



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:15 AM GMT

PDB ID : 1VLD  
Title : Crystal Structure of Pyrogallol-PhloroglucinolTranshydroxylase from Pelobacter acidigallici  
Authors : Messerschmidt, A.; Niessen, H.; Abt, D.; Einsle, O.; Schink, B.; Kroneck, P.M.H.  
Deposited on : 2004-06-03  
Resolution : 2.35 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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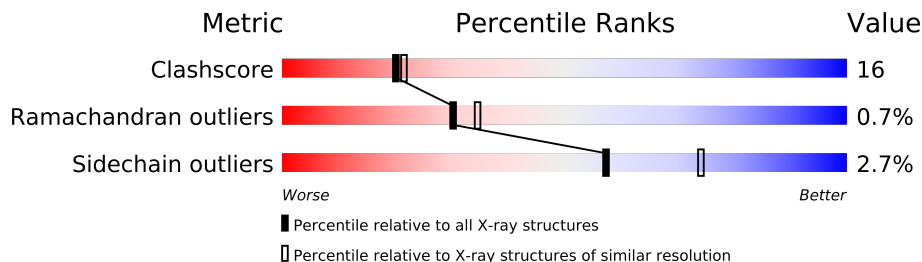
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	M	875	
1	O	875	
1	Q	875	
1	S	875	
1	U	875	
1	W	875	
2	N	274	
2	P	274	
2	R	274	
2	T	274	
2	V	274	
2	X	274	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 61010 atoms, of which 0 are hydrogen and 0 are deuterium.

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	M	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	O	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	Q	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	S	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	U	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			
1	W	875	Total	C	N	O	S	0	2	0
			7018	4477	1192	1301	48			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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.

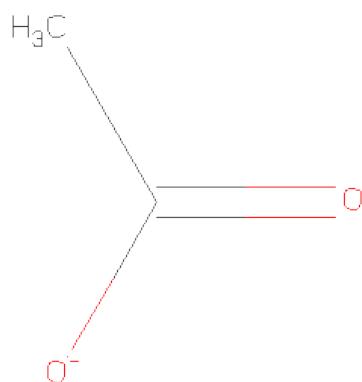
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	P	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	R	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	V	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			
2	X	274	Total	C	N	O	S	0	0	0
			2182	1371	364	423	24			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

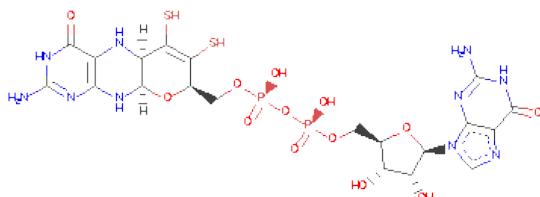


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total	C	O	0	0
			4	2	2		
3	O	1	Total	C	O	0	0
			4	2	2		
3	Q	1	Total	C	O	0	0
			4	2	2		
3	S	1	Total	C	O	0	0
			4	2	2		
3	U	1	Total	C	O	0	0
			4	2	2		
3	W	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Ca 1 1	0	0
4	Q	1	Total Ca 1 1	0	0
4	V	1	Total Ca 1 1	0	0
4	W	1	Total Ca 1 1	0	0
4	T	1	Total Ca 1 1	0	0
4	N	1	Total Ca 1 1	0	0
4	U	1	Total Ca 1 1	0	0
4	X	1	Total Ca 1 1	0	0
4	O	1	Total Ca 1 1	0	0
4	R	1	Total Ca 1 1	0	0
4	S	1	Total Ca 1 1	0	0
4	M	1	Total Ca 1 1	0	0

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONEGUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula:  $C_{20}H_{26}N_{10}O_{13}P_2S_2$ ).

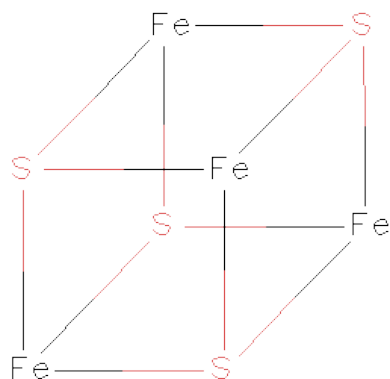


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	M	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	M	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	O	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	O	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	Q	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	Q	1	Total	C	N	O	P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

- Molecule 6 is MOLYBDENUM(IV) ION (three-letter code: 4MO) (formula: Mo).

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

- 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	N	1	Total	Fe	S	0	0
			8	4	4		
7	N	1	Total	Fe	S	0	0
			8	4	4		
7	N	1	Total	Fe	S	0	0
			8	4	4		
7	P	1	Total	Fe	S	0	0
			8	4	4		
7	P	1	Total	Fe	S	0	0
			8	4	4		
7	P	1	Total	Fe	S	0	0
			8	4	4		
7	R	1	Total	Fe	S	0	0
			8	4	4		
7	R	1	Total	Fe	S	0	0
			8	4	4		
7	R	1	Total	Fe	S	0	0
			8	4	4		
7	T	1	Total	Fe	S	0	0
			8	4	4		
7	T	1	Total	Fe	S	0	0
			8	4	4		
7	T	1	Total	Fe	S	0	0
			8	4	4		
7	V	1	Total	Fe	S	0	0
			8	4	4		
7	V	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	M	684	Total 684	O 684	0	0
8	N	162	Total 162	O 162	0	0
8	O	679	Total 679	O 679	0	0
8	P	163	Total 163	O 163	0	0
8	Q	690	Total 690	O 690	0	0
8	R	167	Total 167	O 167	0	0
8	S	679	Total 679	O 679	0	0
8	T	159	Total 159	O 159	0	0
8	U	672	Total 672	O 672	0	0
8	V	163	Total 163	O 163	0	0
8	W	676	Total 676	O 676	0	0
8	X	166	Total 166	O 166	0	0



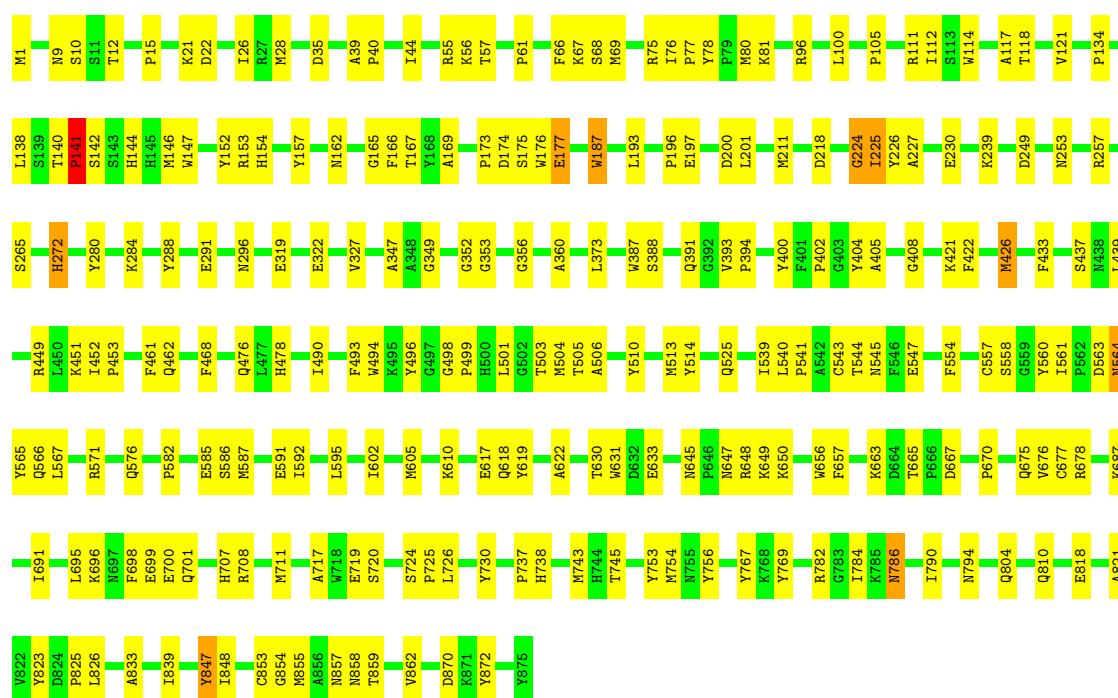
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

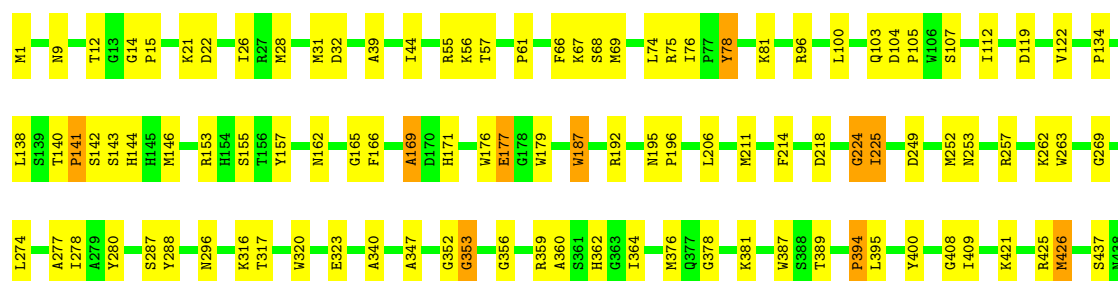
#### • Molecule 1: Pyrogallol hydroxytransferase large subunit

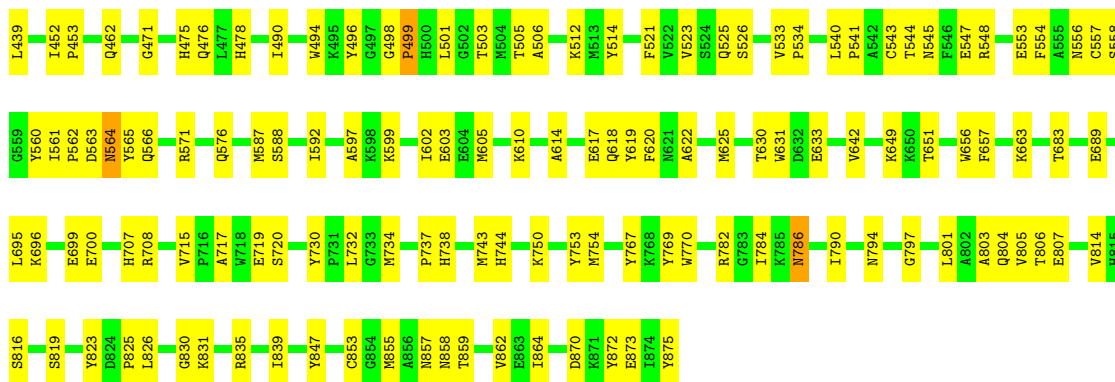
Chain M:



#### • Molecule 1: Pyrogallol hydroxytransferase large subunit

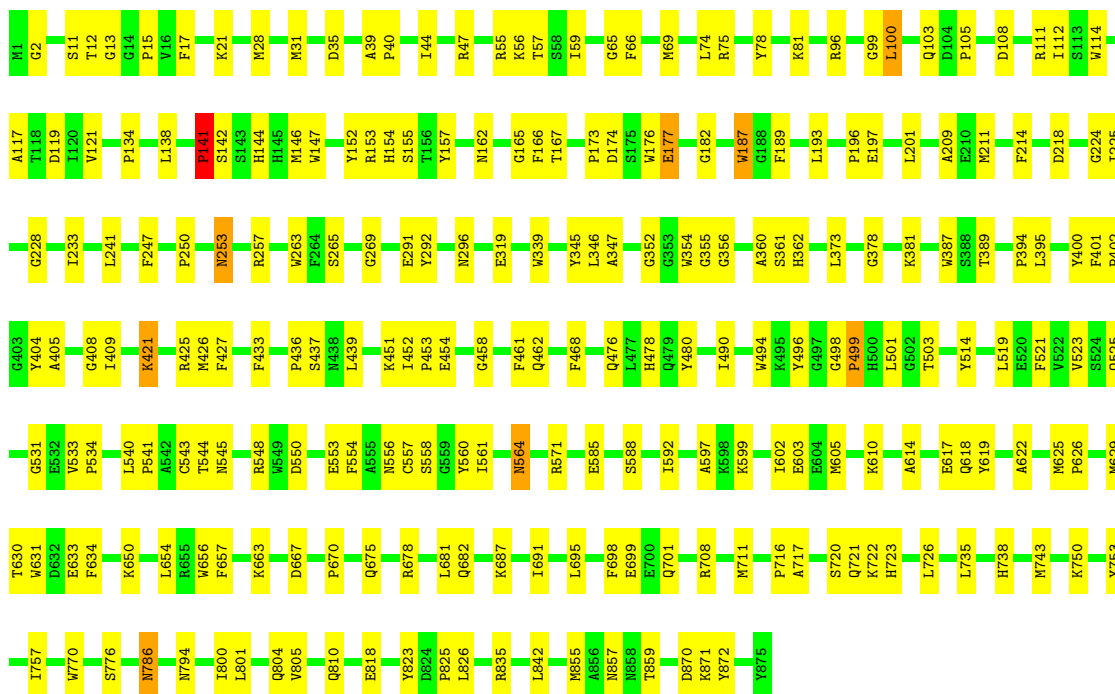
Chain O:





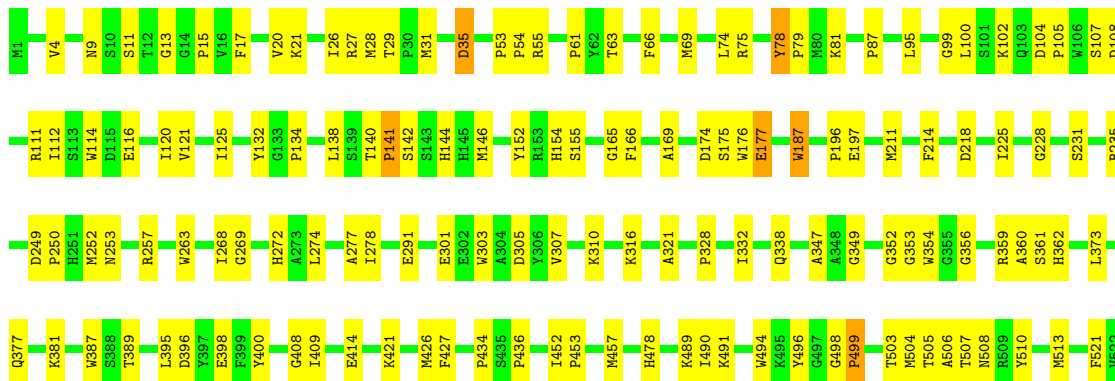
• Molecule 1: Pyrogallol hydroxytransferase large subunit

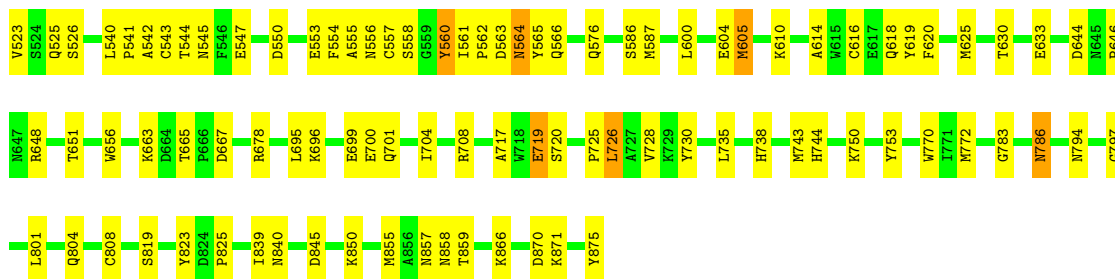
Chain Q:



• Molecule 1: Pyrogallol hydroxytransferase large subunit

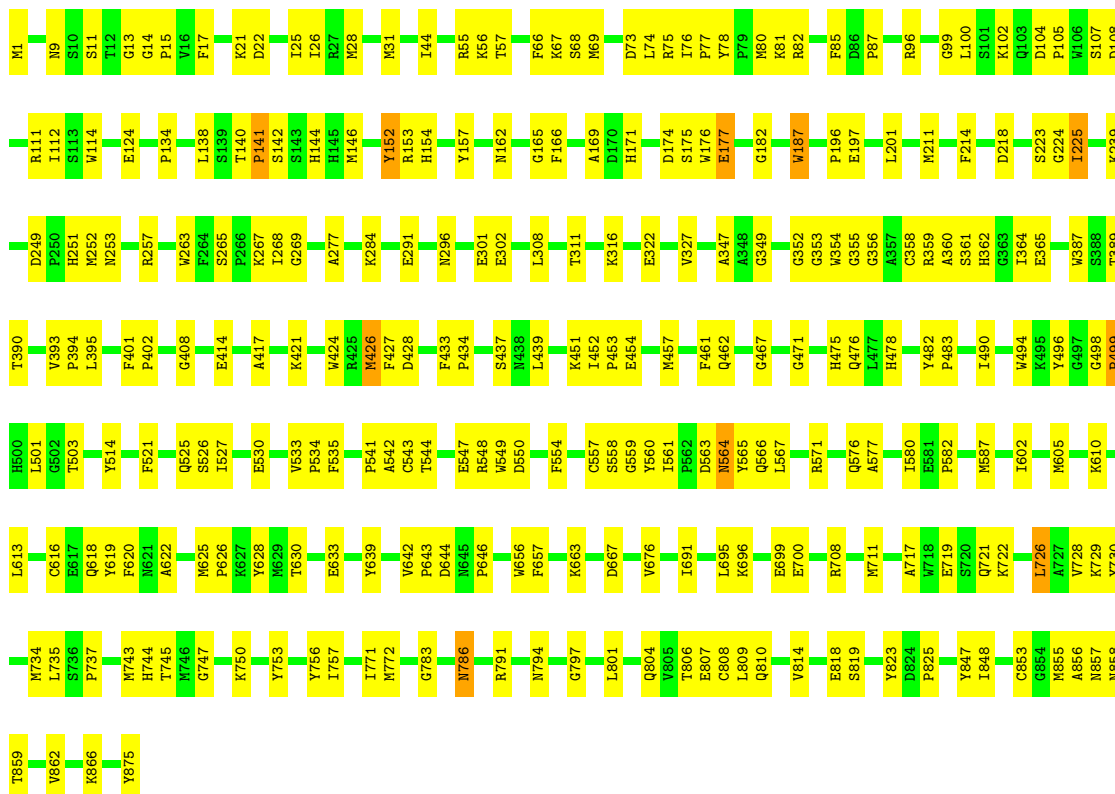
Chain S:





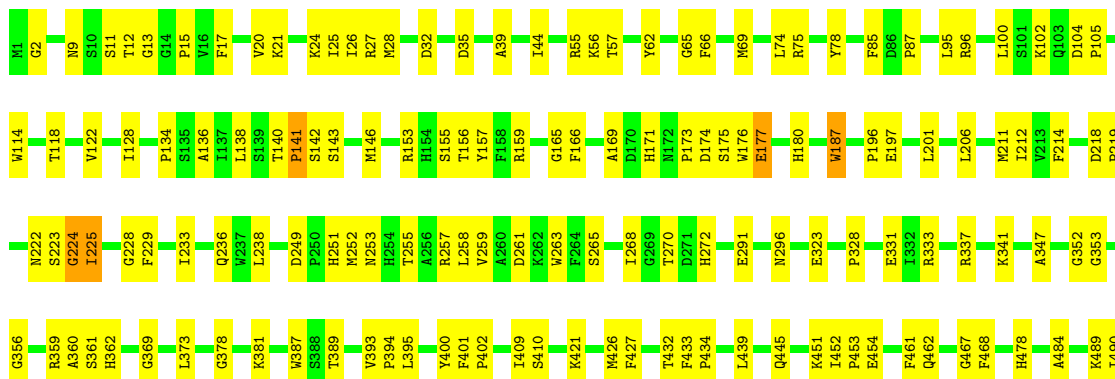
• Molecule 1: Pyrogallol hydroxytransferase large subunit

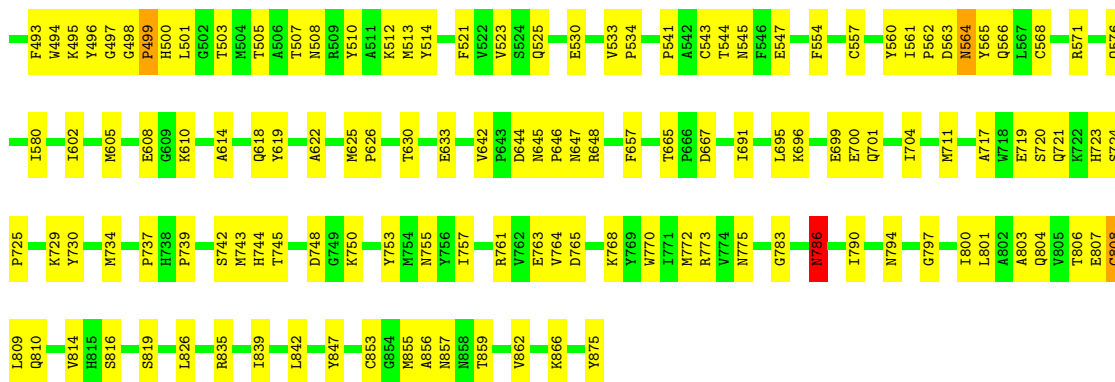
Chain U:



• Molecule 1: Pyrogallol hydroxytransferase large subunit

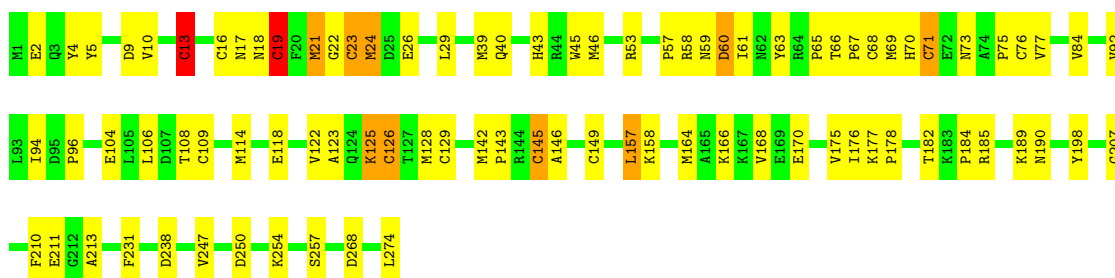
Chain W:





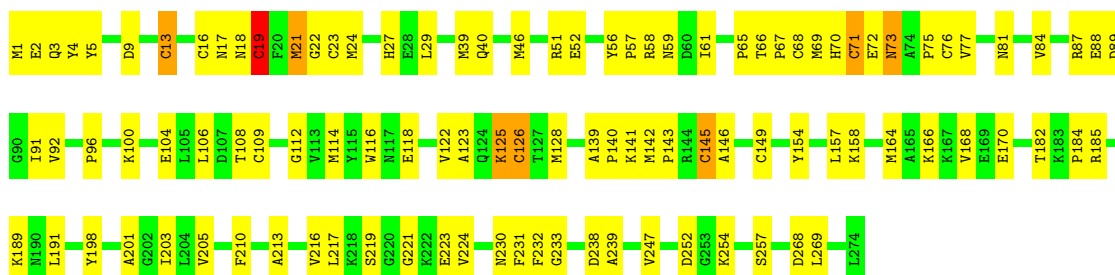
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain N:



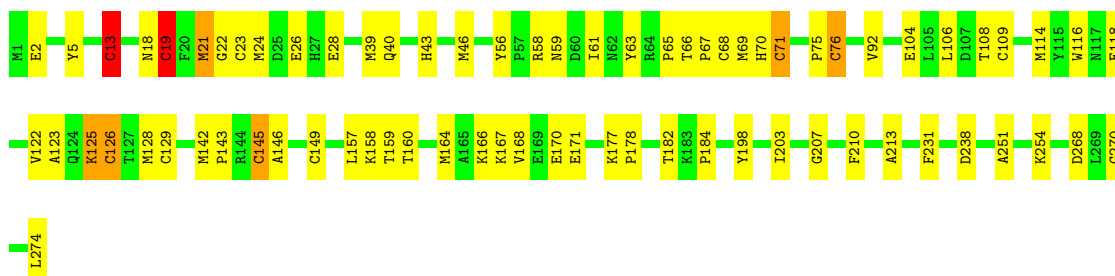
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain P:



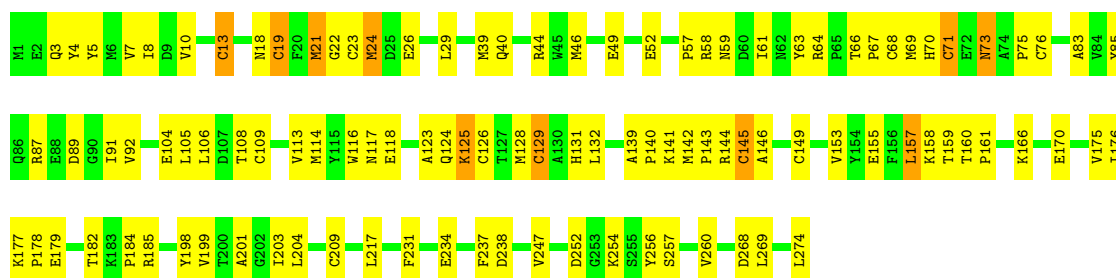
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain R:



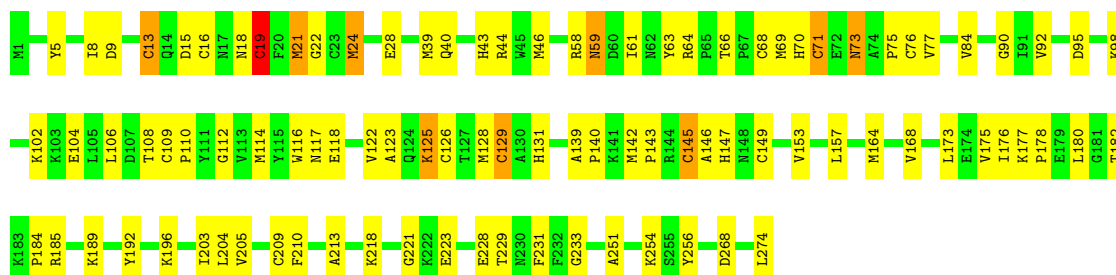
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain T:



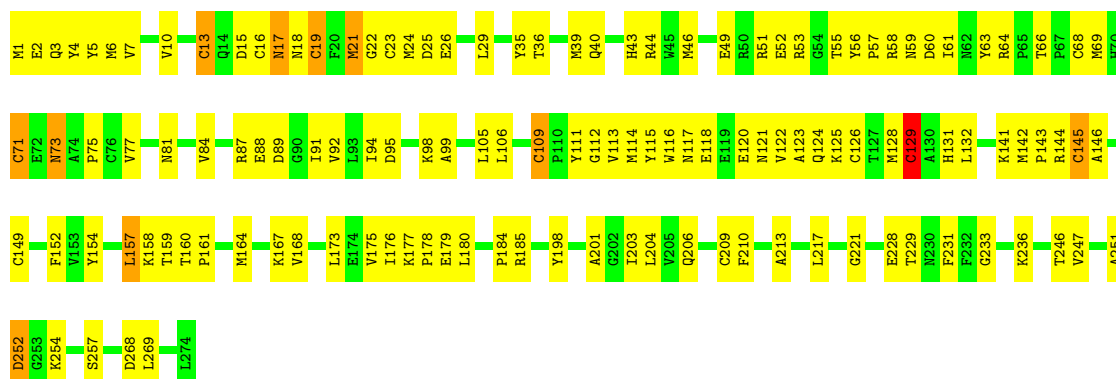
• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain V:



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain X:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.02Å 179.64Å 181.22Å 63.69° 63.98° 64.90°	Depositor
Resolution (Å)	24.98 – 2.35	Depositor
% Data completeness (in resolution range)	86.0 (24.98-2.35)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.198 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	61010	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 4MO, SF4, ACT, 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	M	0.36	0/7240	0.63	3/9815 (0.0%)
1	O	0.34	0/7240	0.62	4/9815 (0.0%)
1	Q	0.35	0/7240	0.62	3/9815 (0.0%)
1	S	0.34	0/7240	0.61	1/9815 (0.0%)
1	U	0.35	0/7240	0.60	1/9815 (0.0%)
1	W	0.33	0/7240	0.59	3/9815 (0.0%)
2	N	0.47	3/2231 (0.1%)	0.66	2/3009 (0.1%)
2	P	0.40	2/2231 (0.1%)	0.61	1/3009 (0.0%)
2	R	0.44	2/2231 (0.1%)	0.66	2/3009 (0.1%)
2	T	0.37	0/2231	0.59	1/3009 (0.0%)
2	V	0.40	1/2231 (0.0%)	0.61	2/3009 (0.1%)
2	X	0.35	0/2231	0.58	1/3009 (0.0%)
All	All	0.36	8/56826 (0.0%)	0.61	24/76944 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	M	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	19	CYS	CB-SG	-8.91	1.67	1.82
2	R	19	CYS	CB-SG	-7.56	1.69	1.82
2	N	126	CYS	CB-SG	-6.80	1.70	1.82
2	V	19	CYS	CB-SG	-6.51	1.71	1.82
2	R	126	CYS	CB-SG	-6.03	1.72	1.82
2	N	23	CYS	CB-SG	-6.02	1.72	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	19	CYS	CB-SG	-5.75	1.72	1.81
2	P	126	CYS	CB-SG	-5.65	1.72	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	352	GLY	N-CA-C	-8.47	91.94	113.10
1	O	352	GLY	N-CA-C	-8.36	92.21	113.10
1	Q	352	GLY	N-CA-C	-8.01	93.08	113.10
1	W	352	GLY	N-CA-C	-7.93	93.28	113.10
1	M	352	GLY	N-CA-C	-7.92	93.31	113.10
1	S	352	GLY	N-CA-C	-7.43	94.52	113.10
2	X	13	CYS	CA-CB-SG	-5.96	103.27	114.00
2	N	13	CYS	CA-CB-SG	-5.85	103.48	114.00
2	N	19	CYS	CB-CA-C	-5.82	98.76	110.40
2	V	13	CYS	CA-CB-SG	-5.72	103.71	114.00
1	M	141	PRO	N-CA-C	-5.69	97.30	112.10
1	M	224	GLY	N-CA-C	-5.55	99.23	113.10
1	Q	224	GLY	N-CA-C	-5.50	99.36	113.10
2	R	19	CYS	CB-CA-C	-5.45	99.51	110.40
1	W	224	GLY	N-CA-C	-5.35	99.73	113.10
2	P	13	CYS	CA-CB-SG	-5.32	104.42	114.00
2	V	16	CYS	CA-CB-SG	-5.32	104.43	114.00
2	R	13	CYS	CA-CB-SG	-5.29	104.47	114.00
1	O	353	GLY	N-CA-C	-5.27	99.91	113.10
1	Q	141	PRO	N-CA-C	-5.27	98.41	112.10
1	W	353	GLY	N-CA-C	-5.24	100.00	113.10
1	O	169	ALA	N-CA-C	-5.20	96.95	111.00
2	T	13	CYS	CA-CB-SG	-5.18	104.68	114.00
1	O	224	GLY	N-CA-C	-5.13	100.27	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	847	TYR	Sidechain

## 5.2 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 hydrogens



added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	7018	0	6645	185	0
1	O	7018	0	6645	194	0
1	Q	7018	0	6645	179	0
1	S	7018	0	6645	188	0
1	U	7018	0	6645	228	0
1	W	7018	0	6645	228	0
2	N	2182	0	2077	82	0
2	P	2182	0	2077	102	0
2	R	2182	0	2077	69	0
2	T	2182	0	2077	100	0
2	V	2182	0	2077	87	0
2	X	2182	0	2077	131	0
3	M	4	0	3	1	0
3	O	4	0	3	2	0
3	Q	4	0	3	1	0
3	S	4	0	3	1	0
3	U	4	0	3	1	0
3	W	4	0	3	2	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	1	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
4	X	1	0	0	0	0
5	M	94	0	44	9	0
5	O	94	0	44	9	0
5	Q	94	0	44	8	0
5	S	94	0	44	9	0
5	U	94	0	44	13	0
5	W	94	0	44	11	0
6	M	1	0	0	0	0
6	O	1	0	0	0	0
6	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	1	0	0	0	0
6	U	1	0	0	0	0
6	W	1	0	0	0	0
7	N	24	0	0	4	0
7	P	24	0	0	6	0
7	R	24	0	0	5	0
7	T	24	0	0	7	0
7	V	24	0	0	4	0
7	X	24	0	0	7	0
8	M	684	0	0	16	0
8	N	162	0	0	5	0
8	O	679	0	0	22	0
8	P	163	0	0	5	0
8	Q	690	0	0	19	0
8	R	167	0	0	2	0
8	S	679	0	0	22	0
8	T	159	0	0	5	0
8	U	672	0	0	26	0
8	V	163	0	0	5	0
8	W	676	0	0	27	0
8	X	166	0	0	12	0
All	All	61010	0	52614	1727	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (1727) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:426:MET:HE1	1:U:618:GLN:HG2	1.30	1.10
2:T:19:CYS:HB3	2:T:145:CYS:HB3	1.37	1.03
1:U:753:TYR:HB3	2:V:24:MET:HE3	1.36	1.03
2:N:2:GLU:HG2	2:N:158:LYS:HG2	1.40	1.02
2:P:19:CYS:HB3	2:P:145:CYS:HB3	1.40	1.01
1:Q:557:CYS:H	1:Q:564:ASN:HD21	1.01	1.00
2:X:69:MET:HB3	2:X:184:PRO:HB3	1.43	1.00
2:P:143:PRO:HB3	7:P:806:SF4:S1	2.03	0.99
2:V:69:MET:HB3	2:V:184:PRO:HB3	1.42	0.99
2:N:207:GLY:HA2	1:S:728:VAL:HG12	1.40	0.99
2:R:207:GLY:HA2	1:U:728:VAL:HG12	1.42	0.99
1:S:557:CYS:H	1:S:564:ASN:HD21	1.01	0.99
2:X:143:PRO:HB3	7:X:806:SF4:S1	2.05	0.97
2:T:128:MET:HA	7:T:806:SF4:S1	2.06	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:426:MET:HE1	1:S:618:GLN:HG2	1.47	0.96
1:M:360:ALA:HB1	1:M:859:THR:HG23	1.48	0.95
1:Q:610:LYS:NZ	1:Q:618:GLN:HE22	1.65	0.94
1:W:360:ALA:HB1	1:W:859:THR:HG23	1.49	0.94
1:U:557:CYS:H	1:U:564:ASN:HD21	1.01	0.94
1:O:753:TYR:HB3	2:P:24:MET:HE3	1.50	0.93
2:N:19:CYS:HB3	2:N:145:CYS:HB3	1.49	0.92
2:T:143:PRO:HB3	7:T:806:SF4:S1	2.10	0.92
2:P:128:MET:HA	7:P:806:SF4:S1	2.10	0.90
2:V:128:MET:HA	7:V:806:SF4:S1	2.12	0.90
2:N:46:MET:HE3	2:N:66:THR:H	1.36	0.89
2:X:40:GLN:NE2	2:X:117:ASN:HA	1.87	0.89
1:M:557:CYS:H	1:M:564:ASN:HD21	1.14	0.89
1:W:561:ILE:HG22	1:W:564:ASN:HB3	1.55	0.89
1:S:561:ILE:HG22	1:S:564:ASN:HB3	1.55	0.89
1:M:66:PHE:CD1	1:M:69:MET:HE3	2.07	0.89
1:W:645:ASN:ND2	1:W:648:ARG:HB3	1.88	0.89
1:O:557:CYS:H	1:O:564:ASN:HD21	1.21	0.88
2:P:70:HIS:HD2	2:P:92:VAL:H	1.20	0.88
2:X:129:CYS:HB3	2:X:131:HIS:CE1	2.08	0.88
1:Q:165:GLY:HA3	1:Q:166:PHE:HB3	1.55	0.88
1:M:426:MET:HE3	1:M:426:MET:HA	1.54	0.88
1:U:610:LYS:NZ	1:U:618:GLN:HE22	1.70	0.87
2:R:46:MET:HE1	2:R:66:THR:N	1.90	0.86
1:S:610:LYS:NZ	1:S:618:GLN:HE22	1.71	0.86
2:X:19:CYS:HB2	2:X:46:MET:HG2	1.55	0.86
1:U:165:GLY:HA3	1:U:166:PHE:HB3	1.55	0.86
1:S:28:MET:HE1	1:S:66:PHE:HB3	1.58	0.85
1:Q:66:PHE:CD1	1:Q:69:MET:HE3	2.11	0.85
1:W:28:MET:HE1	1:W:66:PHE:HB3	1.58	0.85
2:R:70:HIS:HD2	2:R:92:VAL:H	1.23	0.84
1:M:165:GLY:HA3	1:M:166:PHE:HB3	1.58	0.84
2:V:143:PRO:HB3	7:V:806:SF4:S1	2.18	0.84
2:P:73:ASN:OD1	1:S:648:ARG:HA	1.78	0.84
2:X:201:ALA:HB2	2:X:269:LEU:HB2	1.58	0.83
2:N:128:MET:HA	7:N:806:SF4:S1	2.18	0.83
1:O:610:LYS:NZ	1:O:618:GLN:HE22	1.77	0.83
2:X:19:CYS:HB3	2:X:145:CYS:HB3	1.59	0.83
2:R:128:MET:HA	7:R:806:SF4:S1	2.18	0.83
2:N:70:HIS:HD2	2:N:92:VAL:H	1.25	0.83
1:W:258:LEU:HG	1:W:259:VAL:HG13	1.61	0.82
1:W:783:GLY:O	1:W:866:LYS:HD2	1.79	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:138:LEU:HB2	1:O:490:ILE:HD12	1.61	0.82
2:N:46:MET:HE3	2:N:66:THR:N	1.94	0.82
1:O:28:MET:HE1	1:O:67:LYS:N	1.95	0.82
1:W:610:LYS:NZ	1:W:618:GLN:HE22	1.78	0.82
1:Q:503:THR:HG21	5:Q:900:MGD:O2A	1.80	0.82
1:W:32:ASP:OD2	8:W:1564:HOH:O	1.97	0.81
1:O:561:ILE:HG22	1:O:564:ASN:HB3	1.63	0.81
1:S:426:MET:CE	1:S:618:GLN:HG2	2.11	0.81
1:S:360:ALA:HB1	1:S:859:THR:HG23	1.61	0.81
1:M:138:LEU:HB2	1:M:490:ILE:HD12	1.63	0.81
1:W:165:GLY:HA3	1:W:166:PHE:HB3	1.62	0.80
1:W:557:CYS:H	1:W:564:ASN:HD21	1.29	0.80
1:O:794:ASN:HD22	1:O:862:VAL:HG12	1.47	0.80
1:S:557:CYS:N	1:S:564:ASN:HD21	1.80	0.80
1:M:691:ILE:HD11	1:M:711:MET:HE3	1.64	0.79
1:Q:44:ILE:HD11	1:Q:394:PRO:HG2	1.65	0.79
1:Q:610:LYS:HZ1	1:Q:618:GLN:HE22	1.31	0.79
1:O:66:PHE:CD1	1:O:69:MET:HE3	2.18	0.79
2:T:175:VAL:HG23	2:T:178:PRO:HG3	1.65	0.79
1:S:146:MET:HE1	1:S:544:THR:HB	1.65	0.79
1:W:138:LEU:HB2	1:W:490:ILE:HD12	1.63	0.79
1:W:146:MET:HE1	1:W:544:THR:HB	1.63	0.79
2:X:128:MET:HA	7:X:806:SF4:S1	2.22	0.78
1:U:695:LEU:O	1:U:699:GLU:HG2	1.83	0.78
1:S:823:TYR:CZ	1:S:825:PRO:HG3	2.18	0.78
1:U:138:LEU:HB2	1:U:490:ILE:HD12	1.66	0.78
1:Q:360:ALA:HB1	1:Q:859:THR:HG23	1.63	0.77
1:O:66:PHE:HD1	1:O:69:MET:HE3	1.47	0.77
1:Q:319:GLU:HG2	1:U:726:LEU:HD13	1.66	0.77
1:U:426:MET:CE	1:U:618:GLN:HG2	2.14	0.77
1:W:645:ASN:HD21	1:W:648:ARG:HB3	1.49	0.77
1:O:360:ALA:HB1	1:O:859:THR:HG23	1.67	0.76
1:U:557:CYS:N	1:U:564:ASN:HD21	1.80	0.76
2:P:70:HIS:CD2	2:P:92:VAL:H	2.04	0.76
1:U:81:LYS:HB2	1:U:112:ILE:HD13	1.67	0.76
1:M:426:MET:CE	1:M:618:GLN:HG2	2.15	0.76
2:P:68:CYS:HB3	2:P:126:CYS:HB3	1.67	0.76
1:O:61:PRO:HB3	8:P:1017:HOH:O	1.87	0.75
1:U:360:ALA:HB1	1:U:859:THR:HG23	1.67	0.75
1:S:786:ASN:HD21	1:S:804:GLN:HA	1.49	0.75
1:Q:426:MET:HE3	1:Q:426:MET:HA	1.69	0.75
2:R:143:PRO:HB3	7:R:806:SF4:S1	2.27	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:28:MET:HE1	1:M:66:PHE:HB3	1.69	0.74
1:O:719:GLU:HG2	1:O:859:THR:O	1.86	0.74
2:T:68:CYS:HB3	2:T:126:CYS:HB3	1.67	0.74
1:O:823:TYR:CZ	1:O:825:PRO:HG3	2.21	0.74
2:V:70:HIS:HD2	2:V:92:VAL:H	1.36	0.74
1:Q:146:MET:HE1	1:Q:544:THR:HB	1.69	0.74
2:N:143:PRO:HB3	7:N:806:SF4:S1	2.28	0.74
1:O:253:ASN:O	1:O:257:ARG:HG3	1.86	0.74
1:S:66:PHE:CD1	1:S:69:MET:HE3	2.22	0.74
1:W:66:PHE:CD1	1:W:69:MET:HE3	2.22	0.74
2:X:95:ASP:HB3	2:X:98:LYS:HB2	1.69	0.74
2:V:68:CYS:HB3	2:V:126:CYS:HB3	1.70	0.74
1:O:695:LEU:O	1:O:699:GLU:HG2	1.87	0.74
1:S:786:ASN:ND2	1:S:804:GLN:HA	2.02	0.73
2:X:84:VAL:HG22	2:X:94:ILE:HG12	1.69	0.73
2:T:40:GLN:HE22	2:T:118:GLU:H	1.36	0.73
1:W:66:PHE:HD1	1:W:69:MET:HE3	1.54	0.73
1:O:165:GLY:HA3	1:O:166:PHE:HB3	1.68	0.73
2:N:5:TYR:HB2	2:N:157:LEU:CD1	2.18	0.73
1:U:44:ILE:HD11	1:U:394:PRO:HG2	1.70	0.73
2:R:68:CYS:HB2	2:R:126:CYS:HB3	1.70	0.72
2:V:76:CYS:HB3	2:V:108:THR:OG1	1.89	0.72
1:W:328:PRO:HB2	1:W:331:GLU:HG3	1.70	0.72
2:V:19:CYS:HB3	2:V:145:CYS:HB3	1.70	0.72
2:R:40:GLN:HE22	2:R:118:GLU:H	1.35	0.72
2:T:64:ARG:HD2	2:T:176:ILE:HD11	1.71	0.72
2:R:19:CYS:HB3	2:R:145:CYS:HB3	1.70	0.72
1:Q:100:LEU:HD12	1:Q:105:PRO:HG3	1.70	0.72
2:R:68:CYS:CB	2:R:126:CYS:HB3	2.20	0.72
2:T:40:GLN:NE2	2:T:118:GLU:H	1.88	0.72
1:M:61:PRO:HB3	8:N:1016:HOH:O	1.88	0.71
1:O:503:THR:HG21	5:O:900:MGD:O2A	1.89	0.71
2:R:21:MET:HE2	2:R:21:MET:HA	1.72	0.71
1:W:610:LYS:HZ2	1:W:618:GLN:HE22	1.36	0.71
1:O:74:LEU:HD12	1:O:750:LYS:HA	1.71	0.71
2:T:256:TYR:HB2	2:T:274:LEU:HD21	1.72	0.71
1:Q:610:LYS:HB3	1:Q:614:ALA:HB3	1.70	0.71
1:M:610:LYS:NZ	1:M:618:GLN:HE22	1.89	0.71
2:N:76:CYS:HB3	2:N:108:THR:OG1	1.91	0.71
1:U:610:LYS:HZ3	1:U:618:GLN:HE22	1.39	0.70
1:O:146:MET:HG2	5:O:900:MGD:N7	2.06	0.70
2:N:207:GLY:HA2	1:S:728:VAL:CG1	2.18	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:142:MET:HE2	2:N:146:ALA:HB1	1.71	0.70
1:O:96:ARG:HD2	1:O:514:TYR:O	1.91	0.70
1:M:146:MET:HE1	1:M:544:THR:HB	1.73	0.70
1:S:604:GLU:HB3	1:S:605:MET:CE	2.22	0.70
2:N:114:MET:HA	2:N:125:LYS:HB3	1.72	0.70
1:M:557:CYS:N	1:M:564:ASN:HD21	1.89	0.70
1:Q:134:PRO:HB2	1:Q:439:LEU:HD11	1.74	0.70
2:P:69:MET:HB3	2:P:184:PRO:HB3	1.73	0.70
2:V:18:ASN:HB2	7:V:805:SF4:S1	2.31	0.70
1:W:155:SER:OG	1:W:409:ILE:HG12	1.91	0.70
1:W:753:TYR:HB3	2:X:24:MET:HE3	1.74	0.69
2:P:72:GLU:HA	8:P:925:HOH:O	1.91	0.69
1:W:508:ASN:O	1:W:512:LYS:HG3	1.92	0.69
1:M:823:TYR:CZ	1:M:825:PRO:HG3	2.27	0.69
2:P:71:CYS:HA	2:P:184:PRO:HA	1.75	0.69
2:V:58:ARG:HD2	2:V:268:ASP:OD1	1.92	0.69
2:N:106:LEU:HD22	2:N:114:MET:HG3	1.74	0.69
1:W:426:MET:HE1	1:W:618:GLN:HG2	1.74	0.69
2:V:40:GLN:HE22	2:V:118:GLU:H	1.38	0.69
1:M:503:THR:HG21	5:M:900:MGD:O2A	1.93	0.68
1:U:66:PHE:CD1	1:U:69:MET:HE3	2.28	0.68
2:X:175:VAL:HG23	2:X:178:PRO:HG3	1.74	0.68
1:S:610:LYS:HZ3	1:S:618:GLN:HE22	1.41	0.68
1:S:66:PHE:HD1	1:S:69:MET:HE3	1.57	0.68
2:X:10:VAL:HG13	2:X:63:TYR:O	1.92	0.68
1:W:74:LEU:HD12	1:W:750:LYS:HA	1.75	0.68
1:W:757:ILE:HG23	2:X:17:ASN:OD1	1.93	0.68
1:Q:218:ASP:OD2	1:Q:253:ASN:HB2	1.92	0.68
1:Q:599:LYS:HG3	8:Q:1575:HOH:O	1.93	0.68
2:N:53:ARG:HB2	2:N:60:ASP:OD1	1.94	0.68
1:Q:753:TYR:HB3	2:R:24:MET:HE3	1.75	0.68
1:Q:610:LYS:HZ3	1:Q:618:GLN:HE22	1.40	0.68
1:M:356:GLY:H	5:M:901:MGD:H5'2	1.58	0.68
1:Q:426:MET:HE1	1:Q:618:GLN:HG2	1.74	0.67
1:S:558:SER:H	1:S:564:ASN:ND2	1.92	0.67
1:W:143:SER:HB3	3:W:903:ACT:H3	1.76	0.67
2:T:129:CYS:HB3	2:T:131:HIS:CE1	2.28	0.67
2:P:216:VAL:HG13	2:P:223:GLU:HG3	1.77	0.67
1:M:257:ARG:HD3	2:N:61:ILE:HG21	1.77	0.67
2:X:2:GLU:HG2	2:X:158:LYS:HG2	1.75	0.67
2:X:87:ARG:HG3	2:X:91:ILE:O	1.94	0.67
1:W:141:PRO:HA	1:W:496:TYR:HB3	1.77	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:610:LYS:HZ2	1:U:618:GLN:HE22	1.40	0.67
1:Q:426:MET:CE	1:Q:618:GLN:HG2	2.24	0.67
2:N:68:CYS:CB	2:N:126:CYS:HB3	2.25	0.67
2:N:71:CYS:HB2	2:N:182:THR:O	1.95	0.67
1:U:142:SER:HB2	5:U:900:MGD:H5'2	1.77	0.67
1:O:141:PRO:HA	1:O:496:TYR:HB3	1.77	0.67
2:T:49:GLU:HG3	2:T:64:ARG:NH2	2.10	0.67
1:M:786:ASN:ND2	1:M:804:GLN:HA	2.10	0.66
1:Q:870:ASP:HB3	1:Q:872:TYR:CE1	2.31	0.66
2:P:205:VAL:HG13	2:P:254:LYS:NZ	2.10	0.66
1:W:695:LEU:O	1:W:699:GLU:HG2	1.96	0.66
1:Q:319:GLU:HG2	1:U:726:LEU:CD1	2.26	0.66
1:S:75:ARG:HH21	1:S:543:CYS:HA	1.61	0.66
1:U:561:ILE:HG22	1:U:564:ASN:HB3	1.78	0.66
2:X:40:GLN:HE21	2:X:117:ASN:HA	1.60	0.66
2:X:18:ASN:HB2	7:X:805:SF4:S1	2.36	0.66
1:S:610:LYS:HZ2	1:S:618:GLN:HE22	1.43	0.65
1:S:604:GLU:HB3	1:S:605:MET:HE3	1.78	0.65
2:P:21:MET:HA	2:P:21:MET:HE2	1.78	0.65
1:S:695:LEU:O	1:S:699:GLU:HG2	1.95	0.65
2:R:46:MET:CE	2:R:66:THR:N	2.60	0.65
2:N:70:HIS:CD2	2:N:92:VAL:H	2.12	0.65
2:X:71:CYS:HB3	2:X:184:PRO:HA	1.77	0.65
1:O:558:SER:H	1:O:564:ASN:ND2	1.94	0.65
1:Q:356:GLY:H	5:Q:901:MGD:H5'2	1.60	0.65
2:X:164:MET:O	2:X:168:VAL:HG23	1.97	0.65
1:U:823:TYR:CZ	1:U:825:PRO:HG3	2.31	0.65
2:R:40:GLN:NE2	2:R:118:GLU:H	1.93	0.65
1:W:201:LEU:HD13	1:W:387:TRP:HB2	1.78	0.65
2:R:70:HIS:CD2	2:R:92:VAL:H	2.10	0.65
1:O:426:MET:HE1	1:O:618:GLN:O	1.96	0.65
2:V:19:CYS:O	2:V:22:GLY:N	2.28	0.65
1:U:691:ILE:HD11	1:U:711:MET:HE3	1.77	0.65
2:P:68:CYS:CB	2:P:126:CYS:HB3	2.26	0.65
1:O:395:LEU:HD12	1:O:566:GLN:HA	1.78	0.65
2:X:71:CYS:HA	2:X:184:PRO:HA	1.78	0.65
2:N:125:LYS:HD2	2:N:126:CYS:O	1.96	0.65
2:P:2:GLU:HG2	2:P:158:LYS:HG2	1.77	0.65
2:T:69:MET:HB3	2:T:184:PRO:HB3	1.79	0.65
1:W:175:SER:HA	1:W:359:ARG:HH21	1.61	0.64
1:S:630:THR:OG1	1:S:633:GLU:HG3	1.97	0.64
1:O:790:ILE:HD13	1:O:803:ALA:HB2	1.77	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:146:MET:CE	1:S:544:THR:HB	2.26	0.64
1:Q:31:MET:O	1:Q:56:LYS:HG3	1.98	0.64
3:M:903:ACT:H1	8:M:947:HOH:O	1.97	0.64
2:V:229:THR:HB	2:V:233:GLY:HA2	1.79	0.64
2:R:56:TYR:HA	2:R:59:ASN:HD22	1.62	0.64
1:S:81:LYS:HB2	1:S:112:ILE:HD13	1.78	0.64
1:O:770:TRP:HB3	1:O:801:LEU:HD23	1.80	0.64
1:O:187:TRP:CH2	1:O:196:PRO:HB3	2.32	0.64
1:W:610:LYS:NZ	1:W:618:GLN:NE2	2.45	0.64
2:V:75:PRO:HD2	7:V:807:SF4:S4	2.38	0.64
2:X:71:CYS:HB3	2:X:184:PRO:CA	2.27	0.64
2:V:71:CYS:HA	2:V:184:PRO:HA	1.80	0.64
2:V:5:TYR:CD2	2:V:164:MET:HG2	2.33	0.64
1:O:610:LYS:HZ3	1:O:618:GLN:HE22	1.42	0.63
1:W:15:PRO:HD3	1:W:554:PHE:CE1	2.33	0.63
1:M:319:GLU:HG2	1:S:726:LEU:CD1	2.27	0.63
2:V:125:LYS:HD2	2:V:126:CYS:O	1.99	0.63
2:P:21:MET:CE	2:P:21:MET:HA	2.27	0.63
1:M:426:MET:HE2	1:M:618:GLN:HG2	1.78	0.63
1:O:563:ASP:O	1:O:566:GLN:HG2	1.97	0.63
1:W:100:LEU:HD12	1:W:105:PRO:HG3	1.80	0.63
1:W:801:LEU:HD11	1:W:839:ILE:HD11	1.80	0.63
2:N:207:GLY:CA	1:S:728:VAL:HG12	2.22	0.63
1:O:146:MET:HE1	1:O:544:THR:HB	1.80	0.63
1:W:630:THR:OG1	1:W:633:GLU:HG3	1.99	0.63
1:W:369:GLY:O	1:W:373:LEU:HD13	1.98	0.63
2:N:40:GLN:NE2	2:N:118:GLU:H	1.96	0.63
1:U:729:LYS:HD2	8:U:1043:HOH:O	1.99	0.63
1:M:870:ASP:HB3	1:M:872:TYR:CE1	2.34	0.63
2:X:19:CYS:CB	2:X:145:CYS:HB3	2.29	0.63
1:Q:28:MET:HE1	1:Q:66:PHE:HB3	1.81	0.63
1:O:146:MET:CE	1:O:544:THR:HB	2.28	0.63
2:R:76:CYS:HB3	2:R:108:THR:OG1	1.98	0.63
1:Q:557:CYS:H	1:Q:564:ASN:ND2	1.86	0.63
2:X:177:LYS:N	2:X:178:PRO:HD3	2.14	0.63
2:P:40:GLN:HE22	2:P:118:GLU:H	1.45	0.63
2:V:71:CYS:HB2	2:V:182:THR:O	1.97	0.63
2:R:68:CYS:HB2	2:R:126:CYS:CB	2.29	0.62
2:N:40:GLN:HE22	2:N:118:GLU:H	1.47	0.62
2:T:76:CYS:HB3	2:T:108:THR:OG1	1.98	0.62
1:O:100:LEU:HD12	1:O:105:PRO:HG3	1.81	0.62
2:V:95:ASP:HB3	2:V:98:LYS:HB2	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:801:LEU:HD11	1:S:839:ILE:HD11	1.81	0.62
1:M:541:PRO:HB2	1:M:586:SER:HA	1.81	0.62
1:W:218:ASP:OD2	1:W:253:ASN:HB2	1.99	0.62
1:M:146:MET:CE	1:M:544:THR:HB	2.30	0.62
1:M:66:PHE:HD1	1:M:69:MET:HE3	1.63	0.62
2:T:125:LYS:HD2	2:T:126:CYS:O	1.99	0.62
1:S:753:TYR:HB3	2:T:24:MET:HE3	1.80	0.62
1:M:426:MET:HE1	1:M:618:GLN:O	1.99	0.62
2:P:185:ARG:HB3	2:P:185:ARG:CZ	2.29	0.62
1:O:394:PRO:HG3	8:O:1233:HOH:O	1.99	0.62
2:X:56:TYR:HA	2:X:59:ASN:HD22	1.63	0.62
1:Q:153:ARG:O	1:Q:157:TYR:HB3	2.00	0.62
2:N:21:MET:CE	2:N:21:MET:HA	2.29	0.62
1:W:503:THR:HG21	5:W:900:MGD:O2A	2.00	0.62
1:S:165:GLY:HA3	1:S:166:PHE:HB3	1.81	0.62
1:U:786:ASN:HD21	1:U:804:GLN:HA	1.64	0.62
1:Q:141:PRO:HA	1:Q:496:TYR:HB3	1.81	0.62
1:S:553:GLU:HG2	1:S:556:ASN:HB2	1.82	0.62
2:P:114:MET:HB3	2:P:125:LYS:HB3	1.81	0.62
1:U:140:THR:HB	1:U:169:ALA:HB3	1.82	0.62
1:U:478:HIS:HD2	8:U:1116:HOH:O	1.82	0.62
2:N:68:CYS:HB2	2:N:126:CYS:HB3	1.81	0.62
1:W:75:ARG:HH22	1:W:547:GLU:CD	2.01	0.62
2:R:71:CYS:HB2	2:R:182:THR:O	2.00	0.62
1:Q:81:LYS:HB2	1:Q:112:ILE:HD13	1.82	0.62
1:W:212:ILE:HD11	1:W:238:LEU:HD13	1.82	0.62
1:U:134:PRO:HB2	1:U:439:LEU:HD11	1.82	0.61
1:U:166:PHE:N	1:U:439:LEU:HD12	2.15	0.61
2:V:40:GLN:NE2	2:V:117:ASN:HA	2.15	0.61
2:P:19:CYS:HB2	2:P:46:MET:HG2	1.82	0.61
1:Q:610:LYS:NZ	1:Q:618:GLN:NE2	2.44	0.61
2:X:77:VAL:HG22	2:X:84:VAL:HG12	1.81	0.61
1:Q:201:LEU:HD13	1:Q:387:TRP:HB2	1.82	0.61
1:O:452:ILE:HB	1:O:453:PRO:HD3	1.82	0.61
2:R:19:CYS:O	2:R:22:GLY:N	2.33	0.61
1:O:66:PHE:HA	1:O:69:MET:HE2	1.81	0.61
1:W:146:MET:HE2	1:W:545:ASN:H	1.65	0.61
1:W:187:TRP:CH2	1:W:196:PRO:HB3	2.35	0.61
2:X:118:GLU:HG2	8:X:1004:HOH:O	2.00	0.61
1:W:561:ILE:CG2	1:W:564:ASN:HB3	2.29	0.61
1:O:356:GLY:H	5:O:901:MGD:H5'2	1.65	0.61
1:U:100:LEU:HD12	1:U:105:PRO:HG3	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:39:ALA:HB1	8:W:1179:HOH:O	2.00	0.61
1:U:696:LYS:O	1:U:700:GLU:HG3	1.99	0.61
2:N:142:MET:CE	2:N:146:ALA:HB1	2.29	0.61
2:V:218:LYS:HG2	2:V:223:GLU:HA	1.83	0.61
1:U:76:ILE:HG22	1:U:541:PRO:HG3	1.82	0.61
1:U:557:CYS:H	1:U:564:ASN:ND2	1.86	0.61
2:X:94:ILE:HG22	2:X:95:ASP:N	2.15	0.61
1:W:15:PRO:HD2	8:W:907:HOH:O	2.00	0.61
2:P:76:CYS:HB3	2:P:108:THR:OG1	2.00	0.61
2:X:217:LEU:HD12	2:X:246:THR:O	2.01	0.61
2:X:40:GLN:HE22	2:X:117:ASN:HA	1.66	0.60
2:X:19:CYS:HA	2:X:145:CYS:HB3	1.83	0.60
1:O:794:ASN:ND2	1:O:862:VAL:HG12	2.14	0.60
2:V:21:MET:HE2	2:V:21:MET:HA	1.83	0.60
2:P:5:TYR:CD2	2:P:164:MET:HG2	2.36	0.60
1:U:356:GLY:H	5:U:901:MGD:H5'2	1.67	0.60
1:O:252:MET:HE1	8:O:1375:HOH:O	2.01	0.60
2:P:58:ARG:HD2	2:P:268:ASP:OD1	2.00	0.60
1:S:75:ARG:NH2	1:S:543:CYS:HA	2.17	0.60
1:M:66:PHE:HA	1:M:69:MET:CE	2.32	0.60
2:N:68:CYS:HB3	2:N:70:HIS:CE1	2.37	0.60
2:R:43:HIS:ND1	8:R:856:HOH:O	2.31	0.60
1:U:602:ILE:HG23	8:U:983:HOH:O	2.02	0.60
2:P:19:CYS:O	2:P:22:GLY:N	2.34	0.60
1:U:311:THR:HG21	8:U:1410:HOH:O	2.02	0.60
1:W:510:TYR:O	1:W:513:MET:HG2	2.01	0.60
1:S:356:GLY:H	5:S:901:MGD:H5'2	1.66	0.60
1:Q:74:LEU:HD12	1:Q:750:LYS:HA	1.84	0.60
1:M:645:ASN:ND2	1:M:648:ARG:HB3	2.17	0.60
2:T:19:CYS:HB2	2:T:46:MET:HG2	1.84	0.60
1:S:557:CYS:H	1:S:564:ASN:ND2	1.86	0.60
2:R:21:MET:CE	2:R:21:MET:HA	2.32	0.60
1:W:296:ASN:HB3	1:W:657:PHE:CZ	2.36	0.60
2:T:10:VAL:HG13	2:T:63:TYR:O	2.02	0.60
1:U:28:MET:HE1	1:U:67:LYS:N	2.17	0.60
1:O:738:HIS:HE2	5:O:900:MGD:H15	1.50	0.60
2:X:58:ARG:HD2	2:X:268:ASP:OD1	2.02	0.60
1:M:602:ILE:HG21	8:M:978:HOH:O	2.01	0.60
1:Q:66:PHE:HD1	1:Q:69:MET:HE3	1.62	0.59
1:Q:214:PHE:HA	1:Q:347:ALA:HB3	1.84	0.59
1:O:557:CYS:N	1:O:564:ASN:HD21	1.97	0.59
1:W:134:PRO:HB2	1:W:439:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:V:5:TYR:HB2	2:V:157:LEU:CD1	2.32	0.59
1:Q:494:TRP:HE1	1:Q:525:GLN:HE21	1.50	0.59
2:X:129:CYS:HB3	2:X:131:HIS:HE1	1.63	0.59
1:Q:44:ILE:HD11	1:Q:394:PRO:CG	2.31	0.59
1:U:503:THR:HG21	5:U:900:MGD:O2A	2.02	0.59
1:Q:189:PHE:HZ	1:Q:654:LEU:HD21	1.67	0.59
2:V:68:CYS:CB	2:V:126:CYS:HB3	2.32	0.59
1:W:356:GLY:H	5:W:901:MGD:H5'2	1.68	0.59
2:R:56:TYR:HA	2:R:59:ASN:ND2	2.18	0.59
1:M:394:PRO:HG3	8:M:1228:HOH:O	2.02	0.59
2:T:5:TYR:HB2	2:T:157:LEU:CD1	2.31	0.59
1:U:141:PRO:HA	1:U:496:TYR:HB3	1.85	0.59
1:U:257:ARG:HD3	2:V:61:ILE:HG21	1.84	0.59
1:U:722:LYS:HG2	8:U:1471:HOH:O	2.02	0.59
1:U:644:ASP:O	1:U:646:PRO:HD3	2.02	0.59
1:U:395:LEU:HD12	1:U:566:GLN:HA	1.83	0.59
2:P:112:GLY:HA2	8:P:970:HOH:O	2.03	0.59
2:V:59:ASN:ND2	2:V:59:ASN:H	2.01	0.59
1:W:177:GLU:HA	1:W:177:GLU:OE2	2.02	0.59
1:W:765:ASP:HB2	8:W:1073:HOH:O	2.01	0.59
1:Q:211:MET:HE1	2:R:231:PHE:HZ	1.68	0.59
2:P:166:LYS:O	2:P:170:GLU:HG3	2.02	0.59
1:M:494:TRP:HE1	1:M:525:GLN:HE21	1.51	0.59
2:T:166:LYS:HE2	2:T:170:GLU:OE2	2.02	0.59
1:M:100:LEU:HD12	1:M:105:PRO:HG3	1.83	0.59
2:V:102:LYS:HB3	2:V:104:GLU:OE2	2.02	0.59
1:S:400:TYR:CZ	1:S:421:LYS:HD2	2.37	0.59
1:O:426:MET:HE3	1:O:426:MET:HA	1.84	0.58
2:X:53:ARG:HB2	2:X:60:ASP:OD1	2.02	0.58
1:U:848:ILE:HG12	1:U:856:ALA:HB2	1.85	0.58
2:R:46:MET:HE1	2:R:65:PRO:C	2.23	0.58
2:R:207:GLY:HA2	1:U:728:VAL:CG1	2.27	0.58
1:M:44:ILE:HD11	1:M:394:PRO:HG2	1.85	0.58
1:U:408:GLY:HA2	1:U:619:TYR:HE1	1.69	0.58
2:X:105:LEU:HD12	8:X:952:HOH:O	2.03	0.58
1:M:146:MET:HG2	5:M:900:MGD:N7	2.18	0.58
1:U:166:PHE:H	1:U:439:LEU:HD12	1.68	0.58
1:Q:146:MET:CE	1:Q:544:THR:HB	2.33	0.58
1:Q:356:GLY:H	5:Q:901:MGD:C5'	2.17	0.58
1:U:104:ASP:OD2	1:U:107:SER:HB3	2.03	0.58
1:Q:561:ILE:HG22	1:Q:564:ASN:HB3	1.86	0.58
1:W:146:MET:CE	1:W:544:THR:HB	2.32	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:T:70:HIS:HD2	2:T:92:VAL:H	1.50	0.58
2:V:5:TYR:HB2	2:V:157:LEU:HD11	1.85	0.58
2:V:256:TYR:HB2	2:V:274:LEU:HD21	1.85	0.58
1:Q:691:ILE:HD11	1:Q:711:MET:HE3	1.85	0.58
1:Q:823:TYR:CZ	1:Q:825:PRO:HG3	2.38	0.58
1:O:364:ILE:HD13	1:O:708:ARG:HG3	1.86	0.58
2:T:19:CYS:O	2:T:22:GLY:N	2.36	0.58
2:R:46:MET:CE	2:R:66:THR:H	2.17	0.58
2:V:106:LEU:HD11	2:V:116:TRP:HB2	1.84	0.58
2:T:23:CYS:HB3	2:T:39:MET:HE3	1.86	0.58
1:M:81:LYS:HB2	1:M:112:ILE:HD13	1.86	0.58
1:S:503:THR:HG21	5:S:900:MGD:O2A	2.04	0.58
2:T:68:CYS:SG	2:T:113:VAL:HG21	2.44	0.58
1:W:174:ASP:O	1:W:177:GLU:HG2	2.03	0.58
1:U:610:LYS:NZ	1:U:618:GLN:NE2	2.47	0.58
1:O:67:LYS:HE3	2:P:29:LEU:HD12	1.86	0.58
3:U:903:ACT:H1	8:U:951:HOH:O	2.03	0.58
2:X:71:CYS:CA	2:X:184:PRO:HA	2.34	0.57
2:X:19:CYS:CB	2:X:46:MET:HG2	2.33	0.57
1:O:356:GLY:H	5:O:901:MGD:C5'	2.17	0.57
2:X:106:LEU:HD11	2:X:116:TRP:HB2	1.85	0.57
1:W:20:VAL:HG13	1:W:24:LYS:O	2.04	0.57
2:P:18:ASN:HB2	7:P:805:SF4:S1	2.44	0.57
1:S:211:MET:HE1	2:T:231:PHE:HZ	1.69	0.57
2:N:19:CYS:O	2:N:22:GLY:N	2.35	0.57
2:X:19:CYS:HB3	2:X:145:CYS:CB	2.31	0.57
2:N:58:ARG:HD2	2:N:268:ASP:OD1	2.05	0.57
1:M:676:VAL:HG13	8:M:957:HOH:O	2.03	0.57
1:M:134:PRO:HB2	1:M:439:LEU:HD11	1.85	0.57
2:T:75:PRO:HD2	7:T:807:SF4:S4	2.45	0.57
2:X:19:CYS:CA	2:X:145:CYS:HB3	2.35	0.57
1:S:35:ASP:OD1	1:S:55:ARG:HD3	2.04	0.57
1:S:744:HIS:HA	1:S:819:SER:HB3	1.86	0.57
2:X:73:ASN:O	2:X:75:PRO:HD3	2.04	0.57
1:U:265:SER:O	1:U:810:GLN:NE2	2.37	0.57
1:S:400:TYR:CE1	1:S:421:LYS:HD2	2.40	0.57
1:O:134:PRO:HB2	1:O:439:LEU:HD11	1.86	0.57
1:U:825:PRO:HD2	8:U:1247:HOH:O	2.04	0.57
1:U:547:GLU:OE1	1:U:582:PRO:HA	2.04	0.57
1:S:140:THR:HB	1:S:169:ALA:HB3	1.85	0.57
1:M:296:ASN:O	1:M:687:LYS:HB3	2.04	0.57
2:T:18:ASN:HB2	7:T:805:SF4:S1	2.44	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:104:ASP:OD2	1:S:107:SER:HB3	2.03	0.57
2:V:176:ILE:HG22	2:V:177:LYS:HG3	1.87	0.57
1:W:557:CYS:N	1:W:564:ASN:HD21	2.02	0.57
2:T:114:MET:HA	2:T:125:LYS:HB3	1.86	0.57
2:X:4:TYR:CD1	2:X:89:ASP:HB2	2.40	0.57
2:P:201:ALA:HB2	2:P:269:LEU:HB2	1.86	0.57
1:O:786:ASN:ND2	1:O:804:GLN:HA	2.20	0.57
2:R:203:ILE:HD12	2:R:203:ILE:N	2.19	0.57
1:O:426:MET:HE3	1:O:622:ALA:HB2	1.86	0.57
2:N:69:MET:HB3	2:N:184:PRO:HB3	1.86	0.57
1:M:650:LYS:HE3	8:M:1131:HOH:O	2.05	0.57
1:Q:695:LEU:O	1:Q:699:GLU:HG2	2.05	0.57
1:U:177:GLU:OE2	1:U:177:GLU:HA	2.05	0.57
1:O:378:GLY:O	1:O:381:LYS:HG2	2.05	0.57
2:R:114:MET:HA	2:R:125:LYS:HB3	1.86	0.57
1:U:786:ASN:ND2	1:U:804:GLN:HA	2.19	0.57
2:V:177:LYS:N	2:V:178:PRO:HD3	2.19	0.57
1:Q:400:TYR:CZ	1:Q:421:LYS:HD2	2.39	0.57
2:X:17:ASN:N	2:X:17:ASN:HD22	2.01	0.56
1:U:426:MET:HE3	1:U:622:ALA:HB2	1.87	0.56
1:M:66:PHE:HA	1:M:69:MET:HE2	1.87	0.56
2:R:68:CYS:HB3	2:R:70:HIS:CE1	2.40	0.56
2:V:112:GLY:HA2	8:V:970:HOH:O	2.05	0.56
2:T:71:CYS:HB2	2:T:182:THR:O	2.05	0.56
2:V:75:PRO:HG2	2:V:110:PRO:HG2	1.87	0.56
1:M:319:GLU:HG2	1:S:726:LEU:HD13	1.87	0.56
1:S:4:VAL:HG22	1:S:21:LYS:HB2	1.87	0.56
2:X:112:GLY:HA2	8:X:975:HOH:O	2.05	0.56
2:P:106:LEU:HD11	2:P:116:TRP:HB2	1.87	0.56
1:W:387:TRP:CE2	1:W:389:THR:HA	2.41	0.56
2:R:104:GLU:H	2:R:104:GLU:CD	2.09	0.56
1:M:218:ASP:OD2	1:M:253:ASN:HB2	2.06	0.56
2:N:254:LYS:HD2	2:N:274:LEU:OXT	2.06	0.56
1:W:647:ASN:HB2	8:W:1352:HOH:O	2.04	0.56
1:M:587:MET:HE2	1:M:591:GLU:HB3	1.85	0.56
1:M:141:PRO:HA	1:M:496:TYR:HB3	1.87	0.56
1:W:146:MET:HG2	5:W:900:MGD:N7	2.19	0.56
1:Q:15:PRO:HD2	8:Q:907:HOH:O	2.06	0.56
1:W:494:TRP:HE1	1:W:525:GLN:HE21	1.54	0.56
1:U:610:LYS:HA	8:U:1382:HOH:O	2.05	0.56
2:X:92:VAL:HG21	7:X:807:SF4:S1	2.45	0.56
1:W:719:GLU:HG2	1:W:859:THR:O	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:558:SER:H	1:U:564:ASN:ND2	2.03	0.56
2:X:40:GLN:HB3	2:X:43:HIS:CE1	2.41	0.56
1:O:100:LEU:CD1	1:O:105:PRO:HG3	2.36	0.56
2:X:55:THR:HG22	8:X:992:HOH:O	2.04	0.56
1:Q:871:LYS:HG2	8:Q:1140:HOH:O	2.06	0.56
1:U:165:GLY:HA3	1:U:166:PHE:CB	2.26	0.56
1:Q:35:ASP:OD1	1:Q:55:ARG:HD3	2.05	0.56
1:O:602:ILE:HG23	8:O:979:HOH:O	2.06	0.56
1:U:56:LYS:HG2	1:U:57:THR:N	2.21	0.56
1:W:770:TRP:HB3	1:W:801:LEU:HD22	1.88	0.56
2:P:40:GLN:NE2	2:P:118:GLU:H	2.04	0.56
1:S:725:PRO:HD2	8:S:1107:HOH:O	2.06	0.56
1:W:495:LYS:HD2	1:W:514:TYR:OH	2.06	0.56
2:P:205:VAL:HG13	2:P:254:LYS:HZ2	1.68	0.55
1:U:476:GLN:OE1	1:U:708:ARG:NH2	2.39	0.55
2:P:71:CYS:HB2	2:P:182:THR:O	2.06	0.55
2:P:185:ARG:CB	2:P:185:ARG:NH1	2.69	0.55
1:W:85:PHE:CE2	1:W:87:PRO:HG3	2.41	0.55
2:P:19:CYS:CB	2:P:145:CYS:HB3	2.26	0.55
2:P:114:MET:HA	2:P:125:LYS:HB3	1.89	0.55
2:T:114:MET:CB	2:T:125:LYS:HB3	2.35	0.55
1:W:174:ASP:OD1	1:W:175:SER:N	2.38	0.55
1:S:134:PRO:HB3	1:S:165:GLY:HA2	1.89	0.55
1:Q:461:PHE:HA	8:Q:1404:HOH:O	2.05	0.55
1:O:649:LYS:HE3	1:O:651:THR:CG2	2.37	0.55
2:T:52:GLU:HG3	2:T:61:ILE:HD12	1.87	0.55
2:R:114:MET:HE3	2:R:123:ALA:HB1	1.88	0.55
1:U:44:ILE:HD11	1:U:394:PRO:CG	2.35	0.55
1:O:296:ASN:HB3	1:O:657:PHE:CZ	2.41	0.55
1:S:61:PRO:HB3	8:T:1013:HOH:O	2.05	0.55
2:X:204:LEU:HD23	2:X:209:CYS:HA	1.89	0.55
1:S:719:GLU:HG2	1:S:859:THR:O	2.06	0.55
2:V:40:GLN:HB3	2:V:43:HIS:CE1	2.42	0.55
1:M:96:ARG:HD2	1:M:514:TYR:O	2.07	0.55
1:M:707:HIS:HD2	8:M:1291:HOH:O	1.89	0.55
1:U:153:ARG:O	1:U:157:TYR:HB3	2.07	0.55
2:T:58:ARG:HD2	2:T:268:ASP:OD1	2.06	0.55
2:R:58:ARG:HD2	2:R:268:ASP:OD1	2.06	0.55
2:R:142:MET:HE2	2:R:146:ALA:CB	2.37	0.55
1:M:738:HIS:HE2	5:M:900:MGD:H15	1.55	0.55
1:W:32:ASP:HB2	8:W:1564:HOH:O	2.07	0.55
1:W:720:SER:OG	1:W:723:HIS:HB2	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:287:SER:HB2	1:O:340:ALA:HB1	1.89	0.55
1:O:630:THR:OG1	1:O:633:GLU:HG3	2.07	0.55
1:Q:387:TRP:CE2	1:Q:389:THR:HA	2.42	0.55
3:Q:903:ACT:H1	8:Q:947:HOH:O	2.07	0.55
1:S:187:TRP:CH2	1:S:196:PRO:HB3	2.42	0.55
1:Q:165:GLY:CA	1:Q:166:PHE:HB3	2.34	0.54
1:O:610:LYS:HZ2	1:O:618:GLN:HE22	1.53	0.54
2:T:92:VAL:HG11	7:T:807:SF4:S1	2.48	0.54
1:M:504:MET:HE3	8:M:942:HOH:O	2.06	0.54
1:U:526:SER:HB3	8:U:1024:HOH:O	2.06	0.54
1:U:735:LEU:H	1:U:735:LEU:HD23	1.71	0.54
1:M:144:HIS:NE2	5:M:901:MGD:S13	2.80	0.54
2:P:23:CYS:O	2:P:27:HIS:N	2.41	0.54
1:S:15:PRO:HD2	8:S:912:HOH:O	2.06	0.54
1:W:786:ASN:ND2	1:W:804:GLN:HA	2.23	0.54
2:X:19:CYS:O	2:X:22:GLY:N	2.40	0.54
2:T:114:MET:HB3	2:T:125:LYS:HB3	1.88	0.54
1:M:696:LYS:O	1:M:700:GLU:HG3	2.08	0.54
1:M:21:LYS:HB3	1:M:26:ILE:HD11	1.88	0.54
1:W:229:PHE:HA	8:W:1244:HOH:O	2.06	0.54
1:O:176:TRP:O	1:O:177:GLU:C	2.46	0.54
2:N:46:MET:HE1	2:N:65:PRO:HA	1.90	0.54
1:U:533:VAL:HB	1:U:534:PRO:HD3	1.89	0.54
1:W:44:ILE:HD11	1:W:394:PRO:HG2	1.89	0.54
1:Q:155:SER:OG	1:Q:409:ILE:HG12	2.07	0.54
1:M:558:SER:H	1:M:564:ASN:ND2	2.04	0.54
1:O:28:MET:HE1	1:O:67:LYS:H	1.67	0.54
2:P:72:GLU:HG2	2:P:185:ARG:NH2	2.23	0.54
2:X:4:TYR:HD1	2:X:89:ASP:HB2	1.73	0.54
1:M:730:TYR:CZ	1:M:794:ASN:HA	2.42	0.54
2:X:23:CYS:HB3	2:X:39:MET:HE3	1.89	0.54
1:Q:166:PHE:N	1:Q:439:LEU:HD12	2.23	0.54
1:O:426:MET:CE	1:O:618:GLN:HG2	2.37	0.54
1:S:75:ARG:HH22	1:S:547:GLU:CD	2.10	0.54
2:R:23:CYS:HB3	2:R:39:MET:HE3	1.90	0.54
1:Q:610:LYS:HZ1	1:Q:618:GLN:NE2	2.01	0.54
1:U:253:ASN:O	1:U:257:ARG:HG3	2.08	0.54
1:O:119:ASP:OD1	1:O:599:LYS:HE2	2.07	0.54
1:O:717:ALA:HB3	1:O:720:SER:HB3	1.88	0.54
1:U:628:TYR:CE2	1:U:643:PRO:HG2	2.43	0.54
1:U:15:PRO:HD3	1:U:554:PHE:CD1	2.43	0.54
1:U:610:LYS:HZ3	1:U:618:GLN:NE2	2.02	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:772:MET:HB2	1:W:801:LEU:HD13	1.89	0.54
1:O:257:ARG:HD3	2:P:61:ILE:HG21	1.89	0.54
2:V:106:LEU:CD2	2:V:114:MET:HG3	2.38	0.54
1:S:604:GLU:HB3	1:S:605:MET:HE1	1.89	0.54
1:Q:2:GLY:O	1:Q:21:LYS:HE3	2.07	0.54
2:P:157:LEU:HD12	2:P:157:LEU:O	2.08	0.54
2:R:68:CYS:HB3	2:R:126:CYS:HB3	1.90	0.53
2:V:59:ASN:H	2:V:59:ASN:HD22	1.54	0.53
2:X:26:GLU:OE2	2:X:132:LEU:HD21	2.07	0.53
2:T:198:TYR:HB3	2:T:238:ASP:HA	1.90	0.53
2:X:179:GLU:HG2	2:X:180:LEU:N	2.24	0.53
1:M:174:ASP:OD1	1:M:175:SER:N	2.40	0.53
1:M:288:TYR:HA	8:M:1408:HOH:O	2.08	0.53
1:U:165:GLY:CA	1:U:166:PHE:HB3	2.31	0.53
1:W:610:LYS:HB3	1:W:614:ALA:HB3	1.91	0.53
2:P:185:ARG:HB3	2:P:185:ARG:NH1	2.24	0.53
2:T:71:CYS:HA	2:T:184:PRO:HA	1.89	0.53
1:M:100:LEU:CD1	1:M:105:PRO:HG3	2.39	0.53
1:Q:400:TYR:HA	8:Q:1362:HOH:O	2.07	0.53
1:Q:826:LEU:HD21	1:Q:835:ARG:HD3	1.90	0.53
2:N:166:LYS:O	2:N:170:GLU:HG3	2.07	0.53
1:U:772:MET:HB2	1:U:801:LEU:HD13	1.90	0.53
1:M:197:GLU:OE2	1:M:667:ASP:HB2	2.08	0.53
1:Q:233:ILE:HD11	8:Q:1088:HOH:O	2.08	0.53
1:Q:855:MET:HB2	1:Q:857:ASN:OD1	2.09	0.53
1:U:356:GLY:HA2	1:U:359:ARG:NH1	2.23	0.53
2:V:9:ASP:HA	2:V:189:LYS:HB3	1.90	0.53
2:V:19:CYS:HB2	2:V:46:MET:HG2	1.89	0.53
2:R:18:ASN:HB2	7:R:805:SF4:S1	2.48	0.53
2:N:175:VAL:HG23	2:N:178:PRO:HG3	1.91	0.53
1:U:214:PHE:HA	1:U:347:ALA:HB3	1.91	0.53
1:M:12:THR:O	1:M:226:TYR:HA	2.09	0.53
2:R:2:GLU:HG2	2:R:158:LYS:HG2	1.89	0.53
1:S:218:ASP:OD2	1:S:253:ASN:HB2	2.07	0.53
1:M:177:GLU:OE2	1:M:177:GLU:HA	2.09	0.53
1:S:197:GLU:OE2	1:S:667:ASP:HB2	2.09	0.53
1:O:826:LEU:HD21	1:O:835:ARG:HD3	1.91	0.53
1:M:138:LEU:HD12	1:M:167:THR:O	2.07	0.53
1:M:691:ILE:CD1	1:M:711:MET:HE3	2.37	0.53
1:O:323:GLU:HB2	8:O:1482:HOH:O	2.09	0.53
1:S:644:ASP:C	1:S:646:PRO:HD3	2.28	0.53
1:O:478:HIS:HD2	8:O:1114:HOH:O	1.92	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:274:LEU:O	1:O:278:ILE:HG13	2.09	0.53
1:W:800:ILE:N	1:W:800:ILE:HD12	2.24	0.53
1:M:426:MET:HE1	1:M:618:GLN:HG2	1.91	0.53
2:V:19:CYS:CB	2:V:145:CYS:HB3	2.39	0.53
1:M:114:TRP:CZ2	1:M:541:PRO:HD2	2.44	0.53
1:U:218:ASP:OD2	1:U:253:ASN:HB2	2.09	0.53
1:O:526:SER:HB3	8:O:1020:HOH:O	2.09	0.53
1:O:553:GLU:HB3	1:O:556:ASN:CB	2.38	0.53
1:S:735:LEU:HD23	1:S:735:LEU:H	1.73	0.53
2:N:68:CYS:HB3	2:N:126:CYS:HB3	1.89	0.53
1:W:165:GLY:CA	1:W:166:PHE:HB3	2.36	0.53
1:M:501:LEU:HD13	1:M:823:TYR:CD2	2.44	0.53
1:U:563:ASP:HA	1:U:565:TYR:CE1	2.44	0.53
2:T:204:LEU:HD23	2:T:209:CYS:HA	1.90	0.53
1:U:96:ARG:HD3	1:U:535:PHE:O	2.09	0.53
1:U:68:SER:HB3	1:U:753:TYR:CE2	2.44	0.53
2:T:40:GLN:HB2	2:T:117:ASN:ND2	2.24	0.53
1:M:319:GLU:HG2	1:S:726:LEU:HD12	1.90	0.53
1:U:75:ARG:HH22	1:U:547:GLU:CD	2.13	0.53
1:M:211:MET:HE1	2:N:231:PHE:HZ	1.73	0.53
2:R:13:CYS:HB3	2:R:63:TYR:HB2	1.89	0.53
1:O:44:ILE:HD11	1:O:394:PRO:HG2	1.90	0.52
1:M:767:TYR:HB3	1:M:769:TYR:CE1	2.44	0.52
2:P:164:MET:O	2:P:168:VAL:HG23	2.09	0.52
1:W:691:ILE:HD11	1:W:711:MET:HE3	1.92	0.52
1:S:395:LEU:HD12	1:S:566:GLN:HA	1.91	0.52
2:N:46:MET:CE	2:N:66:THR:H	2.17	0.52
1:W:645:ASN:HD22	1:W:648:ARG:HD3	1.73	0.52
2:P:216:VAL:CG1	2:P:223:GLU:HG3	2.40	0.52
1:S:21:LYS:HB3	1:S:26:ILE:HD11	1.92	0.52
1:O:177:GLU:OE2	1:O:177:GLU:HA	2.09	0.52
1:S:414:GLU:HG3	8:S:1350:HOH:O	2.10	0.52
2:P:141:LYS:HA	8:P:952:HOH:O	2.09	0.52
1:S:214:PHE:HA	1:S:347:ALA:HB3	1.91	0.52
2:X:185:ARG:CZ	2:X:185:ARG:HB3	2.39	0.52
1:M:610:LYS:HZ3	1:M:618:GLN:HE22	1.54	0.52
2:V:19:CYS:HA	2:V:145:CYS:HB3	1.92	0.52
1:M:784:ILE:HD13	1:M:790:ILE:HG21	1.92	0.52
1:M:118:THR:HG21	1:M:595:LEU:HD23	1.90	0.52
1:W:197:GLU:OE2	1:W:667:ASP:HB2	2.10	0.52
2:X:68:CYS:HB3	2:X:126:CYS:HB3	1.91	0.52
2:X:122:VAL:HG22	2:X:123:ALA:N	2.24	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:396:ASP:OD2	1:S:398:GLU:HB2	2.09	0.52
2:N:19:CYS:HB2	2:N:46:MET:HG2	1.89	0.52
1:W:564:ASN:N	1:W:564:ASN:HD22	2.06	0.52
1:W:142:SER:HB3	5:W:900:MGD:O1A	2.09	0.52
1:O:786:ASN:HD21	1:O:804:GLN:HA	1.75	0.52
1:M:356:GLY:H	5:M:901:MGD:C5'	2.22	0.52
1:U:176:TRP:O	1:U:177:GLU:C	2.48	0.52
1:U:74:LEU:HD12	1:U:750:LYS:HA	1.91	0.52
1:U:14:GLY:HA2	1:U:554:PHE:CE1	2.44	0.52
2:T:4:TYR:CE2	2:T:158:LYS:HD2	2.44	0.52
1:Q:291:GLU:CD	1:Q:291:GLU:H	2.13	0.52
1:S:291:GLU:CD	1:S:291:GLU:H	2.13	0.52
1:M:561:ILE:HG22	1:M:564:ASN:HB3	1.92	0.52
2:P:70:HIS:HD2	2:P:92:VAL:N	2.00	0.52
1:U:162:ASN:HD22	1:U:166:PHE:HE2	1.56	0.52
2:N:13:CYS:HB3	2:N:63:TYR:HB2	1.90	0.52
1:Q:708:ARG:HD2	8:Q:950:HOH:O	2.09	0.52
1:M:510:TYR:O	1:M:513:MET:HG2	2.10	0.52
1:O:211:MET:HE1	2:P:231:PHE:HZ	1.74	0.52
1:W:323:GLU:HB3	8:W:1016:HOH:O	2.10	0.52
1:O:9:ASN:HA	1:O:576:GLN:HA	1.92	0.52
1:W:100:LEU:CD1	1:W:105:PRO:HG3	2.39	0.52
1:U:141:PRO:HD3	1:U:157:TYR:CZ	2.45	0.52
1:Q:400:TYR:CE1	1:Q:421:LYS:HD2	2.45	0.52
2:R:166:LYS:HG2	2:R:170:GLU:OE2	2.11	0.52
1:M:153:ARG:O	1:M:157:TYR:HB3	2.10	0.52
2:X:71:CYS:CB	2:X:184:PRO:HA	2.39	0.51
1:M:146:MET:HE2	1:M:545:ASN:H	1.75	0.51
2:T:177:LYS:N	2:T:178:PRO:HD3	2.24	0.51
1:W:356:GLY:H	5:W:901:MGD:C5'	2.23	0.51
1:S:144:HIS:NE2	5:S:901:MGD:S13	2.83	0.51
2:N:77:VAL:HG22	2:N:84:VAL:HG12	1.92	0.51
1:W:387:TRP:CZ2	1:W:389:THR:HA	2.45	0.51
1:S:356:GLY:H	5:S:901:MGD:C5'	2.23	0.51
2:T:139:ALA:HB3	2:T:140:PRO:HD3	1.92	0.51
1:S:87:PRO:HB3	8:S:1413:HOH:O	2.10	0.51
1:M:140:THR:HB	1:M:169:ALA:HB3	1.92	0.51
1:W:847:TYR:CZ	1:W:853:CYS:HB3	2.45	0.51
1:S:176:TRP:O	1:S:177:GLU:C	2.47	0.51
2:R:198:TYR:HB3	2:R:238:ASP:HA	1.92	0.51
1:O:21:LYS:HB3	1:O:26:ILE:HD11	1.92	0.51
1:Q:476:GLN:OE1	1:Q:708:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:21:MET:HE3	8:X:1020:HOH:O	2.10	0.51
1:Q:786:ASN:ND2	1:Q:804:GLN:HA	2.24	0.51
2:N:5:TYR:HB2	2:N:157:LEU:HD11	1.91	0.51
2:R:75:PRO:HD2	7:R:807:SF4:S4	2.50	0.51
2:X:99:ALA:HB1	8:X:952:HOH:O	2.10	0.51
2:X:180:LEU:HB2	8:X:976:HOH:O	2.09	0.51
2:T:139:ALA:O	2:T:141:LYS:HG3	2.11	0.51
1:M:753:TYR:HB3	2:N:24:MET:HE3	1.91	0.51
2:N:104:GLU:CD	2:N:104:GLU:H	2.13	0.51
1:W:563:ASP:HA	1:W:565:TYR:CE1	2.45	0.51
1:W:505:THR:HG22	1:W:857:ASN:ND2	2.25	0.51
1:O:165:GLY:CA	1:O:166:PHE:HB3	2.38	0.51
1:S:770:TRP:HB3	1:S:801:LEU:HD23	1.92	0.51
1:Q:211:MET:HE1	2:R:231:PHE:CZ	2.45	0.51
1:W:797:GLY:HA2	1:W:875:TYR:CE2	2.45	0.51
1:Q:738:HIS:HE2	5:Q:900:MGD:H15	1.57	0.51
2:V:21:MET:CE	2:V:21:MET:HA	2.41	0.51
1:U:393:VAL:HG12	1:U:395:LEU:HG	1.93	0.51
1:O:81:LYS:HB2	1:O:112:ILE:HD13	1.93	0.51
1:S:252:MET:HB3	1:S:808:CYS:HB3	1.91	0.51
1:S:349:GLY:HA3	1:S:353:GLY:O	2.11	0.51
1:U:322:GLU:HG3	1:U:327:VAL:O	2.11	0.51
1:O:214:PHE:HA	1:O:347:ALA:HB3	1.93	0.51
1:W:95:LEU:HA	8:W:1443:HOH:O	2.09	0.51
1:O:55:ARG:HD2	8:O:1550:HOH:O	2.10	0.51
2:T:46:MET:HE1	2:T:66:THR:N	2.26	0.51
1:W:610:LYS:HZ2	1:W:618:GLN:NE2	2.07	0.51
2:R:69:MET:HB2	7:R:807:SF4:S2	2.51	0.51
1:U:499:PRO:HB2	1:U:745:THR:HG21	1.93	0.51
1:M:647:ASN:HB2	8:M:1351:HOH:O	2.10	0.51
1:Q:533:VAL:HB	1:Q:534:PRO:HD3	1.93	0.51
2:X:69:MET:HG3	2:X:111:TYR:CE2	2.46	0.51
2:P:219:SER:C	2:P:221:GLY:H	2.14	0.51
1:W:251:HIS:HA	1:W:809:LEU:HD23	1.92	0.51
1:U:174:ASP:OD1	1:U:175:SER:N	2.44	0.51
1:U:356:GLY:H	5:U:901:MGD:C5'	2.23	0.51
1:O:855:MET:HB2	1:O:857:ASN:OD1	2.10	0.51
2:V:77:VAL:HG22	2:V:84:VAL:HG12	1.92	0.51
1:S:303:TRP:O	1:S:307:VAL:HG23	2.11	0.51
2:X:49:GLU:HG3	2:X:64:ARG:NH2	2.26	0.50
2:N:40:GLN:HB3	2:N:43:HIS:CE1	2.46	0.50
1:M:118:THR:HG21	1:M:595:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:T:106:LEU:HD23	2:T:114:MET:HE2	1.93	0.50
2:T:106:LEU:HD11	2:T:116:TRP:HB2	1.93	0.50
1:W:12:THR:HG23	8:W:1236:HOH:O	2.12	0.50
1:S:305:ASP:OD1	1:S:310:LYS:HD2	2.11	0.50
1:U:549:TRP:CE3	1:U:577:ALA:HA	2.46	0.50
2:P:46:MET:HE1	2:P:66:THR:N	2.26	0.50
1:M:146:MET:HE3	1:M:545:ASN:OD1	2.11	0.50
1:Q:452:ILE:HB	1:Q:453:PRO:HD3	1.93	0.50
2:V:213:ALA:O	2:V:228:GLU:HA	2.11	0.50
1:Q:480:TYR:HA	8:Q:1082:HOH:O	2.12	0.50
1:S:269:GLY:HA2	1:S:362:HIS:CE1	2.46	0.50
1:Q:498:GLY:N	1:Q:499:PRO:HD3	2.27	0.50
1:W:233:ILE:O	1:W:236:GLN:HB3	2.12	0.50
1:Q:146:MET:HE3	1:Q:545:ASN:OD1	2.12	0.50
1:W:166:PHE:N	1:W:439:LEU:HD12	2.26	0.50
2:P:114:MET:HE3	2:P:123:ALA:HB1	1.94	0.50
1:U:362:HIS:HB3	1:U:717:ALA:HB2	1.93	0.50
1:S:744:HIS:HA	1:S:819:SER:CB	2.40	0.50
1:S:452:ILE:HB	1:S:453:PRO:HD3	1.92	0.50
1:W:501:LEU:HA	1:W:507:THR:HB	1.92	0.50
1:O:263:TRP:HZ3	2:P:59:ASN:HD21	1.59	0.50
2:X:39:MET:HG2	2:X:40:GLN:N	2.27	0.50
2:R:19:CYS:HB2	2:R:46:MET:HG2	1.92	0.50
1:Q:146:MET:HG2	5:Q:900:MGD:N7	2.27	0.50
2:V:114:MET:HB3	2:V:125:LYS:HB3	1.93	0.50
2:N:43:HIS:ND1	8:N:856:HOH:O	2.35	0.50
1:M:698:PHE:HA	1:M:701:GLN:NE2	2.26	0.50
1:Q:177:GLU:OE2	1:Q:177:GLU:HA	2.12	0.50
1:S:155:SER:OG	1:S:409:ILE:HG12	2.12	0.50
1:M:725:PRO:HA	1:S:704:ILE:HG13	1.93	0.50
2:T:40:GLN:NE2	2:T:117:ASN:HA	2.27	0.50
1:S:563:ASP:HA	1:S:565:TYR:CE1	2.46	0.50
1:Q:138:LEU:HB2	1:Q:490:ILE:HD12	1.94	0.50
2:X:213:ALA:O	2:X:228:GLU:HA	2.12	0.50
1:O:15:PRO:HB2	1:O:31:MET:SD	2.51	0.50
2:T:114:MET:HG2	8:T:968:HOH:O	2.12	0.50
3:S:903:ACT:H1	8:S:951:HOH:O	2.11	0.50
1:W:400:TYR:CZ	1:W:421:LYS:HD2	2.46	0.50
1:W:265:SER:O	1:W:810:GLN:NE2	2.45	0.50
1:S:146:MET:HE2	1:S:545:ASN:H	1.76	0.50
2:V:19:CYS:CA	2:V:145:CYS:HB3	2.42	0.50
2:P:185:ARG:HH11	2:P:185:ARG:HB2	1.77	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:R:5:TYR:CD2	2:R:164:MET:HG2	2.47	0.50
1:M:347:ALA:CB	1:M:388:SER:HA	2.41	0.50
1:M:847:TYR:CZ	1:M:853:CYS:HB3	2.47	0.50
1:U:457:MET:HE3	8:U:906:HOH:O	2.10	0.50
1:M:786:ASN:HD21	1:M:804:GLN:HA	1.76	0.50
1:M:15:PRO:HD3	1:M:554:PHE:CE1	2.47	0.50
1:O:782:ARG:HD3	1:O:864:ILE:O	2.12	0.50
2:N:19:CYS:HA	2:N:145:CYS:HA	1.93	0.49
1:U:76:ILE:CG2	1:U:541:PRO:HG3	2.41	0.49
2:N:210:PHE:HD2	2:N:213:ALA:HB2	1.77	0.49
1:O:75:ARG:HH22	1:O:547:GLU:CD	2.14	0.49
1:Q:173:PRO:HA	1:Q:468:PHE:CE1	2.46	0.49
1:M:15:PRO:HD3	1:M:554:PHE:CD1	2.47	0.49
1:M:322:GLU:HG3	1:M:327:VAL:O	2.11	0.49
1:U:433:PHE:CD1	1:U:433:PHE:N	2.80	0.49
1:Q:800:ILE:HD12	1:Q:800:ILE:N	2.27	0.49
1:O:823:TYR:CE2	1:O:825:PRO:HG3	2.47	0.49
1:U:146:MET:HG2	5:U:900:MGD:N7	2.27	0.49
1:O:476:GLN:HG2	8:O:1191:HOH:O	2.12	0.49
2:P:59:ASN:ND2	2:P:59:ASN:H	2.10	0.49
1:Q:176:TRP:CD2	1:Q:193:LEU:HD12	2.48	0.49
1:U:99:GLY:HA2	1:U:102:LYS:HE2	1.94	0.49
1:U:797:GLY:HA2	1:U:875:TYR:CE2	2.48	0.49
1:M:617:GLU:HG3	1:M:631:TRP:CG	2.47	0.49
1:U:9:ASN:HA	1:U:576:GLN:HA	1.94	0.49
2:T:44:ARG:HG2	2:T:44:ARG:HH11	1.78	0.49
1:W:610:LYS:HZ3	1:W:618:GLN:NE2	2.09	0.49
2:X:105:LEU:HB3	2:X:114:MET:HE1	1.93	0.49
1:O:786:ASN:ND2	1:O:805:VAL:H	2.10	0.49
1:Q:458:GLY:HA3	8:Q:1444:HOH:O	2.12	0.49
1:W:489:LYS:HG3	8:W:1118:HOH:O	2.12	0.49
1:M:56:LYS:HG2	1:M:57:THR:N	2.27	0.49
1:O:76:ILE:HG22	1:O:541:PRO:HG3	1.94	0.49
1:O:78:TYR:C	1:O:541:PRO:HG2	2.31	0.49
1:M:111:ARG:NH2	1:M:585:GLU:OE2	2.37	0.49
1:S:116:GLU:O	1:S:120:ILE:HG13	2.11	0.49
1:O:166:PHE:N	1:O:439:LEU:HD12	2.27	0.49
2:P:21:MET:CE	2:P:21:MET:CA	2.90	0.49
1:Q:451:LYS:HG3	1:Q:461:PHE:CE2	2.47	0.49
2:R:254:LYS:HD2	2:R:274:LEU:OXT	2.13	0.49
1:Q:717:ALA:HB3	1:Q:720:SER:HB3	1.95	0.49
1:Q:17:PHE:CE2	1:Q:31:MET:HE3	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:197:GLU:OE2	1:W:665:THR:OG1	2.26	0.49
2:V:205:VAL:HG13	2:V:254:LYS:NZ	2.28	0.49
1:M:426:MET:CA	1:M:426:MET:HE3	2.36	0.49
2:V:168:VAL:HG13	2:V:173:LEU:HB2	1.94	0.49
1:W:25:ILE:HG13	1:W:580:ILE:CG2	2.43	0.49
2:P:142:MET:HE2	2:P:146:ALA:CB	2.43	0.49
1:O:12:THR:HG23	8:O:1241:HOH:O	2.12	0.49
1:M:855:MET:HB2	1:M:857:ASN:OD1	2.11	0.49
2:P:125:LYS:HD2	2:P:126:CYS:O	2.11	0.49
2:N:18:ASN:HB2	7:N:805:SF4:S1	2.53	0.49
1:M:201:LEU:HD13	1:M:387:TRP:HB2	1.95	0.49
1:Q:735:LEU:HD23	1:Q:735:LEU:H	1.77	0.49
2:R:125:LYS:HD2	2:R:126:CYS:O	2.13	0.49
1:Q:698:PHE:HA	1:Q:701:GLN:NE2	2.27	0.49
1:W:159:ARG:HD2	1:W:409:ILE:O	2.12	0.49
1:U:823:TYR:CE2	1:U:825:PRO:HG3	2.48	0.49
1:U:107:SER:HB3	8:U:1537:HOH:O	2.12	0.49
1:Q:630:THR:OG1	1:Q:633:GLU:HG3	2.13	0.49
1:Q:99:GLY:N	1:Q:108:ASP:OD2	2.39	0.49
1:S:277:ALA:HA	1:S:316:LYS:O	2.13	0.49
2:P:87:ARG:HB2	2:P:89:ASP:OD2	2.13	0.49
1:S:491:LYS:HD3	8:S:1470:HOH:O	2.12	0.49
1:U:301:GLU:CD	1:U:301:GLU:H	2.17	0.49
1:W:393:VAL:HG21	1:W:568:CYS:O	2.13	0.48
1:W:564:ASN:H	1:W:564:ASN:HD22	1.59	0.48
2:N:114:MET:HE3	2:N:123:ALA:HB1	1.95	0.48
1:S:855:MET:HB2	1:S:857:ASN:OD1	2.13	0.48
1:W:356:GLY:HA2	1:W:359:ARG:NH1	2.28	0.48
1:W:763:GLU:HA	1:W:768:LYS:HA	1.95	0.48
1:M:452:ILE:N	1:M:453:PRO:CD	2.76	0.48
1:U:11:SER:C	1:U:13:GLY:H	2.15	0.48
1:O:548:ARG:HB2	8:O:1019:HOH:O	2.13	0.48
1:W:333:ARG:HD3	1:W:337:ARG:NH2	2.27	0.48
1:S:561:ILE:N	1:S:562:PRO:HD3	2.27	0.48
1:Q:166:PHE:H	1:Q:439:LEU:HD12	1.78	0.48
1:M:162:ASN:CG	1:M:437:SER:HB2	2.32	0.48
1:U:644:ASP:C	1:U:646:PRO:HD3	2.33	0.48
2:V:104:GLU:H	2:V:104:GLU:CD	2.15	0.48
1:M:68:SER:HB3	1:M:753:TYR:CE2	2.48	0.48
1:S:231:SER:HB2	1:S:235:ARG:HH12	1.78	0.48
1:W:644:ASP:OD1	1:W:646:PRO:HG3	2.12	0.48
2:N:198:TYR:HB3	2:N:238:ASP:HA	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:296:ASN:O	1:Q:687:LYS:HB3	2.13	0.48
1:U:249:ASP:CG	5:U:901:MGD:H1'	2.34	0.48
1:U:708:ARG:HD3	8:U:954:HOH:O	2.13	0.48
1:W:140:THR:HB	1:W:169:ALA:HB3	1.95	0.48
2:P:247:VAL:O	2:P:257:SER:HA	2.13	0.48
1:S:28:MET:HE1	1:S:66:PHE:CB	2.38	0.48
1:W:28:MET:HE1	1:W:66:PHE:CB	2.37	0.48
1:M:165:GLY:CA	1:M:166:PHE:HB3	2.36	0.48
2:X:201:ALA:CB	2:X:269:LEU:HB2	2.35	0.48
1:S:146:MET:HG2	5:S:900:MGD:N7	2.28	0.48
1:O:563:ASP:HA	1:O:565:TYR:CE1	2.49	0.48
1:S:356:GLY:HA2	1:S:359:ARG:NH1	2.28	0.48
1:Q:65:GLY:HA2	8:Q:1307:HOH:O	2.12	0.48
1:W:610:LYS:HZ3	1:W:618:GLN:HE22	1.57	0.48
1:W:138:LEU:HB2	1:W:490:ILE:CD1	2.39	0.48
2:T:131:HIS:NE2	2:T:132:LEU:HG	2.28	0.48
1:Q:211:MET:CE	2:R:231:PHE:CZ	2.96	0.48
1:S:644:ASP:O	1:S:646:PRO:HD3	2.14	0.48
1:O:553:GLU:HB3	1:O:556:ASN:HB2	1.96	0.48
1:S:457:MET:HE2	8:S:907:HOH:O	2.12	0.48
1:S:656:TRP:CD2	1:S:663:LYS:HA	2.48	0.48
2:X:16:CYS:O	2:X:17:ASN:HB2	2.13	0.48
1:Q:501:LEU:HD13	1:Q:823:TYR:CD2	2.49	0.48
1:M:21:LYS:CB	1:M:26:ILE:HD11	2.44	0.48
1:S:701:GLN:HG3	8:S:1569:HOH:O	2.13	0.48
1:S:870:ASP:OD2	1:S:871:LYS:N	2.47	0.48
3:O:903:ACT:H1	8:O:947:HOH:O	2.13	0.48
1:O:39:ALA:HB1	8:O:1181:HOH:O	2.13	0.48
2:N:9:ASP:HA	2:N:189:LYS:HB3	1.95	0.48
1:M:730:TYR:CE1	1:M:794:ASN:HA	2.49	0.48
1:O:224:GLY:O	1:O:225:ILE:HB	2.14	0.48
1:U:427:PHE:HB3	8:U:936:HOH:O	2.14	0.48
1:Q:776:SER:HA	1:Q:805:VAL:CG1	2.44	0.48
1:M:28:MET:HE1	1:M:67:LYS:N	2.29	0.48
2:N:114:MET:HG2	8:N:971:HOH:O	2.13	0.48
1:W:500:HIS:HA	1:W:503:THR:OG1	2.14	0.48
2:V:106:LEU:HD22	2:V:114:MET:HG3	1.96	0.48
1:Q:56:LYS:HG2	1:Q:57:THR:O	2.14	0.48
1:M:449:ARG:HD2	8:M:942:HOH:O	2.12	0.48
1:O:571:ARG:HB2	1:O:642:VAL:HB	1.96	0.48
2:R:177:LYS:N	2:R:178:PRO:HD3	2.29	0.48
1:Q:111:ARG:NH2	1:Q:585:GLU:OE2	2.41	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:501:LEU:HD13	1:O:823:TYR:CD2	2.48	0.48
1:S:141:PRO:HA	1:S:496:TYR:HB3	1.96	0.48
2:T:142:MET:HE2	2:T:146:ALA:CB	2.44	0.48
1:S:74:LEU:HD12	1:S:750:LYS:HA	1.95	0.48
1:M:677:CYS:C	1:M:678:ARG:HG2	2.34	0.48
2:P:92:VAL:HG11	7:P:807:SF4:S1	2.54	0.48
1:W:142:SER:HB2	5:W:900:MGD:H5'2	1.96	0.48
2:T:68:CYS:HA	2:T:113:VAL:HG11	1.95	0.48
2:N:5:TYR:CD2	2:N:164:MET:HG2	2.49	0.48
1:U:114:TRP:CZ2	1:U:587:MET:HG2	2.48	0.48
2:T:87:ARG:HG3	2:T:91:ILE:O	2.13	0.48
1:M:649:LYS:HA	8:U:905:HOH:O	2.14	0.48
1:U:21:LYS:CB	1:U:26:ILE:HD11	2.43	0.48
2:T:260:VAL:O	2:T:260:VAL:HG13	2.14	0.48
2:P:46:MET:CE	2:P:66:THR:N	2.77	0.47
1:Q:66:PHE:HZ	1:Q:146:MET:HE1	1.78	0.47
1:W:855:MET:HB2	1:W:857:ASN:OD1	2.13	0.47
1:U:146:MET:CE	1:U:544:THR:HB	2.44	0.47
1:U:530:GLU:O	1:U:533:VAL:HG23	2.13	0.47
1:O:15:PRO:HD3	1:O:554:PHE:CD1	2.49	0.47
1:O:75:ARG:NH2	1:O:543:CYS:HA	2.29	0.47
1:S:494:TRP:HE1	1:S:525:GLN:HE21	1.62	0.47
1:M:173:PRO:HA	1:M:468:PHE:CE1	2.49	0.47
1:S:408:GLY:HA2	1:S:619:TYR:HE1	1.78	0.47
1:M:565:TYR:C	1:M:567:LEU:H	2.16	0.47
1:S:66:PHE:HA	1:S:69:MET:HE2	1.95	0.47
2:T:106:LEU:CD2	2:T:114:MET:HG3	2.44	0.47
2:V:39:MET:HG2	2:V:40:GLN:N	2.29	0.47
1:W:772:MET:HB2	1:W:801:LEU:CD1	2.44	0.47
1:U:269:GLY:HA2	1:U:362:HIS:CE1	2.48	0.47
1:S:257:ARG:HD3	2:T:61:ILE:HG21	1.96	0.47
1:U:494:TRP:HE1	1:U:525:GLN:HE21	1.60	0.47
1:Q:13:GLY:O	1:Q:59:ILE:HA	2.13	0.47
1:S:560[A]:TYR:HD1	1:S:561:ILE:HG13	1.80	0.47
1:S:560[B]:TYR:HD1	1:S:561:ILE:HG13	1.80	0.47
1:U:501:LEU:HD13	1:U:823:TYR:CD2	2.49	0.47
1:O:14:GLY:HA2	1:O:554:PHE:CE1	2.48	0.47
2:N:94:ILE:O	2:N:96:PRO:HD3	2.14	0.47
2:X:52:GLU:HG2	2:X:61:ILE:HD12	1.95	0.47
1:M:563:ASP:O	1:M:566:GLN:HG2	2.14	0.47
1:Q:394:PRO:HG3	8:Q:1228:HOH:O	2.13	0.47
2:V:110:PRO:HB3	2:V:180:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:744:HIS:CA	1:S:819:SER:HB3	2.44	0.47
1:U:75:ARG:HG2	8:U:1364:HOH:O	2.13	0.47
2:N:39:MET:HE2	2:N:45:TRP:CD2	2.49	0.47
1:S:9:ASN:HA	1:S:576:GLN:HA	1.97	0.47
1:O:103:GLN:N	1:O:103:GLN:CD	2.68	0.47
2:X:69:MET:HB2	7:X:807:SF4:S2	2.55	0.47
1:Q:66:PHE:HZ	1:Q:146:MET:CE	2.26	0.47
1:O:730:TYR:CE1	1:O:794:ASN:HA	2.50	0.47
2:X:56:TYR:CD1	2:X:57:PRO:HA	2.49	0.47
1:S:521:PHE:CE2	1:S:523:VAL:CG2	2.97	0.47
1:M:476:GLN:OE1	1:M:708:ARG:NH2	2.48	0.47
1:S:717:ALA:HB3	1:S:720:SER:HB3	1.95	0.47
1:Q:557:CYS:N	1:Q:564:ASN:HD21	1.87	0.47
1:U:737:PRO:HG3	5:U:901:MGD:H2'	1.95	0.47
2:X:164:MET:HE2	2:X:168:VAL:HG23	1.96	0.47
2:T:92:VAL:HG21	7:T:807:SF4:S1	2.55	0.47
1:S:563:ASP:O	1:S:566:GLN:HG2	2.14	0.47
1:S:452:ILE:N	1:S:453:PRO:CD	2.78	0.47
1:O:847:TYR:CZ	1:O:853:CYS:HB3	2.49	0.47
1:O:400:TYR:CZ	1:O:421:LYS:HD2	2.50	0.47
2:V:70:HIS:CD2	2:V:92:VAL:H	2.23	0.47
1:Q:691:ILE:HD11	1:Q:711:MET:CE	2.45	0.47
1:W:394:PRO:HG3	8:W:1229:HOH:O	2.14	0.47
2:V:204:LEU:HD23	2:V:209:CYS:HA	1.97	0.47
1:S:11:SER:C	1:S:13:GLY:H	2.17	0.47
1:O:696:LYS:HG3	8:O:945:HOH:O	2.14	0.47
1:W:252:MET:HB3	1:W:808:CYS:HB3	1.97	0.47
1:M:547:GLU:OE1	1:M:582:PRO:HA	2.15	0.47
1:U:365:GLU:OE1	1:U:365:GLU:HA	2.14	0.47
1:Q:540:LEU:HA	1:Q:541:PRO:HD3	1.78	0.47
1:S:600:LEU:HB3	8:S:983:HOH:O	2.15	0.47
2:T:19:CYS:CB	2:T:145:CYS:HB3	2.26	0.47
1:O:561:ILE:CG2	1:O:564:ASN:HB3	2.40	0.47
2:X:44:ARG:C	2:X:46:MET:N	2.67	0.47
2:N:68:CYS:HB2	2:N:126:CYS:CB	2.43	0.47
2:X:94:ILE:HG22	2:X:95:ASP:H	1.78	0.47
1:W:249:ASP:CG	5:W:901:MGD:H1'	2.35	0.47
1:U:361:SER:OG	1:U:717:ALA:HB1	2.15	0.47
1:S:55:ARG:HG3	8:S:1462:HOH:O	2.14	0.47
1:M:197:GLU:OE2	1:M:665:THR:OG1	2.29	0.47
2:P:87:ARG:NH2	2:P:91:ILE:HD12	2.29	0.47
1:S:114:TRP:CZ2	1:S:541:PRO:HD2	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:387:TRP:CZ2	1:S:389:THR:HA	2.50	0.47
1:U:452:ILE:N	1:U:453:PRO:CD	2.78	0.47
1:O:66:PHE:HA	1:O:69:MET:CE	2.45	0.47
1:U:530:GLU:OE2	1:U:750:LYS:NZ	2.48	0.47
1:M:174:ASP:O	1:M:177:GLU:HG2	2.15	0.47
1:M:10:SER:HB3	1:M:147:TRP:HD1	1.80	0.47
1:Q:296:ASN:HB3	1:Q:657:PHE:CZ	2.50	0.47
1:W:721:GLN:NE2	8:W:1191:HOH:O	2.48	0.47
1:W:378:GLY:O	1:W:381:LYS:HG2	2.15	0.47
1:O:262:LYS:HA	8:O:1353:HOH:O	2.14	0.47
1:W:794:ASN:HD21	1:W:842:LEU:HB3	1.79	0.47
2:P:114:MET:CB	2:P:125:LYS:HB3	2.44	0.47
2:T:114:MET:HE3	2:T:123:ALA:HB1	1.97	0.47
2:V:114:MET:HG2	8:V:970:HOH:O	2.15	0.47
2:V:19:CYS:HB3	2:V:145:CYS:CB	2.43	0.47
1:Q:100:LEU:CD1	1:Q:105:PRO:HG3	2.43	0.47
1:O:784:ILE:HD13	1:O:790:ILE:HG21	1.97	0.47
1:Q:174:ASP:O	1:Q:177:GLU:HG2	2.14	0.47
1:O:32:ASP:HB2	8:O:1567:HOH:O	2.14	0.47
1:U:68:SER:HB3	1:U:753:TYR:CD2	2.50	0.46
1:Q:146:MET:CE	1:Q:545:ASN:OD1	2.62	0.46
2:R:106:LEU:HD11	2:R:116:TRP:HB2	1.96	0.46
1:O:426:MET:CE	1:O:426:MET:HA	2.45	0.46
1:W:15:PRO:HD3	1:W:554:PHE:CD1	2.50	0.46
1:S:211:MET:CE	2:T:231:PHE:HZ	2.27	0.46
1:O:122:VAL:HG21	1:O:599:LYS:HG2	1.97	0.46
1:U:21:LYS:HB2	1:U:26:ILE:HD11	1.96	0.46
1:W:794:ASN:HD22	1:W:862:VAL:HG12	1.80	0.46
1:Q:247:PHE:O	1:Q:263:TRP:HA	2.15	0.46
1:W:451:LYS:HG3	1:W:461:PHE:CE2	2.49	0.46
1:U:85:PHE:CE2	1:U:87:PRO:HG3	2.50	0.46
8:S:1242:HOH:O	2:T:29:LEU:HB2	2.15	0.46
1:W:533:VAL:HB	1:W:534:PRO:HD3	1.96	0.46
2:T:8:ILE:HG23	2:T:153:VAL:HG12	1.97	0.46
2:V:71:CYS:CA	2:V:184:PRO:HA	2.44	0.46
1:Q:162:ASN:HD22	1:Q:166:PHE:HE2	1.62	0.46
2:R:21:MET:CE	2:R:21:MET:CA	2.93	0.46
2:X:185:ARG:CB	2:X:185:ARG:NH1	2.79	0.46
1:M:408:GLY:HA2	1:M:619:TYR:HE1	1.80	0.46
2:N:4:TYR:O	2:N:185:ARG:HD3	2.15	0.46
1:O:557:CYS:H	1:O:564:ASN:ND2	2.02	0.46
2:T:114:MET:CA	2:T:125:LYS:HB3	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:737:PRO:CG	5:M:901:MGD:H2'	2.46	0.46
2:X:164:MET:HE3	2:X:167:LYS:HB3	1.97	0.46
2:V:64:ARG:NH1	8:V:869:HOH:O	2.48	0.46
2:P:96:PRO:O	2:P:100:LYS:HG3	2.15	0.46
1:O:533:VAL:HB	1:O:534:PRO:HD3	1.97	0.46
2:X:5:TYR:HB2	2:X:157:LEU:HD11	1.96	0.46
1:U:737:PRO:CG	5:U:901:MGD:H2'	2.44	0.46
1:Q:119:ASP:OD1	1:Q:599:LYS:HE3	2.15	0.46
2:P:3:GLN:O	2:P:158:LYS:HA	2.15	0.46
2:V:175:VAL:HG23	2:V:178:PRO:HG3	1.97	0.46
1:M:587:MET:HG3	1:M:592:ILE:HG13	1.97	0.46
1:Q:176:TRP:O	1:Q:177:GLU:C	2.54	0.46
1:W:27:ARG:HB2	2:X:25:ASP:OD1	2.15	0.46
1:O:195:ASN:OD1	1:O:353:GLY:HA3	2.15	0.46
2:X:124:GLN:HB2	8:X:856:HOH:O	2.16	0.46
1:O:561:ILE:N	1:O:562:PRO:HD3	2.31	0.46
2:P:75:PRO:HD2	7:P:807:SF4:S4	2.56	0.46
1:U:81:LYS:HG2	1:U:82:ARG:N	2.31	0.46
1:O:218:ASP:OD2	1:O:253:ASN:HB2	2.16	0.46
2:T:85:TYR:HB2	8:T:1004:HOH:O	2.15	0.46
1:U:783:GLY:O	1:U:866:LYS:HD2	2.15	0.46
1:W:114:TRP:CZ2	1:W:541:PRO:HD2	2.50	0.46
2:P:198:TYR:HB3	2:P:238:ASP:HA	1.98	0.46
1:M:478:HIS:HD2	8:M:1110:HOH:O	1.98	0.46
2:X:142:MET:HE2	2:X:146:ALA:CB	2.46	0.46
2:N:142:MET:HE1	2:N:146:ALA:C	2.36	0.46
1:U:142:SER:HB3	5:U:900:MGD:O1A	2.15	0.46
1:W:495:LYS:HD3	8:W:1013:HOH:O	2.15	0.46
1:Q:114:TRP:CZ2	1:Q:541:PRO:HD2	2.50	0.46
1:O:155:SER:OG	1:O:409:ILE:HG12	2.15	0.46
1:M:200:ASP:HB3	8:M:963:HOH:O	2.15	0.46
1:S:301:GLU:CD	1:S:301:GLU:H	2.19	0.46
1:S:253:ASN:O	1:S:257:ARG:HG3	2.14	0.46
1:W:337:ARG:O	1:W:341:LYS:HG2	2.15	0.46
1:O:143:SER:HB3	3:O:903:ACT:H3	1.97	0.46
1:W:78:TYR:HA	1:W:541:PRO:HG2	1.97	0.46
2:X:252:ASP:HB3	2:X:254:LYS:HE2	1.96	0.46
1:W:452:ILE:N	1:W:453:PRO:CD	2.78	0.46
1:U:239:LYS:HE3	8:U:1001:HOH:O	2.15	0.46
1:U:417:ALA:CB	1:U:559:GLY:HA2	2.45	0.46
2:X:71:CYS:HB3	2:X:184:PRO:N	2.31	0.46
2:V:110:PRO:CB	2:V:180:LEU:HD13	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:696:LYS:HD3	8:O:1583:HOH:O	2.15	0.46
1:W:268:ILE:O	1:W:270:THR:HG23	2.16	0.46
1:M:1:MET:H3	1:M:22:ASP:CG	2.19	0.46
1:M:187:TRP:CH2	1:M:196:PRO:HB3	2.51	0.46
1:U:387:TRP:CE2	1:U:389:THR:HA	2.50	0.46
1:U:527:ILE:HG23	1:U:542:ALA:O	2.16	0.46
1:O:620:PHE:CZ	1:O:625:MET:HB3	2.51	0.46
1:Q:427:PHE:HB3	8:Q:932:HOH:O	2.14	0.46
2:P:104:GLU:CD	2:P:104:GLU:H	2.18	0.46
1:M:138:LEU:HB2	1:M:490:ILE:CD1	2.42	0.46
2:X:164:MET:HE2	2:X:168:VAL:CG2	2.46	0.46
2:X:168:VAL:HG21	8:X:980:HOH:O	2.15	0.46
2:P:5:TYR:CE2	2:P:164:MET:HG2	2.51	0.46
1:U:284:LYS:HE2	1:U:308:LEU:HD22	1.98	0.46
1:U:124:GLU:HG3	1:U:521:PHE:CD2	2.51	0.46
1:M:726:LEU:HD23	8:M:1279:HOH:O	2.15	0.46
1:S:121:VAL:O	1:S:125:ILE:HG13	2.15	0.46
2:P:126:CYS:HB2	8:P:916:HOH:O	2.16	0.46
1:W:764:VAL:O	1:W:765:ASP:HB2	2.16	0.46
1:M:296:ASN:HB3	1:M:657:PHE:CZ	2.51	0.46
1:W:495:LYS:HE3	1:W:497:GLY:O	2.16	0.46
1:W:11:SER:C	1:W:13:GLY:H	2.18	0.46
2:V:15:ASP:HB2	2:V:63:TYR:CD2	2.51	0.46
1:U:1:MET:HB2	1:U:22:ASP:OD1	2.16	0.46
1:Q:152:TYR:CD2	1:Q:154:HIS:HD2	2.34	0.46
2:X:69:MET:N	7:X:807:SF4:S2	2.89	0.45
1:W:222:ASN:HA	5:W:901:MGD:H22	1.81	0.45
1:O:737:PRO:CG	5:O:901:MGD:H2'	2.46	0.45
1:W:498:GLY:N	1:W:499:PRO:HD3	2.31	0.45
2:T:83:ALA:HB1	2:T:105:LEU:HD11	1.98	0.45
1:Q:75:ARG:HH21	1:Q:543:CYS:HA	1.79	0.45
1:W:173:PRO:HG3	1:W:180:HIS:CG	2.51	0.45
1:M:162:ASN:HD22	1:M:166:PHE:HE2	1.65	0.45
2:X:3:GLN:HB3	2:X:89:ASP:O	2.17	0.45
1:S:250:PRO:HD3	5:S:901:MGD:C2	2.46	0.45
1:Q:451:LYS:HA	1:Q:454:GLU:OE1	2.16	0.45
1:S:15:PRO:HB2	1:S:31:MET:SD	2.56	0.45
1:U:744:HIS:HA	1:U:819:SER:HB3	1.98	0.45
1:M:630:THR:OG1	1:M:633:GLU:HG3	2.16	0.45
1:M:75:ARG:HH21	1:M:543:CYS:HA	1.80	0.45
1:U:620:PHE:CZ	1:U:625:MET:HB3	2.51	0.45
1:U:162:ASN:ND2	1:U:437:SER:HB2	2.31	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:608:GLU:HB3	1:W:610:LYS:HE3	1.97	0.45
2:P:39:MET:HG2	2:P:40:GLN:N	2.30	0.45
2:N:21:MET:HE2	2:N:21:MET:HA	1.98	0.45
1:Q:501:LEU:HD13	1:Q:823:TYR:CG	2.51	0.45
2:X:68:CYS:CB	2:X:113:VAL:HG21	2.46	0.45
1:M:756:TYR:HB2	2:N:24:MET:HE1	1.98	0.45
1:U:482:TYR:CD1	1:U:483:PRO:HA	2.52	0.45
1:M:239:LYS:HE2	8:M:1507:HOH:O	2.16	0.45
2:T:247:VAL:O	2:T:257:SER:HA	2.16	0.45
1:U:721:GLN:HG3	8:U:1215:HOH:O	2.15	0.45
1:O:734:MET:HB2	1:O:814:VAL:HG23	1.99	0.45
1:S:268:ILE:O	1:S:268:ILE:HG13	2.14	0.45
2:N:122:VAL:HG22	2:N:123:ALA:N	2.31	0.45
2:X:64:ARG:HD2	2:X:176:ILE:HD11	1.97	0.45
1:U:75:ARG:NH2	1:U:543:CYS:HA	2.31	0.45
1:S:13:GLY:HA3	1:S:63:THR:OG1	2.16	0.45
1:O:262:LYS:HG2	2:P:232:PHE:CE1	2.51	0.45
1:Q:721:GLN:NE2	8:Q:1190:HOH:O	2.50	0.45
1:S:29:THR:HG22	2:T:144:ARG:HH21	1.81	0.45
1:Q:670:PRO:HB3	1:Q:682:GLN:HB2	1.99	0.45
1:M:745:THR:HB	1:M:821:ALA:HB2	1.98	0.45
1:S:478:HIS:HD2	8:S:1118:HOH:O	1.99	0.45
2:V:73:ASN:HA	2:V:73:ASN:HD22	1.64	0.45
1:U:561:ILE:CG2	1:U:564:ASN:HB3	2.45	0.45
1:M:557:CYS:H	1:M:564:ASN:ND2	1.96	0.45
1:M:165:GLY:HA3	1:M:166:PHE:CB	2.30	0.45
1:O:44:ILE:HG21	1:O:206:LEU:HD12	1.98	0.45
1:S:55:ARG:HD2	8:S:1552:HOH:O	2.17	0.45
1:Q:265:SER:O	1:Q:810:GLN:NE2	2.50	0.45
1:W:725:PRO:HD2	8:W:1101:HOH:O	2.17	0.45
1:M:717:ALA:HB3	1:M:720:SER:HB3	1.98	0.45
1:O:505:THR:O	1:O:506:ALA:C	2.55	0.45
1:U:421:LYS:HA	1:U:424:TRP:HD1	1.82	0.45
1:S:100:LEU:CD1	1:S:105:PRO:HG3	2.46	0.45
1:O:269:GLY:HA2	1:O:362:HIS:CG	2.51	0.45
1:W:701:GLN:HG3	8:W:1565:HOH:O	2.17	0.45
1:S:79:PRO:HB2	1:S:112:ILE:O	2.15	0.45
2:R:69:MET:HB3	2:R:184:PRO:HB3	1.99	0.45
1:O:15:PRO:HD2	8:O:907:HOH:O	2.16	0.45
1:W:62:TYR:HB3	1:W:742:SER:HA	1.99	0.45
1:S:434:PRO:O	1:S:436:PRO:HD3	2.16	0.45
1:W:56:LYS:HG2	1:W:57:THR:N	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:265:SER:O	1:M:810:GLN:NE2	2.48	0.45
1:W:214:PHE:HA	1:W:347:ALA:HB3	1.99	0.45
1:W:773:ARG:HH11	1:W:773:ARG:HG3	1.81	0.45
1:Q:426:MET:HE2	1:Q:618:GLN:HG2	1.98	0.45
1:O:425:ARG:HD3	1:O:622:ALA:O	2.16	0.45
2:P:4:TYR:CZ	2:P:158:LYS:HD2	2.52	0.45
1:Q:617:GLU:HG3	1:Q:631:TRP:CG	2.52	0.45
1:M:498:GLY:N	1:M:499:PRO:HD3	2.32	0.45
2:X:141:LYS:HA	8:X:956:HOH:O	2.15	0.45
1:M:839:ILE:HA	1:M:839:ILE:HD13	1.86	0.45
1:O:359:ARG:O	1:O:359:ARG:HG3	2.17	0.45
2:N:70:HIS:HD2	2:N:92:VAL:N	2.03	0.45
1:U:144:HIS:HB2	5:U:900:MGD:O1B	2.17	0.45
1:S:772:MET:HB2	1:S:801:LEU:HD13	1.98	0.45
1:W:253:ASN:O	1:W:257:ARG:HG3	2.17	0.45
1:U:642:VAL:HA	1:U:643:PRO:HD3	1.84	0.45
1:W:730:TYR:CE1	1:W:794:ASN:HA	2.52	0.45
1:S:505:THR:O	1:S:506:ALA:C	2.56	0.45
2:N:247:VAL:O	2:N:257:SER:HA	2.17	0.45
1:S:99:GLY:HA2	1:S:102:LYS:HG2	1.98	0.45
1:Q:103:GLN:CD	1:Q:103:GLN:N	2.70	0.45
1:U:426:MET:HA	1:U:426:MET:CE	2.47	0.45
1:W:426:MET:HE1	1:W:618:GLN:CG	2.44	0.45
1:U:224:GLY:O	1:U:225:ILE:HB	2.17	0.45
1:W:75:ARG:HH21	1:W:543:CYS:HA	1.82	0.45
1:W:95:LEU:HD21	8:W:1397:HOH:O	2.17	0.45
1:W:730:TYR:CZ	1:W:794:ASN:HA	2.52	0.45
1:Q:152:TYR:HD2	1:Q:154:HIS:HD2	1.64	0.45
1:O:683:THR:HB	1:O:689:GLU:OE1	2.17	0.45
2:P:210:PHE:O	2:P:233:GLY:HA2	2.17	0.45
2:T:252:ASP:C	2:T:254:LYS:H	2.19	0.45
2:V:8:ILE:HG23	2:V:153:VAL:CG1	2.47	0.45
2:N:59:ASN:ND2	2:N:59:ASN:H	2.15	0.45
1:W:857:ASN:HB3	5:W:900:MGD:N19	2.32	0.45
2:N:164:MET:O	2:N:168:VAL:HG23	2.18	0.45
1:U:857:ASN:HB3	5:U:900:MGD:N19	2.31	0.45
1:Q:253:ASN:O	1:Q:257:ARG:HG3	2.16	0.45
1:Q:257:ARG:HD3	2:R:61:ILE:HG21	1.98	0.45
1:O:249:ASP:CG	5:O:901:MGD:H1'	2.37	0.45
2:T:141:LYS:HA	8:T:950:HOH:O	2.17	0.45
1:U:454:GLU:HA	8:U:906:HOH:O	2.16	0.45
2:T:87:ARG:HB2	2:T:89:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:387:TRP:CE2	1:S:389:THR:HA	2.52	0.45
2:T:217:LEU:HB2	2:T:237:PHE:CE1	2.52	0.45
1:W:806:THR:OG1	1:W:807:GLU:N	2.49	0.45
1:M:433:PHE:CD1	1:M:433:PHE:N	2.85	0.45
1:M:426:MET:HE3	1:M:622:ALA:HB2	1.99	0.44
1:O:28:MET:CE	1:O:67:LYS:H	2.28	0.44
2:X:84:VAL:CG2	2:X:94:ILE:HG12	2.40	0.44
1:O:166:PHE:H	1:O:439:LEU:HD12	1.82	0.44
1:W:816:SER:OG	1:W:839:ILE:HG13	2.18	0.44
1:M:452:ILE:HB	1:M:453:PRO:HD3	1.99	0.44
1:Q:656:TRP:CD2	1:Q:663:LYS:HA	2.51	0.44
1:W:704:ILE:HG23	8:W:1554:HOH:O	2.17	0.44
1:W:393:VAL:HG23	1:W:566:GLN:O	2.17	0.44
1:Q:857:ASN:HB3	5:Q:900:MGD:N19	2.32	0.44
2:P:252:ASP:C	2:P:254:LYS:H	2.21	0.44
1:W:770:TRP:HB3	1:W:801:LEU:CD2	2.47	0.44
1:W:212:ILE:CD1	1:W:238:LEU:HD13	2.47	0.44
2:X:51:ARG:O	2:X:61:ILE:HG13	2.16	0.44
1:U:847:TYR:CZ	1:U:853:CYS:HB3	2.52	0.44
1:S:797:GLY:HA2	1:S:875:TYR:CE2	2.52	0.44
1:W:224:GLY:O	1:W:225:ILE:HB	2.17	0.44
1:M:291:GLU:H	1:M:291:GLU:CD	2.21	0.44
1:M:391:GLN:HG2	1:M:567:LEU:CD2	2.47	0.44
1:O:277:ALA:HA	1:O:316:LYS:O	2.16	0.44
2:P:77:VAL:HG22	2:P:84:VAL:HG12	1.97	0.44
1:W:576:GLN:HB3	8:W:1012:HOH:O	2.17	0.44
1:W:790:ILE:HD13	1:W:803:ALA:HB2	1.99	0.44
1:W:445:GLN:HB2	1:W:484:ALA:HB3	1.99	0.44
1:U:756:TYR:HD1	2:V:24:MET:HE1	1.82	0.44
2:T:70:HIS:CD2	2:T:92:VAL:H	2.33	0.44
2:P:23:CYS:HB3	2:P:39:MET:HE1	1.98	0.44
1:U:393:VAL:CG1	1:U:395:LEU:HG	2.47	0.44
1:M:730:TYR:HB3	1:M:862:VAL:CA	2.48	0.44
1:Q:776:SER:HA	1:Q:805:VAL:HG13	1.99	0.44
1:U:201:LEU:HD13	1:U:387:TRP:HB2	2.00	0.44
1:M:9:ASN:HA	1:M:576:GLN:HA	1.99	0.44
1:M:564:ASN:HD22	1:M:564:ASN:H	1.65	0.44
2:N:17:ASN:HB2	8:N:1016:HOH:O	2.16	0.44
1:U:66:PHE:HZ	1:U:146:MET:CE	2.30	0.44
2:X:3:GLN:NE2	2:X:161:PRO:HG3	2.32	0.44
2:R:23:CYS:O	2:R:26:GLU:N	2.48	0.44
1:O:15:PRO:HD3	1:O:554:PHE:CE1	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:X:157:LEU:HD12	2:X:157:LEU:O	2.18	0.44
1:W:9:ASN:HA	1:W:576:GLN:HA	1.98	0.44
1:O:471:GLY:HA3	1:O:475:HIS:CE1	2.53	0.44
1:U:302:GLU:OE1	1:U:302:GLU:N	2.46	0.44
1:U:414:GLU:O	1:U:414:GLU:CG	2.65	0.44
2:X:203:ILE:HD12	2:X:203:ILE:N	2.32	0.44
2:T:185:ARG:HB3	2:T:185:ARG:CZ	2.48	0.44
1:U:753:TYR:CE1	2:V:28:GLU:HG3	2.53	0.44
1:S:27:ARG:NH2	2:T:132:LEU:HD21	2.31	0.44
2:X:126:CYS:HB2	8:X:922:HOH:O	2.18	0.44
1:S:656:TRP:CG	1:S:663:LYS:HA	2.53	0.44
2:X:247:VAL:O	2:X:257:SER:HA	2.18	0.44
1:Q:757:ILE:HD11	8:R:1021:HOH:O	2.16	0.44
1:M:571:ARG:HA	8:M:930:HOH:O	2.18	0.44
1:O:610:LYS:HB3	1:O:614:ALA:HB3	1.98	0.44
2:T:49:GLU:HG3	2:T:64:ARG:HH21	1.80	0.44
1:U:144:HIS:CE1	1:U:225:ILE:HD11	2.53	0.44
2:R:142:MET:CE	2:R:146:ALA:HB1	2.48	0.44
1:U:452:ILE:HB	1:U:453:PRO:HD3	2.00	0.44
1:U:676:VAL:HG13	8:U:962:HOH:O	2.18	0.44
1:O:588:SER:HA	8:O:1274:HOH:O	2.18	0.44
1:W:118:THR:O	1:W:122:VAL:HG23	2.18	0.44
1:Q:770:TRP:HB3	1:Q:801:LEU:HD23	2.00	0.44
1:Q:716:PRO:HB3	1:Q:723:HIS:CD2	2.53	0.44
2:P:46:MET:HE1	2:P:65:PRO:CA	2.47	0.44
1:O:68:SER:HB3	1:O:753:TYR:CD2	2.52	0.44
1:Q:28:MET:CE	1:Q:66:PHE:HB3	2.47	0.44
2:R:70:HIS:HD2	2:R:92:VAL:N	2.03	0.44
1:W:748:ASP:O	1:W:750:LYS:HG3	2.17	0.44
2:T:129:CYS:HB3	2:T:131:HIS:HE1	1.79	0.44
1:W:737:PRO:CG	5:W:901:MGD:H2'	2.48	0.44
2:T:21:MET:CE	2:T:24:MET:HE2	2.48	0.44
1:W:75:ARG:NH2	1:W:547:GLU:OE1	2.43	0.44
1:U:76:ILE:HA	1:U:77:PRO:HD3	1.82	0.44
1:W:362:HIS:HB3	1:W:717:ALA:HB2	1.99	0.44
1:Q:47:ARG:HD2	1:Q:241:LEU:HD22	2.00	0.44
1:S:426:MET:HE3	1:S:426:MET:HA	1.99	0.44
1:U:28:MET:CE	1:U:67:LYS:N	2.81	0.44
2:X:73:ASN:HD22	2:X:73:ASN:C	2.21	0.44
2:N:176:ILE:HG22	2:N:177:LYS:HG3	1.99	0.44
2:N:211:GLU:HB2	2:N:231:PHE:HA	1.99	0.44
2:P:59:ASN:HD22	2:P:59:ASN:H	1.64	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:427:PHE:CG	1:S:434:PRO:HG3	2.53	0.44
2:V:129:CYS:HB3	2:V:131:HIS:CE1	2.53	0.44
2:X:152:PHE:CD1	2:X:152:PHE:N	2.86	0.44
2:T:177:LYS:HA	2:T:179:GLU:OE1	2.18	0.43
1:U:571:ARG:HA	8:U:934:HOH:O	2.18	0.43
2:X:179:GLU:HG2	2:X:180:LEU:H	1.81	0.43
1:S:277:ALA:HB2	1:S:321:ALA:HB2	2.00	0.43
1:Q:39:ALA:HA	1:Q:40:PRO:HD3	1.88	0.43
1:U:353:GLY:O	1:U:354:TRP:HB2	2.18	0.43
2:X:1:MET:SD	2:X:88:GLU:HB3	2.58	0.43
1:W:156:THR:HB	8:W:1206:HOH:O	2.18	0.43
1:Q:339:TRP:CH2	1:Q:346:LEU:HD13	2.54	0.43
1:W:564:ASN:C	1:W:566:GLN:N	2.72	0.43
1:U:182:GLY:HA3	1:U:364:ILE:HG23	2.00	0.43
1:Q:452:ILE:N	1:Q:453:PRO:CD	2.81	0.43
2:N:23:CYS:HB3	2:N:39:MET:HE3	2.00	0.43
1:W:452:ILE:HB	1:W:453:PRO:HD3	2.00	0.43
1:Q:670:PRO:HG2	1:Q:675:GLN:CD	2.39	0.43
2:V:90:GLY:HA3	2:V:185:ARG:CZ	2.48	0.43
1:S:138:LEU:HB2	1:S:490:ILE:HD12	2.00	0.43
1:U:187:TRP:CH2	1:U:196:PRO:HB3	2.53	0.43
1:U:197:GLU:OE2	1:U:667:ASP:HB2	2.19	0.43
2:T:106:LEU:HD23	2:T:114:MET:CE	2.48	0.43
2:X:56:TYR:HA	2:X:59:ASN:ND2	2.33	0.43
2:T:201:ALA:HB2	2:T:269:LEU:HB2	2.00	0.43
1:Q:176:TRP:CE2	1:Q:193:LEU:HD12	2.54	0.43
2:R:159:THR:OG1	2:R:160:THR:N	2.52	0.43
2:V:142:MET:HE2	2:V:146:ALA:C	2.39	0.43
2:R:213:ALA:HB1	2:R:251:ALA:HB2	2.00	0.43
1:Q:11:SER:HA	1:Q:147:TRP:HB2	2.00	0.43
1:M:404:TYR:CD1	1:M:405:ALA:N	2.86	0.43
1:S:263:TRP:HZ3	2:T:59:ASN:HD21	1.67	0.43
2:X:46:MET:HE1	2:X:66:THR:N	2.34	0.43
2:X:4:TYR:CZ	2:X:158:LYS:HD2	2.53	0.43
2:V:5:TYR:CE2	2:V:164:MET:HG2	2.53	0.43
1:U:223:SER:HB2	8:U:940:HOH:O	2.17	0.43
1:Q:96:ARG:HH12	1:Q:519:LEU:HB3	1.81	0.43
1:U:630:THR:OG1	1:U:633:GLU:HG3	2.18	0.43
2:X:210:PHE:CE2	2:X:251:ALA:HB1	2.52	0.43
1:Q:597:ALA:HB1	1:Q:603:GLU:HA	2.00	0.43
1:S:610:LYS:HB3	1:S:614:ALA:HB3	1.99	0.43
1:W:104:ASP:N	1:W:105:PRO:HD3	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:269:GLY:HA2	1:U:362:HIS:CG	2.52	0.43
1:W:25:ILE:HG13	1:W:580:ILE:HG21	1.99	0.43
1:U:744:HIS:HA	1:U:819:SER:CB	2.49	0.43
1:U:349:GLY:HA3	1:U:353:GLY:O	2.18	0.43
2:R:210:PHE:HD2	2:R:213:ALA:HB2	1.84	0.43
1:Q:478:HIS:HD2	8:Q:1112:HOH:O	2.00	0.43
1:O:797:GLY:HA2	1:O:875:TYR:CE2	2.54	0.43
1:O:656:TRP:CD2	1:O:663:LYS:HA	2.54	0.43
1:Q:558:SER:H	1:Q:564:ASN:ND2	2.16	0.43
1:O:69:MET:HE1	1:O:754:MET:HE3	2.00	0.43
1:S:738:HIS:HE2	5:S:900:MGD:H15	1.66	0.43
1:S:249:ASP:CG	5:S:901:MGD:H1'	2.39	0.43
2:X:106:LEU:HD22	2:X:114:MET:O	2.18	0.43
1:U:571:ARG:HB2	1:U:642:VAL:HB	2.01	0.43
2:X:26:GLU:HB2	2:X:144:ARG:NH1	2.34	0.43
1:U:498:GLY:N	1:U:499:PRO:HD3	2.33	0.43
1:Q:657:PHE:CE1	1:Q:681:LEU:HG	2.54	0.43
1:Q:408:GLY:HA2	1:Q:619:TYR:HE1	1.83	0.43
2:P:56:TYR:CD1	2:P:57:PRO:HA	2.54	0.43
1:M:152:TYR:CD2	1:M:154:HIS:HD2	2.36	0.43
1:U:730:TYR:HB3	1:U:862:VAL:C	2.39	0.43
1:S:550:ASP:HA	1:S:616:CYS:SG	2.58	0.43
1:M:117:ALA:O	1:M:121:VAL:HG23	2.19	0.43
2:V:210:PHE:CE2	2:V:251:ALA:HB1	2.54	0.43
1:S:850:LYS:NZ	8:S:1190:HOH:O	2.51	0.43
2:P:46:MET:HE1	2:P:65:PRO:HA	1.99	0.43
1:O:28:MET:CE	1:O:66:PHE:HB3	2.49	0.43
1:W:530:GLU:OE1	1:W:750:LYS:NZ	2.50	0.43
2:T:76:CYS:HA	2:T:108:THR:HB	2.01	0.43
1:M:347:ALA:HB1	1:M:388:SER:HA	2.01	0.43
1:W:219:PRO:HD2	1:W:255:THR:HG21	1.99	0.43
1:S:504:MET:HE3	8:S:947:HOH:O	2.17	0.43
1:W:696:LYS:O	1:W:700:GLU:HG3	2.19	0.43
1:O:816:SER:OG	1:O:839:ILE:HG13	2.18	0.43
1:S:542:ALA:HA	1:S:587:MET:O	2.19	0.43
1:M:66:PHE:HA	1:M:69:MET:HE3	2.00	0.43
1:M:825:PRO:HD2	8:M:1243:HOH:O	2.18	0.43
1:M:10:SER:HA	1:M:15:PRO:HA	2.00	0.43
1:S:361:SER:OG	1:S:717:ALA:HB1	2.19	0.43
1:W:724:SER:HA	1:W:725:PRO:HD3	1.86	0.43
1:S:730:TYR:CE1	1:S:794:ASN:HA	2.53	0.43
2:V:139:ALA:HB3	2:V:140:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:152:TYR:CD2	1:U:154:HIS:HD2	2.36	0.43
1:S:696:LYS:O	1:S:700:GLU:HG3	2.19	0.43
2:X:176:ILE:HG22	2:X:177:LYS:HG3	2.01	0.43
1:W:222:ASN:HA	5:W:901:MGD:N22	2.34	0.43
2:R:58:ARG:NH1	2:R:270:GLY:HA2	2.34	0.43
1:O:262:LYS:HD2	8:O:1353:HOH:O	2.19	0.43
2:T:26:GLU:HB2	2:T:144:ARG:HH11	1.84	0.43
1:Q:378:GLY:O	1:Q:381:LYS:HG2	2.18	0.43
1:O:831:LYS:O	1:O:873:GLU:HA	2.18	0.43
1:Q:395:LEU:HD13	1:Q:571:ARG:CG	2.49	0.43
1:S:377:GLN:O	1:S:381:LYS:HE2	2.19	0.43
1:M:224:GLY:O	1:M:225:ILE:HB	2.17	0.43
1:W:291:GLU:CD	1:W:291:GLU:H	2.22	0.43
2:T:104:GLU:CD	2:T:104:GLU:H	2.22	0.43
1:S:146:MET:HE1	1:S:544:THR:CB	2.45	0.43
1:W:146:MET:HE3	1:W:545:ASN:OD1	2.19	0.43
1:O:499:PRO:HG3	5:O:900:MGD:O5'	2.19	0.43
2:P:185:ARG:CZ	2:P:185:ARG:CB	2.96	0.43
2:X:7:VAL:HG21	2:X:167:LYS:HZ2	1.84	0.43
1:M:176:TRP:CE2	1:M:193:LEU:HD12	2.54	0.43
1:U:549:TRP:CG	1:U:613:LEU:HD13	2.54	0.43
1:M:56:LYS:HG2	1:M:57:THR:O	2.19	0.43
1:W:56:LYS:HG2	1:W:57:THR:O	2.18	0.43
1:W:773:ARG:HG3	1:W:773:ARG:NH1	2.34	0.43
1:U:401:PHE:HA	1:U:402:PRO:HD3	1.80	0.43
1:Q:588:SER:O	1:Q:592:ILE:HG13	2.19	0.43
1:O:617:GLU:HG3	1:O:631:TRP:CG	2.54	0.43
1:Q:401:PHE:HA	1:Q:402:PRO:HD3	1.84	0.43
2:V:114:MET:CB	2:V:125:LYS:HB3	2.49	0.42
2:V:126:CYS:HB2	8:V:919:HOH:O	2.18	0.42
1:M:786:ASN:HD22	1:M:786:ASN:HA	1.58	0.42
1:U:501:LEU:HB2	8:U:1274:HOH:O	2.18	0.42
2:V:5:TYR:HB2	2:V:157:LEU:HD12	2.01	0.42
1:O:104:ASP:OD2	1:O:107:SER:HB3	2.18	0.42
2:X:109:CYS:HB2	2:X:114:MET:SD	2.59	0.42
2:T:201:ALA:O	2:T:234:GLU:HA	2.19	0.42
1:W:44:ILE:HG21	1:W:206:LEU:HD12	2.01	0.42
1:U:549:TRP:CZ3	1:U:577:ALA:HA	2.54	0.42
2:R:164:MET:O	2:R:168:VAL:HG23	2.18	0.42
1:O:732:LEU:CD1	1:O:864:ILE:HG12	2.49	0.42
2:P:87:ARG:HG3	2:P:91:ILE:O	2.18	0.42
1:O:696:LYS:O	1:O:700:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Q:96:ARG:HD2	1:Q:514:TYR:O	2.19	0.42
1:W:478:HIS:CD2	8:W:1112:HOH:O	2.71	0.42
2:V:122:VAL:HG22	2:V:123:ALA:N	2.34	0.42
1:W:602:ILE:CG2	8:W:978:HOH:O	2.66	0.42
1:Q:146:MET:HE2	1:Q:545:ASN:H	1.84	0.42
1:W:28:MET:HE2	8:W:1308:HOH:O	2.19	0.42
1:M:176:TRP:O	1:M:177:GLU:C	2.57	0.42
1:W:65:GLY:HA3	2:X:21:MET:HG3	2.01	0.42
1:U:267:LYS:HB3	1:U:721:GLN:NE2	2.33	0.42
1:O:870:ASP:HB3	1:O:872:TYR:CE1	2.53	0.42
2:X:6:MET:CE	2:X:143:PRO:HG2	2.49	0.42
1:M:166:PHE:N	1:M:439:LEU:HD12	2.34	0.42
1:O:730:TYR:HB3	1:O:862:VAL:CA	2.49	0.42
2:X:175:VAL:CG2	2:X:178:PRO:HG3	2.43	0.42
1:O:540:LEU:HA	1:O:541:PRO:HD3	1.78	0.42
1:W:478:HIS:HD2	8:W:1112:HOH:O	2.02	0.42
1:W:2:GLY:O	1:W:21:LYS:HE3	2.18	0.42
1:S:20:VAL:HG12	8:S:1512:HOH:O	2.19	0.42
2:N:250:ASP:HB2	8:N:990:HOH:O	2.19	0.42
1:W:211:MET:HE3	2:X:231:PHE:CZ	2.54	0.42
1:M:69:MET:HE2	1:M:754:MET:HE1	2.01	0.42
1:S:360:ALA:HB1	1:S:859:THR:CG2	2.40	0.42
1:S:165:GLY:CA	1:S:166:PHE:HB3	2.49	0.42
1:U:78:TYR:O	1:U:80:MET:HG3	2.20	0.42
2:V:21:MET:CE	2:V:21:MET:CA	2.97	0.42
1:U:263:TRP:CZ2	1:U:265:SER:HB2	2.53	0.42
1:Q:354:TRP:HB3	1:Q:355:GLY:H	1.64	0.42
1:S:708:ARG:CD	8:S:954:HOH:O	2.67	0.42
1:O:162:ASN:CG	1:O:437:SER:HB2	2.40	0.42
1:M:402:PRO:HG2	1:M:422:PHE:CE1	2.54	0.42
1:Q:602:ILE:HG23	8:Q:979:HOH:O	2.20	0.42
2:X:159:THR:OG1	2:X:160:THR:N	2.51	0.42
2:P:191:LEU:HD12	2:P:191:LEU:O	2.20	0.42
2:P:203:ILE:N	2:P:203:ILE:HD12	2.35	0.42
1:W:557:CYS:H	1:W:564:ASN:ND2	2.08	0.42
1:W:563:ASP:O	1:W:566:GLN:HG2	2.19	0.42
2:X:44:ARG:HH11	2:X:44:ARG:HG2	1.84	0.42
2:P:52:GLU:HG3	2:P:61:ILE:HD12	2.02	0.42
2:T:69:MET:HB2	7:T:807:SF4:S2	2.59	0.42
1:S:249:ASP:O	1:S:250:PRO:C	2.58	0.42
1:O:75:ARG:HH21	1:O:543:CYS:HA	1.84	0.42
1:S:508:ASN:HB2	8:S:1206:HOH:O	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:80:MET:HB2	1:M:539:ILE:HB	2.01	0.42
1:Q:209:ALA:HB2	1:Q:345:TYR:CE1	2.54	0.42
1:O:494:TRP:HE1	1:O:525:GLN:HE21	1.67	0.42
1:W:625:MET:N	1:W:626:PRO:CD	2.82	0.42
2:V:44:ARG:HG2	2:V:44:ARG:HH11	1.85	0.42
1:Q:425:ARG:HD3	1:Q:622:ALA:O	2.20	0.42
1:M:146:MET:CE	1:M:545:ASN:OD1	2.68	0.42
1:W:426:MET:CE	1:W:618:GLN:HG2	2.47	0.42
1:Q:319:GLU:CG	1:U:726:LEU:HD13	2.43	0.42
2:V:46:MET:HE1	2:V:66:THR:N	2.34	0.42
1:U:144:HIS:NE2	5:U:901:MGD:S13	2.92	0.42
1:U:78:TYR:CD1	1:U:111:ARG:HG3	2.54	0.42
2:N:177:LYS:N	2:N:178:PRO:HD3	2.34	0.42
1:W:745:THR:HG22	1:W:819:SER:O	2.19	0.42
1:O:597:ALA:HB1	1:O:603:GLU:HA	2.02	0.42
1:U:251:HIS:HA	1:U:809:LEU:HD23	2.00	0.42
2:R:207:GLY:CA	1:U:728:VAL:HG12	2.31	0.42
1:O:74:LEU:HD12	1:O:750:LYS:CA	2.43	0.42
2:X:229:THR:HB	2:X:233:GLY:HA2	2.00	0.42
1:Q:197:GLU:OE2	1:Q:667:ASP:HB2	2.20	0.42
1:U:291:GLU:CD	1:U:291:GLU:H	2.23	0.42
1:W:454:GLU:CD	1:W:454:GLU:H	2.21	0.42
2:X:111:TYR:CD1	2:X:111:TYR:N	2.87	0.42
1:S:857:ASN:HB3	5:S:900:MGD:N19	2.35	0.42
1:M:249:ASP:OD2	5:M:901:MGD:H1'	2.19	0.42
1:U:77:PRO:HB2	1:U:78:TYR:CD2	2.54	0.42
1:W:96:ARG:HD2	1:W:514:TYR:O	2.20	0.42
1:S:177:GLU:HA	1:S:177:GLU:OE2	2.20	0.42
1:W:263:TRP:CZ2	1:W:265:SER:HB2	2.55	0.42
1:U:625:MET:N	1:U:626:PRO:CD	2.82	0.42
1:M:349:GLY:HA3	1:M:353:GLY:O	2.19	0.42
2:T:159:THR:OG1	2:T:160:THR:N	2.51	0.42
1:M:826:LEU:HD12	1:M:833:ALA:HB3	2.02	0.42
1:U:806:THR:OG1	1:U:807:GLU:N	2.53	0.42
1:M:848:ILE:HG13	1:M:854:GLY:O	2.19	0.42
1:M:782:ARG:HH11	1:M:782:ARG:HG3	1.84	0.42
2:N:21:MET:HE3	2:N:21:MET:HA	2.02	0.42
2:N:10:VAL:HG13	2:N:63:TYR:O	2.20	0.42
1:O:21:LYS:CB	1:O:26:ILE:HD11	2.49	0.42
1:Q:361:SER:OG	1:Q:717:ALA:HB1	2.19	0.42
1:Q:292:TYR:CD2	1:Q:378:GLY:HA2	2.55	0.42
2:P:9:ASP:HA	2:P:189:LYS:HB3	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:53:PRO:HA	1:S:54:PRO:HD3	1.87	0.42
1:O:288:TYR:HB2	1:O:376:MET:O	2.20	0.42
1:Q:433:PHE:CD1	1:Q:433:PHE:N	2.88	0.42
2:T:73:ASN:C	2:T:73:ASN:HD22	2.23	0.42
2:R:40:GLN:HB3	2:R:43:HIS:CE1	2.55	0.42
2:R:166:LYS:HE2	2:R:170:GLU:OE2	2.20	0.42
1:W:739:PRO:HG2	1:W:742:SER:O	2.20	0.42
2:P:210:PHE:HD2	2:P:213:ALA:HB2	1.85	0.42
1:Q:269:GLY:HA2	1:Q:362:HIS:ND1	2.35	0.42
1:O:587:MET:HG3	1:O:592:ILE:CG1	2.49	0.42
1:U:471:GLY:HA3	1:U:475:HIS:CE1	2.54	0.42
1:Q:404:TYR:CD1	1:Q:405:ALA:N	2.88	0.42
1:W:521:PHE:CE2	1:W:523:VAL:CG2	3.03	0.42
1:O:56:LYS:HG2	1:O:57:THR:O	2.20	0.42
1:W:561:ILE:N	1:W:562:PRO:HD3	2.34	0.41
1:O:564:ASN:H	1:O:564:ASN:HD22	1.66	0.41
1:U:162:ASN:ND2	1:U:166:PHE:HE2	2.17	0.41
2:X:168:VAL:O	2:X:168:VAL:HG12	2.20	0.41
2:T:76:CYS:HB3	2:T:108:THR:CB	2.49	0.41
2:T:5:TYR:HB2	2:T:157:LEU:HD12	1.99	0.41
1:W:44:ILE:HD11	1:W:394:PRO:CG	2.49	0.41
1:U:499:PRO:CB	1:U:745:THR:HG21	2.49	0.41
1:W:224:GLY:HA2	8:W:1235:HOH:O	2.20	0.41
2:V:142:MET:HE2	2:V:147:HIS:N	2.35	0.41
1:S:730:TYR:CZ	1:S:794:ASN:HA	2.55	0.41
1:M:505:THR:O	1:M:506:ALA:C	2.58	0.41
1:U:277:ALA:HA	1:U:316:LYS:O	2.20	0.41
1:O:140:THR:HB	1:O:169:ALA:HB3	2.02	0.41
2:P:16:CYS:O	2:P:17:ASN:HB2	2.20	0.41
1:M:670:PRO:HG2	1:M:675:GLN:CD	2.40	0.41
1:M:76:ILE:HA	1:M:77:PRO:HD3	1.82	0.41
2:V:203:ILE:HD12	2:V:203:ILE:N	2.35	0.41
1:M:272:HIS:N	1:M:272:HIS:ND1	2.67	0.41
1:S:610:LYS:HZ3	1:S:618:GLN:NE2	2.14	0.41
1:M:66:PHE:HZ	1:M:146:MET:CE	2.33	0.41
1:O:498:GLY:N	1:O:499:PRO:HD3	2.35	0.41
2:N:142:MET:HE2	2:N:146:ALA:CB	2.44	0.41
1:U:855:MET:HB2	1:U:857:ASN:OD1	2.20	0.41
1:W:74:LEU:HD12	1:W:750:LYS:CA	2.45	0.41
1:W:143:SER:CB	3:W:903:ACT:H3	2.49	0.41
1:O:144:HIS:NE2	5:O:901:MGD:S13	2.93	0.41
1:M:211:MET:CE	2:N:231:PHE:HZ	2.33	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:826:LEU:HD21	1:W:835:ARG:HD3	2.01	0.41
1:W:171:HIS:O	1:W:467:GLY:HA2	2.20	0.41
2:X:198:TYR:CD1	2:X:236:LYS:HE3	2.55	0.41
2:P:217:LEU:O	2:P:224:VAL:N	2.42	0.41
1:S:489:LYS:HD3	8:S:929:HOH:O	2.20	0.41
1:U:31:MET:HE1	1:U:639:TYR:CG	2.55	0.41
1:S:354:TRP:CZ2	1:S:561:ILE:HD11	2.55	0.41
1:W:176:TRP:O	1:W:177:GLU:C	2.59	0.41
1:U:361:SER:N	1:U:856:ALA:HB1	2.36	0.41
1:U:730:TYR:CE1	1:U:794:ASN:HA	2.56	0.41
1:U:757:ILE:HD11	8:V:1017:HOH:O	2.20	0.41
1:Q:521:PHE:CE2	1:Q:523:VAL:HG22	2.55	0.41
1:Q:548:ARG:NH1	1:Q:550:ASP:OD2	2.47	0.41
1:M:39:ALA:HA	1:M:40:PRO:HD3	1.85	0.41
1:O:171:HIS:HD2	8:O:1368:HOH:O	2.03	0.41
1:U:734:MET:HB2	1:U:814:VAL:HG23	2.01	0.41
2:P:81:ASN:O	2:P:81:ASN:OD1	2.39	0.41
2:V:106:LEU:HD23	2:V:114:MET:HG3	2.01	0.41
2:X:87:ARG:HB2	2:X:89:ASP:OD2	2.20	0.41
2:P:205:VAL:HG13	2:P:254:LYS:HZ1	1.82	0.41
1:U:28:MET:CE	1:U:67:LYS:H	2.32	0.41
1:O:364:ILE:HB	8:O:1254:HOH:O	2.20	0.41
2:P:154:TYR:CE1	7:P:805:SF4:S4	3.14	0.41
1:S:744:HIS:C	1:S:819:SER:HB3	2.40	0.41
2:P:238:ASP:O	2:P:239:ALA:HB3	2.20	0.41
1:O:316:LYS:HD2	1:O:320:TRP:CH2	2.55	0.41
1:Q:794:ASN:ND2	1:Q:842:LEU:HB3	2.34	0.41
1:U:390:THR:HB	1:U:567:LEU:CD2	2.50	0.41
1:Q:117:ALA:O	1:Q:121:VAL:HG23	2.20	0.41
1:O:744:HIS:HA	1:O:819:SER:HB3	2.02	0.41
1:O:744:HIS:HA	1:O:819:SER:CB	2.50	0.41
1:U:548:ARG:NH1	8:U:1110:HOH:O	2.44	0.41
2:R:122:VAL:HG22	2:R:123:ALA:N	2.35	0.41
1:O:426:MET:HE3	1:O:622:ALA:CB	2.50	0.41
1:M:138:LEU:HA	1:M:167:THR:O	2.20	0.41
2:X:94:ILE:CG2	2:X:95:ASP:N	2.82	0.41
2:N:73:ASN:HB3	2:N:182:THR:HA	2.02	0.41
1:U:364:ILE:HD13	1:U:708:ARG:HG3	2.03	0.41
1:U:96:ARG:HD2	1:U:514:TYR:O	2.21	0.41
2:X:185:ARG:NH1	2:X:185:ARG:HB3	2.34	0.41
1:U:433:PHE:HA	1:U:434:PRO:HD3	1.91	0.41
2:P:230:ASN:OD1	2:P:232:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:744:HIS:HA	1:W:819:SER:CB	2.51	0.41
1:U:211:MET:HE1	2:V:231:PHE:HZ	1.85	0.41
2:T:3:GLN:NE2	2:T:161:PRO:HG3	2.36	0.41
2:T:203:ILE:HD12	2:T:203:ILE:N	2.35	0.41
1:S:272:HIS:N	1:S:272:HIS:ND1	2.69	0.41
1:W:426:MET:HE3	1:W:622:ALA:HB2	2.02	0.41
1:U:69:MET:HE1	1:U:747:GLY:HA2	2.02	0.41
2:X:154:TYR:HE1	7:X:805:SF4:S4	2.43	0.41
1:Q:138:LEU:HD12	1:Q:167:THR:O	2.21	0.41
1:W:744:HIS:HA	1:W:819:SER:HB3	2.03	0.41
1:S:526:SER:HB3	8:S:1024:HOH:O	2.19	0.41
1:S:174:ASP:OD1	1:S:175:SER:N	2.52	0.41
1:O:512:LYS:HE3	1:O:830:GLY:O	2.21	0.41
1:M:400:TYR:CE1	1:M:421:LYS:HD2	2.56	0.41
1:O:426:MET:HE1	1:O:618:GLN:HG2	2.01	0.41
2:P:122:VAL:HG22	2:P:123:ALA:N	2.35	0.41
1:U:69:MET:SD	1:U:747:GLY:HA2	2.60	0.41
1:O:452:ILE:N	1:O:453:PRO:CD	2.83	0.41
1:O:476:GLN:OE1	1:O:708:ARG:NH2	2.53	0.41
2:V:192:TYR:HA	2:V:196:LYS:HG2	2.02	0.41
1:M:451:LYS:HG3	1:M:461:PHE:CE2	2.55	0.41
1:O:707:HIS:HA	1:O:715:VAL:HG11	2.01	0.41
1:U:268:ILE:HG13	1:U:268:ILE:O	2.20	0.41
2:T:175:VAL:CG2	2:T:178:PRO:HG3	2.44	0.41
1:U:355:GLY:N	5:U:901:MGD:O2A	2.50	0.41
1:M:393:VAL:HA	1:M:394:PRO:HD3	1.76	0.41
2:X:68:CYS:HB2	2:X:113:VAL:HG21	2.03	0.41
2:P:1:MET:HG2	2:P:88:GLU:O	2.21	0.41
1:O:280:TYR:CE2	1:O:317:THR:HG22	2.56	0.41
2:N:46:MET:HE1	2:N:65:PRO:CA	2.51	0.41
2:R:106:LEU:HA	2:R:114:MET:HG3	2.03	0.41
2:P:51:ARG:O	2:P:61:ILE:HG13	2.21	0.41
2:T:117:ASN:HB2	2:T:124:GLN:OE1	2.20	0.41
1:O:165:GLY:HA3	1:O:166:PHE:CB	2.35	0.41
1:U:66:PHE:HD1	1:U:69:MET:HE3	1.81	0.41
2:X:15:ASP:HB2	2:X:63:TYR:CG	2.56	0.41
1:Q:144:HIS:NE2	5:Q:901:MGD:S13	2.93	0.41
2:V:229:THR:HB	2:V:233:GLY:CA	2.47	0.41
1:U:269:GLY:HA2	1:U:362:HIS:ND1	2.36	0.41
1:S:338:GLN:HG2	2:T:231:PHE:CZ	2.56	0.41
1:W:495:LYS:CD	1:W:514:TYR:OH	2.69	0.41
2:R:142:MET:HE2	2:R:146:ALA:C	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:U:11:SER:C	1:U:13:GLY:N	2.74	0.41
1:W:499:PRO:HB2	1:W:745:THR:HG21	2.02	0.41
2:X:210:PHE:O	2:X:233:GLY:HA2	2.20	0.41
1:U:296:ASN:HB3	1:U:657:PHE:CZ	2.55	0.41
2:X:120:GLU:O	2:X:121:ASN:C	2.58	0.41
1:S:498:GLY:N	1:S:499:PRO:HD3	2.35	0.41
1:W:433:PHE:HA	1:W:434:PRO:HD3	1.89	0.41
1:S:95:LEU:HD21	8:S:1407:HOH:O	2.20	0.41
1:M:35:ASP:OD1	1:M:55:ARG:HD3	2.20	0.41
1:O:387:TRP:CE2	1:O:389:THR:HA	2.56	0.41
1:Q:625:MET:N	1:Q:626:PRO:CD	2.84	0.41
2:N:4:TYR:CE2	2:N:158:LYS:HD2	2.56	0.41
1:S:558:SER:H	1:S:564:ASN:HD22	1.66	0.41
1:Q:753:TYR:CE1	2:R:28:GLU:HG3	2.56	0.41
2:P:23:CYS:HB3	2:P:39:MET:CE	2.51	0.41
1:Q:691:ILE:HG12	1:Q:711:MET:HB2	2.03	0.41
1:O:176:TRP:O	1:O:179:TRP:N	2.54	0.41
2:T:44:ARG:NH1	2:T:44:ARG:HG2	2.36	0.41
1:Q:722:LYS:HD3	8:Q:1467:HOH:O	2.20	0.41
1:Q:436:PRO:HG3	8:Q:1365:HOH:O	2.21	0.41
1:O:408:GLY:HA2	1:O:619:TYR:HE1	1.86	0.41
1:W:755:ASN:OD1	1:W:761:ARG:HD2	2.21	0.41
1:U:428:ASP:HB2	8:U:1141:HOH:O	2.21	0.41
1:W:128:ILE:CG2	1:W:136:ALA:HB3	2.51	0.41
1:U:550:ASP:HA	1:U:616:CYS:SG	2.61	0.41
1:U:451:LYS:HG3	1:U:461:PHE:CE2	2.56	0.41
1:M:162:ASN:ND2	1:M:437:SER:HB2	2.36	0.40
2:N:16:CYS:O	2:N:17:ASN:HB2	2.21	0.40
2:X:7:VAL:HG13	2:X:173:LEU:HD22	2.02	0.40
1:U:771:ILE:HG22	1:U:772:MET:N	2.35	0.40
1:U:454:GLU:CD	1:U:454:GLU:N	2.74	0.40
2:N:75:PRO:HD2	7:N:807:SF4:S4	2.61	0.40
1:W:734:MET:HB2	1:W:814:VAL:HG23	2.03	0.40
1:W:571:ARG:HB2	1:W:642:VAL:HB	2.02	0.40
1:U:791:ARG:NH2	8:U:1493:HOH:O	2.36	0.40
1:O:806:THR:OG1	1:O:807:GLU:N	2.54	0.40
1:U:25:ILE:HG13	1:U:580:ILE:HG21	2.02	0.40
1:M:656:TRP:CD2	1:M:663:LYS:HA	2.56	0.40
1:S:783:GLY:O	1:S:866:LYS:HD2	2.22	0.40
1:W:468:PHE:N	1:W:468:PHE:CD1	2.89	0.40
1:O:1:MET:H3	1:O:22:ASP:CG	2.23	0.40
1:S:845:ASP:N	1:S:845:ASP:OD2	2.48	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:192:ARG:NH2	1:O:562:PRO:HB2	2.37	0.40
2:T:106:LEU:HD23	2:T:114:MET:HG3	2.03	0.40
1:S:699:GLU:H	1:S:699:GLU:HG2	1.63	0.40
1:W:222:ASN:O	1:W:223:SER:OG	2.32	0.40
2:V:164:MET:O	2:V:168:VAL:HG23	2.22	0.40
1:O:104:ASP:N	1:O:105:PRO:HD3	2.36	0.40
1:Q:15:PRO:HD3	1:Q:554:PHE:CE1	2.57	0.40
1:U:730:TYR:HB3	1:U:862:VAL:CA	2.51	0.40
1:W:729:LYS:HD2	8:W:1038:HOH:O	2.19	0.40
1:W:361:SER:N	1:W:856:ALA:HB1	2.35	0.40
1:U:73:ASP:HB3	8:U:1532:HOH:O	2.20	0.40
2:X:35:TYR:O	2:X:36:THR:HB	2.21	0.40
1:Q:12:THR:HG23	8:Q:1235:HOH:O	2.21	0.40
2:P:139:ALA:N	2:P:140:PRO:CD	2.85	0.40
1:O:153:ARG:O	1:O:157:TYR:HB3	2.21	0.40
1:W:402:PRO:HB2	1:W:619:TYR:OH	2.22	0.40
1:W:401:PHE:HA	1:W:402:PRO:HD3	1.94	0.40
1:S:503:THR:HA	1:S:840:ASN:ND2	2.35	0.40
1:O:146:MET:HE2	1:O:545:ASN:H	1.86	0.40
1:W:155:SER:O	1:W:410:SER:HB3	2.20	0.40
2:X:26:GLU:HB2	2:X:144:ARG:HH11	1.84	0.40
1:M:724:SER:HA	1:M:725:PRO:HD3	1.99	0.40
1:U:454:GLU:H	1:U:454:GLU:CD	2.25	0.40
2:N:189:LYS:O	2:N:190:ASN:HB2	2.22	0.40
2:T:142:MET:HE1	8:T:882:HOH:O	2.21	0.40
1:S:541:PRO:HB2	1:S:586:SER:HA	2.03	0.40
1:S:540:LEU:HA	1:S:541:PRO:HD3	1.79	0.40
1:S:99:GLY:N	1:S:108:ASP:OD2	2.44	0.40
1:W:21:LYS:HB2	1:W:26:ILE:HD11	2.04	0.40
1:W:395:LEU:HD13	1:W:571:ARG:HG2	2.03	0.40
1:M:695:LEU:O	1:M:699:GLU:HG2	2.22	0.40
1:S:328:PRO:O	1:S:332:ILE:HG13	2.21	0.40
1:S:510:TYR:O	1:S:513:MET:HG2	2.21	0.40
1:O:767:TYR:HB3	1:O:769:TYR:CE1	2.56	0.40
1:Q:187:TRP:CH2	1:Q:196:PRO:HB3	2.56	0.40
1:Q:650:LYS:HG2	8:S:909:HOH:O	2.21	0.40
1:S:620:PHE:CZ	1:S:625:MET:HB3	2.56	0.40
1:M:280:TYR:OH	1:M:284:LYS:HE3	2.21	0.40
1:O:521:PHE:CE2	1:O:523:VAL:CG2	3.04	0.40
2:X:206:GLN:N	8:X:879:HOH:O	2.55	0.40
1:W:153:ARG:O	1:W:157:TYR:HB3	2.21	0.40
2:T:199:VAL:O	2:T:199:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:227:ALA:O	1:M:230:GLU:HG2	2.20	0.40
2:P:46:MET:CE	2:P:66:THR:H	2.34	0.40
1:Q:162:ASN:ND2	1:Q:437:SER:HB2	2.36	0.40
1:M:540:LEU:HA	1:M:541:PRO:HD3	1.74	0.40
2:T:166:LYS:HG2	2:T:170:GLU:OE2	2.22	0.40
1:O:553:GLU:HB3	1:O:556:ASN:HB3	2.04	0.40
2:N:23:CYS:O	2:N:26:GLU:N	2.55	0.40
1:W:775:ASN:HA	1:W:806:THR:O	2.21	0.40
1:U:211:MET:CE	2:V:231:PHE:CZ	3.05	0.40
1:U:211:MET:CE	2:V:231:PHE:HZ	2.34	0.40
1:Q:629:MET:HE1	1:Q:634:PHE:HA	2.03	0.40
2:R:167:LYS:HG3	2:R:171:GLU:OE2	2.20	0.40
1:S:152:TYR:CD2	1:S:154:HIS:HD2	2.40	0.40
1:U:656:TRP:CD2	1:U:663:LYS:HA	2.56	0.40
1:S:651:THR:HB	1:S:665:THR:HG22	2.04	0.40
1:W:427:PHE:HA	1:W:432:THR:HG23	2.04	0.40
2:T:7:VAL:HB	2:T:155:GLU:HB3	2.03	0.40
1:M:146:MET:HE1	1:M:544:THR:CB	2.46	0.40
2:P:73:ASN:O	2:P:75:PRO:HD3	2.21	0.40
1:M:737:PRO:HG3	5:M:901:MGD:H2'	2.03	0.40
2:P:21:MET:HE3	2:P:21:MET:N	2.36	0.40
1:Q:250:PRO:HD3	5:Q:901:MGD:C2	2.51	0.40
1:O:602:ILE:CG2	8:O:979:HOH:O	2.68	0.40
1:O:649:LYS:HE3	1:O:651:THR:HG22	2.04	0.40
2:T:58:ARG:NE	2:T:234:GLU:OE2	2.51	0.40
1:S:132:TYR:CD2	1:S:491:LYS:HG3	2.57	0.40
1:Q:553:GLU:HB3	1:Q:556:ASN:HB2	2.03	0.40
1:W:102:LYS:HE2	8:W:1393:HOH:O	2.21	0.40
1:S:274:LEU:O	1:S:278:ILE:HG13	2.22	0.40
1:U:252:MET:HB3	1:U:808:CYS:HB3	2.03	0.40
1:S:78:TYR:CD1	1:S:111:ARG:HG3	2.57	0.40
1:U:171:HIS:O	1:U:467:GLY:HA2	2.21	0.40
2:X:115:TYR:N	2:X:115:TYR:CD1	2.89	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	M	875/875 (100%)	814 (93%)	57 (6%)	4 (0%)	38	45
1	O	875/875 (100%)	819 (94%)	51 (6%)	5 (1%)	33	39
1	Q	875/875 (100%)	815 (93%)	52 (6%)	8 (1%)	25	27
1	S	875/875 (100%)	815 (93%)	52 (6%)	8 (1%)	25	27
1	U	875/875 (100%)	808 (92%)	63 (7%)	4 (0%)	38	45
1	W	875/875 (100%)	803 (92%)	65 (7%)	7 (1%)	27	31
2	N	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	43	52
2	P	272/274 (99%)	254 (93%)	17 (6%)	1 (0%)	43	52
2	R	272/274 (99%)	259 (95%)	12 (4%)	1 (0%)	43	52
2	T	272/274 (99%)	251 (92%)	20 (7%)	1 (0%)	43	52
2	V	272/274 (99%)	257 (94%)	13 (5%)	2 (1%)	30	34
2	X	272/274 (99%)	239 (88%)	30 (11%)	3 (1%)	21	21
All	All	6882/6894 (100%)	6392 (93%)	445 (6%)	45 (1%)	30	34

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	141	PRO
1	O	177	GLU
1	Q	177	GLU
1	S	177	GLU
1	U	177	GLU
1	W	177	GLU
1	M	177	GLU
1	O	225	ILE
1	Q	225	ILE
1	S	141	PRO
1	U	225	ILE
1	W	141	PRO
1	M	141	PRO
2	P	67	PRO
1	Q	141	PRO
1	Q	228	GLY
1	S	35	ASP
1	U	141	PRO
1	U	858	ASN

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Mol	Chain	Res	Type
1	W	225	ILE
1	M	225	ILE
1	M	858	ASN
2	N	67	PRO
1	S	507	THR
1	S	555	ALA
1	S	858	ASN
1	W	35	ASP
2	X	81	ASN
2	X	221	GLY
1	O	858	ASN
1	Q	253	ASN
1	Q	421	LYS
2	R	67	PRO
1	S	225	ILE
2	V	19	CYS
1	W	786	ASN
1	W	808	CYS
1	S	228	GLY
2	V	221	GLY
2	X	129	CYS
1	Q	182	GLY
1	Q	531	GLY
1	W	228	GLY
1	O	394	PRO
2	T	67	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	731/729 (100%)	715 (98%)	16 (2%)	64	81
1	O	731/729 (100%)	719 (98%)	12 (2%)	75	87
1	Q	731/729 (100%)	715 (98%)	16 (2%)	64	81
1	S	731/729 (100%)	715 (98%)	16 (2%)	64	81
1	U	731/729 (100%)	713 (98%)	18 (2%)	60	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	731/729 (100%)	717 (98%)	14 (2%)	69	84
2	N	235/235 (100%)	221 (94%)	14 (6%)	27	32
2	P	235/235 (100%)	226 (96%)	9 (4%)	44	59
2	R	235/235 (100%)	224 (95%)	11 (5%)	36	46
2	T	235/235 (100%)	222 (94%)	13 (6%)	30	36
2	V	235/235 (100%)	223 (95%)	12 (5%)	33	41
2	X	235/235 (100%)	221 (94%)	14 (6%)	27	32
All	All	5796/5784 (100%)	5631 (97%)	165 (3%)	57	73

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	78	TYR
1	M	142	SER
1	M	187	TRP
1	M	272	HIS
1	M	373	LEU
1	M	426	MET
1	M	462	GLN
1	M	493	PHE
1	M	560[A]	TYR
1	M	560[B]	TYR
1	M	564	ASN
1	M	605	MET
1	M	719	GLU
1	M	743	MET
1	M	786	ASN
1	M	818	GLU
2	N	13	CYS
2	N	19	CYS
2	N	21	MET
2	N	24	MET
2	N	29	LEU
2	N	57	PRO
2	N	60	ASP
2	N	71	CYS
2	N	109	CYS
2	N	125	LYS
2	N	129	CYS
2	N	145	CYS

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Mol	Chain	Res	Type
2	N	149	CYS
2	N	157	LEU
1	O	78	TYR
1	O	142	SER
1	O	187	TRP
1	O	426	MET
1	O	462	GLN
1	O	499	PRO
1	O	560[A]	TYR
1	O	560[B]	TYR
1	O	564	ASN
1	O	605	MET
1	O	743	MET
1	O	786	ASN
2	P	13	CYS
2	P	19	CYS
2	P	21	MET
2	P	71	CYS
2	P	73	ASN
2	P	109	CYS
2	P	125	LYS
2	P	145	CYS
2	P	149	CYS
1	Q	78	TYR
1	Q	100	LEU
1	Q	142	SER
1	Q	187	TRP
1	Q	373	LEU
1	Q	462	GLN
1	Q	499	PRO
1	Q	560[A]	TYR
1	Q	560[B]	TYR
1	Q	564	ASN
1	Q	605	MET
1	Q	678	ARG
1	Q	726	LEU
1	Q	743	MET
1	Q	786	ASN
1	Q	818	GLU
2	R	13	CYS
2	R	19	CYS
2	R	21	MET

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Mol	Chain	Res	Type
2	R	71	CYS
2	R	76	CYS
2	R	109	CYS
2	R	125	LYS
2	R	129	CYS
2	R	145	CYS
2	R	149	CYS
2	R	157	LEU
1	S	17	PHE
1	S	78	TYR
1	S	142	SER
1	S	187	TRP
1	S	373	LEU
1	S	499	PRO
1	S	554	PHE
1	S	560[A]	TYR
1	S	560[B]	TYR
1	S	564	ASN
1	S	605	MET
1	S	678	ARG
1	S	719	GLU
1	S	726	LEU
1	S	743	MET
1	S	786	ASN
2	T	13	CYS
2	T	19	CYS
2	T	21	MET
2	T	24	MET
2	T	57	PRO
2	T	71	CYS
2	T	73	ASN
2	T	109	CYS
2	T	125	LYS
2	T	129	CYS
2	T	145	CYS
2	T	149	CYS
2	T	157	LEU
1	U	17	PHE
1	U	55	ARG
1	U	108	ASP
1	U	152	TYR
1	U	187	TRP

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Mol	Chain	Res	Type
1	U	358	CYS
1	U	426	MET
1	U	462	GLN
1	U	499	PRO
1	U	560[A]	TYR
1	U	560[B]	TYR
1	U	564	ASN
1	U	605	MET
1	U	719	GLU
1	U	726	LEU
1	U	743	MET
1	U	786	ASN
1	U	818	GLU
2	V	13	CYS
2	V	19	CYS
2	V	21	MET
2	V	24	MET
2	V	59	ASN
2	V	71	CYS
2	V	73	ASN
2	V	109	CYS
2	V	125	LYS
2	V	129	CYS
2	V	145	CYS
2	V	149	CYS
1	W	17	PHE
1	W	55	ARG
1	W	187	TRP
1	W	261	ASP
1	W	272	HIS
1	W	462	GLN
1	W	493	PHE
1	W	499	PRO
1	W	560[A]	TYR
1	W	560[B]	TYR
1	W	564	ASN
1	W	605	MET
1	W	743	MET
1	W	786	ASN
2	X	13	CYS
2	X	17	ASN
2	X	19	CYS

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Mol	Chain	Res	Type
2	X	21	MET
2	X	29	LEU
2	X	71	CYS
2	X	73	ASN
2	X	109	CYS
2	X	125	LYS
2	X	129	CYS
2	X	145	CYS
2	X	149	CYS
2	X	157	LEU
2	X	252	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	154	HIS
1	M	162	ASN
1	M	222	ASN
1	M	440	ASN
1	M	462	GLN
1	M	478	HIS
1	M	525	GLN
1	M	564	ASN
1	M	618	GLN
1	M	645	ASN
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
2	N	81	ASN
1	O	154	HIS
1	O	162	ASN
1	O	171	HIS
1	O	222	ASN
1	O	478	HIS
1	O	525	GLN

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Mol	Chain	Res	Type
1	O	564	ASN
1	O	618	GLN
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
2	P	81	ASN
1	Q	154	HIS
1	Q	162	ASN
1	Q	478	HIS
1	Q	525	GLN
1	Q	564	ASN
1	Q	618	GLN
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
2	R	81	ASN
1	S	154	HIS
1	S	162	ASN
1	S	462	GLN
1	S	478	HIS
1	S	525	GLN
1	S	564	ASN
1	S	618	GLN
1	S	697	ASN
1	S	701	GLN
1	S	707	HIS
1	S	721	GLN
1	S	786	ASN
2	T	3	GLN
2	T	27	HIS

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

### 5.3.3 RNA ⓘ

There are no RNA chains 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 54 ligands modelled in this entry, 18 are monoatomic - leaving 36 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	$\# Z  > 2$
5	MGD	M	900	6	52,52,52	2.12	16 (30%)	72,81,81	3.29	19 (26%)
5	MGD	M	901	6	52,52,52	2.19	18 (34%)	72,81,81	2.96	16 (22%)
3	ACT	M	903	6	1,3,3	3.29	1 (100%)	0,3,3	0.00	-
7	SF4	N	805	2	12,12,12	10.14	9 (75%)	0,24,24	0.00	-
7	SF4	N	806	2	12,12,12	10.97	9 (75%)	0,24,24	0.00	-
7	SF4	N	807	2	12,12,12	9.27	10 (83%)	0,24,24	0.00	-
5	MGD	O	900	6	52,52,52	2.23	19 (36%)	72,81,81	2.97	14 (19%)
5	MGD	O	901	6	52,52,52	2.22	18 (34%)	72,81,81	3.18	15 (20%)
3	ACT	O	903	6	1,3,3	3.54	1 (100%)	0,3,3	0.00	-
7	SF4	P	805	2	12,12,12	10.64	9 (75%)	0,24,24	0.00	-
7	SF4	P	806	2	12,12,12	9.85	10 (83%)	0,24,24	0.00	-
7	SF4	P	807	2	12,12,12	8.80	9 (75%)	0,24,24	0.00	-
5	MGD	Q	900	6	52,52,52	2.15	19 (36%)	72,81,81	2.70	17 (23%)
5	MGD	Q	901	6	52,52,52	2.19	19 (36%)	72,81,81	2.94	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ACT	Q	903	6	1,3,3	2.97	1 (100%)	0,3,3	0.00	-
7	SF4	R	805	2	12,12,12	9.92	10 (83%)	0,24,24	0.00	-
7	SF4	R	806	2	12,12,12	11.23	9 (75%)	0,24,24	0.00	-
7	SF4	R	807	2	12,12,12	8.96	9 (75%)	0,24,24	0.00	-
5	MGD	S	900	6	52,52,52	2.10	17 (32%)	72,81,81	2.89	16 (22%)
5	MGD	S	901	6	52,52,52	2.23	18 (34%)	72,81,81	2.88	13 (18%)
3	ACT	S	903	6	1,3,3	3.83	1 (100%)	0,3,3	0.00	-
7	SF4	T	805	2	12,12,12	10.88	10 (83%)	0,24,24	0.00	-
7	SF4	T	806	2	12,12,12	10.50	11 (91%)	0,24,24	0.00	-
7	SF4	T	807	2	12,12,12	8.85	9 (75%)	0,24,24	0.00	-
5	MGD	U	900	6	52,52,52	2.26	22 (42%)	72,81,81	2.66	18 (25%)
5	MGD	U	901	6	52,52,52	2.15	16 (30%)	72,81,81	3.10	12 (16%)
3	ACT	U	903	6	1,3,3	3.67	1 (100%)	0,3,3	0.00	-
7	SF4	V	805	2	12,12,12	10.03	9 (75%)	0,24,24	0.00	-
7	SF4	V	806	2	12,12,12	10.25	9 (75%)	0,24,24	0.00	-
7	SF4	V	807	2	12,12,12	8.60	9 (75%)	0,24,24	0.00	-
5	MGD	W	900	6	52,52,52	2.29	20 (38%)	72,81,81	2.56	16 (22%)
5	MGD	W	901	6	52,52,52	2.18	17 (32%)	72,81,81	2.87	15 (20%)
3	ACT	W	903	6	1,3,3	4.07	1 (100%)	0,3,3	0.00	-
7	SF4	X	805	2	12,12,12	10.33	9 (75%)	0,24,24	0.00	-
7	SF4	X	806	2	12,12,12	10.58	11 (91%)	0,24,24	0.00	-
7	SF4	X	807	2	12,12,12	9.00	10 (83%)	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
5	MGD	M	900	6	-	0/22/66/66	0/1/6/6
5	MGD	M	901	6	-	0/22/66/66	0/1/6/6
3	ACT	M	903	6	-	0/0/0/0	0/0/0/0
7	SF4	N	805	2	-	0/0/48/48	0/0/5/5
7	SF4	N	806	2	-	0/0/48/48	0/0/5/5
7	SF4	N	807	2	-	0/0/48/48	0/0/5/5
5	MGD	O	900	6	-	0/22/66/66	0/1/6/6
5	MGD	O	901	6	-	0/22/66/66	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACT	O	903	6	-	0/0/0/0	0/0/0/0
7	SF4	P	805	2	-	0/0/48/48	0/0/5/5
7	SF4	P	806	2	-	0/0/48/48	0/0/5/5
7	SF4	P	807	2	-	0/0/48/48	0/0/5/5
5	MGD	Q	900	6	-	0/22/66/66	0/1/6/6
5	MGD	Q	901	6	-	0/22/66/66	0/1/6/6
3	ACT	Q	903	6	-	0/0/0/0	0/0/0/0
7	SF4	R	805	2	-	0/0/48/48	0/0/5/5
7	SF4	R	806	2	-	0/0/48/48	0/0/5/5
7	SF4	R	807	2	-	0/0/48/48	0/0/5/5
5	MGD	S	900	6	-	0/22/66/66	0/1/6/6
5	MGD	S	901	6	-	0/22/66/66	0/1/6/6
3	ACT	S	903	6	-	0/0/0/0	0/0/0/0
7	SF4	T	805	2	-	0/0/48/48	0/0/5/5
7	SF4	T	806	2	-	0/0/48/48	0/0/5/5
7	SF4	T	807	2	-	0/0/48/48	0/0/5/5
5	MGD	U	900	6	-	0/22/66/66	0/1/6/6
5	MGD	U	901	6	-	0/22/66/66	0/1/6/6
3	ACT	U	903	6	-	0/0/0/0	0/0/0/0
7	SF4	V	805	2	-	0/0/48/48	0/0/5/5
7	SF4	V	806	2	-	0/0/48/48	0/0/5/5
7	SF4	V	807	2	-	0/0/48/48	0/0/5/5
5	MGD	W	900	6	-	0/22/66/66	0/1/6/6
5	MGD	W	901	6	-	0/22/66/66	0/1/6/6
3	ACT	W	903	6	-	0/0/0/0	0/0/0/0
7	SF4	X	805	2	-	0/0/48/48	0/0/5/5
7	SF4	X	806	2	-	0/0/48/48	0/0/5/5
7	SF4	X	807	2	-	0/0/48/48	0/0/5/5

All (396) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	805	SF4	S1-FE4	-20.09	2.19	2.33
7	T	805	SF4	S1-FE4	-19.93	2.19	2.33
7	N	805	SF4	S1-FE4	-19.79	2.19	2.33
7	X	806	SF4	S1-FE4	-19.46	2.20	2.33
7	P	805	SF4	S1-FE4	-19.39	2.20	2.33
7	R	805	SF4	S1-FE4	-19.35	2.20	2.33
7	T	806	SF4	S1-FE4	-18.96	2.20	2.33
7	N	806	SF4	S1-FE4	-18.68	2.20	2.33
7	V	806	SF4	S1-FE4	-18.62	2.20	2.33
7	V	805	SF4	S1-FE4	-18.01	2.21	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	807	SF4	S1-FE4	-18.00	2.21	2.33
7	P	806	SF4	S1-FE4	-18.00	2.21	2.33
7	R	806	SF4	S1-FE4	-17.68	2.21	2.33
7	N	805	SF4	S4-FE1	-17.42	2.21	2.33
7	R	807	SF4	S1-FE4	-17.33	2.21	2.33
7	X	807	SF4	S1-FE4	-17.31	2.21	2.33
7	T	805	SF4	S4-FE1	-17.22	2.21	2.33
7	T	805	SF4	S3-FE1	-16.99	2.21	2.33
7	R	805	SF4	S4-FE1	-16.95	2.21	2.33
7	P	807	SF4	S1-FE4	-16.76	2.22	2.33
7	P	805	SF4	S3-FE1	-16.58	2.22	2.33
7	V	805	SF4	S3-FE1	-16.44	2.22	2.33
7	V	807	SF4	S1-FE4	-16.36	2.22	2.33
7	T	807	SF4	S1-FE4	-16.33	2.22	2.33
7	P	805	SF4	S4-FE1	-16.26	2.22	2.33
7	R	806	SF4	S3-FE1	-15.84	2.22	2.33
7	T	807	SF4	S3-FE4	-15.38	2.22	2.33
7	X	805	SF4	S3-FE1	-15.19	2.23	2.33
7	T	806	SF4	S3-FE1	-15.14	2.23	2.33
7	R	806	SF4	S2-FE1	-14.92	2.23	2.33
7	N	806	SF4	S1-FE3	-14.91	2.23	2.33
7	R	805	SF4	S3-FE1	-14.86	2.23	2.33
7	V	806	SF4	S3-FE1	-14.84	2.23	2.33
7	V	805	SF4	S4-FE1	-14.81	2.23	2.33
7	X	805	SF4	S4-FE1	-14.61	2.23	2.33
7	N	807	SF4	S3-FE4	-14.47	2.23	2.33
7	X	807	SF4	S3-FE4	-14.41	2.23	2.33
7	N	806	SF4	S3-FE1	-14.33	2.23	2.33
7	R	806	SF4	S1-FE3	-14.16	2.23	2.33
7	N	806	SF4	S2-FE1	-13.89	2.23	2.33
7	T	805	SF4	S2-FE1	-13.82	2.24	2.33
7	T	806	SF4	S2-FE4	-13.80	2.24	2.33
7	P	807	SF4	S3-FE4	-13.78	2.24	2.33
7	V	807	SF4	S3-FE4	-13.59	2.24	2.33
7	X	806	SF4	S3-FE1	-13.52	2.24	2.33
7	X	806	SF4	S2-FE4	-13.51	2.24	2.33
7	P	806	SF4	S3-FE1	-13.41	2.24	2.33
7	N	805	SF4	S2-FE1	-13.30	2.24	2.33
7	R	806	SF4	S4-FE1	-13.26	2.24	2.33
7	X	806	SF4	S3-FE4	-13.16	2.24	2.33
7	P	805	SF4	S2-FE1	-13.13	2.24	2.33
7	R	805	SF4	S2-FE1	-13.12	2.24	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	805	SF4	S2-FE1	-13.04	2.24	2.33
7	N	806	SF4	S2-FE4	-12.98	2.24	2.33
7	T	806	SF4	S1-FE3	-12.94	2.24	2.33
7	N	805	SF4	S3-FE1	-12.92	2.24	2.33
7	R	807	SF4	S3-FE1	-12.71	2.24	2.33
7	X	806	SF4	S4-FE1	-12.68	2.24	2.33
7	N	806	SF4	S4-FE1	-12.68	2.24	2.33
7	V	806	SF4	S2-FE4	-12.55	2.24	2.33
7	N	807	SF4	S3-FE1	-12.44	2.24	2.33
7	R	807	SF4	S3-FE4	-12.42	2.24	2.33
7	R	806	SF4	S2-FE4	-12.40	2.24	2.33
7	R	806	SF4	S3-FE4	-12.32	2.25	2.33
7	P	807	SF4	S3-FE1	-12.10	2.25	2.33
7	X	805	SF4	S2-FE1	-11.76	2.25	2.33
7	T	807	SF4	S3-FE1	-11.62	2.25	2.33
7	V	806	SF4	S1-FE3	-11.58	2.25	2.33
7	P	806	SF4	S4-FE1	-11.47	2.25	2.33
7	P	806	SF4	S2-FE4	-11.44	2.25	2.33
7	P	807	SF4	S4-FE1	-11.40	2.25	2.33
7	X	807	SF4	S4-FE1	-11.40	2.25	2.33
7	T	806	SF4	S3-FE4	-11.38	2.25	2.33
7	V	806	SF4	S4-FE1	-11.35	2.25	2.33
7	V	806	SF4	S3-FE4	-11.27	2.25	2.33
7	R	807	SF4	S4-FE1	-11.23	2.25	2.33
7	P	806	SF4	S3-FE4	-11.21	2.25	2.33
7	P	806	SF4	S1-FE3	-11.19	2.25	2.33
7	V	807	SF4	S3-FE1	-11.17	2.25	2.33
7	X	806	SF4	S1-FE3	-10.76	2.26	2.33
7	X	807	SF4	S3-FE1	-10.67	2.26	2.33
7	N	807	SF4	S4-FE1	-10.63	2.26	2.33
7	N	806	SF4	S3-FE4	-10.49	2.26	2.33
7	T	806	SF4	S4-FE1	-10.25	2.26	2.33
7	R	807	SF4	S2-FE1	-10.19	2.26	2.33
7	V	807	SF4	S4-FE1	-10.15	2.26	2.33
7	N	807	SF4	S2-FE1	-10.01	2.26	2.33
7	V	806	SF4	S2-FE1	-9.56	2.26	2.33
7	P	806	SF4	S2-FE1	-9.37	2.26	2.33
7	T	807	SF4	S2-FE4	-9.31	2.27	2.33
7	T	806	SF4	S2-FE1	-9.17	2.27	2.33
7	X	805	SF4	S3-FE4	-9.08	2.27	2.33
7	X	807	SF4	S2-FE4	-9.04	2.27	2.33
7	X	805	SF4	S2-FE4	-8.86	2.27	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	805	SF4	S1-FE3	-8.82	2.27	2.33
7	N	805	SF4	S3-FE4	-8.77	2.27	2.33
7	X	805	SF4	S1-FE3	-8.60	2.27	2.33
7	V	807	SF4	S2-FE1	-8.58	2.27	2.33
7	P	805	SF4	S2-FE4	-8.50	2.27	2.33
7	T	805	SF4	S2-FE4	-8.31	2.27	2.33
7	T	805	SF4	S3-FE4	-8.29	2.27	2.33
7	T	807	SF4	S4-FE1	-8.29	2.27	2.33
7	V	805	SF4	S2-FE4	-8.25	2.27	2.33
7	T	807	SF4	S2-FE1	-8.12	2.27	2.33
7	P	805	SF4	S3-FE4	-8.07	2.27	2.33
7	P	807	SF4	S2-FE1	-7.96	2.27	2.33
7	V	807	SF4	S2-FE4	-7.86	2.28	2.33
7	N	807	SF4	S4-FE3	-7.42	2.28	2.33
7	P	807	SF4	S2-FE4	-7.28	2.28	2.33
7	V	805	SF4	S1-FE3	-7.11	2.28	2.33
7	T	805	SF4	S1-FE3	-7.07	2.28	2.33
7	R	807	SF4	S4-FE3	-7.02	2.28	2.33
7	X	807	SF4	S2-FE1	-6.99	2.28	2.33
7	V	805	SF4	S4-FE3	-6.98	2.28	2.33
7	N	807	SF4	S2-FE4	-6.97	2.28	2.33
7	X	807	SF4	S4-FE3	-6.97	2.28	2.33
7	P	805	SF4	S4-FE3	-6.85	2.28	2.33
7	R	805	SF4	S3-FE4	-6.75	2.28	2.33
7	X	806	SF4	S2-FE1	-6.66	2.28	2.33
7	T	807	SF4	S4-FE3	-6.66	2.28	2.33
7	V	805	SF4	S3-FE4	-6.57	2.28	2.33
7	N	805	SF4	S1-FE3	-6.53	2.28	2.33
7	P	807	SF4	S4-FE3	-6.35	2.29	2.33
7	R	807	SF4	S2-FE4	-6.35	2.29	2.33
7	X	806	SF4	S1-FE2	6.22	2.37	2.33
5	U	901	MGD	C14-N15	6.18	1.54	1.45
7	X	806	SF4	S4-FE3	-6.17	2.29	2.33
5	S	901	MGD	C14-N15	6.10	1.54	1.45
7	V	807	SF4	S4-FE3	-6.09	2.29	2.33
7	R	805	SF4	S1-FE3	-6.08	2.29	2.33
7	R	806	SF4	S4-FE3	-6.07	2.29	2.33
5	Q	901	MGD	C14-N15	6.01	1.54	1.45
5	W	901	MGD	O11-C11	5.91	1.52	1.43
7	T	805	SF4	S4-FE3	-5.87	2.29	2.33
7	P	806	SF4	S4-FE3	-5.80	2.29	2.33
5	M	901	MGD	C14-N15	5.71	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	901	MGD	C14-N15	5.71	1.53	1.45
7	N	805	SF4	S4-FE3	-5.68	2.29	2.33
7	V	806	SF4	S4-FE3	-5.65	2.29	2.33
5	O	900	MGD	O11-C11	5.57	1.52	1.43
5	W	900	MGD	C14-N15	5.56	1.53	1.45
7	T	806	SF4	S4-FE3	-5.50	2.29	2.33
7	N	805	SF4	S2-FE4	-5.39	2.29	2.33
5	W	901	MGD	C14-N15	5.32	1.53	1.45
7	X	805	SF4	S4-FE3	-5.27	2.29	2.33
5	Q	900	MGD	C14-N15	5.23	1.53	1.45
5	W	900	MGD	O11-C11	5.20	1.51	1.43
7	X	805	SF4	S1-FE2	5.19	2.36	2.33
5	U	900	MGD	O11-C11	5.17	1.51	1.43
5	S	900	MGD	O11-C11	5.15	1.51	1.43
7	N	806	SF4	S4-FE3	-5.13	2.29	2.33
5	O	900	MGD	C14-N15	5.13	1.53	1.45
5	O	901	MGD	O11-C11	5.11	1.51	1.43
7	T	807	SF4	S1-FE3	-5.06	2.29	2.33
7	R	805	SF4	S2-FE4	-5.04	2.29	2.33
5	Q	900	MGD	O11-C11	4.94	1.51	1.43
5	U	900	MGD	C14-N15	4.93	1.52	1.45
5	M	901	MGD	C17-N18	4.86	1.45	1.37
5	M	900	MGD	C17-N18	4.76	1.45	1.37
5	Q	901	MGD	O11-C11	4.69	1.50	1.43
7	P	806	SF4	S1-FE2	4.61	2.36	2.33
5	Q	901	MGD	C17-N18	4.56	1.44	1.37
5	Q	900	MGD	C17-N18	4.56	1.44	1.37
5	S	901	MGD	O11-C11	4.52	1.50	1.43
5	U	900	MGD	C17-N18	4.52	1.44	1.37
5	U	901	MGD	O11-C11	4.51	1.50	1.43
5	M	901	MGD	O11-C11	4.45	1.50	1.43
5	M	900	MGD	O11-C11	4.43	1.50	1.43
7	V	807	SF4	S1-FE3	-4.43	2.30	2.33
5	M	900	MGD	C14-N15	4.42	1.52	1.45
5	S	901	MGD	C17-N18	4.38	1.44	1.37
7	V	806	SF4	S1-FE2	4.38	2.36	2.33
5	S	900	MGD	C14-N15	4.37	1.51	1.45
5	W	900	MGD	C17-N18	4.36	1.44	1.37
5	O	900	MGD	C17-N18	4.36	1.44	1.37
5	U	901	MGD	C17-N18	4.36	1.44	1.37
7	R	807	SF4	S1-FE3	-4.30	2.30	2.33
5	S	900	MGD	C17-N18	4.29	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	X	807	SF4	S1-FE3	-4.26	2.30	2.33
7	X	806	SF4	S3-FE2	-4.21	2.30	2.33
5	O	901	MGD	C14-C13	4.14	1.56	1.50
5	O	901	MGD	C17-N18	4.14	1.44	1.37
5	M	901	MGD	C14-C13	4.10	1.56	1.50
3	W	903	ACT	CH3-C	4.07	1.54	1.48
5	W	901	MGD	O11-C23	4.07	1.49	1.44
5	M	900	MGD	C6-N1	3.95	1.43	1.37
7	N	807	SF4	S1-FE3	-3.96	2.30	2.33
5	Q	900	MGD	C8-N9	3.95	1.42	1.36
7	P	807	SF4	S1-FE3	-3.94	2.30	2.33
5	S	901	MGD	C6-N1	3.94	1.43	1.37
5	S	901	MGD	C14-C13	3.93	1.56	1.50
5	O	901	MGD	C6-N1	3.91	1.43	1.37
5	U	901	MGD	C6-N1	3.86	1.43	1.37
5	Q	901	MGD	C14-C13	3.85	1.56	1.50
7	X	807	SF4	S3-FE2	-3.83	2.30	2.33
3	S	903	ACT	CH3-C	3.83	1.54	1.48
5	W	900	MGD	C21-N22	3.80	1.42	1.35
5	O	900	MGD	C6-N1	3.80	1.43	1.37
5	S	901	MGD	O11-C23	3.79	1.49	1.44
5	W	900	MGD	C2-N2	3.77	1.38	1.32
5	W	901	MGD	C17-N18	3.77	1.43	1.37
5	Q	900	MGD	C2-N2	3.76	1.38	1.32
5	O	901	MGD	O11-C23	3.75	1.49	1.44
5	S	900	MGD	C2-N2	3.74	1.38	1.32
7	T	806	SF4	S1-FE2	3.73	2.35	2.33
5	M	900	MGD	C2-N2	3.68	1.38	1.32
3	U	903	ACT	CH3-C	3.67	1.54	1.48
5	U	900	MGD	C2-N2	3.64	1.38	1.32
5	O	900	MGD	C2-N1	3.60	1.42	1.36
5	M	900	MGD	C2-N1	3.56	1.42	1.36
5	W	900	MGD	C8-N9	3.56	1.41	1.36
3	O	903	ACT	CH3-C	3.54	1.53	1.48
5	Q	900	MGD	C6-N1	3.54	1.43	1.37
5	S	901	MGD	C21-N20	3.54	1.41	1.34
5	Q	901	MGD	C6-N1	3.53	1.43	1.37
5	M	900	MGD	C19-N19	3.50	1.37	1.32
5	U	900	MGD	C8-N9	3.50	1.41	1.36
5	S	901	MGD	C2-N2	3.49	1.37	1.32
5	W	901	MGD	C6-N1	3.48	1.43	1.37
5	W	901	MGD	C2-N2	3.48	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	901	MGD	C2-N1	3.48	1.42	1.36
5	U	900	MGD	C21-N20	3.48	1.41	1.34
5	O	900	MGD	C2-N2	3.46	1.37	1.32
5	W	900	MGD	C21-N20	3.46	1.41	1.34
5	Q	901	MGD	C2-N2	3.45	1.37	1.32
5	U	901	MGD	O11-C23	3.45	1.48	1.44
7	T	805	SF4	S4-FE2	3.43	2.35	2.33
5	M	901	MGD	C21-N20	3.42	1.41	1.34
5	S	900	MGD	C2-N1	3.41	1.42	1.36
5	U	900	MGD	C6-N1	3.41	1.42	1.37
5	M	901	MGD	PA-O3B	3.40	1.66	1.59
5	U	901	MGD	C2-N1	3.39	1.42	1.36
5	M	900	MGD	C8-N9	3.37	1.41	1.36
5	S	900	MGD	C8-N9	3.36	1.41	1.36
7	T	805	SF4	S3-FE2	-3.36	2.31	2.33
5	U	901	MGD	C14-C13	3.36	1.55	1.50
5	S	900	MGD	O4'-C1'	3.35	1.46	1.41
5	W	901	MGD	C2-N1	3.34	1.42	1.36
5	U	901	MGD	C21-N22	3.33	1.41	1.35
5	M	900	MGD	O4'-C1'	3.32	1.46	1.41
5	M	901	MGD	C6-N1	3.32	1.42	1.37
5	S	900	MGD	C6-N1	3.32	1.42	1.37
5	U	901	MGD	C2-N2	3.31	1.37	1.32
5	Q	901	MGD	C8-N9	3.30	1.41	1.36
5	Q	901	MGD	O11-C23	3.30	1.48	1.44
3	M	903	ACT	CH3-C	3.29	1.53	1.48
5	W	901	MGD	C21-N22	3.29	1.41	1.35
5	U	900	MGD	C6-C5	3.29	1.46	1.41
5	M	901	MGD	C19-N19	3.26	1.37	1.32
5	Q	901	MGD	C21-N20	3.26	1.41	1.34
5	O	901	MGD	C21-N22	3.26	1.41	1.35
5	O	900	MGD	O4'-C1'	3.25	1.46	1.41
5	U	900	MGD	C2-N1	3.25	1.41	1.36
7	X	806	SF4	S2-FE3	-3.23	2.31	2.33
5	U	900	MGD	C4-N9	3.21	1.42	1.37
5	S	901	MGD	C21-N22	3.21	1.41	1.35
5	Q	900	MGD	O4'-C1'	3.19	1.46	1.41
5	O	900	MGD	C8-N9	3.18	1.41	1.36
5	W	900	MGD	C6-C5	3.18	1.46	1.41
5	Q	901	MGD	C6-C5	3.17	1.46	1.41
5	W	900	MGD	C6-N1	3.15	1.42	1.37
5	O	901	MGD	C6-C5	3.15	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	900	MGD	C19-N19	3.14	1.37	1.32
5	W	900	MGD	C4-N9	3.14	1.42	1.37
5	Q	900	MGD	C16-N15	3.13	1.48	1.38
5	O	901	MGD	C2-N2	3.13	1.37	1.32
5	M	901	MGD	C2-N2	3.12	1.37	1.32
5	O	900	MGD	C21-N22	3.12	1.41	1.35
5	W	901	MGD	C8-N9	3.12	1.41	1.36
5	M	901	MGD	C16-N15	3.11	1.48	1.38
5	W	900	MGD	O4'-C1'	3.10	1.46	1.41
5	M	900	MGD	C21-N20	3.10	1.40	1.34
5	Q	901	MGD	C16-N15	3.09	1.48	1.38
5	Q	900	MGD	C2-N1	3.09	1.41	1.36
5	U	900	MGD	C21-N22	3.09	1.40	1.35
7	N	805	SF4	S4-FE2	3.09	2.35	2.33
5	S	900	MGD	C21-N20	3.08	1.40	1.34
5	Q	901	MGD	C19-N19	3.07	1.37	1.32
5	M	901	MGD	O11-C23	3.06	1.48	1.44
5	S	901	MGD	C6-C5	3.05	1.46	1.41
5	U	900	MGD	O4'-C1'	3.05	1.46	1.41
5	O	900	MGD	C21-N20	3.05	1.40	1.34
5	S	901	MGD	C19-N19	3.03	1.37	1.32
5	W	901	MGD	C14-C13	3.01	1.55	1.50
5	Q	900	MGD	C19-N19	3.01	1.37	1.32
5	U	901	MGD	C21-N20	3.01	1.40	1.34
5	U	901	MGD	C23-C14	3.00	1.59	1.53
7	V	805	SF4	S2-FE3	-3.00	2.31	2.33
5	O	901	MGD	C21-N20	2.99	1.40	1.34
5	Q	901	MGD	C2-N1	2.98	1.41	1.36
3	Q	903	ACT	CH3-C	2.97	1.53	1.48
5	O	901	MGD	C2-N1	2.97	1.41	1.36
5	U	900	MGD	C19-N19	2.97	1.37	1.32
5	W	900	MGD	C19-N19	2.96	1.37	1.32
5	O	901	MGD	C16-N15	2.95	1.48	1.38
5	M	900	MGD	C21-N22	2.95	1.40	1.35
5	S	900	MGD	C16-N15	2.94	1.48	1.38
5	Q	900	MGD	C21-N22	2.93	1.40	1.35
5	Q	900	MGD	C21-N20	2.93	1.40	1.34
5	M	900	MGD	PA-O3B	2.91	1.65	1.59
7	R	805	SF4	S4-FE3	-2.90	2.31	2.33
5	O	901	MGD	C8-N9	2.90	1.40	1.36
5	Q	901	MGD	C21-N22	2.88	1.40	1.35
5	M	901	MGD	C2-N1	2.85	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	W	901	MGD	C19-N19	2.84	1.36	1.32
5	S	900	MGD	C19-N19	2.84	1.36	1.32
5	U	900	MGD	C16-N15	2.83	1.47	1.38
5	M	901	MGD	C21-N22	2.82	1.40	1.35
5	U	900	MGD	PA-O3B	2.81	1.65	1.59
5	S	901	MGD	C8-N9	2.80	1.40	1.36
5	W	901	MGD	C21-N20	2.78	1.40	1.34
5	S	900	MGD	C6-C5	2.78	1.45	1.41
5	O	901	MGD	C19-N19	2.77	1.36	1.32
5	M	901	MGD	C8-N9	2.76	1.40	1.36
5	M	900	MGD	C23-N22	2.75	1.50	1.44
5	M	900	MGD	C16-N15	2.75	1.47	1.38
5	W	900	MGD	C16-N15	2.75	1.47	1.38
5	S	901	MGD	C16-N15	2.74	1.47	1.38
7	P	807	SF4	S3-FE2	-2.73	2.31	2.33
5	O	900	MGD	C16-N15	2.73	1.47	1.38
5	O	900	MGD	C4-N9	2.69	1.41	1.37
5	U	901	MGD	C8-N9	2.69	1.40	1.36
5	S	900	MGD	C4-N9	2.68	1.41	1.37
5	U	900	MGD	C14-C13	2.67	1.54	1.50
5	W	900	MGD	C2-N1	2.67	1.41	1.36
5	O	900	MGD	C6-C5	2.66	1.45	1.41
5	W	900	MGD	PA-O3B	2.66	1.64	1.59
5	W	901	MGD	C6-C5	2.64	1.45	1.41
5	W	900	MGD	O11-C23	2.64	1.47	1.44
5	W	901	MGD	C16-N15	2.63	1.47	1.38
7	X	807	SF4	S1-FE2	2.62	2.35	2.33
5	W	900	MGD	C11-C12	2.61	1.56	1.51
5	U	901	MGD	C16-N15	2.58	1.47	1.38
5	U	901	MGD	C19-N19	2.58	1.36	1.32
5	S	900	MGD	C21-N22	2.57	1.39	1.35
7	T	807	SF4	S4-FE2	2.56	2.35	2.33
5	O	901	MGD	C23-C14	2.56	1.58	1.53
5	O	900	MGD	C14-C13	2.56	1.54	1.50
5	M	901	MGD	C6-C5	2.55	1.45	1.41
5	Q	900	MGD	C19-N18	2.54	1.40	1.36
5	W	900	MGD	C19-N20	2.50	1.36	1.33
5	W	900	MGD	C23-N22	2.49	1.49	1.44
5	S	900	MGD	C23-N22	2.49	1.49	1.44
7	V	807	SF4	S4-FE2	2.49	2.34	2.33
7	T	806	SF4	S3-FE2	-2.48	2.31	2.33
5	S	901	MGD	C23-N22	2.47	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	900	MGD	C19-N20	2.45	1.36	1.33
5	Q	900	MGD	C23-N22	2.42	1.49	1.44
5	W	901	MGD	C23-C14	2.42	1.58	1.53
5	U	900	MGD	C23-N22	2.41	1.49	1.44
5	Q	900	MGD	C4-N9	2.37	1.41	1.37
5	U	900	MGD	C2-N3	2.36	1.36	1.33
5	U	901	MGD	C6-C5	2.34	1.45	1.41
5	S	901	MGD	PA-O3B	2.33	1.64	1.59
5	W	900	MGD	C14-C13	2.33	1.54	1.50
7	R	807	SF4	S3-FE2	-2.32	2.31	2.33
5	M	900	MGD	C19-N18	2.32	1.40	1.36
5	M	900	MGD	C4-N9	2.30	1.41	1.37
5	O	901	MGD	C2'-C1'	2.29	1.56	1.53
5	O	900	MGD	C23-N22	2.30	1.49	1.44
5	O	900	MGD	C19-N20	2.28	1.36	1.33
7	R	805	SF4	S2-FE3	-2.27	2.31	2.33
5	W	901	MGD	C2'-C1'	2.25	1.56	1.53
7	N	806	SF4	S3-FE2	-2.25	2.31	2.33
5	Q	900	MGD	C14-C13	2.24	1.54	1.50
5	Q	901	MGD	C19-N20	2.22	1.36	1.33
5	U	900	MGD	C12-S12	2.20	1.82	1.74
7	P	805	SF4	S4-FE2	2.20	2.34	2.33
7	R	806	SF4	S3-FE2	-2.20	2.31	2.33
5	M	901	MGD	C19-N18	2.19	1.40	1.36
5	W	901	MGD	C23-N22	2.19	1.49	1.44
5	O	901	MGD	C23-N22	2.19	1.49	1.44
7	N	807	SF4	S4-FE2	2.18	2.34	2.33
5	Q	900	MGD	C11-C12	2.18	1.55	1.51
5	O	900	MGD	O11-C23	2.18	1.47	1.44
5	U	901	MGD	C23-N22	2.18	1.49	1.44
5	Q	901	MGD	C23-N22	2.17	1.49	1.44
5	O	901	MGD	C2-N3	2.16	1.36	1.33
5	S	900	MGD	C2-N3	2.16	1.36	1.33
5	S	901	MGD	C19-N20	2.15	1.36	1.33
5	Q	901	MGD	C19-N18	2.15	1.40	1.36
5	Q	901	MGD	C2-N3	2.15	1.36	1.33
5	S	901	MGD	C23-C14	2.15	1.57	1.53
5	Q	900	MGD	C6-C5	2.14	1.44	1.41
5	Q	900	MGD	C2-N3	2.13	1.36	1.33
7	N	807	SF4	S3-FE2	-2.13	2.31	2.33
5	U	900	MGD	C11-C12	2.13	1.55	1.51
7	T	806	SF4	S4-FE2	-2.13	2.31	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	901	MGD	C23-N22	2.12	1.49	1.44
5	O	900	MGD	C2-N3	2.12	1.36	1.33
7	P	806	SF4	S3-FE2	-2.11	2.31	2.33
5	M	901	MGD	C4-N3	2.10	1.39	1.35
7	R	805	SF4	S1-FE2	2.07	2.34	2.33
5	S	900	MGD	C11-C12	2.06	1.55	1.51
5	U	900	MGD	C19-N18	2.03	1.40	1.36
5	Q	901	MGD	C23-C14	2.00	1.57	1.53

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	901	MGD	C6-C5-N7	-23.56	130.97	134.14
5	U	901	MGD	C6-C5-N7	-23.03	131.04	134.14
5	M	900	MGD	C6-C5-N7	-22.72	131.08	134.14
5	M	901	MGD	C6-C5-N7	-21.06	131.30	134.14
5	Q	901	MGD	C6-C5-N7	-20.81	131.34	134.14
5	S	901	MGD	C6-C5-N7	-20.65	131.36	134.14
5	W	901	MGD	C6-C5-N7	-20.47	131.38	134.14
5	O	900	MGD	C6-C5-N7	-19.82	131.47	134.14
5	S	900	MGD	C6-C5-N7	-19.01	131.58	134.14
5	Q	900	MGD	C6-C5-N7	-16.22	131.96	134.14
5	U	900	MGD	C6-C5-N7	-15.97	131.99	134.14
5	W	900	MGD	C6-C5-N7	-15.20	132.09	134.14
5	Q	900	MGD	O2A-PA-O3B	-5.75	77.85	105.14
5	O	900	MGD	O2A-PA-O3B	-5.68	78.16	105.14
5	S	900	MGD	O2A-PA-O3B	-5.57	78.71	105.14
5	M	900	MGD	O2A-PA-O3B	-5.55	78.82	105.14
5	U	900	MGD	O2A-PA-O3B	-5.30	79.99	105.14
5	W	900	MGD	O2A-PA-O3A	-5.27	81.94	108.51
5	M	900	MGD	O2A-PA-O3A	-5.26	82.01	108.51
5	O	900	MGD	O2A-PA-O3A	-5.18	82.40	108.51
5	U	900	MGD	O2A-PA-O3A	-5.14	82.59	108.51
5	W	900	MGD	O2A-PA-O3B	-5.08	81.04	105.14
5	Q	900	MGD	O2A-PA-O3A	-4.96	83.52	108.51
5	S	900	MGD	O2A-PA-O3A	-4.58	85.44	108.51
5	M	900	MGD	C17-C16-C21	4.53	118.75	114.56
5	W	900	MGD	C17-C16-C21	4.50	118.73	114.56
5	O	900	MGD	C17-C16-C21	4.37	118.61	114.56
5	U	901	MGD	C17-C16-C21	4.35	118.59	114.56
5	W	901	MGD	C17-C16-C21	4.34	118.58	114.56
5	S	900	MGD	O2A-PA-O1A	-4.15	89.01	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	900	MGD	C17-C16-C21	4.15	118.41	114.56
5	Q	900	MGD	O4'-C1'-N9	-4.10	104.63	108.44
5	Q	901	MGD	O4'-C1'-N9	-4.10	104.63	108.44
5	O	900	MGD	O4'-C1'-N9	-4.08	104.64	108.44
5	U	901	MGD	C13-C14-N15	-4.07	104.02	111.70
5	S	900	MGD	C17-C16-C21	4.07	118.33	114.56
5	S	901	MGD	C13-C14-N15	-4.06	104.04	111.70
5	M	900	MGD	O4'-C1'-N9	-3.97	104.74	108.44
5	O	901	MGD	C17-C16-C21	3.96	118.23	114.56
5	S	900	MGD	C23-C14-N15	3.96	113.48	108.44
5	S	901	MGD	C17-C16-C21	3.96	118.22	114.56
5	Q	901	MGD	C17-C16-C21	3.94	118.21	114.56
5	W	900	MGD	O2A-PA-O1A	-3.94	90.19	112.21
5	M	901	MGD	O4'-C4'-C5'	-3.93	95.32	109.36
5	U	900	MGD	O2A-PA-O1A	-3.93	90.27	112.21
5	Q	900	MGD	C17-C16-C21	3.89	118.16	114.56
5	M	901	MGD	C17-C16-C21	3.84	118.12	114.56
5	Q	901	MGD	C13-C14-N15	-3.84	104.45	111.70
5	M	901	MGD	O4'-C1'-N9	-3.83	104.88	108.44
5	O	900	MGD	O3B-PA-O3A	3.81	120.46	103.41
5	Q	900	MGD	O2A-PA-O1A	-3.81	90.95	112.21
5	O	901	MGD	C13-C14-N15	-3.80	104.53	111.70
5	W	900	MGD	C13-C14-N15	-3.77	104.58	111.70
5	Q	900	MGD	O3B-PA-O3A	3.76	120.21	103.41
5	M	900	MGD	O2A-PA-O1A	-3.74	91.33	112.21
5	Q	901	MGD	O4'-C4'-C5'	-3.73	96.03	109.36
5	W	901	MGD	C13-C14-N15	-3.72	104.68	111.70
5	S	900	MGD	C16-N15-C14	-3.72	108.90	118.60
5	M	900	MGD	C23-C14-N15	3.71	113.15	108.44
5	Q	900	MGD	C16-N15-C14	-3.71	108.94	118.60
5	M	900	MGD	O3B-PA-O3A	3.69	119.89	103.41
5	U	901	MGD	O4'-C4'-C5'	-3.69	96.20	109.36
5	U	900	MGD	O3B-PA-O3A	3.63	119.63	103.41
5	W	900	MGD	O3B-PA-O3A	3.62	119.61	103.41
5	M	900	MGD	C16-N15-C14	-3.59	109.24	118.60
5	U	900	MGD	C16-N15-C14	-3.59	109.23	118.60
5	O	900	MGD	O2A-PA-O1A	-3.53	92.52	112.21
5	O	900	MGD	C23-C14-N15	3.51	112.90	108.44
5	O	901	MGD	O4'-C4'-C5'	-3.47	96.97	109.36
5	S	901	MGD	O4'-C4'-C5'	-3.43	97.11	109.36
5	U	900	MGD	O4'-C1'-N9	-3.38	105.29	108.44
5	Q	900	MGD	C23-C14-N15	3.37	112.72	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	901	MGD	C16-N15-C14	-3.31	109.98	118.60
5	U	900	MGD	C23-C14-N15	3.30	112.63	108.44
5	W	900	MGD	C16-N15-C14	-3.28	110.06	118.60
5	O	900	MGD	C16-N15-C14	-3.27	110.08	118.60
5	S	901	MGD	C5-C4-N3	3.21	130.59	125.94
5	W	901	MGD	C16-N15-C14	-3.21	110.25	118.60
5	S	900	MGD	O3B-PA-O3A	3.19	117.67	103.41
5	M	901	MGD	C13-C14-N15	-3.19	105.69	111.70
5	O	901	MGD	C16-N15-C14	-3.17	110.34	118.60
5	W	900	MGD	O4'-C1'-N9	-3.16	105.50	108.44
5	Q	901	MGD	C16-N15-C14	-3.14	110.43	118.60
5	U	900	MGD	O3A-C10-C11	-3.08	100.54	108.53
5	W	901	MGD	O4'-C4'-C5'	-3.06	98.45	109.36
5	U	901	MGD	C16-N15-C14	-3.05	110.66	118.60
5	M	900	MGD	C13-C14-N15	-3.02	106.01	111.70
5	Q	901	MGD	C5-C4-N3	2.96	130.24	125.94
5	M	901	MGD	C4'-O4'-C1'	2.95	112.95	109.75
5	U	901	MGD	O4'-C1'-N9	-2.91	105.73	108.44
5	W	900	MGD	C23-C14-N15	2.90	112.12	108.44
5	O	900	MGD	C13-C14-N15	-2.90	106.23	111.70
5	S	901	MGD	C16-N15-C14	-2.83	111.21	118.60
5	M	901	MGD	O11-C23-C14	-2.83	105.66	109.50
5	W	901	MGD	O4'-C1'-N9	-2.80	105.83	108.44
5	M	900	MGD	C5-C4-N3	2.71	129.88	125.94
5	M	901	MGD	C5-C4-N3	2.70	129.86	125.94
5	W	901	MGD	C5-C4-N3	2.68	129.84	125.94
5	S	901	MGD	O4'-C1'-N9	-2.68	105.95	108.44
5	M	901	MGD	C2-N3-C4	-2.66	111.35	115.09
5	O	901	MGD	C5-C4-N3	2.66	129.80	125.94
5	Q	900	MGD	C5-C4-N3	2.66	129.80	125.94
5	O	901	MGD	O4'-C1'-N9	-2.61	106.01	108.44
5	O	901	MGD	O11-C23-C14	-2.60	105.96	109.50
5	Q	900	MGD	C2-N3-C4	-2.60	111.44	115.09
5	Q	901	MGD	C2-N3-C4	-2.57	111.49	115.09
5	U	901	MGD	C5-C4-N3	2.54	129.63	125.94
5	O	901	MGD	C3'-C2'-C1'	2.52	104.84	100.91
5	Q	901	MGD	O11-C23-C14	-2.51	106.08	109.50
5	Q	901	MGD	C4'-O4'-C1'	2.51	112.47	109.75
5	S	901	MGD	C2-N3-C4	-2.50	111.57	115.09
5	U	900	MGD	O4'-C4'-C5'	-2.50	100.42	109.36
5	Q	900	MGD	O4'-C4'-C5'	-2.49	100.45	109.36
5	U	900	MGD	C13-C14-N15	-2.49	106.99	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	900	MGD	O3A-C10-C11	-2.49	102.08	108.53
5	S	900	MGD	C5-C4-N3	2.49	129.55	125.94
5	Q	900	MGD	C16-C21-N20	2.44	125.41	121.50
5	W	900	MGD	C10-C11-C12	2.43	113.85	110.98
5	O	901	MGD	C2-N3-C4	-2.42	111.70	115.09
5	W	901	MGD	C4'-O4'-C1'	2.40	112.36	109.75
5	O	900	MGD	C5-C4-N3	2.40	129.42	125.94
5	M	900	MGD	O3A-C10-C11	-2.40	102.33	108.53
5	U	900	MGD	C5-C4-N3	2.39	129.40	125.94
5	M	901	MGD	C16-C21-N20	2.38	125.31	121.50
5	S	900	MGD	C2-N3-C4	-2.38	111.75	115.09
5	M	900	MGD	O4'-C4'-C5'	-2.36	100.92	109.36
5	O	901	MGD	C4'-O4'-C1'	2.36	112.31	109.75
5	S	901	MGD	C17-N18-C19	2.35	123.63	119.51
5	Q	901	MGD	C16-C21-N20	2.34	125.25	121.50
5	W	900	MGD	C5-C4-N3	2.34	129.34	125.94
5	W	901	MGD	C10-C11-C12	-2.34	108.22	110.98
5	U	901	MGD	C3'-C2'-C1'	2.34	104.57	100.91
5	M	900	MGD	C16-C21-N20	2.33	125.23	121.50
5	S	901	MGD	C3'-C2'-C1'	2.31	104.52	100.91
5	S	900	MGD	C16-C21-N20	2.30	125.17	121.50
5	U	901	MGD	C11-C12-C13	2.30	125.12	117.86
5	O	901	MGD	C11-C12-C13	2.27	125.04	117.86
5	Q	901	MGD	C10-C11-C12	-2.25	108.33	110.98
5	Q	900	MGD	C13-C14-N15	-2.24	107.47	111.70
5	U	900	MGD	C16-C21-N20	2.24	125.08	121.50
5	M	900	MGD	C2-N3-C4	-2.24	111.95	115.09
5	M	901	MGD	C17-N18-C19	2.22	123.39	119.51
5	M	900	MGD	C4-C5-N7	2.22	111.42	109.52
5	U	900	MGD	N1-C2-N3	2.22	124.89	121.78
5	U	901	MGD	C17-N18-C19	2.22	123.39	119.51
5	U	900	MGD	C2-N3-C4	-2.22	111.98	115.09
5	W	901	MGD	C11-C12-C13	2.21	124.85	117.86
5	S	901	MGD	O3A-C10-C11	2.21	114.25	108.53
5	S	900	MGD	C17-N18-C19	2.21	123.38	119.51
5	O	901	MGD	C17-N18-C19	2.20	123.36	119.51
5	S	900	MGD	O4'-C4'-C5'	-2.20	101.50	109.36
5	S	900	MGD	N1-C2-N3	2.20	124.86	121.78
5	W	901	MGD	C2-N3-C4	-2.20	112.01	115.09
5	O	900	MGD	C2-N3-C4	-2.19	112.01	115.09
5	Q	901	MGD	C17-N18-C19	2.19	123.33	119.51
5	U	901	MGD	C2-N3-C4	-2.18	112.03	115.09

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	901	MGD	C16-C21-N20	2.18	124.98	121.50
5	Q	900	MGD	N1-C2-N3	2.17	124.83	121.78
5	M	901	MGD	C3'-C2'-C1'	2.17	104.30	100.91
5	S	900	MGD	O3A-C10-C11	-2.17	102.91	108.53
5	S	901	MGD	C11-C12-C13	2.16	124.69	117.86
5	O	901	MGD	C16-C21-N20	2.16	124.96	121.50
5	M	901	MGD	C11-C12-C13	2.16	124.67	117.86
5	U	900	MGD	C17-N18-C19	2.15	123.27	119.51
5	Q	901	MGD	C11-C12-C13	2.14	124.61	117.86
5	M	900	MGD	C17-N18-C19	2.14	123.25	119.51
5	U	901	MGD	C16-C21-N20	2.14	124.92	121.50
5	W	901	MGD	C3'-C2'-C1'	2.14	104.25	100.91
5	W	901	MGD	C17-N18-C19	2.14	123.25	119.51
5	M	900	MGD	O4'-C1'-C2'	-2.12	103.52	106.77
5	U	900	MGD	C14-C13-C12	2.11	123.92	116.27
5	W	901	MGD	C16-C21-N20	2.11	124.87	121.50
5	O	901	MGD	N1-C2-N3	2.10	124.72	121.78
5	O	900	MGD	C16-C21-N20	2.09	124.85	121.50
5	M	900	MGD	C14-C13-C12	2.08	123.81	116.27
5	O	900	MGD	C14-C13-C12	2.07	123.78	116.27
5	W	900	MGD	C14-C13-C12	2.06	123.75	116.27
5	M	901	MGD	C6-N1-C2	2.06	123.11	119.51
5	W	900	MGD	O4'-C4'-C5'	-2.06	102.02	109.36
5	W	900	MGD	C17-N18-C19	2.05	123.10	119.51
5	Q	901	MGD	N1-C2-N3	2.04	124.65	121.78
5	Q	900	MGD	C17-N18-C19	2.05	123.09	119.51
5	M	901	MGD	C4-C5-N7	2.04	111.27	109.52
5	W	901	MGD	C6-N1-C2	2.04	123.08	119.51
5	Q	901	MGD	O3A-C10-C11	2.04	113.80	108.53
5	W	900	MGD	C2-N3-C4	-2.03	112.23	115.09
5	S	900	MGD	C14-C13-C12	2.03	123.63	116.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.