD3	2.34	0.42
1:I:262:LYS:HG2	2:J:232:PHE:CE1	2.54	0.42
1:K:269:GLY:HA2	1:K:362:HIS:CG	2.54	0.42
1:M:364:ILE:HD13	1:M:708:ARG:HG3	2.01	0.42
2:N:126:CYS:HB2	8:N:466:HOH:O	2.20	0.42
1:O:239:LYS:HE2	8:O:1595:HOH:O	2.20	0.42
2:P:46:MET:HE3	2:P:66:THR:N	2.35	0.42
1:Q:103:GLN:CD	1:Q:103:GLN:N	2.73	0.42
1:Q:730:TYR:CZ	1:Q:794:ASN:HA	2.54	0.42
1:S:250:PRO:HD3	4:S:903:MGD:C2	2.49	0.42
1:U:554:PHE:HB3	8:U:1031:HOH:O	2.20	0.42
1:W:427:PHE:HB3	8:W:1027:HOH:O	2.20	0.42
1:W:744:HIS:HA	1:W:819:SER:HB3	2.02	0.42
1:A:328:PRO:HB2	1:A:331:GLU:HG3	2.02	0.42
1:A:521:PHE:CE2	1:A:523:VAL:CG2	3.02	0.42
2:B:124:GLN:O	2:B:125:LYS:HB3	2.20	0.42
1:C:426:MET:HA	1:C:426:MET:CE	2.44	0.42
1:C:76:ILE:HA	1:C:77:PRO:HD3	1.77	0.42
1:E:68:SER:HB3	1:E:753:TYR:CE2	2.55	0.42
1:G:565:TYR:C	1:G:567:LEU:H	2.23	0.42
1:G:730:TYR:HB3	1:G:862:VAL:CA	2.50	0.42
1:G:211:MET:CE	2:H:231:PHE:CZ	3.02	0.42
1:K:66:PHE:HA	1:K:69:MET:HE2	2.02	0.42
1:K:76:ILE:HA	1:K:77:PRO:HD3	1.73	0.42
1:K:250:PRO:HD3	4:K:903:MGD:C2	2.50	0.42
1:M:69:MET:HE1	1:M:754:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:166:LYS:HG2	2:N:170:GLU:OE2	2.20	0.42
1:O:510:TYR:O	1:O:513:MET:HG2	2.20	0.42
1:Q:625:MET:N	1:Q:626:PRO:CD	2.83	0.42
1:S:163:MET:CE	1:S:606:PHE:HA	2.50	0.42
1:S:426:MET:HE3	1:S:622:ALA:HB2	2.01	0.42
2:T:70:HIS:HD2	2:T:92:VAL:N	2.00	0.42
1:U:673:ASN:ND2	1:U:673:ASN:H	2.18	0.42
2:V:191:LEU:HG	2:V:195:GLU:HG3	2.01	0.42
1:W:729:LYS:HD2	8:W:1132:HOH:O	2.18	0.42
1:W:528:TRP:CD2	1:W:750:LYS:HD3	2.55	0.42
1:A:565:TYR:C	1:A:567:LEU:H	2.24	0.42
1:A:69:MET:HE2	1:A:754:MET:HE1	2.02	0.42
1:C:737:PRO:CG	4:C:903:MGD:H2'	2.50	0.42
1:E:571:ARG:HA	8:E:1026:HOH:O	2.20	0.42
1:G:736:SER:O	4:G:902:MGD:N18	2.53	0.42
1:I:501:LEU:HD13	1:I:823:TYR:CG	2.55	0.42
1:I:847:TYR:CZ	1:I:853:CYS:HB3	2.55	0.42
1:K:505:THR:HB	1:K:845:ASP:HA	2.01	0.42
1:M:763:GLU:HA	1:M:768:LYS:HA	2.01	0.42
1:O:114:TRP:CZ2	1:O:587:MET:HG2	2.54	0.42
1:O:162:ASN:HD22	1:O:166:PHE:HE2	1.68	0.42
1:O:401:PHE:HA	1:O:402:PRO:HD3	1.86	0.42
1:O:770:TRP:HB3	1:O:801:LEU:HD23	2.02	0.42
1:O:249:ASP:CG	4:O:903:MGD:H1'	2.40	0.42
2:P:166:LYS:HE2	2:P:170:GLU:OE2	2.20	0.42
2:P:81:ASN:O	2:P:81:ASN:OD1	2.36	0.42
1:Q:620:PHE:CZ	1:Q:625:MET:HB3	2.55	0.42
2:R:122:VAL:HG22	2:R:123:ALA:N	2.35	0.42
2:R:164:MET:O	2:R:168:VAL:HG23	2.20	0.42
1:S:563:ASP:O	1:S:566:GLN:HG2	2.19	0.42
1:S:56:LYS:HG2	1:S:57:THR:O	2.20	0.42
1:S:69:MET:CE	1:S:754:MET:HE3	2.49	0.42
2:T:53:ARG:HB2	2:T:60:ASP:OD1	2.20	0.42
1:U:173:PRO:HG3	1:U:180:HIS:CG	2.55	0.42
1:U:396:ASP:OD2	1:U:398:GLU:HB2	2.20	0.42
1:U:498:GLY:N	1:U:499:PRO:HD3	2.35	0.42
1:U:786:ASN:HD22	1:U:805:VAL:N	2.16	0.42
1:W:338:GLN:OE1	1:W:341:LYS:HE3	2.19	0.42
1:W:387:TRP:CZ2	1:W:389:THR:HA	2.54	0.42
2:X:139:ALA:O	2:X:141:LYS:HG3	2.19	0.42
1:A:12:THR:HB	1:A:743:MET:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:ASN:HD22	2:B:59:ASN:H	1.67	0.42
1:C:540:LEU:HA	1:C:541:PRO:HD3	1.83	0.42
1:C:557:CYS:H	1:C:564:ASN:ND2	1.94	0.42
1:C:691:ILE:HD11	1:C:711:MET:CE	2.50	0.42
1:E:288:TYR:HB2	1:E:376:MET:O	2.20	0.42
1:G:76:ILE:HG22	1:G:541:PRO:HG3	2.02	0.42
1:I:452:ILE:HB	1:I:453:PRO:HD3	2.02	0.42
1:I:605:MET:N	1:I:605:MET:SD	2.91	0.42
1:K:498:GLY:N	1:K:499:PRO:HD3	2.35	0.42
1:O:56:LYS:HG2	1:O:57:THR:N	2.35	0.42
1:O:605:MET:SD	1:O:605:MET:N	2.90	0.42
1:O:262:LYS:HG2	2:P:232:PHE:CE1	2.55	0.42
2:P:46:MET:HE1	2:P:65:PRO:C	2.39	0.42
1:Q:74:LEU:HA	1:Q:74:LEU:HD23	1.90	0.42
1:Q:782:ARG:HD3	1:Q:864:ILE:O	2.20	0.42
1:S:401:PHE:HA	1:S:402:PRO:HD3	1.79	0.42
2:T:40:GLN:NE2	2:T:118:GLU:H	2.14	0.42
1:S:67:LYS:NZ	2:T:25:ASP:O	2.49	0.42
2:V:74:ALA:HA	2:V:75:PRO:HD3	1.93	0.42
1:W:13:GLY:HA3	1:W:63:THR:OG1	2.20	0.42
1:W:495:LYS:HD2	1:W:514:TYR:OH	2.20	0.42
1:W:782:ARG:HG3	1:W:782:ARG:HH11	1.85	0.42
2:B:39:MET:HE2	2:B:45:TRP:CD2	2.55	0.41
1:C:744:HIS:HA	1:C:819:SER:HB3	2.02	0.41
2:D:270:GLY:HA2	8:D:534:HOH:O	2.20	0.41
1:E:521:PHE:CE2	1:E:523:VAL:CG2	3.03	0.41
1:E:748:ASP:O	1:E:750:LYS:HG3	2.20	0.41
2:F:114:MET:HA	2:F:125:LYS:HB3	2.01	0.41
2:F:94:ILE:HG13	2:F:125:LYS:HE3	2.02	0.41
1:G:404:TYR:CD1	1:G:405:ALA:N	2.88	0.41
1:I:644:ASP:C	1:I:646:PRO:HD3	2.39	0.41
2:J:2:GLU:HG3	2:J:159:THR:C	2.40	0.41
1:K:35:ASP:OD1	1:K:55:ARG:HD3	2.20	0.41
1:K:563:ASP:O	1:K:566:GLN:HG2	2.20	0.41
1:M:460:LYS:HG3	8:M:1230:HOH:O	2.18	0.41
1:O:218:ASP:OD2	1:O:253:ASN:HB2	2.20	0.41
1:O:15:PRO:HD3	1:O:554:PHE:CE1	2.55	0.41
2:P:40:GLN:NE2	8:P:441:HOH:O	2.52	0.41
1:S:387:TRP:CZ2	1:S:389:THR:HA	2.55	0.41
1:S:296:ASN:O	1:S:687:LYS:HB3	2.20	0.41
2:T:19:CYS:HA	2:T:145:CYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:489:LYS:HG3	8:W:1212:HOH:O	2.19	0.41
1:A:553:GLU:HG2	1:A:556:ASN:HB2	2.02	0.41
1:C:404:TYR:CD1	1:C:405:ALA:N	2.88	0.41
1:C:55:ARG:HG3	8:C:1548:HOH:O	2.19	0.41
1:C:776:SER:HA	1:C:805:VAL:HG13	2.01	0.41
1:C:868:ASP:OD1	1:C:870:ASP:HB2	2.20	0.41
1:E:249:ASP:OD2	4:E:903:MGD:H1'	2.19	0.41
1:I:737:PRO:CG	4:I:903:MGD:H2'	2.50	0.41
1:K:269:GLY:HA2	1:K:362:HIS:CE1	2.55	0.41
1:M:76:ILE:CG2	1:M:541:PRO:HG3	2.50	0.41
1:Q:649:LYS:HE2	8:Q:1454:HOH:O	2.20	0.41
1:Q:76:ILE:HA	1:Q:77:PRO:HD3	1.75	0.41
1:U:107:SER:HB3	8:U:1624:HOH:O	2.20	0.41
1:E:13:GLY:HA3	1:E:63:THR:OG1	2.20	0.41
1:G:296:ASN:O	1:G:687:LYS:HB3	2.21	0.41
2:H:105:LEU:HB3	2:H:114:MET:HE3	2.02	0.41
1:I:39:ALA:HA	1:I:40:PRO:HD3	1.87	0.41
2:J:60:ASP:OD1	2:J:60:ASP:C	2.59	0.41
1:M:269:GLY:HA2	1:M:362:HIS:CE1	2.55	0.41
1:M:402:PRO:HG2	1:M:422:PHE:CE1	2.55	0.41
1:O:78:TYR:C	1:O:541:PRO:HG2	2.40	0.41
2:P:19:CYS:O	2:P:22:GLY:N	2.53	0.41
1:Q:56:LYS:HE2	8:Q:1461:HOH:O	2.20	0.41
1:Q:716:PRO:HB3	1:Q:723:HIS:CD2	2.55	0.41
1:Q:724:SER:HA	1:Q:725:PRO:HD3	1.91	0.41
1:U:252:MET:HE3	8:V:965:HOH:O	2.20	0.41
2:V:213:ALA:O	2:V:228:GLU:HA	2.20	0.41
1:W:770:TRP:HB3	1:W:801:LEU:HD23	2.01	0.41
1:W:9:ASN:HA	1:W:576:GLN:HA	2.01	0.41
2:X:135:ASP:OD1	2:X:137:SER:HB2	2.19	0.41
1:A:735:LEU:HD23	1:A:735:LEU:H	1.84	0.41
1:A:770:TRP:HB3	1:A:801:LEU:HD23	2.02	0.41
2:B:23:CYS:HB3	2:B:39:MET:CE	2.51	0.41
1:C:224:GLY:O	1:C:225:ILE:HB	2.20	0.41
1:E:233:ILE:HD11	8:E:1179:HOH:O	2.19	0.41
1:E:35:ASP:OD1	1:E:55:ARG:HD3	2.20	0.41
1:G:12:THR:HG23	8:G:1326:HOH:O	2.20	0.41
1:I:656:TRP:CG	1:I:663:LYS:HA	2.54	0.41
1:K:128:ILE:CD1	1:K:492:MET:HB2	2.50	0.41
1:K:323:GLU:HB2	8:K:1567:HOH:O	2.20	0.41
1:M:257:ARG:HD3	2:N:61:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:561:ILE:CG2	1:O:564:ASN:HB3	2.51	0.41
1:Q:587:MET:HG3	1:Q:592:ILE:CG1	2.51	0.41
1:S:175:SER:HB2	1:S:176:TRP:CE3	2.55	0.41
1:S:74:LEU:HD12	1:S:750:LYS:HA	2.02	0.41
2:T:46:MET:HE1	2:T:65:PRO:HA	2.02	0.41
1:U:66:PHE:CZ	1:U:146:MET:CE	3.03	0.41
1:U:549:TRP:CG	1:U:613:LEU:HD13	2.55	0.41
1:U:708:ARG:HD2	8:U:1049:HOH:O	2.19	0.41
1:W:722:LYS:HE3	1:W:722:LYS:HB2	1.88	0.41
1:W:250:PRO:HD3	4:W:903:MGD:C2	2.51	0.41
1:W:96:ARG:HD2	1:W:514:TYR:O	2.20	0.41
2:X:124:GLN:O	2:X:125:LYS:HB3	2.19	0.41
1:A:21:LYS:CB	1:A:26:ILE:HD11	2.50	0.41
1:E:347:ALA:CB	1:E:388:SER:HA	2.51	0.41
1:E:69:MET:HE1	1:E:754:MET:HE3	2.02	0.41
1:I:625:MET:N	1:I:626:PRO:CD	2.84	0.41
1:I:69:MET:CE	1:I:754:MET:HE3	2.51	0.41
2:J:204:LEU:HD23	2:J:209:CYS:HA	2.01	0.41
1:M:625:MET:N	1:M:626:PRO:CD	2.83	0.41
1:M:249:ASP:OD2	4:M:903:MGD:HI1'	2.21	0.41
1:Q:13:GLY:O	1:Q:59:ILE:HA	2.20	0.41
1:Q:277:ALA:HB2	1:Q:321:ALA:HB2	2.01	0.41
1:Q:613:LEU:HA	1:Q:613:LEU:HD12	1.94	0.41
1:S:166:PHE:N	1:S:439:LEU:HD12	2.36	0.41
1:S:724:SER:HA	1:S:725:PRO:HD3	1.94	0.41
1:U:201:LEU:HD13	1:U:387:TRP:HB2	2.02	0.41
1:U:426:MET:CE	1:U:426:MET:HA	2.50	0.41
1:W:142:SER:HB3	4:W:902:MGD:O1A	2.20	0.41
1:W:173:PRO:HG3	1:W:180:HIS:CG	2.56	0.41
1:W:476:GLN:OE1	1:W:708:ARG:NH2	2.54	0.41
1:W:143:SER:N	4:W:902:MGD:O1A	2.53	0.41
2:X:5:TYR:CD2	2:X:164:MET:HG2	2.55	0.41
1:A:396:ASP:OD2	1:A:398:GLU:HB2	2.21	0.41
1:C:402:PRO:HG2	1:C:422:PHE:CE1	2.55	0.41
1:C:56:LYS:HG2	1:C:57:THR:O	2.20	0.41
1:C:211:MET:HE3	2:D:231:PHE:CZ	2.55	0.41
1:E:28:MET:HE3	1:E:63:THR:O	2.21	0.41
1:E:114:TRP:CZ2	1:E:587:MET:HG2	2.56	0.41
1:K:225:ILE:HG12	1:K:226:TYR:CD1	2.55	0.41
2:L:142:MET:CE	2:L:146:ALA:HB1	2.49	0.41
2:L:210:PHE:HD2	2:L:213:ALA:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:736:SER:O	4:M:902:MGD:N18	2.53	0.41
2:N:154:TYR:CE1	7:N:302:SF4:S4	3.13	0.41
1:O:269:GLY:HA2	1:O:362:HIS:ND1	2.36	0.41
1:O:95:LEU:HD23	1:O:95:LEU:HA	1.89	0.41
2:P:218:LYS:HG2	2:P:223:GLU:N	2.36	0.41
1:Q:44:ILE:HD11	1:Q:394:PRO:CG	2.50	0.41
1:S:786:ASN:HD21	1:S:804:GLN:HA	1.85	0.41
2:T:40:GLN:HB3	2:T:43:HIS:CE1	2.56	0.41
1:U:105:PRO:HD2	8:U:1425:HOH:O	2.21	0.41
1:W:162:ASN:HD22	1:W:166:PHE:HE2	1.69	0.41
1:W:554:PHE:HB3	8:W:1025:HOH:O	2.20	0.41
2:X:173:LEU:HB3	2:X:187:TYR:HB3	2.03	0.41
1:A:404:TYR:CD1	1:A:405:ALA:N	2.88	0.41
2:B:125:LYS:HD2	2:B:126:CYS:O	2.20	0.41
1:C:76:ILE:CG2	1:C:541:PRO:HG3	2.50	0.41
1:E:617:GLU:HG3	1:E:631:TRP:CG	2.55	0.41
2:F:210:PHE:CE2	2:F:251:ALA:HB1	2.55	0.41
1:G:176:TRP:CD1	1:G:193:LEU:HB2	2.55	0.41
2:H:21:MET:CA	2:H:21:MET:HE3	2.51	0.41
1:M:21:LYS:CB	1:M:26:ILE:HD11	2.50	0.41
1:M:597:ALA:HB1	1:M:603:GLU:HA	2.03	0.41
1:M:175:SER:OG	6:M:905:PYG:C1	2.68	0.41
1:O:734:MET:HB2	1:O:814:VAL:HG23	2.03	0.41
2:P:124:GLN:O	2:P:125:LYS:HB3	2.20	0.41
2:R:13:CYS:HB3	2:R:63:TYR:HB2	2.02	0.41
1:A:211:MET:HE1	2:B:231:PHE:CZ	2.54	0.41
1:A:263:TRP:CZ2	1:A:265:SER:HB2	2.55	0.41
1:C:138:LEU:HB2	1:C:490:ILE:CD1	2.50	0.41
1:C:272:HIS:N	1:C:272:HIS:ND1	2.67	0.41
1:C:670:PRO:HG2	1:C:675:GLN:CD	2.41	0.41
1:E:10:SER:HA	1:E:15:PRO:HA	2.03	0.41
2:F:106:LEU:HD22	2:F:114:MET:HB3	2.02	0.41
2:H:166:LYS:HE2	2:H:170:GLU:OE2	2.19	0.41
1:I:155:SER:HA	1:I:407:GLY:O	2.21	0.41
2:J:106:LEU:HA	2:J:114:MET:HG3	2.02	0.41
2:J:198:TYR:HB3	2:J:238:ASP:HA	2.03	0.41
1:M:501:LEU:HB2	8:M:1360:HOH:O	2.20	0.41
2:N:26:GLU:HB2	2:N:144:ARG:HH11	1.84	0.41
1:O:11:SER:HA	1:O:147:TRP:HB2	2.02	0.41
1:O:153:ARG:O	1:O:157:TYR:HB3	2.20	0.41
1:O:391:GLN:HG2	1:O:567:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:870:ASP:HB3	1:O:872:TYR:CE1	2.55	0.41
1:Q:691:ILE:HD11	1:Q:711:MET:CE	2.51	0.41
1:S:426:MET:CA	1:S:426:MET:HE3	2.33	0.41
1:U:99:GLY:HA2	1:U:102:LYS:HG2	2.01	0.41
1:U:867:TRP:CE2	1:U:869:GLY:HA2	2.55	0.41
1:W:21:LYS:HB3	1:W:26:ILE:HD11	2.02	0.41
1:C:356:GLY:H	4:C:903:MGD:C5'	2.26	0.41
1:C:433:PHE:HA	1:C:434:PRO:HD3	1.81	0.41
1:C:739:PRO:HG2	1:C:742:SER:O	2.21	0.41
2:D:13:CYS:HB3	2:D:63:TYR:HB2	2.03	0.41
2:D:16:CYS:O	2:D:17:ASN:HB2	2.21	0.41
2:D:46:MET:HE1	2:D:66:THR:H	1.80	0.41
1:E:501:LEU:HA	1:E:507:THR:HB	2.02	0.41
1:E:187:TRP:HB2	1:E:681:LEU:HD13	2.03	0.41
1:I:100:LEU:HD12	1:I:105:PRO:HG3	2.02	0.41
1:K:328:PRO:HB2	1:K:331:GLU:HG3	2.02	0.41
1:O:356:GLY:HA2	1:O:359:ARG:NH1	2.36	0.41
1:Q:287:SER:HB2	1:Q:340:ALA:HB1	2.02	0.41
1:Q:39:ALA:HA	1:Q:40:PRO:HD3	1.91	0.41
1:Q:565:TYR:C	1:Q:567:LEU:N	2.74	0.41
1:Q:249:ASP:OD2	4:Q:903:MGD:H1'	2.21	0.41
1:S:263:TRP:CZ2	1:S:265:SER:HB2	2.55	0.41
1:S:39:ALA:HA	1:S:40:PRO:HD3	1.90	0.41
1:S:737:PRO:HB3	4:S:903:MGD:H3'	2.03	0.41
1:U:146:MET:HE3	8:U:1475:HOH:O	2.21	0.41
1:U:719:GLU:HG2	1:U:859:THR:O	2.21	0.41
2:V:39:MET:HE2	2:V:45:TRP:CD2	2.55	0.41
2:X:46:MET:CE	2:X:66:THR:H	2.33	0.41
1:A:425:ARG:HD3	1:A:622:ALA:O	2.20	0.41
1:C:565:TYR:C	1:C:567:LEU:H	2.24	0.41
1:E:426:MET:HE1	1:E:618:GLN:C	2.41	0.41
2:F:19:CYS:O	2:F:22:GLY:N	2.53	0.41
2:F:77:VAL:HG22	2:F:84:VAL:HG12	2.02	0.41
1:G:277:ALA:HA	1:G:316:LYS:O	2.21	0.41
2:H:106:LEU:CD2	2:H:114:MET:HB3	2.50	0.41
2:H:216:VAL:HG13	2:H:223:GLU:HG3	2.03	0.41
2:H:254:LYS:HD2	2:H:274:LEU:OXT	2.21	0.41
1:I:146:MET:CE	1:I:545:ASN:OD1	2.68	0.41
2:J:245:TYR:HB2	2:J:260:VAL:CG1	2.51	0.41
1:K:561:ILE:N	1:K:562:PRO:HD3	2.36	0.41
2:P:1:MET:HG3	2:P:88:GLU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:165:GLY:CA	1:Q:166:PHE:HB3	2.43	0.41
1:S:96:ARG:HD2	1:S:514:TYR:O	2.21	0.41
1:S:670:PRO:HG2	1:S:675:GLN:CD	2.41	0.41
2:V:204:LEU:HD23	2:V:209:CYS:HA	2.02	0.41
1:W:171:HIS:HD2	8:W:1457:HOH:O	2.04	0.41
1:W:645:ASN:HD22	1:W:648:ARG:HB3	1.84	0.41
1:W:144:HIS:HB2	4:W:902:MGD:O1B	2.21	0.41
2:X:60:ASP:C	2:X:60:ASP:OD1	2.59	0.41
2:B:105:LEU:HB3	2:B:114:MET:CE	2.51	0.41
1:C:100:LEU:HD22	1:C:534:PRO:HB2	2.02	0.41
2:D:118:GLU:O	2:D:121:ASN:ND2	2.54	0.41
1:E:162:ASN:HD22	1:E:166:PHE:HE2	1.68	0.41
1:E:175:SER:HB2	1:E:176:TRP:CZ3	2.56	0.41
1:E:828:THR:HG21	1:E:831:LYS:HD2	2.03	0.41
1:G:66:PHE:HZ	1:G:146:MET:CE	2.34	0.41
1:G:165:GLY:HA3	1:G:166:PHE:CB	2.37	0.41
1:I:146:MET:HG2	4:I:902:MGD:N7	2.36	0.41
1:K:565:TYR:C	1:K:567:LEU:H	2.24	0.41
1:M:263:TRP:CZ2	1:M:265:SER:HB2	2.56	0.41
1:M:498:GLY:N	1:M:499:PRO:HD3	2.36	0.41
1:O:274:LEU:O	1:O:278:ILE:HG13	2.21	0.41
2:P:105:LEU:HB3	2:P:114:MET:HE2	2.03	0.41
2:P:167:LYS:HZ3	2:P:171:GLU:CD	2.24	0.41
1:Q:140:THR:HB	1:Q:169:ALA:HB3	2.02	0.41
1:Q:61:PRO:HG3	2:R:16:CYS:HB2	2.03	0.41
1:Q:66:PHE:CZ	1:Q:146:MET:CE	3.04	0.41
1:S:107:SER:HB3	8:S:1619:HOH:O	2.20	0.41
1:U:301:GLU:CD	1:U:301:GLU:H	2.24	0.41
1:W:439:LEU:HD21	1:W:487:TYR:CE2	2.56	0.41
1:W:704:ILE:HG23	8:W:1646:HOH:O	2.21	0.41
2:X:216:VAL:HG13	2:X:223:GLU:HG3	2.03	0.41
2:X:99:ALA:O	2:X:100:LYS:C	2.59	0.41
1:A:347:ALA:CB	1:A:388:SER:HA	2.51	0.40
1:A:395:LEU:HD13	1:A:571:ARG:CG	2.51	0.40
1:A:691:ILE:HD11	1:A:711:MET:CE	2.50	0.40
1:C:274:LEU:O	1:C:278:ILE:HG13	2.20	0.40
1:C:387:TRP:CZ2	1:C:389:THR:HA	2.56	0.40
1:E:565:TYR:C	1:E:567:LEU:N	2.74	0.40
2:F:18:ASN:HB2	7:F:302:SF4:S1	2.61	0.40
1:G:476:GLN:HG2	8:G:1279:HOH:O	2.20	0.40
1:G:730:TYR:HB3	1:G:862:VAL:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:100:LEU:HD22	1:K:534:PRO:HB2	2.03	0.40
2:L:1:MET:CG	2:L:88:GLU:HB3	2.49	0.40
1:M:128:ILE:HD12	1:M:492:MET:HB2	2.01	0.40
1:M:695:LEU:HD22	1:M:708:ARG:HD3	2.03	0.40
1:O:426:MET:HE2	1:O:618:GLN:CG	2.47	0.40
1:O:610:LYS:NZ	1:O:618:GLN:NE2	2.57	0.40
1:Q:647:ASN:HB2	8:Q:1437:HOH:O	2.20	0.40
1:Q:95:LEU:HD23	1:Q:95:LEU:HA	1.90	0.40
1:S:347:ALA:CB	1:S:388:SER:HA	2.51	0.40
1:U:393:VAL:HA	1:U:394:PRO:HD3	1.86	0.40
2:V:139:ALA:HB3	2:V:140:PRO:HD3	2.03	0.40
2:V:29:LEU:HD23	2:V:29:LEU:HA	1.91	0.40
1:A:604:GLU:HB3	1:A:605:MET:CE	2.52	0.40
1:C:393:VAL:HA	1:C:394:PRO:HD3	1.78	0.40
1:C:13:GLY:HA3	1:C:63:THR:OG1	2.21	0.40
1:E:540:LEU:HA	1:E:541:PRO:HD3	1.83	0.40
1:I:192:ARG:CZ	1:I:562:PRO:HD2	2.51	0.40
1:K:75:ARG:HH22	1:K:547:GLU:CD	2.24	0.40
1:K:786:ASN:HD22	1:K:805:VAL:H	1.66	0.40
1:M:378:GLY:O	1:M:381:LYS:HG2	2.21	0.40
1:M:782:ARG:HH11	1:M:782:ARG:HG3	1.85	0.40
1:O:630:THR:OG1	1:O:633:GLU:HG3	2.20	0.40
1:O:670:PRO:HB3	1:O:682:GLN:HB2	2.03	0.40
1:O:767:TYR:HB3	1:O:769:TYR:CE1	2.57	0.40
2:P:210:PHE:HD2	2:P:213:ALA:HB2	1.87	0.40
1:Q:670:PRO:HG2	1:Q:675:GLN:CD	2.41	0.40
1:S:211:MET:HE1	2:T:231:PHE:CZ	2.56	0.40
1:U:499:PRO:CB	1:U:745:THR:HG21	2.51	0.40
1:W:155:SER:OG	1:W:409:ILE:HG12	2.20	0.40
1:W:258:LEU:HG	1:W:259:VAL:HG13	2.02	0.40
1:W:354:TRP:HB3	1:W:355:GLY:H	1.76	0.40
2:B:139:ALA:HB3	2:B:140:PRO:HD3	2.03	0.40
1:C:541:PRO:HB2	1:C:586:SER:HA	2.03	0.40
1:C:62:TYR:HB3	1:C:742:SER:HA	2.03	0.40
1:C:724:SER:HA	1:C:725:PRO:HD3	1.94	0.40
2:D:210:PHE:O	2:D:233:GLY:HA2	2.21	0.40
1:E:642:VAL:HA	1:E:643:PRO:HD3	1.96	0.40
1:E:738:HIS:ND1	4:E:903:MGD:N15	2.70	0.40
1:E:92:ASN:N	1:E:93:PRO:HD3	2.36	0.40
1:G:714:TYR:O	1:G:716:PRO:HD3	2.22	0.40
1:I:249:ASP:OD2	4:I:903:MGD:H1'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:716:PRO:HB3	1:K:723:HIS:CG	2.56	0.40
2:N:159:THR:OG1	2:N:160:THR:N	2.52	0.40
2:N:95:ASP:HB3	2:N:98:LYS:HB2	2.04	0.40
1:Q:165:GLY:HA3	1:Q:166:PHE:CB	2.36	0.40
1:Q:200:ASP:HB3	8:Q:1055:HOH:O	2.21	0.40
1:Q:826:LEU:HD21	1:Q:835:ARG:HD3	2.04	0.40
2:T:52:GLU:CG	2:T:61:ILE:HD12	2.52	0.40
1:U:138:LEU:HB2	1:U:490:ILE:CD1	2.51	0.40
1:U:426:MET:O	1:U:426:MET:HE2	2.21	0.40
1:W:452:ILE:HB	1:W:453:PRO:HD3	2.04	0.40
1:A:433:PHE:CD1	1:A:433:PHE:N	2.88	0.40
1:A:505:THR:HG22	1:A:857:ASN:ND2	2.36	0.40
1:C:187:TRP:CH2	1:C:196:PRO:HB3	2.56	0.40
1:C:396:ASP:OD2	1:C:398:GLU:HB2	2.21	0.40
1:C:729:LYS:HD2	8:C:1131:HOH:O	2.21	0.40
1:E:15:PRO:HD2	8:E:1003:HOH:O	2.20	0.40
1:G:146:MET:CE	1:G:545:ASN:OD1	2.70	0.40
2:H:52:GLU:CG	2:H:61:ILE:HD12	2.52	0.40
1:I:2:GLY:N	1:I:22:ASP:OD1	2.55	0.40
1:K:328:PRO:O	1:K:332:ILE:HG13	2.21	0.40
1:M:491:LYS:HD3	8:M:1557:HOH:O	2.21	0.40
2:N:19:CYS:HA	2:N:145:CYS:HA	2.04	0.40
1:O:201:LEU:HD13	1:O:387:TRP:HB2	2.03	0.40
1:O:786:ASN:HD21	1:O:805:VAL:N	2.19	0.40
1:Q:10:SER:HA	1:Q:15:PRO:HA	2.04	0.40
1:S:362:HIS:HB3	1:S:717:ALA:HB2	2.03	0.40
1:S:378:GLY:O	1:S:381:LYS:HG2	2.22	0.40
1:S:722:LYS:HE3	1:S:722:LYS:HB2	1.87	0.40
1:U:353:GLY:O	1:U:354:TRP:HB2	2.21	0.40
1:U:211:MET:HE2	2:V:231:PHE:HZ	1.86	0.40
1:W:426:MET:HA	1:W:426:MET:CE	2.46	0.40
1:W:460:LYS:HE3	8:W:1232:HOH:O	2.22	0.40
1:W:141:PRO:CA	1:W:496:TYR:HB3	2.47	0.40
1:W:542:ALA:HA	1:W:587:MET:O	2.21	0.40
2:B:74:ALA:HA	2:B:75:PRO:HD3	1.85	0.40
1:C:356:GLY:HA2	1:C:359:ARG:NH1	2.36	0.40
2:D:105:LEU:HB3	2:D:114:MET:HE1	2.03	0.40
2:D:251:ALA:O	2:D:254:LYS:HB2	2.22	0.40
1:G:867:TRP:CE2	1:G:869:GLY:HA2	2.56	0.40
2:J:21:MET:HE3	2:J:21:MET:HA	2.02	0.40
1:K:274:LEU:O	1:K:278:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:528:TRP:CD2	1:K:750:LYS:HD3	2.57	0.40
2:L:142:MET:HB2	2:L:142:MET:HE2	1.85	0.40
1:K:211:MET:CE	2:L:231:PHE:CZ	3.04	0.40
1:M:176:TRP:CD1	1:M:193:LEU:HB2	2.57	0.40
1:M:180:HIS:HD2	1:M:193:LEU:HD22	1.86	0.40
1:O:347:ALA:CB	1:O:388:SER:HA	2.52	0.40
1:O:77:PRO:HB2	1:O:78:TYR:CD2	2.57	0.40
2:P:9:ASP:HA	2:P:189:LYS:HB3	2.04	0.40
2:P:23:CYS:O	2:P:27:HIS:N	2.47	0.40
1:Q:347:ALA:CB	1:Q:388:SER:HA	2.52	0.40
1:Q:628:TYR:CE2	1:Q:643:PRO:HG2	2.56	0.40
2:R:207:GLY:CA	1:U:728:VAL:HG12	2.31	0.40
2:V:106:LEU:CD2	2:V:114:MET:HG3	2.51	0.40
2:V:46:MET:CE	2:V:66:THR:H	2.33	0.40
1:W:404:TYR:CD1	1:W:405:ALA:N	2.90	0.40
1:W:426:MET:HE1	1:W:618:GLN:C	2.41	0.40
1:W:499:PRO:HB2	1:W:745:THR:HG21	2.04	0.40
1:W:598:LYS:HA	1:W:603:GLU:HB2	2.03	0.40
1:W:249:ASP:CG	4:W:903:MGD:H1'	2.42	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	873/875 (100%)	815 (93%)	54 (6%)	4 (0%)	32	34
1	C	873/875 (100%)	822 (94%)	46 (5%)	5 (1%)	28	29
1	E	873/875 (100%)	820 (94%)	50 (6%)	3 (0%)	44	49
1	G	873/875 (100%)	823 (94%)	46 (5%)	4 (0%)	32	34
1	I	873/875 (100%)	821 (94%)	49 (6%)	3 (0%)	44	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	873/875 (100%)	822 (94%)	48 (6%)	3 (0%)	44	49
1	M	873/875 (100%)	825 (94%)	45 (5%)	3 (0%)	44	49
1	O	873/875 (100%)	816 (94%)	51 (6%)	6 (1%)	25	24
1	Q	873/875 (100%)	821 (94%)	48 (6%)	4 (0%)	32	34
1	S	873/875 (100%)	814 (93%)	52 (6%)	7 (1%)	22	21
1	U	873/875 (100%)	820 (94%)	49 (6%)	4 (0%)	32	34
1	W	873/875 (100%)	815 (93%)	55 (6%)	3 (0%)	44	49
2	B	272/274 (99%)	261 (96%)	10 (4%)	1 (0%)	38	41
2	D	272/274 (99%)	256 (94%)	14 (5%)	2 (1%)	25	24
2	F	272/274 (99%)	257 (94%)	14 (5%)	1 (0%)	38	41
2	H	272/274 (99%)	258 (95%)	11 (4%)	3 (1%)	17	13
2	J	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	38	41
2	L	272/274 (99%)	259 (95%)	11 (4%)	2 (1%)	25	24
2	N	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	38	41
2	P	272/274 (99%)	256 (94%)	15 (6%)	1 (0%)	38	41
2	R	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	38	41
2	T	272/274 (99%)	259 (95%)	12 (4%)	1 (0%)	38	41
2	V	272/274 (99%)	258 (95%)	12 (4%)	2 (1%)	25	24
2	X	272/274 (99%)	245 (90%)	25 (9%)	2 (1%)	25	24
All	All	13740/13788 (100%)	12921 (94%)	752 (6%)	67 (0%)	32	34

All (67) 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	I	177	GLU
1	I	225	ILE
1	K	177	GLU
1	M	177	GLU
1	O	177	GLU
1	Q	177	GLU
1	S	141	PRO

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Mol	Chain	Res	Type
1	S	177	GLU
1	U	177	GLU
1	W	177	GLU
1	A	141	PRO
1	C	141	PRO
1	E	141	PRO
1	I	141	PRO
1	K	141	PRO
1	M	141	PRO
1	O	141	PRO
1	O	647	ASN
1	Q	141	PRO
1	S	648	ARG
1	U	141	PRO
1	W	141	PRO
2	D	67	PRO
2	D	179	GLU
1	G	141	PRO
1	S	225	ILE
2	X	221	GLY
1	C	225	ILE
1	C	858	ASN
2	H	19	CYS
2	N	67	PRO
1	O	646	PRO
2	P	67	PRO
1	S	737	PRO
2	V	67	PRO
1	A	394	PRO
2	B	67	PRO
2	F	67	PRO
1	G	421	LYS
2	H	67	PRO
2	J	67	PRO
1	O	858	ASN
2	R	67	PRO
1	S	858	ASN
2	T	67	PRO
1	U	225	ILE
2	V	129	CYS
2	X	67	PRO
1	K	225	ILE

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Mol	Chain	Res	Type
1	M	225	ILE
1	O	225	ILE
1	U	858	ASN
1	A	225	ILE
1	E	225	ILE
2	L	67	PRO
1	W	225	ILE
2	L	221	GLY
1	C	394	PRO
1	G	225	ILE
2	H	221	GLY
1	Q	225	ILE
1	Q	394	PRO
1	S	182	GLY

### 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%)	715 (98%)	14 (2%)	62	76
1	C	729/729 (100%)	712 (98%)	17 (2%)	56	69
1	E	729/729 (100%)	714 (98%)	15 (2%)	59	72
1	G	729/729 (100%)	717 (98%)	12 (2%)	68	81
1	I	729/729 (100%)	714 (98%)	15 (2%)	59	72
1	K	729/729 (100%)	715 (98%)	14 (2%)	62	76
1	M	729/729 (100%)	714 (98%)	15 (2%)	59	72
1	O	729/729 (100%)	711 (98%)	18 (2%)	53	65
1	Q	729/729 (100%)	715 (98%)	14 (2%)	62	76
1	S	729/729 (100%)	716 (98%)	13 (2%)	64	77
1	U	729/729 (100%)	716 (98%)	13 (2%)	64	77
1	W	729/729 (100%)	713 (98%)	16 (2%)	57	70
2	B	235/235 (100%)	223 (95%)	12 (5%)	28	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	235/235 (100%)	223 (95%)	12 (5%)	28	33
2	F	235/235 (100%)	223 (95%)	12 (5%)	28	33
2	H	235/235 (100%)	224 (95%)	11 (5%)	30	37
2	J	235/235 (100%)	221 (94%)	14 (6%)	22	25
2	L	235/235 (100%)	222 (94%)	13 (6%)	25	29
2	N	235/235 (100%)	226 (96%)	9 (4%)	38	47
2	P	235/235 (100%)	222 (94%)	13 (6%)	25	29
2	R	235/235 (100%)	223 (95%)	12 (5%)	28	33
2	T	235/235 (100%)	222 (94%)	13 (6%)	25	29
2	V	235/235 (100%)	223 (95%)	12 (5%)	28	33
2	X	235/235 (100%)	225 (96%)	10 (4%)	33	41
All	All	11568/11568 (100%)	11249 (97%)	319 (3%)	49	61

All (319) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	78	TYR
1	A	108	ASP
1	A	142	SER
1	A	187	TRP
1	A	358	CYS
1	A	373	LEU
1	A	493	PHE
1	A	499	PRO
1	A	554	PHE
1	A	564	ASN
1	A	605	MET
1	A	743	MET
1	A	818	GLU
2	B	13	CYS
2	B	19	CYS
2	B	21	MET
2	B	24	MET
2	B	71	CYS
2	B	76	CYS
2	B	104	GLU
2	B	109	CYS

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Mol	Chain	Res	Type
2	B	125	LYS
2	B	145	CYS
2	B	149	CYS
2	B	157	LEU
1	C	55	ARG
1	C	78	TYR
1	C	119	ASP
1	C	142	SER
1	C	187	TRP
1	C	358	CYS
1	C	426	MET
1	C	462	GLN
1	C	493	PHE
1	C	499	PRO
1	C	554	PHE
1	C	564	ASN
1	C	605	MET
1	C	743	MET
1	C	786	ASN
1	C	818	GLU
1	C	870	ASP
2	D	13	CYS
2	D	19	CYS
2	D	21	MET
2	D	71	CYS
2	D	73	ASN
2	D	76	CYS
2	D	109	CYS
2	D	125	LYS
2	D	145	CYS
2	D	149	CYS
2	D	157	LEU
2	D	179	GLU
1	E	55	ARG
1	E	78	TYR
1	E	142	SER
1	E	187	TRP
1	E	358	CYS
1	E	426	MET
1	E	462	GLN
1	E	493	PHE
1	E	499	PRO

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Mol	Chain	Res	Type
1	E	564	ASN
1	E	605	MET
1	E	673	ASN
1	E	719	GLU
1	E	743	MET
1	E	818	GLU
2	F	13	CYS
2	F	19	CYS
2	F	21	MET
2	F	24	MET
2	F	29	LEU
2	F	71	CYS
2	F	76	CYS
2	F	109	CYS
2	F	125	LYS
2	F	129	CYS
2	F	145	CYS
2	F	149	CYS
1	G	17	PHE
1	G	78	TYR
1	G	100	LEU
1	G	142	SER
1	G	187	TRP
1	G	373	LEU
1	G	462	GLN
1	G	493	PHE
1	G	564	ASN
1	G	726	LEU
1	G	743	MET
1	G	818	GLU
2	H	13	CYS
2	H	21	MET
2	H	24	MET
2	H	57	PRO
2	H	71	CYS
2	H	76	CYS
2	H	109	CYS
2	H	125	LYS
2	H	145	CYS
2	H	149	CYS
2	H	157	LEU
1	I	55	ARG

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Mol	Chain	Res	Type
1	I	78	TYR
1	I	142	SER
1	I	187	TRP
1	I	426	MET
1	I	462	GLN
1	I	492	MET
1	I	493	PHE
1	I	499	PRO
1	I	554	PHE
1	I	564	ASN
1	I	605	MET
1	I	726	LEU
1	I	743	MET
1	I	818	GLU
2	J	13	CYS
2	J	19	CYS
2	J	21	MET
2	J	24	MET
2	J	71	CYS
2	J	76	CYS
2	J	104	GLU
2	J	109	CYS
2	J	125	LYS
2	J	126	CYS
2	J	129	CYS
2	J	145	CYS
2	J	149	CYS
2	J	157	LEU
1	K	78	TYR
1	K	142	SER
1	K	187	TRP
1	K	286	ASP
1	K	493	PHE
1	K	499	PRO
1	K	554	PHE
1	K	564	ASN
1	K	605	MET
1	K	708	ARG
1	K	719	GLU
1	K	726	LEU
1	K	786	ASN
1	K	818	GLU

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Mol	Chain	Res	Type
2	L	13	CYS
2	L	19	CYS
2	L	21	MET
2	L	59	ASN
2	L	71	CYS
2	L	73	ASN
2	L	76	CYS
2	L	109	CYS
2	L	125	LYS
2	L	129	CYS
2	L	145	CYS
2	L	149	CYS
2	L	157	LEU
1	M	55	ARG
1	M	78	TYR
1	M	142	SER
1	M	187	TRP
1	M	358	CYS
1	M	426	MET
1	M	462	GLN
1	M	493	PHE
1	M	499	PRO
1	M	564	ASN
1	M	605	MET
1	M	708	ARG
1	M	726	LEU
1	M	743	MET
1	M	786	ASN
2	N	2	GLU
2	N	13	CYS
2	N	21	MET
2	N	71	CYS
2	N	76	CYS
2	N	109	CYS
2	N	125	LYS
2	N	145	CYS
2	N	149	CYS
1	O	55	ARG
1	O	78	TYR
1	O	100	LEU
1	O	142	SER
1	O	187	TRP

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Mol	Chain	Res	Type
1	O	272	HIS
1	O	426	MET
1	O	462	GLN
1	O	493	PHE
1	O	499	PRO
1	O	554	PHE
1	O	564	ASN
1	O	605	MET
1	O	673	ASN
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	59	ASN
2	P	71	CYS
2	P	73	ASN
2	P	76	CYS
2	P	104	GLU
2	P	109	CYS
2	P	125	LYS
2	P	129	CYS
2	P	145	CYS
2	P	149	CYS
2	P	157	LEU
1	Q	78	TYR
1	Q	100	LEU
1	Q	142	SER
1	Q	187	TRP
1	Q	373	LEU
1	Q	426	MET
1	Q	462	GLN
1	Q	493	PHE
1	Q	499	PRO
1	Q	564	ASN
1	Q	605	MET
1	Q	726	LEU
1	Q	743	MET
1	Q	786	ASN
2	R	13	CYS
2	R	19	CYS

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Mol	Chain	Res	Type
2	R	21	MET
2	R	24	MET
2	R	71	CYS
2	R	76	CYS
2	R	109	CYS
2	R	125	LYS
2	R	126	CYS
2	R	145	CYS
2	R	149	CYS
2	R	157	LEU
1	S	55	ARG
1	S	73	ASP
1	S	78	TYR
1	S	142	SER
1	S	187	TRP
1	S	426	MET
1	S	493	PHE
1	S	499	PRO
1	S	554	PHE
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	24	MET
2	T	71	CYS
2	T	73	ASN
2	T	76	CYS
2	T	109	CYS
2	T	125	LYS
2	T	126	CYS
2	T	145	CYS
2	T	149	CYS
2	T	157	LEU
1	U	17	PHE
1	U	78	TYR
1	U	142	SER
1	U	187	TRP
1	U	358	CYS
1	U	462	GLN

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Mol	Chain	Res	Type
1	U	499	PRO
1	U	554	PHE
1	U	564	ASN
1	U	605	MET
1	U	719	GLU
1	U	726	LEU
1	U	743	MET
2	V	13	CYS
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	125	LYS
2	V	129	CYS
2	V	145	CYS
2	V	149	CYS
1	W	55	ARG
1	W	142	SER
1	W	187	TRP
1	W	426	MET
1	W	462	GLN
1	W	493	PHE
1	W	499	PRO
1	W	554	PHE
1	W	564	ASN
1	W	605	MET
1	W	708	ARG
1	W	743	MET
1	W	786	ASN
1	W	801	LEU
1	W	818	GLU
1	W	849	SER
2	X	13	CYS
2	X	19	CYS
2	X	21	MET
2	X	71	CYS
2	X	109	CYS
2	X	125	LYS
2	X	129	CYS

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Mol	Chain	Res	Type
2	X	145	CYS
2	X	149	CYS
2	X	157	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (241) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	171	HIS
1	A	222	ASN
1	A	462	GLN
1	A	478	HIS
1	A	525	GLN
1	A	564	ASN
1	A	618	GLN
1	A	673	ASN
1	A	697	ASN
1	A	701	GLN
1	A	721	GLN
1	A	786	ASN
2	B	27	HIS
2	B	40	GLN
2	B	59	ASN
2	B	70	HIS
2	B	73	ASN
2	B	81	ASN
1	C	162	ASN
1	C	171	HIS
1	C	222	ASN
1	C	462	GLN
1	C	478	HIS
1	C	525	GLN
1	C	564	ASN
1	C	618	GLN
1	C	673	ASN
1	C	674	ASN
1	C	697	ASN
1	C	701	GLN
1	C	721	GLN
1	C	786	ASN
2	D	27	HIS
2	D	40	GLN

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Mol	Chain	Res	Type
2	D	59	ASN
2	D	70	HIS
2	D	73	ASN
2	D	81	ASN
2	D	121	ASN
1	E	162	ASN
1	E	171	HIS
1	E	222	ASN
1	E	462	GLN
1	E	478	HIS
1	E	525	GLN
1	E	564	ASN
1	E	576	GLN
1	E	618	GLN
1	E	647	ASN
1	E	673	ASN
1	E	674	ASN
1	E	697	ASN
1	E	701	GLN
1	E	721	GLN
1	E	786	ASN
2	F	27	HIS
2	F	40	GLN
2	F	59	ASN
2	F	70	HIS
2	F	73	ASN
2	F	81	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	697	ASN
1	G	701	GLN
1	G	721	GLN
1	G	786	ASN

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Mol	Chain	Res	Type
2	H	27	HIS
2	H	40	GLN
2	H	59	ASN
2	H	70	HIS
2	H	73	ASN
2	H	81	ASN
1	I	130	HIS
1	I	162	ASN
1	I	171	HIS
1	I	222	ASN
1	I	462	GLN
1	I	478	HIS
1	I	525	GLN
1	I	564	ASN
1	I	576	GLN
1	I	618	GLN
1	I	673	ASN
1	I	697	ASN
1	I	701	GLN
1	I	721	GLN
1	I	786	ASN
2	J	27	HIS
2	J	40	GLN
2	J	59	ASN
2	J	70	HIS
2	J	73	ASN
2	J	81	ASN
1	K	162	ASN
1	K	171	HIS
1	K	222	ASN
1	K	462	GLN
1	K	478	HIS
1	K	525	GLN
1	K	564	ASN
1	K	618	GLN
1	K	673	ASN
1	K	697	ASN
1	K	701	GLN
1	K	721	GLN
1	K	786	ASN
2	L	27	HIS
2	L	40	GLN

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Mol	Chain	Res	Type
2	L	59	ASN
2	L	70	HIS
2	L	73	ASN
2	L	81	ASN
2	L	121	ASN
1	M	162	ASN
1	M	171	HIS
1	M	222	ASN
1	M	462	GLN
1	M	478	HIS
1	M	525	GLN
1	M	564	ASN
1	M	618	GLN
1	M	673	ASN
1	M	697	ASN
1	M	701	GLN
1	M	721	GLN
1	M	786	ASN
2	N	27	HIS
2	N	40	GLN
2	N	59	ASN
2	N	70	HIS
2	N	73	ASN
1	O	130	HIS
1	O	162	ASN
1	O	171	HIS
1	O	222	ASN
1	O	478	HIS
1	O	525	GLN
1	O	564	ASN
1	O	576	GLN
1	O	618	GLN
1	O	645	ASN
1	O	673	ASN
1	O	697	ASN
1	O	701	GLN
1	O	721	GLN
1	O	786	ASN
2	P	27	HIS
2	P	40	GLN
2	P	59	ASN
2	P	70	HIS

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Mol	Chain	Res	Type
2	P	81	ASN
2	P	86	GLN
1	Q	162	ASN
1	Q	171	HIS
1	Q	222	ASN
1	Q	462	GLN
1	Q	478	HIS
1	Q	525	GLN
1	Q	564	ASN
1	Q	618	GLN
1	Q	673	ASN
1	Q	697	ASN
1	Q	701	GLN
1	Q	721	GLN
1	Q	786	ASN
2	R	27	HIS
2	R	40	GLN
2	R	59	ASN
2	R	70	HIS
2	R	73	ASN
1	S	130	HIS
1	S	162	ASN
1	S	171	HIS
1	S	222	ASN
1	S	462	GLN
1	S	478	HIS
1	S	525	GLN
1	S	564	ASN
1	S	618	GLN
1	S	673	ASN
1	S	697	ASN
1	S	701	GLN
1	S	721	GLN
1	S	786	ASN
2	T	27	HIS
2	T	40	GLN
2	T	59	ASN
2	T	70	HIS
2	T	73	ASN
2	T	81	ASN
1	U	130	HIS
1	U	162	ASN

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Mol	Chain	Res	Type
1	U	171	HIS
1	U	222	ASN
1	U	462	GLN
1	U	478	HIS
1	U	525	GLN
1	U	564	ASN
1	U	618	GLN
1	U	673	ASN
1	U	674	ASN
1	U	697	ASN
1	U	701	GLN
1	U	721	GLN
1	U	786	ASN
2	V	27	HIS
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	222	ASN
1	W	478	HIS
1	W	525	GLN
1	W	564	ASN
1	W	618	GLN
1	W	645	ASN
1	W	673	ASN
1	W	697	ASN
1	W	701	GLN
1	W	721	GLN
1	W	786	ASN
2	X	27	HIS
2	X	40	GLN
2	X	59	ASN
2	X	70	HIS
2	X	73	ASN
2	X	86	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 107 ligands modelled in this entry, 35 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	$\# Z  > 2$
4	MGD	A	902	5	41,52,52	2.66	13 (31%)	37,81,81	2.62	14 (37%)
4	MGD	A	903	5	41,52,52	2.60	11 (26%)	37,81,81	3.29	14 (37%)
6	PYG	A	905	5	9,9,9	4.63	9 (100%)	12,12,12	3.03	4 (33%)
7	SF4	B	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	304	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	C	902	5	41,52,52	2.67	11 (26%)	37,81,81	2.56	13 (35%)
4	MGD	C	903	5	41,52,52	2.76	14 (34%)	37,81,81	2.51	12 (32%)
6	PYG	C	905	5	9,9,9	4.59	9 (100%)	12,12,12	3.08	5 (41%)
7	SF4	D	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	D	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	D	304	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	E	902	5	41,52,52	2.58	13 (31%)	37,81,81	2.59	14 (37%)
4	MGD	E	903	5	41,52,52	2.64	13 (31%)	37,81,81	2.61	13 (35%)
6	PYG	E	905	5	9,9,9	4.65	9 (100%)	12,12,12	3.06	4 (33%)
7	SF4	F	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	F	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	F	304	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	G	902	5	41,52,52	2.65	11 (26%)	37,81,81	2.58	14 (37%)
4	MGD	G	903	5	41,52,52	2.63	14 (34%)	37,81,81	2.79	11 (29%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PYG	G	905	5	9,9,9	4.59	9 (100%)	12,12,12	3.06	4 (33%)
7	SF4	H	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	H	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	H	304	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	I	902	5	41,52,52	2.54	14 (34%)	37,81,81	2.62	14 (37%)
4	MGD	I	903	5	41,52,52	2.63	13 (31%)	37,81,81	2.74	12 (32%)
6	PYG	I	905	5	9,9,9	4.63	9 (100%)	12,12,12	3.07	5 (41%)
7	SF4	J	301	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	J	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	J	303	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	K	902	5	41,52,52	2.60	12 (29%)	37,81,81	2.54	12 (32%)
4	MGD	K	903	5	41,52,52	2.59	12 (29%)	37,81,81	3.18	14 (37%)
6	PYG	K	905	5	9,9,9	4.66	9 (100%)	12,12,12	3.09	4 (33%)
7	SF4	L	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	L	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	L	304	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	M	902	5	41,52,52	2.52	13 (31%)	37,81,81	2.59	14 (37%)
4	MGD	M	903	5	41,52,52	2.65	13 (31%)	37,81,81	2.60	13 (35%)
6	PYG	M	905	5	9,9,9	4.64	9 (100%)	12,12,12	3.06	5 (41%)
7	SF4	N	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	N	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	N	304	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	O	902	5	41,52,52	2.57	13 (31%)	37,81,81	2.57	14 (37%)
4	MGD	O	903	5	41,52,52	2.66	13 (31%)	37,81,81	2.55	13 (35%)
6	PYG	O	905	5	9,9,9	4.64	9 (100%)	12,12,12	3.10	5 (41%)
7	SF4	P	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	P	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	P	304	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	Q	902	5	41,52,52	2.54	11 (26%)	37,81,81	2.55	13 (35%)
4	MGD	Q	903	5	41,52,52	2.61	12 (29%)	37,81,81	2.69	13 (35%)
6	PYG	Q	905	5	9,9,9	4.63	9 (100%)	12,12,12	3.05	4 (33%)
7	SF4	R	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	R	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	R	304	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	S	902	5	41,52,52	2.56	14 (34%)	37,81,81	2.58	13 (35%)
4	MGD	S	903	5	41,52,52	2.64	11 (26%)	37,81,81	2.63	13 (35%)
6	PYG	S	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.04	4 (33%)
7	SF4	T	302	2	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SF4	T	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	T	304	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	U	902	5	41,52,52	2.68	14 (34%)	37,81,81	2.62	14 (37%)
4	MGD	U	903	5	41,52,52	2.66	11 (26%)	37,81,81	2.55	13 (35%)
6	PYG	U	905	5	9,9,9	4.60	9 (100%)	12,12,12	3.07	4 (33%)
7	SF4	V	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	V	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	V	304	2	0,12,12	0.00	-	0,24,24	0.00	-
4	MGD	W	902	5	41,52,52	2.57	11 (26%)	37,81,81	2.54	15 (40%)
4	MGD	W	903	5	41,52,52	2.73	11 (26%)	37,81,81	2.45	12 (32%)
6	PYG	W	905	5	9,9,9	4.64	9 (100%)	12,12,12	3.14	5 (41%)
7	SF4	X	302	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	X	303	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	X	304	2	0,12,12	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MGD	A	902	5	-	0/18/66/66	0/6/6/6
4	MGD	A	903	5	-	0/18/66/66	0/6/6/6
6	PYG	A	905	5	-	0/0/0/0	0/1/1/1
7	SF4	B	302	2	-	0/0/48/48	0/6/5/5
7	SF4	B	303	2	-	0/0/48/48	0/6/5/5
7	SF4	B	304	2	-	0/0/48/48	0/6/5/5
4	MGD	C	902	5	-	0/18/66/66	0/6/6/6
4	MGD	C	903	5	-	0/18/66/66	0/6/6/6
6	PYG	C	905	5	-	0/0/0/0	0/1/1/1
7	SF4	D	302	2	-	0/0/48/48	0/6/5/5
7	SF4	D	303	2	-	0/0/48/48	0/6/5/5
7	SF4	D	304	2	-	0/0/48/48	0/6/5/5
4	MGD	E	902	5	-	0/18/66/66	0/6/6/6
4	MGD	E	903	5	-	0/18/66/66	0/6/6/6
6	PYG	E	905	5	-	0/0/0/0	0/1/1/1
7	SF4	F	302	2	-	0/0/48/48	0/6/5/5
7	SF4	F	303	2	-	0/0/48/48	0/6/5/5
7	SF4	F	304	2	-	0/0/48/48	0/6/5/5
4	MGD	G	902	5	-	0/18/66/66	0/6/6/6
4	MGD	G	903	5	-	0/18/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PYG	G	905	5	-	0/0/0/0	0/1/1/1
7	SF4	H	302	2	-	0/0/48/48	0/6/5/5
7	SF4	H	303	2	-	0/0/48/48	0/6/5/5
7	SF4	H	304	2	-	0/0/48/48	0/6/5/5
4	MGD	I	902	5	-	0/18/66/66	0/6/6/6
4	MGD	I	903	5	-	0/18/66/66	0/6/6/6
6	PYG	I	905	5	-	0/0/0/0	0/1/1/1
7	SF4	J	301	2	-	0/0/48/48	0/6/5/5
7	SF4	J	302	2	-	0/0/48/48	0/6/5/5
7	SF4	J	303	2	-	0/0/48/48	0/6/5/5
4	MGD	K	902	5	-	0/18/66/66	0/6/6/6
4	MGD	K	903	5	-	0/18/66/66	0/6/6/6
6	PYG	K	905	5	-	0/0/0/0	0/1/1/1
7	SF4	L	302	2	-	0/0/48/48	0/6/5/5
7	SF4	L	303	2	-	0/0/48/48	0/6/5/5
7	SF4	L	304	2	-	0/0/48/48	0/6/5/5
4	MGD	M	902	5	-	0/18/66/66	0/6/6/6
4	MGD	M	903	5	-	0/18/66/66	0/6/6/6
6	PYG	M	905	5	-	0/0/0/0	0/1/1/1
7	SF4	N	302	2	-	0/0/48/48	0/6/5/5
7	SF4	N	303	2	-	0/0/48/48	0/6/5/5
7	SF4	N	304	2	-	0/0/48/48	0/6/5/5
4	MGD	O	902	5	-	0/18/66/66	0/6/6/6
4	MGD	O	903	5	-	0/18/66/66	0/6/6/6
6	PYG	O	905	5	-	0/0/0/0	0/1/1/1
7	SF4	P	302	2	-	0/0/48/48	0/6/5/5
7	SF4	P	303	2	-	0/0/48/48	0/6/5/5
7	SF4	P	304	2	-	0/0/48/48	0/6/5/5
4	MGD	Q	902	5	-	0/18/66/66	0/6/6/6
4	MGD	Q	903	5	-	0/18/66/66	0/6/6/6
6	PYG	Q	905	5	-	0/0/0/0	0/1/1/1
7	SF4	R	302	2	-	0/0/48/48	0/6/5/5
7	SF4	R	303	2	-	0/0/48/48	0/6/5/5
7	SF4	R	304	2	-	0/0/48/48	0/6/5/5
4	MGD	S	902	5	-	0/18/66/66	0/6/6/6
4	MGD	S	903	5	-	0/18/66/66	0/6/6/6
6	PYG	S	905	5	-	0/0/0/0	0/1/1/1
7	SF4	T	302	2	-	0/0/48/48	0/6/5/5
7	SF4	T	303	2	-	0/0/48/48	0/6/5/5
7	SF4	T	304	2	-	0/0/48/48	0/6/5/5
4	MGD	U	902	5	-	0/18/66/66	0/6/6/6
4	MGD	U	903	5	-	0/18/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PYG	U	905	5	-	0/0/0/0	0/1/1/1
7	SF4	V	302	2	-	0/0/48/48	0/6/5/5
7	SF4	V	303	2	-	0/0/48/48	0/6/5/5
7	SF4	V	304	2	-	0/0/48/48	0/6/5/5
4	MGD	W	902	5	-	0/18/66/66	0/6/6/6
4	MGD	W	903	5	-	0/18/66/66	0/6/6/6
6	PYG	W	905	5	-	0/0/0/0	0/1/1/1
7	SF4	X	302	2	-	0/0/48/48	0/6/5/5
7	SF4	X	303	2	-	0/0/48/48	0/6/5/5
7	SF4	X	304	2	-	0/0/48/48	0/6/5/5

All (406) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	902	MGD	O11-C23	2.00	1.46	1.43
4	K	902	MGD	C23-N22	2.02	1.48	1.44
4	Q	903	MGD	C2-N2	2.02	1.38	1.34
4	E	902	MGD	O3'-C3'	2.03	1.47	1.43
4	G	903	MGD	O4'-C1'	2.03	1.44	1.41
4	I	902	MGD	C6-C5	2.03	1.45	1.41
4	Q	903	MGD	C23-N22	2.06	1.48	1.44
4	K	903	MGD	C23-N22	2.06	1.48	1.44
4	W	902	MGD	C2-N2	2.06	1.38	1.34
4	C	903	MGD	C2-N2	2.07	1.38	1.34
4	A	903	MGD	C2-N2	2.07	1.38	1.34
4	C	903	MGD	C4-N3	2.07	1.39	1.35
4	I	902	MGD	C2-N2	2.08	1.38	1.34
4	O	902	MGD	C19-N18	2.08	1.39	1.35
4	U	902	MGD	C6-C5	2.08	1.45	1.41
4	O	902	MGD	C6-C5	2.08	1.45	1.41
4	M	902	MGD	C4-N3	2.09	1.39	1.35
4	I	903	MGD	C2-N2	2.09	1.38	1.34
4	C	903	MGD	O4'-C1'	2.13	1.44	1.41
4	M	903	MGD	C3'-C4'	2.13	1.58	1.53
4	U	902	MGD	C10-C11	2.15	1.55	1.52
4	E	903	MGD	C2-N2	2.21	1.38	1.34
4	S	902	MGD	C19-N18	2.21	1.39	1.35
4	S	903	MGD	C23-N22	2.21	1.49	1.44
4	A	902	MGD	C4-N3	2.22	1.39	1.35
6	M	905	PYG	C4-C3	2.23	1.43	1.39
4	G	903	MGD	C23-N22	2.24	1.49	1.44
4	K	903	MGD	C19-N18	2.25	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	902	MGD	C6-C5	2.25	1.45	1.41
4	I	902	MGD	C19-N18	2.25	1.39	1.35
6	G	905	PYG	C4-C3	2.28	1.43	1.39
6	K	905	PYG	C4-C3	2.28	1.43	1.39
4	M	903	MGD	C2-N2	2.28	1.38	1.34
4	O	903	MGD	C19-N18	2.29	1.39	1.35
4	O	902	MGD	C23-N22	2.29	1.49	1.44
6	I	905	PYG	C4-C3	2.29	1.43	1.39
4	S	902	MGD	C4-N3	2.30	1.39	1.35
4	I	902	MGD	C4-N3	2.30	1.39	1.35
4	I	903	MGD	C23-N22	2.30	1.49	1.44
4	E	903	MGD	C23-N22	2.31	1.49	1.44
4	M	903	MGD	C4-N3	2.31	1.39	1.35
4	U	903	MGD	C23-N22	2.32	1.49	1.44
4	C	902	MGD	C23-N22	2.33	1.49	1.44
6	C	905	PYG	C4-C3	2.34	1.43	1.39
4	C	903	MGD	C19-N18	2.34	1.39	1.35
4	A	902	MGD	O11-C23	2.34	1.47	1.43
4	S	902	MGD	C6-C5	2.34	1.45	1.41
4	O	902	MGD	C4-N3	2.35	1.39	1.35
6	Q	905	PYG	C4-C3	2.36	1.43	1.39
4	O	903	MGD	C2-N2	2.36	1.38	1.34
4	I	903	MGD	C19-N18	2.36	1.39	1.35
4	S	902	MGD	O3'-C3'	2.37	1.48	1.43
4	M	902	MGD	C19-N18	2.37	1.39	1.35
6	O	905	PYG	C4-C3	2.38	1.43	1.39
4	Q	902	MGD	C23-N22	2.38	1.49	1.44
6	G	905	PYG	C5-C4	2.38	1.43	1.38
6	U	905	PYG	C4-C3	2.38	1.43	1.39
4	A	902	MGD	C19-N18	2.38	1.39	1.35
6	W	905	PYG	C4-C3	2.39	1.43	1.39
4	E	902	MGD	C4-N3	2.39	1.39	1.35
4	S	903	MGD	C19-N18	2.39	1.39	1.35
4	I	902	MGD	C23-N22	2.39	1.49	1.44
4	I	903	MGD	O4'-C1'	2.40	1.44	1.41
4	U	902	MGD	C19-N18	2.40	1.39	1.35
6	E	905	PYG	C5-C4	2.43	1.43	1.38
6	S	905	PYG	C4-C3	2.44	1.43	1.39
6	A	905	PYG	C4-C3	2.44	1.43	1.39
4	C	902	MGD	C19-N18	2.45	1.39	1.35
4	O	903	MGD	C3'-C4'	2.45	1.59	1.53
4	U	902	MGD	O3'-C3'	2.45	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	MGD	C19-N18	2.46	1.39	1.35
4	U	903	MGD	C19-N18	2.46	1.39	1.35
6	E	905	PYG	C4-C3	2.47	1.44	1.39
4	E	903	MGD	C19-N18	2.48	1.39	1.35
4	G	903	MGD	C2-N2	2.48	1.39	1.34
6	U	905	PYG	O1-C1	2.49	1.41	1.36
4	K	903	MGD	C2'-C3'	2.50	1.60	1.53
6	M	905	PYG	C5-C4	2.50	1.43	1.38
4	M	902	MGD	C23-N22	2.51	1.49	1.44
4	E	902	MGD	C19-N18	2.52	1.39	1.35
4	E	902	MGD	C23-N22	2.53	1.49	1.44
4	S	902	MGD	C23-N22	2.53	1.49	1.44
6	M	905	PYG	O2-C2	2.54	1.42	1.37
4	G	903	MGD	C4-N3	2.54	1.39	1.35
4	K	902	MGD	C19-N18	2.55	1.40	1.35
6	C	905	PYG	O2-C2	2.55	1.42	1.37
6	C	905	PYG	O1-C1	2.55	1.41	1.36
4	G	903	MGD	C19-N18	2.55	1.40	1.35
4	W	903	MGD	C19-N18	2.56	1.40	1.35
4	A	902	MGD	C23-N22	2.57	1.49	1.44
4	W	902	MGD	C23-N22	2.58	1.49	1.44
6	E	905	PYG	O2-C2	2.58	1.43	1.37
4	I	903	MGD	O11-C23	2.59	1.47	1.43
4	E	903	MGD	C3'-C4'	2.59	1.59	1.53
4	O	903	MGD	C23-N22	2.60	1.49	1.44
6	A	905	PYG	C5-C4	2.60	1.43	1.38
4	G	902	MGD	C19-N18	2.60	1.40	1.35
6	K	905	PYG	C5-C4	2.60	1.43	1.38
6	I	905	PYG	C5-C4	2.61	1.43	1.38
6	S	905	PYG	C5-C4	2.63	1.43	1.38
4	Q	902	MGD	C19-N18	2.63	1.40	1.35
6	I	905	PYG	O2-C2	2.64	1.43	1.37
4	A	903	MGD	C2'-C3'	2.64	1.60	1.53
6	W	905	PYG	O2-C2	2.65	1.43	1.37
6	U	905	PYG	C5-C4	2.66	1.44	1.38
6	O	905	PYG	O1-C1	2.66	1.41	1.36
6	C	905	PYG	C5-C4	2.66	1.44	1.38
4	G	902	MGD	C23-N22	2.66	1.50	1.44
6	Q	905	PYG	C5-C4	2.68	1.44	1.38
6	W	905	PYG	C5-C4	2.68	1.44	1.38
6	O	905	PYG	C5-C4	2.69	1.44	1.38
6	O	905	PYG	O2-C2	2.69	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	903	MGD	C19-N18	2.69	1.40	1.35
4	U	902	MGD	C23-N22	2.70	1.50	1.44
6	A	905	PYG	O2-C2	2.72	1.43	1.37
6	S	905	PYG	O2-C2	2.73	1.43	1.37
6	G	905	PYG	O2-C2	2.73	1.43	1.37
6	Q	905	PYG	O2-C2	2.74	1.43	1.37
6	K	905	PYG	O1-C1	2.74	1.42	1.36
6	W	905	PYG	O1-C1	2.75	1.42	1.36
4	M	903	MGD	C19-N18	2.75	1.40	1.35
6	K	905	PYG	O2-C2	2.75	1.43	1.37
6	S	905	PYG	O1-C1	2.76	1.42	1.36
4	K	903	MGD	C2'-C1'	2.80	1.58	1.53
4	C	903	MGD	C23-N22	2.81	1.50	1.44
6	U	905	PYG	O2-C2	2.82	1.43	1.37
4	W	903	MGD	C23-N22	2.90	1.50	1.44
6	Q	905	PYG	O1-C1	3.02	1.42	1.36
6	A	905	PYG	O1-C1	3.03	1.42	1.36
4	Q	903	MGD	O11-C23	3.05	1.48	1.43
4	S	902	MGD	O4'-C1'	3.11	1.45	1.41
6	I	905	PYG	O1-C1	3.15	1.42	1.36
4	K	903	MGD	O11-C11	3.18	1.48	1.43
4	G	902	MGD	O4'-C1'	3.23	1.45	1.41
6	G	905	PYG	O1-C1	3.32	1.43	1.36
4	A	903	MGD	O11-C11	3.33	1.48	1.43
4	S	902	MGD	C2-N1	3.34	1.41	1.35
6	M	905	PYG	O1-C1	3.35	1.43	1.36
6	E	905	PYG	O1-C1	3.37	1.43	1.36
6	S	905	PYG	C5-C6	3.41	1.45	1.38
4	Q	902	MGD	O4'-C1'	3.42	1.46	1.41
4	G	903	MGD	O11-C23	3.43	1.48	1.43
6	C	905	PYG	C5-C6	3.44	1.45	1.38
4	K	902	MGD	C2-N1	3.46	1.41	1.35
6	Q	905	PYG	C5-C6	3.46	1.45	1.38
6	E	905	PYG	C5-C6	3.48	1.45	1.38
6	U	905	PYG	C5-C6	3.48	1.45	1.38
6	O	905	PYG	C5-C6	3.48	1.45	1.38
6	G	905	PYG	C5-C6	3.49	1.45	1.38
4	E	903	MGD	O11-C23	3.51	1.48	1.43
6	A	905	PYG	C5-C6	3.51	1.45	1.38
6	K	905	PYG	C5-C6	3.53	1.45	1.38
6	W	905	PYG	C5-C6	3.53	1.45	1.38
4	Q	902	MGD	C2-N1	3.54	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	905	PYG	C5-C6	3.54	1.45	1.38
4	O	903	MGD	C21-N20	3.56	1.40	1.34
4	W	902	MGD	C2-N1	3.60	1.41	1.35
6	M	905	PYG	C5-C6	3.60	1.45	1.38
4	E	902	MGD	C21-N20	3.61	1.40	1.34
4	U	902	MGD	C2-N1	3.61	1.41	1.35
4	A	902	MGD	C2-N1	3.63	1.42	1.35
4	M	903	MGD	C21-N20	3.63	1.40	1.34
4	O	902	MGD	C2-N1	3.63	1.42	1.35
4	C	902	MGD	C2-N1	3.64	1.42	1.35
4	M	902	MGD	C21-N20	3.64	1.40	1.34
4	I	902	MGD	C2-N1	3.65	1.42	1.35
4	U	903	MGD	C2-N1	3.66	1.42	1.35
4	Q	903	MGD	C2-N1	3.70	1.42	1.35
4	M	903	MGD	O11-C23	3.70	1.49	1.43
4	W	903	MGD	C2-N1	3.72	1.42	1.35
4	O	903	MGD	O11-C23	3.75	1.49	1.43
4	G	902	MGD	C2-N1	3.79	1.42	1.35
4	A	902	MGD	O4'-C1'	3.79	1.46	1.41
4	I	902	MGD	C21-N20	3.79	1.41	1.34
4	U	903	MGD	O11-C23	3.82	1.49	1.43
4	S	903	MGD	C21-N20	3.82	1.41	1.34
4	O	902	MGD	C21-N20	3.82	1.41	1.34
4	W	902	MGD	C21-N20	3.83	1.41	1.34
4	K	902	MGD	C21-N20	3.84	1.41	1.34
4	Q	902	MGD	C21-N20	3.85	1.41	1.34
4	K	903	MGD	C21-N20	3.87	1.41	1.34
4	M	902	MGD	C2-N1	3.89	1.42	1.35
4	M	902	MGD	O4'-C1'	3.89	1.46	1.41
4	Q	903	MGD	C21-N20	3.90	1.41	1.34
4	U	902	MGD	O4'-C1'	3.91	1.46	1.41
4	E	902	MGD	C2-N1	3.91	1.42	1.35
4	G	903	MGD	C21-N20	3.91	1.41	1.34
4	U	902	MGD	C21-N20	3.92	1.41	1.34
4	G	903	MGD	C2-N1	3.98	1.42	1.35
4	W	902	MGD	O4'-C1'	3.99	1.46	1.41
4	C	903	MGD	O11-C23	4.02	1.49	1.43
4	I	902	MGD	O4'-C1'	4.03	1.46	1.41
4	A	903	MGD	C21-N20	4.05	1.41	1.34
4	C	903	MGD	C2-N1	4.05	1.42	1.35
4	E	902	MGD	O4'-C1'	4.06	1.46	1.41
4	S	903	MGD	C2-N1	4.07	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	902	MGD	C14-N15	4.08	1.51	1.45
4	E	903	MGD	C21-N20	4.09	1.41	1.34
4	G	902	MGD	C21-N20	4.09	1.41	1.34
4	O	903	MGD	C2-N1	4.11	1.42	1.35
4	A	903	MGD	C2-N1	4.11	1.42	1.35
4	E	903	MGD	C2-N1	4.12	1.42	1.35
4	C	903	MGD	C21-N20	4.12	1.41	1.34
4	U	903	MGD	C21-N20	4.13	1.41	1.34
4	W	902	MGD	C14-N15	4.13	1.51	1.45
4	I	903	MGD	C21-N20	4.14	1.41	1.34
4	I	902	MGD	C14-N15	4.17	1.51	1.45
4	S	903	MGD	O11-C23	4.17	1.49	1.43
4	E	902	MGD	C16-N15	4.18	1.47	1.37
4	O	902	MGD	O4'-C1'	4.21	1.47	1.41
4	K	902	MGD	C14-N15	4.22	1.51	1.45
4	I	902	MGD	C16-N15	4.23	1.47	1.37
4	K	903	MGD	C2-N1	4.26	1.43	1.35
4	A	902	MGD	C21-N20	4.27	1.41	1.34
4	W	903	MGD	C21-N20	4.28	1.41	1.34
4	O	902	MGD	C16-N15	4.31	1.47	1.37
4	M	902	MGD	C16-N15	4.31	1.47	1.37
4	Q	902	MGD	C16-N15	4.31	1.47	1.37
4	C	902	MGD	O4'-C1'	4.31	1.47	1.41
4	C	902	MGD	C21-N20	4.32	1.42	1.34
4	M	903	MGD	C2-N1	4.33	1.43	1.35
4	U	903	MGD	C16-N15	4.33	1.47	1.37
4	I	903	MGD	C2-N1	4.36	1.43	1.35
4	S	902	MGD	C21-N20	4.36	1.42	1.34
4	M	902	MGD	C14-N15	4.37	1.51	1.45
4	O	903	MGD	C16-N15	4.40	1.47	1.37
4	Q	902	MGD	O11-C11	4.42	1.50	1.43
4	K	902	MGD	O4'-C1'	4.42	1.47	1.41
4	S	902	MGD	C14-N15	4.43	1.51	1.45
4	W	903	MGD	C16-N15	4.44	1.47	1.37
4	W	902	MGD	C16-N15	4.44	1.47	1.37
4	C	903	MGD	C16-N15	4.45	1.47	1.37
6	U	905	PYG	C6-C1	4.46	1.47	1.39
4	G	903	MGD	C16-N15	4.46	1.47	1.37
4	K	903	MGD	C16-N15	4.48	1.47	1.37
4	U	902	MGD	C14-N15	4.51	1.51	1.45
4	A	902	MGD	C14-N15	4.54	1.51	1.45
4	E	903	MGD	C16-N15	4.56	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	902	MGD	O11-C11	4.57	1.50	1.43
4	S	902	MGD	C16-N15	4.58	1.48	1.37
6	G	905	PYG	C6-C1	4.59	1.47	1.39
4	G	902	MGD	C16-N15	4.61	1.48	1.37
6	C	905	PYG	C6-C1	4.61	1.47	1.39
4	U	903	MGD	C6-N1	4.61	1.41	1.33
4	M	903	MGD	C16-N15	4.61	1.48	1.37
4	S	903	MGD	C16-N15	4.62	1.48	1.37
4	K	902	MGD	C16-N15	4.62	1.48	1.37
4	C	902	MGD	C16-N15	4.63	1.48	1.37
4	S	903	MGD	O11-C11	4.63	1.50	1.43
6	I	905	PYG	C6-C1	4.64	1.47	1.39
6	M	905	PYG	C6-C1	4.65	1.47	1.39
4	M	903	MGD	O11-C11	4.66	1.50	1.43
6	Q	905	PYG	C6-C1	4.67	1.48	1.39
4	O	902	MGD	C14-N15	4.68	1.51	1.45
4	C	902	MGD	C14-N15	4.69	1.51	1.45
6	O	905	PYG	C6-C1	4.69	1.48	1.39
4	E	902	MGD	C14-N15	4.71	1.51	1.45
4	I	903	MGD	O11-C11	4.71	1.50	1.43
4	U	902	MGD	C16-N15	4.73	1.48	1.37
6	A	905	PYG	C6-C1	4.75	1.48	1.39
6	W	905	PYG	C6-C1	4.78	1.48	1.39
6	K	905	PYG	C6-C1	4.78	1.48	1.39
6	E	905	PYG	C6-C1	4.78	1.48	1.39
4	W	903	MGD	O11-C23	4.82	1.50	1.43
6	S	905	PYG	C6-C1	4.83	1.48	1.39
4	A	903	MGD	C16-N15	4.83	1.48	1.37
4	Q	903	MGD	C16-N15	4.85	1.48	1.37
4	I	902	MGD	O11-C11	4.92	1.50	1.43
4	A	902	MGD	C16-N15	4.94	1.48	1.37
4	I	903	MGD	C16-N15	4.94	1.48	1.37
4	G	902	MGD	C14-N15	4.96	1.52	1.45
4	E	903	MGD	C6-N1	4.96	1.42	1.33
4	Q	903	MGD	O11-C11	4.99	1.50	1.43
4	W	902	MGD	O11-C11	5.01	1.50	1.43
4	O	903	MGD	C6-N1	5.05	1.42	1.33
4	E	902	MGD	O11-C11	5.10	1.50	1.43
4	Q	903	MGD	C6-N1	5.15	1.42	1.33
4	O	903	MGD	O11-C11	5.16	1.51	1.43
4	W	903	MGD	C6-N1	5.19	1.42	1.33
4	S	903	MGD	C6-N1	5.21	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	903	MGD	O11-C11	5.22	1.51	1.43
4	G	903	MGD	O11-C11	5.25	1.51	1.43
4	I	903	MGD	C6-N1	5.25	1.42	1.33
4	S	902	MGD	O11-C11	5.25	1.51	1.43
4	O	902	MGD	O11-C11	5.31	1.51	1.43
4	A	903	MGD	C6-N1	5.31	1.42	1.33
4	U	903	MGD	O11-C11	5.37	1.51	1.43
4	C	903	MGD	C6-N1	5.38	1.42	1.33
6	E	905	PYG	O3-C3	5.38	1.47	1.36
6	G	905	PYG	O3-C3	5.40	1.47	1.36
6	U	905	PYG	O3-C3	5.40	1.47	1.36
6	M	905	PYG	O3-C3	5.41	1.47	1.36
4	M	902	MGD	O11-C11	5.45	1.51	1.43
4	K	903	MGD	C6-N1	5.46	1.42	1.33
6	O	905	PYG	O3-C3	5.46	1.47	1.36
4	G	903	MGD	C6-N1	5.46	1.42	1.33
6	Q	905	PYG	O3-C3	5.46	1.47	1.36
6	I	905	PYG	O3-C3	5.47	1.47	1.36
4	M	903	MGD	C6-N1	5.48	1.43	1.33
4	C	902	MGD	O11-C11	5.51	1.51	1.43
6	S	905	PYG	O3-C3	5.54	1.47	1.36
6	A	905	PYG	O3-C3	5.54	1.47	1.36
4	W	903	MGD	O11-C11	5.54	1.51	1.43
6	K	905	PYG	O3-C3	5.55	1.47	1.36
4	S	902	MGD	C6-N1	5.55	1.43	1.33
6	C	905	PYG	O3-C3	5.56	1.47	1.36
4	M	902	MGD	C23-C14	5.56	1.57	1.53
6	I	905	PYG	C3-C2	5.61	1.46	1.39
4	E	903	MGD	C23-C14	5.61	1.57	1.53
6	Q	905	PYG	C3-C2	5.62	1.46	1.39
6	W	905	PYG	O3-C3	5.65	1.47	1.36
4	K	902	MGD	C6-N1	5.67	1.43	1.33
4	M	903	MGD	C23-C14	5.68	1.57	1.53
4	A	902	MGD	O11-C11	5.69	1.51	1.43
4	C	903	MGD	O11-C11	5.69	1.51	1.43
4	I	903	MGD	C23-C14	5.71	1.57	1.53
6	C	905	PYG	C3-C2	5.72	1.46	1.39
6	E	905	PYG	C3-C2	5.73	1.46	1.39
4	G	903	MGD	C23-C14	5.75	1.57	1.53
4	Q	903	MGD	C23-C14	5.77	1.57	1.53
6	G	905	PYG	C3-C2	5.80	1.46	1.39
4	E	902	MGD	C23-C14	5.80	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	902	MGD	O11-C11	5.83	1.52	1.43
6	A	905	PYG	C3-C2	5.83	1.46	1.39
4	S	902	MGD	C23-C14	5.86	1.57	1.53
4	G	902	MGD	O11-C11	5.87	1.52	1.43
4	W	902	MGD	C6-N1	5.87	1.43	1.33
6	U	905	PYG	C3-C2	5.91	1.46	1.39
6	O	905	PYG	C3-C2	5.95	1.46	1.39
4	S	903	MGD	C23-C14	5.95	1.57	1.53
6	M	905	PYG	C3-C2	6.00	1.46	1.39
4	G	902	MGD	C6-N1	6.00	1.43	1.33
4	M	902	MGD	C17-N18	6.00	1.43	1.33
4	O	902	MGD	C6-N1	6.01	1.43	1.33
4	U	902	MGD	C6-N1	6.03	1.44	1.33
4	U	902	MGD	C23-C14	6.04	1.58	1.53
4	M	902	MGD	C6-N1	6.04	1.44	1.33
6	K	905	PYG	C3-C2	6.05	1.46	1.39
4	K	903	MGD	C17-N18	6.08	1.44	1.33
4	Q	902	MGD	C6-N1	6.12	1.44	1.33
4	C	902	MGD	C6-N1	6.13	1.44	1.33
4	I	902	MGD	C6-N1	6.15	1.44	1.33
6	S	905	PYG	C3-C2	6.15	1.46	1.39
4	W	902	MGD	C17-N18	6.17	1.44	1.33
4	O	903	MGD	C17-N18	6.17	1.44	1.33
4	A	902	MGD	C23-C14	6.17	1.58	1.53
4	O	902	MGD	C17-N18	6.18	1.44	1.33
4	G	902	MGD	C23-C14	6.18	1.58	1.53
4	A	902	MGD	C6-N1	6.19	1.44	1.33
4	I	902	MGD	C17-N18	6.22	1.44	1.33
4	E	902	MGD	C6-N1	6.22	1.44	1.33
4	E	902	MGD	C17-N18	6.24	1.44	1.33
4	W	903	MGD	C23-C14	6.25	1.58	1.53
6	W	905	PYG	C3-C2	6.26	1.47	1.39
4	E	903	MGD	C17-N18	6.28	1.44	1.33
4	A	902	MGD	C17-N18	6.30	1.44	1.33
4	U	903	MGD	C17-N18	6.32	1.44	1.33
4	C	903	MGD	C17-N18	6.32	1.44	1.33
4	G	903	MGD	C14-N15	6.34	1.54	1.45
4	A	903	MGD	C23-C14	6.35	1.58	1.53
4	O	902	MGD	C23-C14	6.36	1.58	1.53
4	G	902	MGD	C17-N18	6.39	1.44	1.33
4	S	902	MGD	C17-N18	6.39	1.44	1.33
4	S	903	MGD	C17-N18	6.45	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	903	MGD	C17-N18	6.46	1.44	1.33
4	K	903	MGD	C23-C14	6.47	1.58	1.53
4	I	902	MGD	C23-C14	6.48	1.58	1.53
4	C	902	MGD	C17-N18	6.49	1.44	1.33
4	O	903	MGD	C14-N15	6.50	1.54	1.45
4	M	903	MGD	C14-N15	6.51	1.54	1.45
4	W	903	MGD	C14-N15	6.53	1.54	1.45
4	U	903	MGD	C23-C14	6.53	1.58	1.53
4	I	903	MGD	C17-N18	6.54	1.44	1.33
4	A	903	MGD	C17-N18	6.56	1.44	1.33
4	I	903	MGD	C14-N15	6.57	1.54	1.45
4	C	903	MGD	C14-N15	6.57	1.54	1.45
4	G	903	MGD	C17-N18	6.58	1.45	1.33
4	Q	902	MGD	C17-N18	6.59	1.45	1.33
4	U	902	MGD	C17-N18	6.65	1.45	1.33
4	K	902	MGD	C17-N18	6.68	1.45	1.33
4	Q	903	MGD	C14-N15	6.69	1.54	1.45
4	C	902	MGD	C23-C14	6.70	1.58	1.53
4	O	903	MGD	C23-C14	6.72	1.58	1.53
4	E	903	MGD	C14-N15	6.76	1.54	1.45
4	Q	903	MGD	C17-N18	6.77	1.45	1.33
4	Q	902	MGD	C23-C14	6.77	1.58	1.53
4	M	903	MGD	C17-N18	6.79	1.45	1.33
4	A	903	MGD	C14-N15	6.84	1.54	1.45
4	K	903	MGD	C14-N15	6.96	1.55	1.45
4	C	903	MGD	C23-C14	7.05	1.58	1.53
4	W	902	MGD	C23-C14	7.08	1.58	1.53
4	U	903	MGD	C14-N15	7.12	1.55	1.45
4	K	902	MGD	C23-C14	7.17	1.58	1.53
4	S	903	MGD	C14-N15	7.26	1.55	1.45
6	W	905	PYG	C1-C2	7.72	1.48	1.39
6	A	905	PYG	C1-C2	8.01	1.49	1.39
6	G	905	PYG	C1-C2	8.03	1.49	1.39
6	M	905	PYG	C1-C2	8.07	1.49	1.39
6	S	905	PYG	C1-C2	8.12	1.49	1.39
6	K	905	PYG	C1-C2	8.12	1.49	1.39
6	O	905	PYG	C1-C2	8.19	1.49	1.39
6	C	905	PYG	C1-C2	8.20	1.49	1.39
6	U	905	PYG	C1-C2	8.21	1.49	1.39
6	E	905	PYG	C1-C2	8.23	1.49	1.39
6	I	905	PYG	C1-C2	8.26	1.49	1.39
6	Q	905	PYG	C1-C2	8.29	1.49	1.39

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	903	MGD	O11-C23-C14	-10.46	101.98	108.96
4	K	903	MGD	O11-C23-C14	-9.78	102.44	108.96
4	I	903	MGD	O11-C23-C14	-7.56	103.92	108.96
6	W	905	PYG	O1-C1-C2	-7.55	98.12	117.86
6	K	905	PYG	O1-C1-C2	-7.41	98.48	117.86
6	C	905	PYG	O1-C1-C2	-7.39	98.54	117.86
6	O	905	PYG	O1-C1-C2	-7.36	98.60	117.86
6	U	905	PYG	O1-C1-C2	-7.31	98.75	117.86
6	A	905	PYG	O1-C1-C2	-7.26	98.87	117.86
6	S	905	PYG	O1-C1-C2	-7.19	99.05	117.86
6	I	905	PYG	O1-C1-C2	-7.15	99.16	117.86
6	G	905	PYG	O1-C1-C2	-7.13	99.22	117.86
6	E	905	PYG	O1-C1-C2	-7.12	99.23	117.86
4	G	903	MGD	O11-C23-C14	-7.12	104.21	108.96
4	S	902	MGD	C5-C6-N1	-7.10	113.38	123.48
6	Q	905	PYG	O1-C1-C2	-7.09	99.30	117.86
4	A	903	MGD	C5-C6-N1	-7.08	113.40	123.48
4	K	903	MGD	C5-C6-N1	-7.08	113.41	123.48
4	E	902	MGD	C5-C6-N1	-7.07	113.41	123.48
4	Q	902	MGD	C5-C6-N1	-7.06	113.43	123.48
4	I	902	MGD	C5-C6-N1	-7.06	113.44	123.48
6	M	905	PYG	O1-C1-C2	-7.03	99.47	117.86
4	G	903	MGD	C5-C6-N1	-7.01	113.50	123.48
4	G	902	MGD	C5-C6-N1	-6.96	113.57	123.48
4	K	902	MGD	C5-C6-N1	-6.96	113.57	123.48
4	A	902	MGD	C5-C6-N1	-6.96	113.58	123.48
4	S	903	MGD	C5-C6-N1	-6.94	113.60	123.48
4	W	902	MGD	C5-C6-N1	-6.94	113.61	123.48
4	O	902	MGD	C5-C6-N1	-6.94	113.61	123.48
4	U	902	MGD	C5-C6-N1	-6.92	113.62	123.48
4	I	903	MGD	C5-C6-N1	-6.92	113.63	123.48
4	A	903	MGD	O4'-C4'-C5'	-6.90	86.10	109.40
4	C	902	MGD	C5-C6-N1	-6.86	113.71	123.48
4	M	902	MGD	C5-C6-N1	-6.74	113.88	123.48
4	O	903	MGD	C5-C6-N1	-6.74	113.89	123.48
4	K	903	MGD	O4'-C4'-C5'	-6.62	87.06	109.40
4	Q	903	MGD	C5-C6-N1	-6.60	114.09	123.48
4	M	903	MGD	C5-C6-N1	-6.59	114.10	123.48
4	E	903	MGD	C5-C6-N1	-6.53	114.19	123.48
4	C	903	MGD	C5-C6-N1	-6.50	114.22	123.48
4	W	903	MGD	C5-C6-N1	-6.40	114.37	123.48
4	U	903	MGD	C5-C6-N1	-6.32	114.48	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	903	MGD	O11-C23-C14	-6.21	104.82	108.96
4	M	903	MGD	O11-C23-C14	-5.89	105.03	108.96
4	C	902	MGD	O2A-PA-O3A	-5.49	82.20	108.14
4	M	902	MGD	O2A-PA-O3A	-5.45	82.40	108.14
4	A	902	MGD	O2A-PA-O3A	-5.42	82.57	108.14
4	I	902	MGD	O2A-PA-O3A	-5.33	82.96	108.14
4	Q	903	MGD	O4'-C4'-C5'	-5.30	91.50	109.40
4	S	903	MGD	O11-C23-C14	-5.29	105.44	108.96
4	U	902	MGD	O2A-PA-O3A	-5.26	83.30	108.14
4	G	903	MGD	O4'-C4'-C5'	-5.20	91.84	109.40
4	W	902	MGD	O2A-PA-O3A	-5.17	83.75	108.14
4	Q	902	MGD	O2A-PA-O3A	-5.15	83.82	108.14
4	E	903	MGD	O4'-C4'-C5'	-5.13	92.08	109.40
4	U	903	MGD	O11-C23-C14	-5.12	105.55	108.96
4	E	902	MGD	O2A-PA-O3A	-5.10	84.08	108.14
4	K	902	MGD	O2A-PA-O3A	-5.07	84.18	108.14
4	E	903	MGD	O11-C23-C14	-5.04	105.60	108.96
4	G	902	MGD	O2A-PA-O3A	-5.04	84.36	108.14
4	O	902	MGD	O2A-PA-O3A	-4.97	84.69	108.14
4	S	903	MGD	O4'-C4'-C5'	-4.95	92.69	109.40
4	I	903	MGD	O4'-C4'-C5'	-4.90	92.84	109.40
4	S	902	MGD	O2A-PA-O3A	-4.85	85.24	108.14
4	O	903	MGD	O11-C23-C14	-4.60	105.89	108.96
4	S	902	MGD	O2A-PA-O1A	-4.59	88.52	112.28
4	O	903	MGD	O4'-C4'-C5'	-4.54	94.06	109.40
4	U	902	MGD	O2A-PA-O1A	-4.50	88.97	112.28
4	M	903	MGD	O4'-C4'-C5'	-4.44	94.40	109.40
4	C	903	MGD	O11-C23-C14	-4.40	106.03	108.96
4	E	902	MGD	O2A-PA-O1A	-4.39	89.55	112.28
4	U	903	MGD	O4'-C4'-C5'	-4.34	94.75	109.40
4	G	903	MGD	C6-C5-C4	-4.33	116.54	120.84
4	C	903	MGD	O4'-C4'-C5'	-4.32	94.81	109.40
4	Q	903	MGD	C6-C5-C4	-4.30	116.57	120.84
4	M	902	MGD	O2A-PA-O1A	-4.29	90.06	112.28
4	G	903	MGD	C2-N3-C4	-4.25	110.20	115.16
4	G	902	MGD	O2A-PA-O1A	-4.22	90.43	112.28
4	A	902	MGD	O2A-PA-O1A	-4.20	90.53	112.28
4	A	903	MGD	C6-C5-C4	-4.19	116.68	120.84
4	W	903	MGD	C6-C5-C4	-4.17	116.70	120.84
4	K	903	MGD	C6-C5-C4	-4.16	116.71	120.84
4	W	903	MGD	O4'-C4'-C5'	-4.11	95.54	109.40
4	C	902	MGD	O2A-PA-O1A	-4.06	91.28	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	903	MGD	C6-C5-C4	-4.03	116.84	120.84
4	E	903	MGD	C6-C5-C4	-4.03	116.84	120.84
6	M	905	PYG	C6-C1-C2	-3.99	115.80	120.08
4	I	903	MGD	C6-C5-C4	-3.97	116.90	120.84
4	U	903	MGD	C6-C5-C4	-3.96	116.91	120.84
6	E	905	PYG	C6-C1-C2	-3.93	115.87	120.08
6	M	905	PYG	O3-C3-C4	-3.92	108.69	119.35
4	I	902	MGD	O2A-PA-O1A	-3.91	92.02	112.28
6	E	905	PYG	O3-C3-C4	-3.91	108.71	119.35
6	G	905	PYG	C6-C1-C2	-3.90	115.89	120.08
6	I	905	PYG	O3-C3-C4	-3.90	108.72	119.35
6	G	905	PYG	O3-C3-C4	-3.90	108.73	119.35
6	I	905	PYG	C6-C1-C2	-3.88	115.91	120.08
6	O	905	PYG	O3-C3-C4	-3.88	108.79	119.35
6	W	905	PYG	O3-C3-C4	-3.87	108.80	119.35
4	O	902	MGD	O2A-PA-O1A	-3.87	92.24	112.28
6	Q	905	PYG	O3-C3-C4	-3.87	108.80	119.35
6	Q	905	PYG	C6-C1-C2	-3.86	115.94	120.08
6	S	905	PYG	O3-C3-C4	-3.86	108.84	119.35
6	K	905	PYG	O3-C3-C4	-3.85	108.86	119.35
6	W	905	PYG	C6-C1-C2	-3.85	115.95	120.08
6	K	905	PYG	C6-C1-C2	-3.84	115.95	120.08
6	O	905	PYG	C6-C1-C2	-3.83	115.97	120.08
6	U	905	PYG	O3-C3-C4	-3.83	108.92	119.35
6	C	905	PYG	O3-C3-C4	-3.82	108.94	119.35
6	A	905	PYG	O3-C3-C4	-3.82	108.95	119.35
6	U	905	PYG	C6-C1-C2	-3.77	116.03	120.08
6	C	905	PYG	C6-C1-C2	-3.76	116.04	120.08
6	S	905	PYG	C6-C1-C2	-3.75	116.05	120.08
4	K	902	MGD	O2A-PA-O1A	-3.73	92.97	112.28
4	O	903	MGD	C6-C5-C4	-3.73	117.14	120.84
6	A	905	PYG	C6-C1-C2	-3.64	116.17	120.08
4	Q	902	MGD	O2A-PA-O1A	-3.63	93.48	112.28
4	W	902	MGD	O2A-PA-O1A	-3.61	93.59	112.28
4	M	903	MGD	C6-C5-C4	-3.61	117.25	120.84
4	C	903	MGD	C6-C5-C4	-3.61	117.26	120.84
4	W	903	MGD	O11-C23-C14	-3.51	106.63	108.96
4	E	903	MGD	C2-N3-C4	-3.36	111.24	115.16
4	S	903	MGD	C2-N3-C4	-3.33	111.27	115.16
4	Q	903	MGD	C2-N3-C4	-3.12	111.52	115.16
4	C	903	MGD	C2-N3-C4	-3.12	111.52	115.16
4	I	903	MGD	C2-N3-C4	-3.06	111.58	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	902	MGD	C16-C17-N18	-3.04	114.96	123.91
4	Q	903	MGD	C16-C17-N18	-3.04	114.97	123.91
4	U	903	MGD	C2-N3-C4	-3.03	111.62	115.16
4	W	902	MGD	C16-C17-N18	-3.03	115.00	123.91
4	Q	902	MGD	C16-C17-N18	-3.03	115.00	123.91
4	K	902	MGD	C16-C17-N18	-3.03	115.00	123.91
4	E	902	MGD	C16-C17-N18	-3.03	115.02	123.91
4	C	902	MGD	C16-C17-N18	-3.02	115.02	123.91
4	M	902	MGD	C16-C17-N18	-3.02	115.03	123.91
4	I	902	MGD	C16-C17-N18	-3.01	115.05	123.91
4	S	902	MGD	C16-C17-N18	-3.01	115.06	123.91
4	K	903	MGD	C16-C17-N18	-3.01	115.08	123.91
4	U	902	MGD	C16-C17-N18	-3.01	115.08	123.91
4	W	902	MGD	C6-C5-C4	-3.00	117.86	120.84
4	A	902	MGD	C16-C17-N18	-2.99	115.11	123.91
4	C	903	MGD	C16-C17-N18	-2.99	115.14	123.91
4	M	903	MGD	C16-C17-N18	-2.98	115.15	123.91
4	G	903	MGD	C16-C17-N18	-2.98	115.16	123.91
4	M	902	MGD	C6-C5-C4	-2.97	117.89	120.84
4	O	903	MGD	C16-C17-N18	-2.97	115.17	123.91
4	I	903	MGD	C16-C17-N18	-2.97	115.18	123.91
4	A	903	MGD	C16-C17-N18	-2.97	115.19	123.91
4	O	902	MGD	C16-C17-N18	-2.97	115.19	123.91
4	W	903	MGD	C16-C17-N18	-2.96	115.20	123.91
4	U	903	MGD	C16-C17-N18	-2.96	115.21	123.91
4	S	903	MGD	C16-C17-N18	-2.96	115.21	123.91
4	O	903	MGD	C2-N3-C4	-2.96	111.70	115.16
4	E	903	MGD	C16-C17-N18	-2.95	115.23	123.91
4	M	903	MGD	C2-N3-C4	-2.92	111.75	115.16
4	G	902	MGD	C6-C5-C4	-2.91	117.95	120.84
4	A	903	MGD	C2-N3-C4	-2.91	111.76	115.16
4	U	902	MGD	C6-C5-C4	-2.90	117.96	120.84
4	S	902	MGD	O4'-C4'-C5'	-2.90	99.62	109.40
4	I	902	MGD	C6-C5-C4	-2.88	117.98	120.84
4	Q	902	MGD	C6-C5-C4	-2.87	117.99	120.84
4	K	902	MGD	C6-C5-C4	-2.87	118.00	120.84
4	G	902	MGD	O4'-C4'-C5'	-2.84	99.80	109.40
4	W	903	MGD	C2-N3-C4	-2.82	111.87	115.16
4	C	902	MGD	C6-C5-C4	-2.81	118.05	120.84
4	K	903	MGD	C2-N3-C4	-2.80	111.89	115.16
4	O	902	MGD	C6-C5-C4	-2.80	118.06	120.84
4	U	902	MGD	O4'-C4'-C5'	-2.79	99.97	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	902	MGD	N3-C2-N1	-2.71	123.50	127.46
4	U	902	MGD	N3-C2-N1	-2.68	123.54	127.46
4	A	902	MGD	C6-C5-C4	-2.66	118.20	120.84
4	K	902	MGD	N3-C2-N1	-2.65	123.59	127.46
4	O	902	MGD	C2-N3-C4	-2.59	112.14	115.16
4	M	903	MGD	N3-C2-N1	-2.59	123.68	127.46
4	I	902	MGD	O4'-C4'-C5'	-2.58	100.69	109.40
4	W	903	MGD	N3-C2-N1	-2.57	123.71	127.46
4	S	902	MGD	C6-C5-C4	-2.55	118.31	120.84
4	E	902	MGD	C2-N3-C4	-2.55	112.19	115.16
4	E	902	MGD	C6-C5-C4	-2.54	118.32	120.84
4	I	903	MGD	N3-C2-N1	-2.51	123.80	127.46
4	A	902	MGD	C2-N3-C4	-2.51	112.23	115.16
4	O	902	MGD	N3-C2-N1	-2.50	123.80	127.46
4	Q	902	MGD	N3-C2-N1	-2.50	123.81	127.46
4	Q	903	MGD	N3-C2-N1	-2.50	123.81	127.46
4	W	902	MGD	N3-C2-N1	-2.50	123.81	127.46
4	G	902	MGD	N3-C2-N1	-2.49	123.82	127.46
4	U	903	MGD	N3-C2-N1	-2.49	123.83	127.46
4	I	902	MGD	N3-C2-N1	-2.48	123.83	127.46
4	C	903	MGD	N3-C2-N1	-2.46	123.86	127.46
4	E	902	MGD	O4'-C4'-C5'	-2.46	101.11	109.40
4	A	903	MGD	N3-C2-N1	-2.46	123.87	127.46
4	M	902	MGD	C2-N3-C4	-2.45	112.30	115.16
4	M	902	MGD	N3-C2-N1	-2.41	123.94	127.46
4	C	902	MGD	N3-C2-N1	-2.40	123.95	127.46
4	A	902	MGD	N3-C2-N1	-2.39	123.97	127.46
4	G	902	MGD	C2-N3-C4	-2.37	112.40	115.16
4	E	902	MGD	N3-C2-N1	-2.36	124.01	127.46
4	Q	902	MGD	C2-N3-C4	-2.35	112.42	115.16
4	A	902	MGD	O4'-C4'-C5'	-2.35	101.47	109.40
4	E	903	MGD	N3-C2-N1	-2.35	124.03	127.46
4	I	902	MGD	C2-N3-C4	-2.34	112.42	115.16
4	W	902	MGD	C2-N3-C4	-2.34	112.43	115.16
4	O	903	MGD	N3-C2-N1	-2.34	124.04	127.46
4	Q	902	MGD	O4'-C4'-C5'	-2.33	101.52	109.40
4	K	903	MGD	N3-C2-N1	-2.33	124.06	127.46
4	S	902	MGD	C2-N3-C4	-2.30	112.47	115.16
4	W	902	MGD	O4'-C4'-C5'	-2.27	101.74	109.40
4	S	903	MGD	N3-C2-N1	-2.26	124.16	127.46
4	O	902	MGD	O4'-C4'-C5'	-2.25	101.79	109.40
4	C	902	MGD	C2-N3-C4	-2.19	112.60	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	902	MGD	O4'-C4'-C5'	-2.19	102.02	109.40
4	K	902	MGD	O4'-C4'-C5'	-2.17	102.08	109.40
4	K	903	MGD	O2B-PB-O5'	-2.15	97.98	108.14
4	U	902	MGD	C2-N3-C4	-2.12	112.68	115.16
4	W	902	MGD	O5'-C5'-C4'	-2.09	101.58	109.00
4	A	903	MGD	O2B-PB-O5'	-2.06	98.41	108.14
6	M	905	PYG	C3-C2-C1	2.00	120.79	119.50
4	W	902	MGD	C4-C5-N7	2.02	111.36	109.41
6	C	905	PYG	C3-C2-C1	2.03	120.81	119.50
4	W	902	MGD	O11-C23-C14	2.04	110.32	108.96
6	I	905	PYG	C3-C2-C1	2.07	120.83	119.50
4	U	902	MGD	C4-C5-N7	2.07	111.41	109.41
6	O	905	PYG	C3-C2-C1	2.09	120.84	119.50
4	Q	902	MGD	C4-C5-N7	2.10	111.44	109.41
4	U	903	MGD	C4'-O4'-C1'	2.10	112.01	109.77
4	E	902	MGD	C4-C5-N7	2.11	111.45	109.41
6	W	905	PYG	C3-C2-C1	2.15	120.88	119.50
4	C	902	MGD	C4-C5-N7	2.16	111.49	109.41
4	O	902	MGD	C4-C5-N7	2.20	111.53	109.41
4	G	902	MGD	C4-C5-N7	2.20	111.54	109.41
4	Q	903	MGD	C4'-O4'-C1'	2.25	112.16	109.77
4	I	903	MGD	O4'-C4'-C3'	2.28	109.69	105.17
4	M	902	MGD	C4-C5-N7	2.28	111.62	109.41
4	O	903	MGD	C4'-O4'-C1'	2.30	112.21	109.77
4	I	902	MGD	C4-C5-N7	2.31	111.64	109.41
4	M	903	MGD	C4-C5-N7	2.36	111.69	109.41
4	A	902	MGD	C4-C5-N7	2.36	111.69	109.41
4	W	903	MGD	C4-C5-N7	2.40	111.72	109.41
4	Q	903	MGD	C4-C5-N7	2.41	111.74	109.41
4	O	903	MGD	C4-C5-N7	2.42	111.75	109.41
4	K	902	MGD	O11-C23-C14	2.47	110.61	108.96
4	S	903	MGD	C4-C5-N7	2.49	111.81	109.41
4	G	903	MGD	C4-C5-N7	2.51	111.84	109.41
4	S	903	MGD	C4'-O4'-C1'	2.56	112.49	109.77
4	M	903	MGD	C4'-O4'-C1'	2.58	112.51	109.77
4	E	903	MGD	C4-C5-N7	2.58	111.90	109.41
4	E	903	MGD	C4'-O4'-C1'	2.62	112.56	109.77
4	C	903	MGD	C4-C5-N7	2.68	112.00	109.41
4	M	902	MGD	O11-C23-C14	2.69	110.76	108.96
4	U	903	MGD	C4-C5-N7	2.71	112.03	109.41
4	C	902	MGD	O11-C23-C14	2.74	110.79	108.96
4	E	902	MGD	O11-C23-C14	2.76	110.81	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	903	MGD	C16-C21-N22	2.79	120.68	118.17
4	S	902	MGD	O11-C23-C14	2.80	110.83	108.96
4	I	902	MGD	O11-C23-C14	2.80	110.83	108.96
4	E	903	MGD	C16-C21-N22	2.80	120.69	118.17
4	G	903	MGD	C16-C21-N22	2.96	120.83	118.17
4	C	903	MGD	C16-C21-N22	2.97	120.84	118.17
4	I	903	MGD	C16-C21-N22	3.02	120.88	118.17
4	U	903	MGD	C16-C21-N22	3.03	120.89	118.17
4	S	902	MGD	C16-C21-N22	3.04	120.90	118.17
4	O	902	MGD	O11-C23-C14	3.07	111.01	108.96
4	A	902	MGD	C16-C21-N22	3.07	120.93	118.17
4	U	902	MGD	O11-C23-C14	3.11	111.04	108.96
4	Q	903	MGD	C16-C21-N22	3.12	120.97	118.17
4	O	903	MGD	C16-C21-N22	3.13	120.98	118.17
4	Q	902	MGD	C16-C21-N22	3.13	120.98	118.17
4	I	902	MGD	C16-C21-N22	3.14	120.99	118.17
4	E	902	MGD	C16-C21-N22	3.15	121.00	118.17
4	A	903	MGD	C16-C21-N22	3.16	121.01	118.17
4	W	902	MGD	C16-C21-N22	3.18	121.03	118.17
4	U	902	MGD	C16-C21-N22	3.20	121.05	118.17
4	G	902	MGD	C16-C21-N22	3.20	121.05	118.17
4	M	902	MGD	C16-C21-N22	3.24	121.08	118.17
4	C	902	MGD	C16-C21-N22	3.26	121.10	118.17
4	O	902	MGD	C16-C21-N22	3.28	121.12	118.17
4	G	902	MGD	O11-C23-C14	3.31	111.17	108.96
4	M	903	MGD	C16-C21-N22	3.34	121.17	118.17
4	K	903	MGD	C16-C21-N22	3.34	121.17	118.17
4	K	902	MGD	C16-C21-N22	3.35	121.18	118.17
4	K	903	MGD	O5'-C5'-C4'	3.39	121.04	109.00
4	S	903	MGD	C16-C21-N22	3.52	121.33	118.17
4	A	903	MGD	O5'-C5'-C4'	3.55	121.59	109.00
4	A	902	MGD	O11-C23-C14	3.76	111.47	108.96
4	S	903	MGD	C17-C16-C21	4.09	118.27	114.56
4	I	903	MGD	C17-C16-C21	4.30	118.46	114.56
4	M	903	MGD	C17-C16-C21	4.35	118.50	114.56
4	K	903	MGD	C4'-O4'-C1'	4.39	114.44	109.77
4	Q	903	MGD	C17-C16-C21	4.39	118.54	114.56
4	A	903	MGD	C17-C16-C21	4.40	118.55	114.56
4	K	903	MGD	C17-C16-C21	4.43	118.57	114.56
4	E	903	MGD	C17-C16-C21	4.51	118.64	114.56
4	C	902	MGD	C6-N1-C2	4.59	122.66	116.06
4	M	902	MGD	C6-N1-C2	4.63	122.72	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	903	MGD	C17-C16-C21	4.66	118.78	114.56
6	A	905	PYG	O3-C3-C2	4.66	130.05	117.86
6	Q	905	PYG	O3-C3-C2	4.67	130.07	117.86
6	G	905	PYG	O3-C3-C2	4.67	130.08	117.86
6	S	905	PYG	O3-C3-C2	4.68	130.10	117.86
6	K	905	PYG	O3-C3-C2	4.68	130.11	117.86
6	E	905	PYG	O3-C3-C2	4.68	130.12	117.86
6	C	905	PYG	O3-C3-C2	4.69	130.13	117.86
6	U	905	PYG	O3-C3-C2	4.69	130.15	117.86
6	M	905	PYG	O3-C3-C2	4.70	130.15	117.86
4	U	903	MGD	C17-C16-C21	4.71	118.83	114.56
6	I	905	PYG	O3-C3-C2	4.72	130.22	117.86
4	K	902	MGD	C17-N18-C19	4.75	122.89	116.06
6	W	905	PYG	O3-C3-C2	4.75	130.29	117.86
6	O	905	PYG	O3-C3-C2	4.75	130.29	117.86
4	O	902	MGD	C17-N18-C19	4.75	122.90	116.06
4	C	903	MGD	C17-C16-C21	4.78	118.89	114.56
4	G	902	MGD	C6-N1-C2	4.79	122.95	116.06
4	E	902	MGD	C17-N18-C19	4.80	122.96	116.06
4	A	902	MGD	C6-N1-C2	4.80	122.96	116.06
4	U	902	MGD	C17-N18-C19	4.80	122.96	116.06
4	Q	902	MGD	C17-N18-C19	4.80	122.97	116.06
4	W	903	MGD	C17-N18-C19	4.80	122.97	116.06
4	A	903	MGD	C4'-O4'-C1'	4.81	114.89	109.77
4	O	903	MGD	C17-C16-C21	4.81	118.92	114.56
4	M	903	MGD	C17-N18-C19	4.82	122.99	116.06
4	W	902	MGD	C6-N1-C2	4.86	123.05	116.06
4	E	902	MGD	C6-N1-C2	4.86	123.05	116.06
4	O	903	MGD	C17-N18-C19	4.87	123.07	116.06
4	C	902	MGD	C17-C16-C21	4.88	118.98	114.56
4	U	902	MGD	C6-N1-C2	4.88	123.08	116.06
4	K	902	MGD	C6-N1-C2	4.89	123.09	116.06
4	G	903	MGD	C17-N18-C19	4.90	123.11	116.06
4	C	903	MGD	C6-N1-C2	4.90	123.11	116.06
4	I	902	MGD	C17-N18-C19	4.91	123.12	116.06
4	A	902	MGD	C17-C16-C21	4.93	119.03	114.56
4	Q	902	MGD	C6-N1-C2	4.93	123.15	116.06
4	M	902	MGD	C17-N18-C19	4.94	123.17	116.06
4	U	903	MGD	C17-N18-C19	4.95	123.18	116.06
4	C	903	MGD	C17-N18-C19	4.95	123.18	116.06
4	W	903	MGD	C6-N1-C2	4.96	123.19	116.06
4	O	902	MGD	C6-N1-C2	4.96	123.19	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	902	MGD	C17-C16-C21	4.96	119.06	114.56
4	G	902	MGD	C17-N18-C19	4.97	123.20	116.06
4	S	902	MGD	C17-N18-C19	4.97	123.21	116.06
4	W	903	MGD	C17-C16-C21	4.98	119.07	114.56
4	W	902	MGD	C17-N18-C19	4.98	123.23	116.06
4	W	902	MGD	C17-C16-C21	4.98	119.08	114.56
4	Q	903	MGD	C17-N18-C19	4.99	123.23	116.06
4	S	903	MGD	C17-N18-C19	5.00	123.25	116.06
4	I	902	MGD	C6-N1-C2	5.00	123.25	116.06
4	E	903	MGD	C6-N1-C2	5.01	123.27	116.06
4	A	903	MGD	C17-N18-C19	5.02	123.28	116.06
4	U	903	MGD	C6-N1-C2	5.02	123.28	116.06
4	G	902	MGD	C17-C16-C21	5.02	119.11	114.56
4	M	903	MGD	C6-N1-C2	5.03	123.30	116.06
4	S	902	MGD	C17-C16-C21	5.03	119.12	114.56
4	E	903	MGD	C17-N18-C19	5.04	123.31	116.06
4	O	903	MGD	C6-N1-C2	5.04	123.31	116.06
4	I	903	MGD	C17-N18-C19	5.06	123.33	116.06
4	K	903	MGD	C6-N1-C2	5.06	123.33	116.06
4	C	902	MGD	C17-N18-C19	5.07	123.35	116.06
4	A	902	MGD	C17-N18-C19	5.09	123.38	116.06
4	S	903	MGD	C6-N1-C2	5.10	123.39	116.06
4	M	902	MGD	C17-C16-C21	5.12	119.20	114.56
4	K	902	MGD	C17-C16-C21	5.13	119.21	114.56
4	O	902	MGD	C17-C16-C21	5.15	119.22	114.56
4	K	903	MGD	C17-N18-C19	5.15	123.47	116.06
4	Q	903	MGD	C6-N1-C2	5.16	123.49	116.06
4	S	902	MGD	C6-N1-C2	5.17	123.50	116.06
4	I	903	MGD	C6-N1-C2	5.18	123.51	116.06
4	I	902	MGD	C17-C16-C21	5.20	119.27	114.56
4	E	902	MGD	C17-C16-C21	5.26	119.32	114.56
4	G	903	MGD	C6-N1-C2	5.27	123.64	116.06
4	A	903	MGD	C6-N1-C2	5.31	123.69	116.06
4	Q	902	MGD	C17-C16-C21	5.31	119.37	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

67 monomers are involved in 203 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	MGD	5	0
4	A	903	MGD	8	0
6	A	905	PYG	1	0
7	B	302	SF4	1	0
7	B	303	SF4	2	0
7	B	304	SF4	1	0
4	C	902	MGD	8	0
4	C	903	MGD	5	0
7	D	302	SF4	1	0
7	D	303	SF4	2	0
7	D	304	SF4	1	0
4	E	902	MGD	9	0
4	E	903	MGD	5	0
6	E	905	PYG	1	0
7	F	302	SF4	1	0
7	F	303	SF4	2	0
7	F	304	SF4	1	0
4	G	902	MGD	6	0
4	G	903	MGD	4	0
7	H	302	SF4	1	0
7	H	303	SF4	2	0
7	H	304	SF4	1	0
4	I	902	MGD	6	0
4	I	903	MGD	6	0
6	I	905	PYG	1	0
7	J	301	SF4	1	0
7	J	302	SF4	2	0
7	J	303	SF4	1	0
4	K	902	MGD	5	0
4	K	903	MGD	8	0
7	L	302	SF4	1	0
7	L	303	SF4	2	0
7	L	304	SF4	1	0
4	M	902	MGD	8	0
4	M	903	MGD	7	0
6	M	905	PYG	1	0
7	N	302	SF4	2	0
7	N	303	SF4	2	0
7	N	304	SF4	1	0
4	O	902	MGD	7	0
4	O	903	MGD	4	0
6	O	905	PYG	1	0
7	P	302	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	P	303	SF4	2	0
7	P	304	SF4	1	0
4	Q	902	MGD	6	0
4	Q	903	MGD	4	0
6	Q	905	PYG	1	0
7	R	303	SF4	2	0
7	R	304	SF4	1	0
4	S	902	MGD	4	0
4	S	903	MGD	6	0
6	S	905	PYG	1	0
7	T	302	SF4	1	0
7	T	303	SF4	2	0
7	T	304	SF4	1	0
4	U	902	MGD	8	0
4	U	903	MGD	5	0
6	U	905	PYG	1	0
7	V	302	SF4	1	0
7	V	303	SF4	2	0
7	V	304	SF4	1	0
4	W	902	MGD	8	0
4	W	903	MGD	4	0
7	X	302	SF4	1	0
7	X	303	SF4	2	0
7	X	304	SF4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.