Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:20 PM EDT

PDB ID	:	4V4D / pdb_00004v4d
Title	:	Crystal Structure of Pyrogallol-Phloroglucinol Transhydroxylase from Pelobacter acidigallici complexed with pyrogallol
Authors	:	Messerschmidt, A.; Niessen, H.; Abt, D.; Einsle, O.; Schink, B.; Kroneck, P.M.H.
Deposited on	:	2004-06-02
Resolution	:	2.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

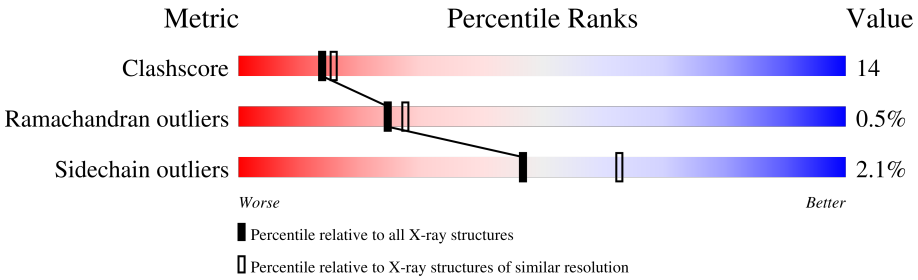
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	875	74% 24% ·
1	C	875	71% 27% ·
1	E	875	75% 23% ·
1	G	875	76% 22% ·
1	I	875	74% 23% ·
1	K	875	74% 24% ·
1	M	875	73% 25% ·
1	O	875	72% 25% ·

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Mol	Chain	Length	Quality of chain
1	Q	875	72% 25%
1	S	875	73% 26%
1	U	875	72% 26%
1	W	875	71% 26%
2	B	274	67% 29%
2	D	274	64% 32%
2	F	274	68% 30%
2	H	274	69% 27%
2	J	274	69% 26% 5%
2	L	274	65% 31%
2	N	274	67% 28%
2	P	274	63% 33%
2	R	274	69% 27%
2	T	274	62% 34%
2	V	274	66% 31%
2	X	274	55% 41%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PYG	A	905	-	X	-	-
6	PYG	C	905	-	X	-	-
6	PYG	E	905	-	X	-	-
6	PYG	G	905	-	X	-	-
6	PYG	I	905	-	X	-	-
6	PYG	K	905	-	X	-	-
6	PYG	M	905	-	X	-	-
6	PYG	O	905	-	X	-	-
6	PYG	Q	905	-	X	-	-
6	PYG	S	905	-	X	-	-

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

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 121808 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	C	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	E	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	G	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	I	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	K	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	M	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	O	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	Q	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	S	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	U	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			
1	W	875	Total	C	N	O	S	0	0	0
			6998	4464	1189	1297	48			

There are 12 discrepancies between the modelled and reference sequences:

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

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

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

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

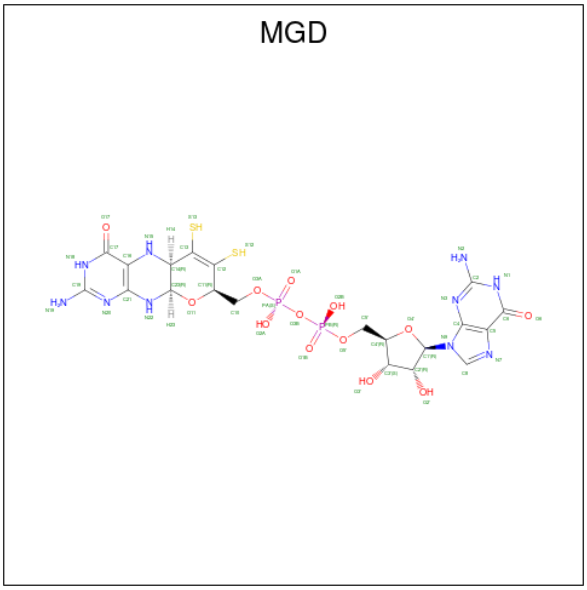
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

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

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



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

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

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

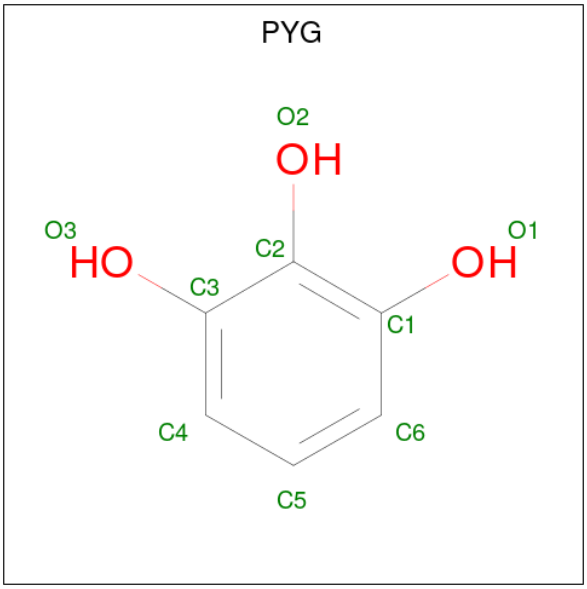
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mo	0	0
			1	1		
5	C	1	Total	Mo	0	0
			1	1		
5	E	1	Total	Mo	0	0
			1	1		
5	G	1	Total	Mo	0	0
			1	1		
5	I	1	Total	Mo	0	0
			1	1		
5	K	1	Total	Mo	0	0
			1	1		
5	M	1	Total	Mo	0	0
			1	1		

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

- Molecule 6 is BENZENE-1,2,3-TRIOL (CCD ID: PYG) (formula: $C_6H_6O_3$).



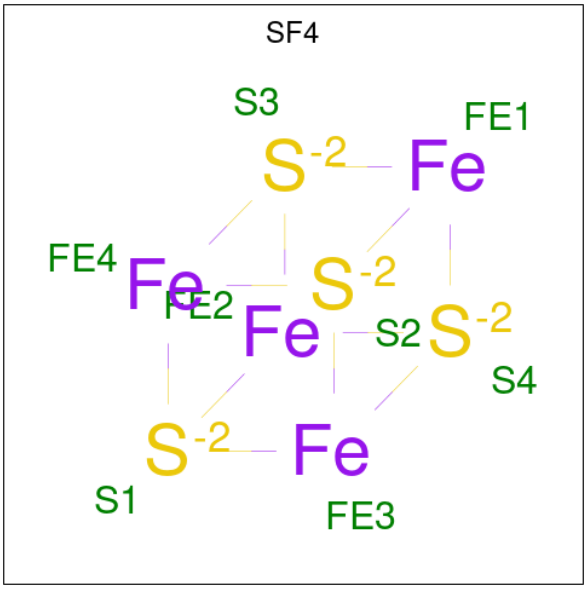
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 9 6 3	0	0
6	C	1	Total C O 9 6 3	0	0
6	E	1	Total C O 9 6 3	0	0
6	G	1	Total C O 9 6 3	0	0
6	I	1	Total C O 9 6 3	0	0
6	K	1	Total C O 9 6 3	0	0

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

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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

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

- Molecule 8 is water.

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

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

3 Residue-property plots (i)

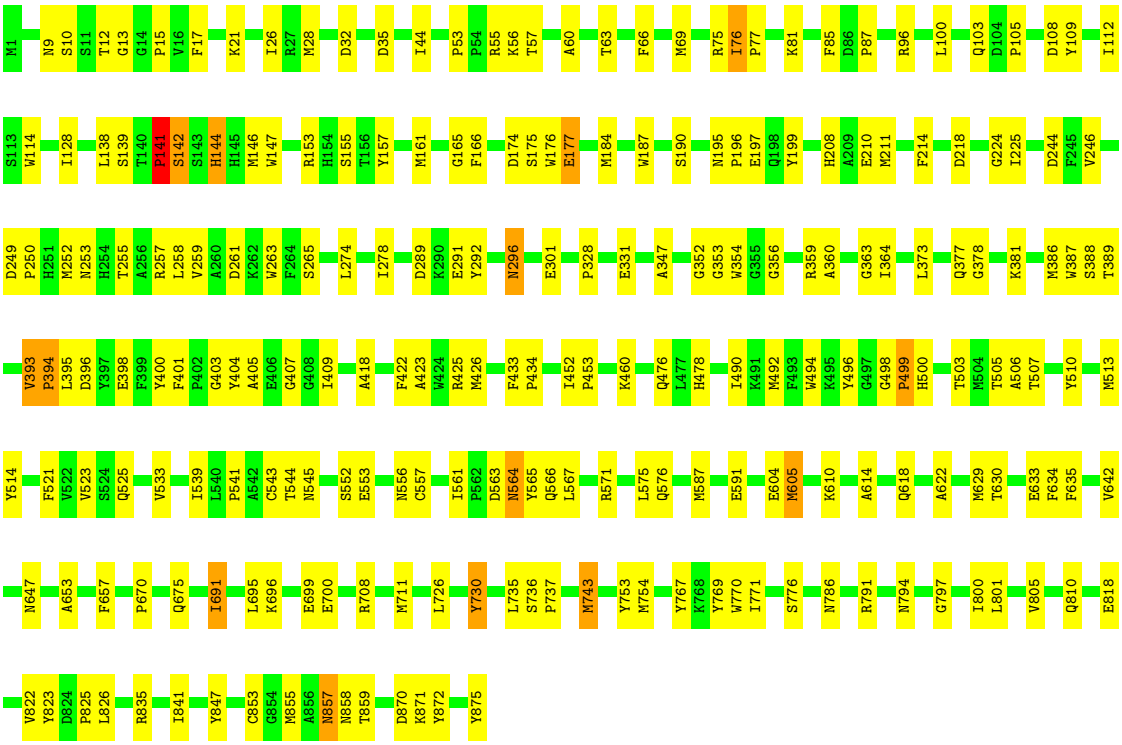
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain A:

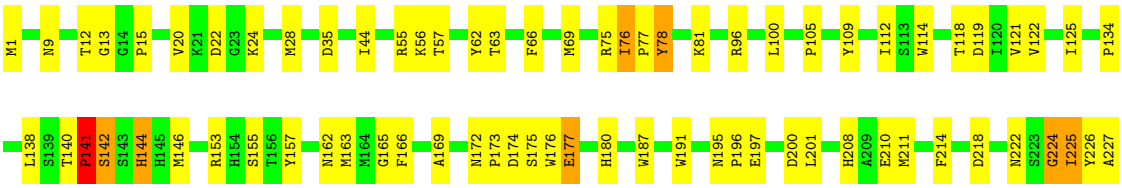


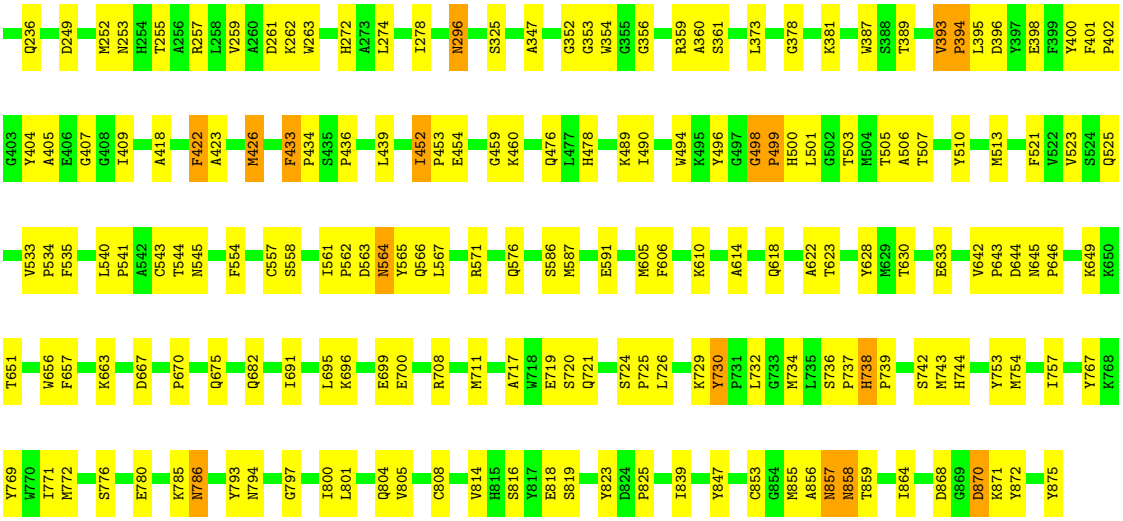


• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain C:



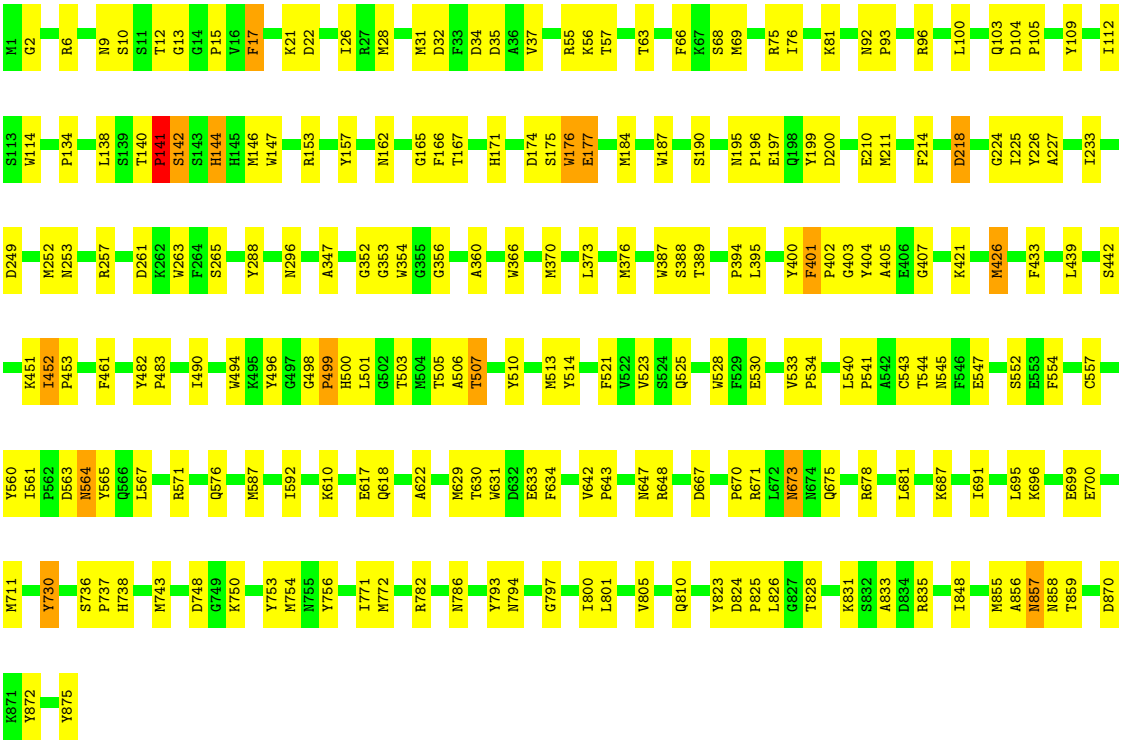




• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain E:

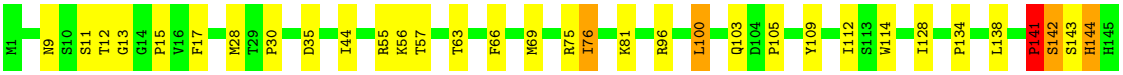


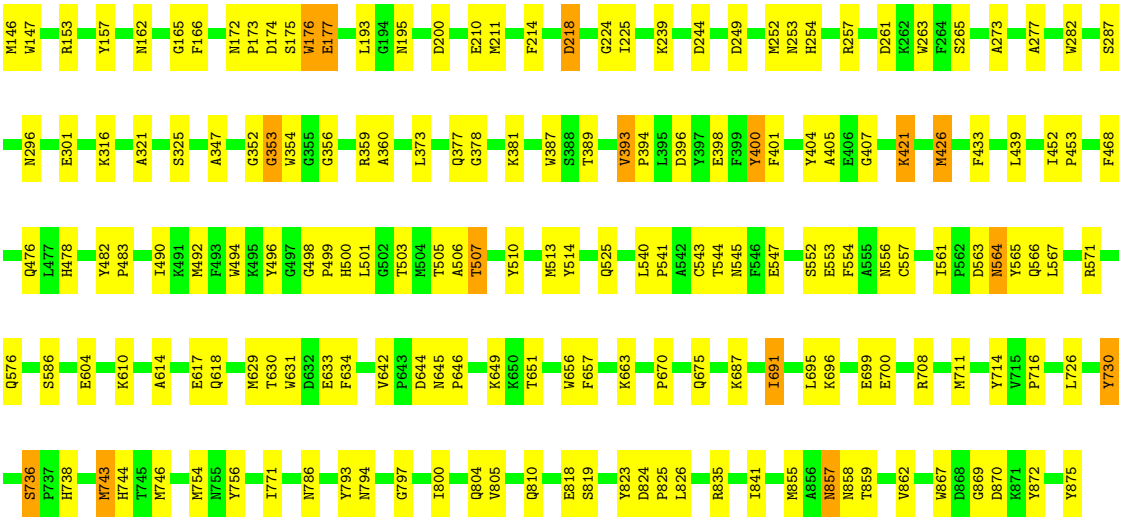


• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain G:



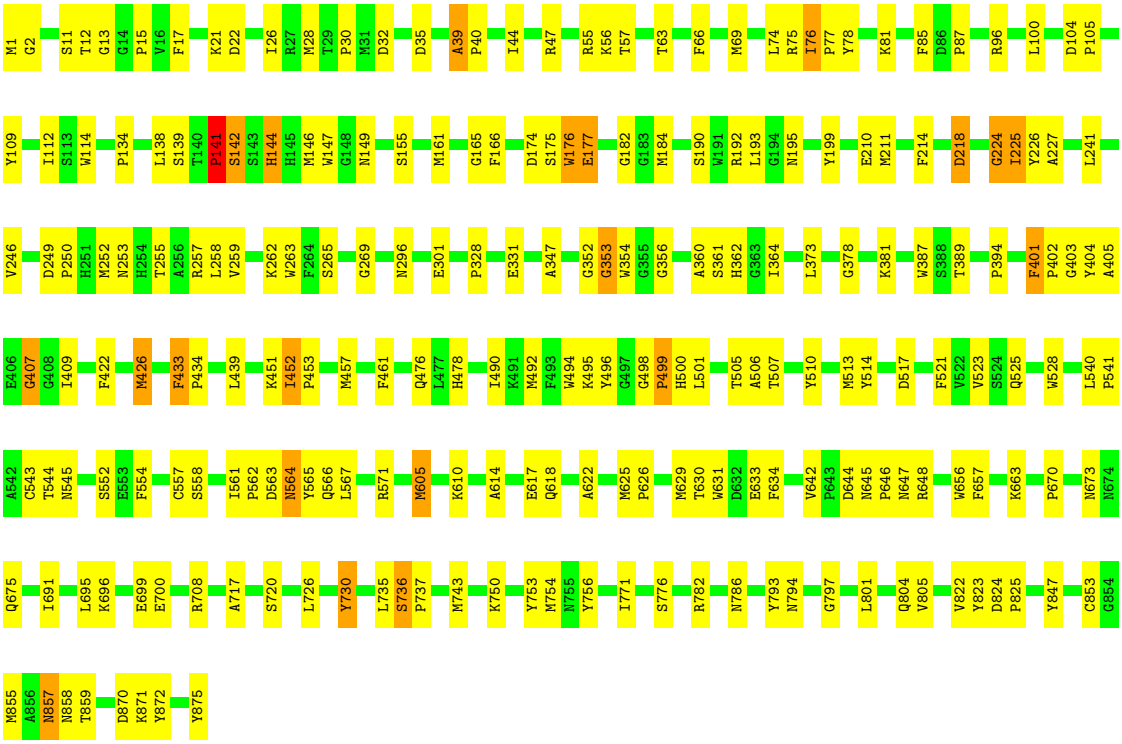




• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain I:

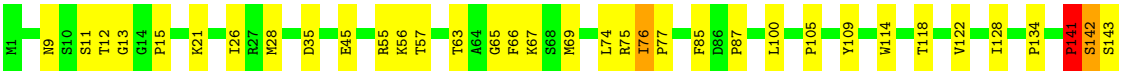


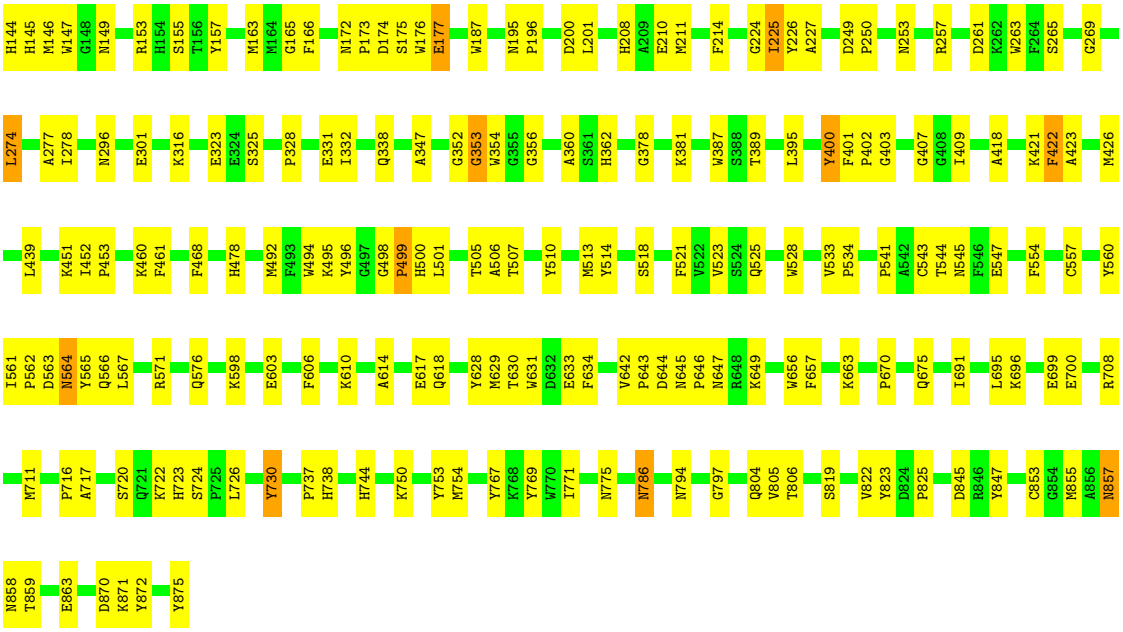


• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain K:



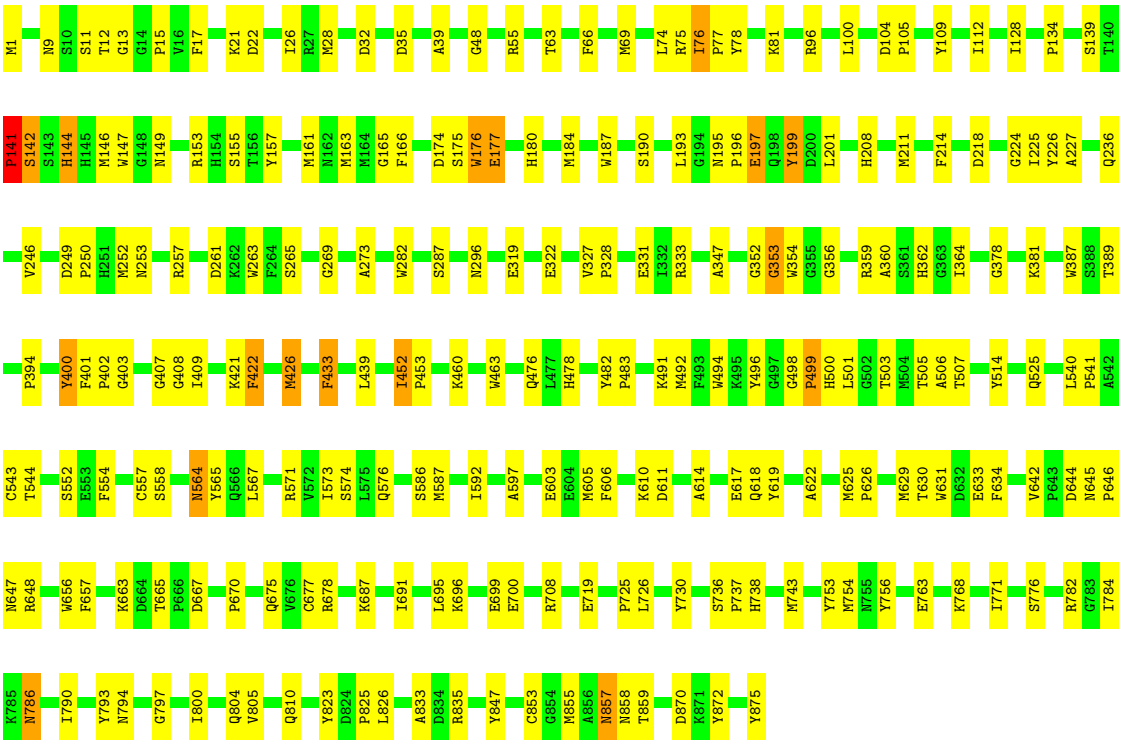




• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain M:

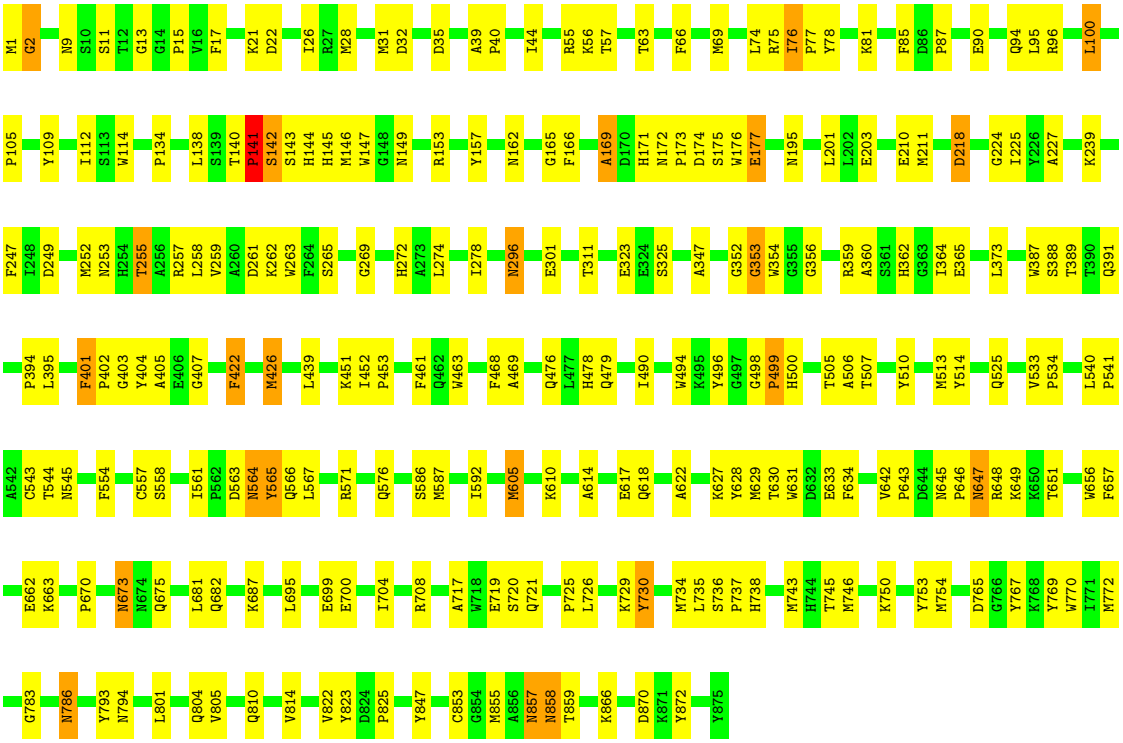




• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain O:

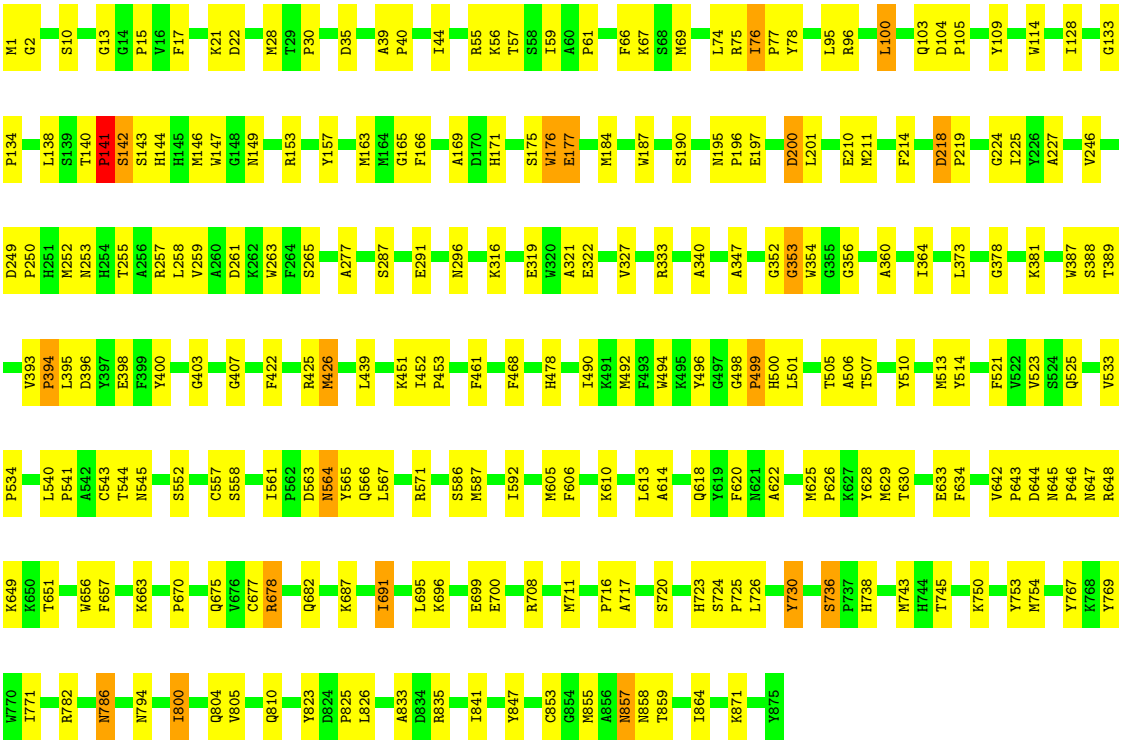




• Molecule 1: Pyrogallol hydroxytransferase large subunit

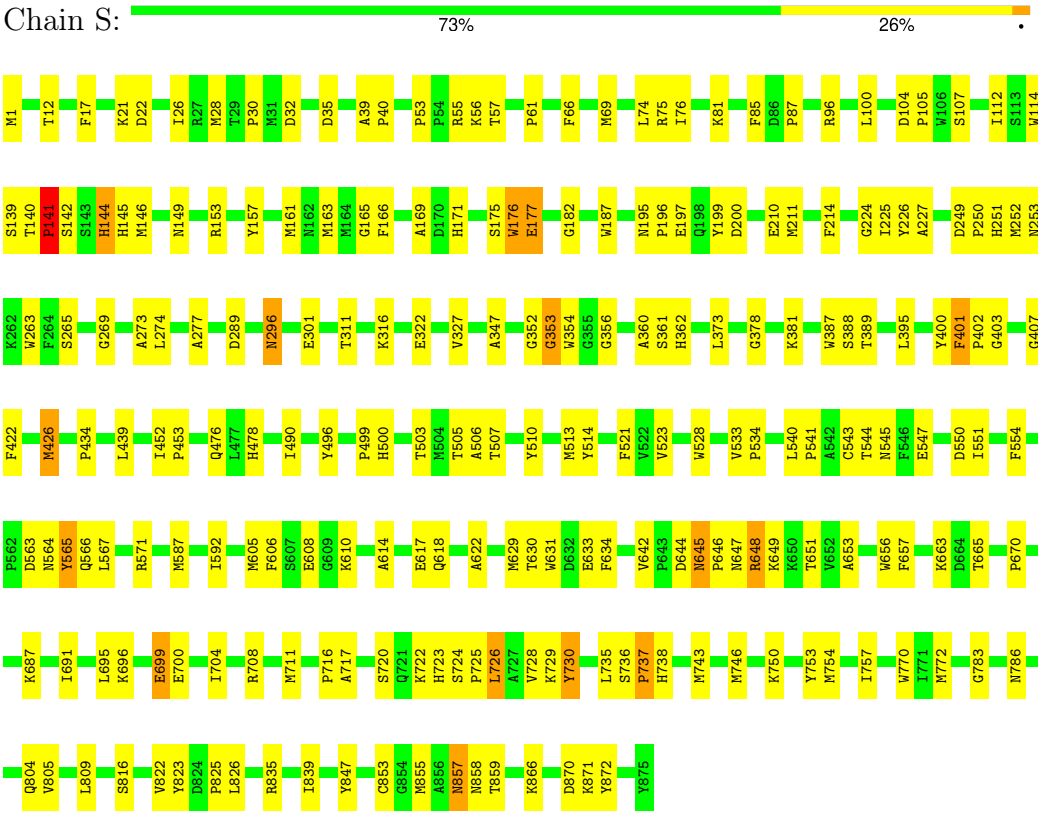
Chain Q:





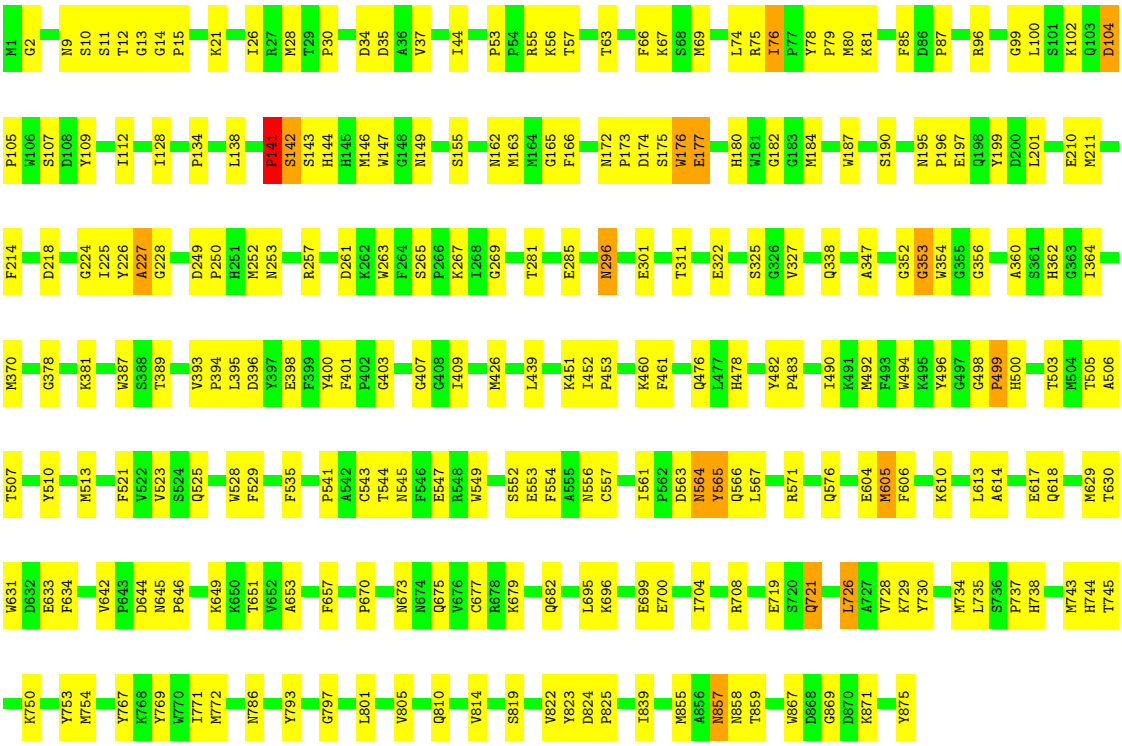
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain S:



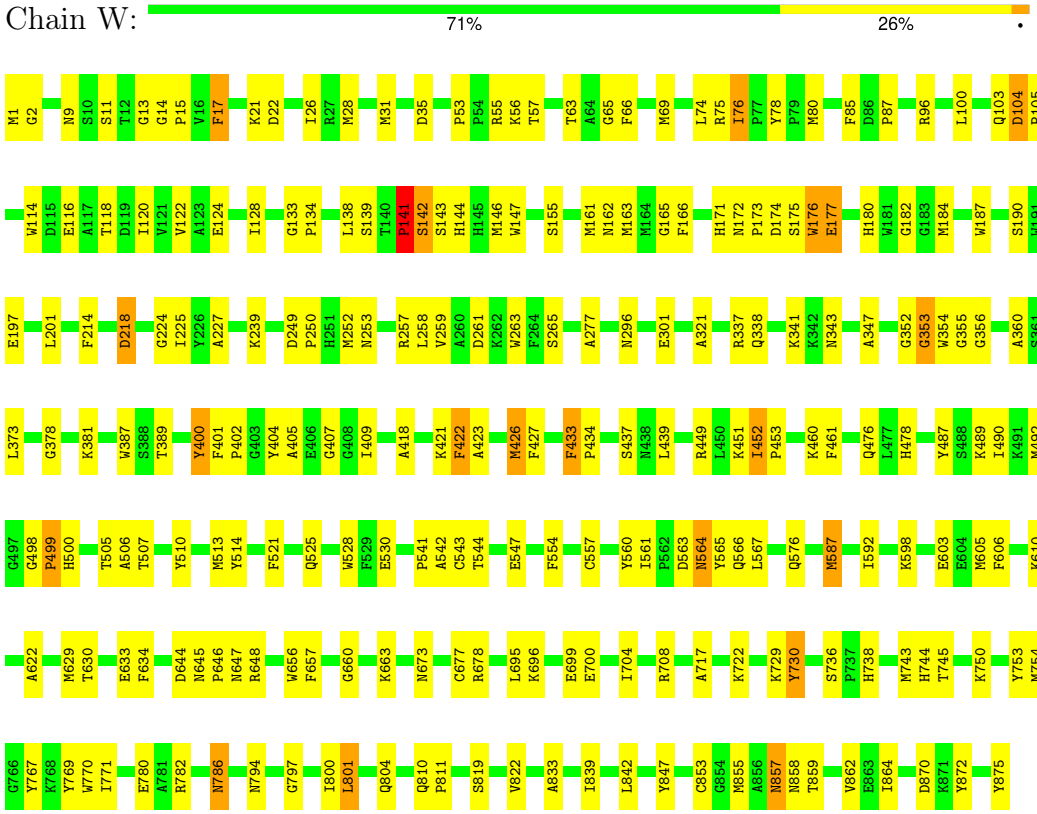
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain U:



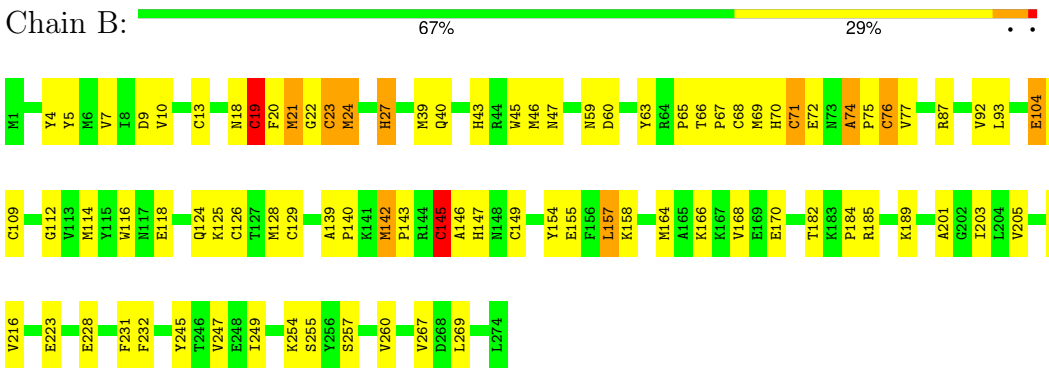
• Molecule 1: Pyrogallol hydroxytransferase large subunit

Chain W:



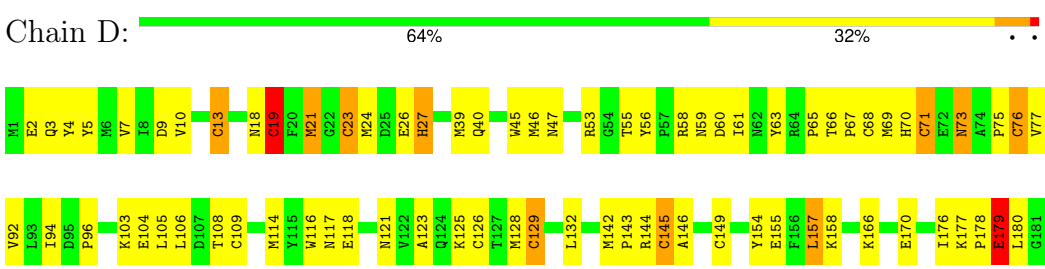
• Molecule 2: Pyrogallol hydroxytransferase small subunit

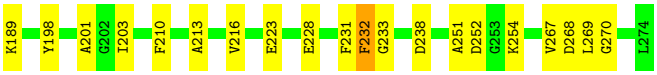
Chain B:



• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain D:

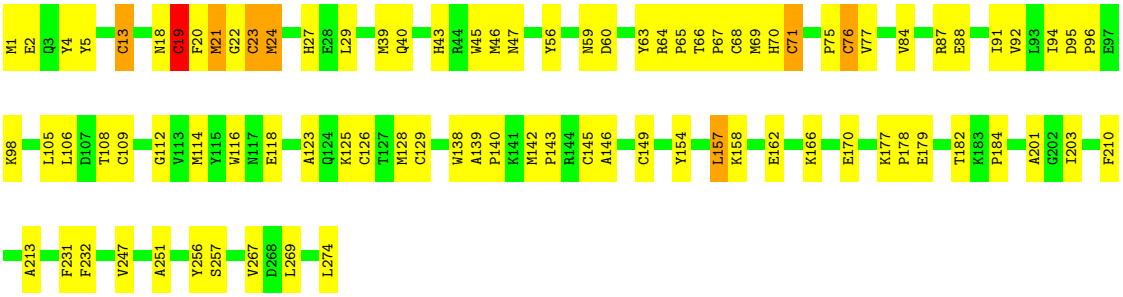




• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain F:





• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain H:

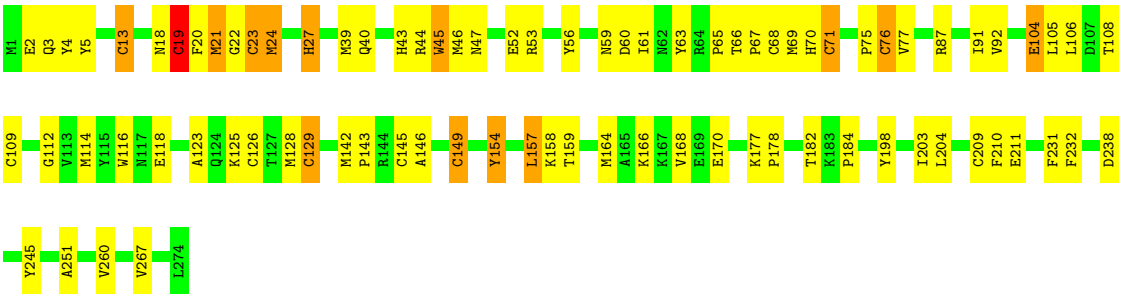




• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain J:

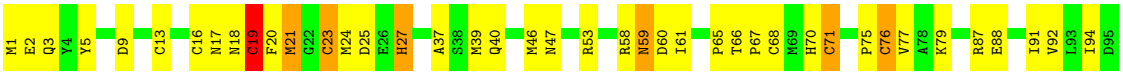


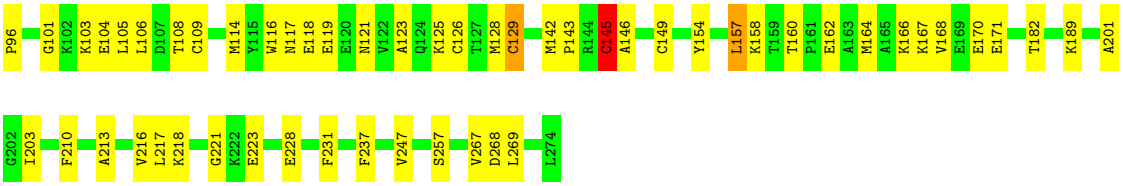


• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain L:



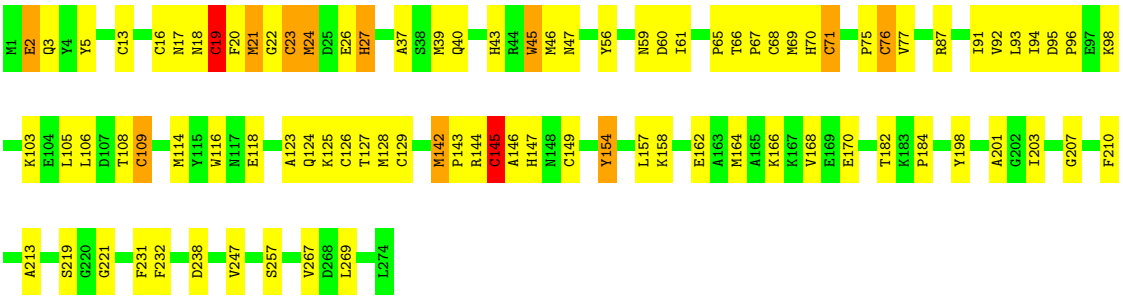




• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain N:

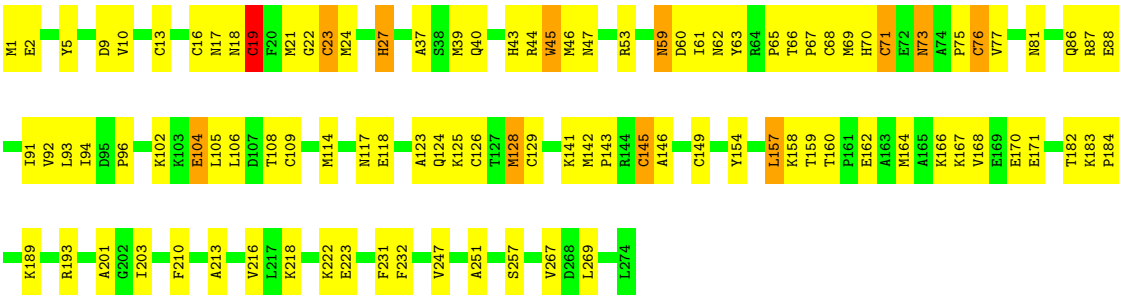




• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain P:

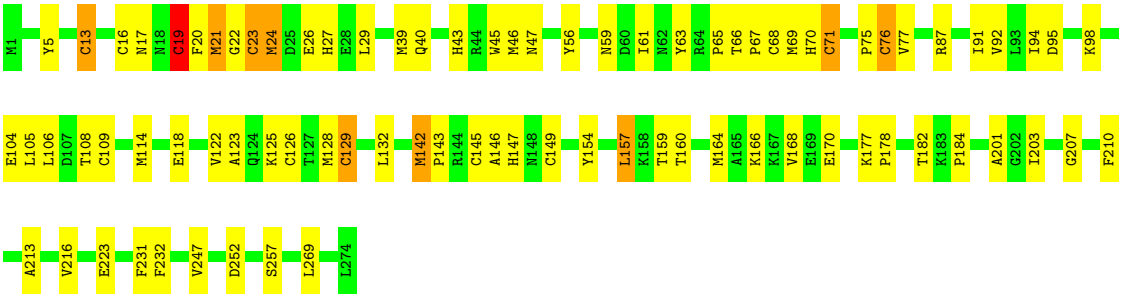




• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain R:

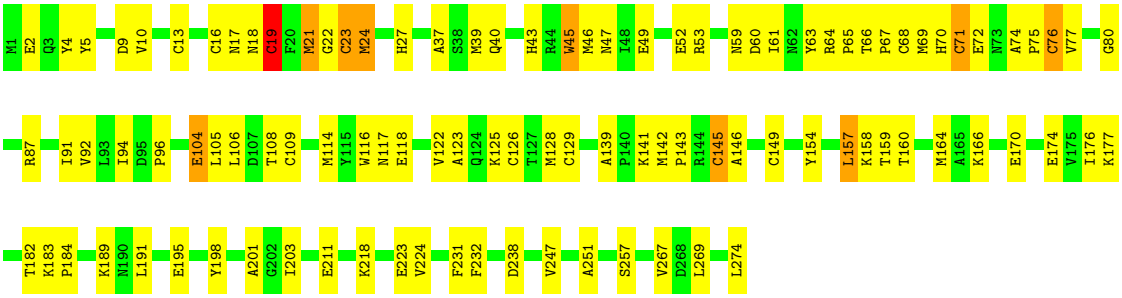




• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain T:

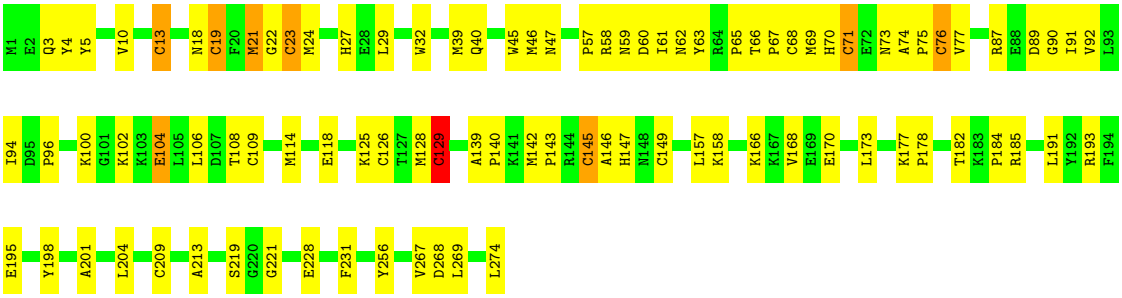




• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain V:

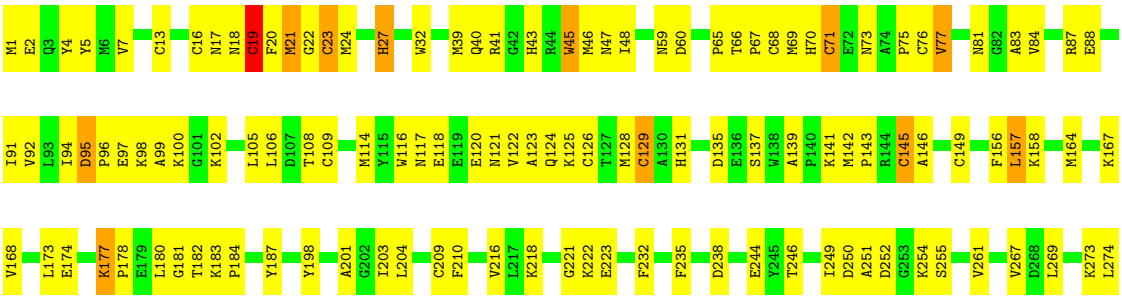




• Molecule 2: Pyrogallol hydroxytransferase small subunit

Chain X:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	172.47Å 178.14Å 179.05Å 64.11° 64.45° 65.11°	Depositor
Resolution (Å)	24.99 – 2.20	Depositor
% Data completeness (in resolution range)	96.7 (24.99-2.20)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	121808	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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, MGD, CA, SF4, PYG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.38	0/7219	0.98	41/9786 (0.4%)
1	C	0.37	0/7219	0.97	45/9786 (0.5%)
1	E	0.38	0/7219	0.97	36/9786 (0.4%)
1	G	0.38	0/7219	0.98	45/9786 (0.5%)
1	I	0.37	0/7219	0.97	45/9786 (0.5%)
1	K	0.39	0/7219	0.97	37/9786 (0.4%)
1	M	0.38	0/7219	0.97	43/9786 (0.4%)
1	O	0.38	0/7219	0.96	42/9786 (0.4%)
1	Q	0.38	0/7219	0.97	44/9786 (0.4%)
1	S	0.37	0/7219	0.97	39/9786 (0.4%)
1	U	0.37	0/7219	0.97	42/9786 (0.4%)
1	W	0.37	0/7219	0.97	41/9786 (0.4%)
2	B	0.47	1/2231 (0.0%)	0.97	10/3009 (0.3%)
2	D	0.39	0/2231	0.92	8/3009 (0.3%)
2	F	0.45	0/2231	0.96	6/3009 (0.2%)
2	H	0.44	0/2231	0.97	9/3009 (0.3%)
2	J	0.43	0/2231	0.95	8/3009 (0.3%)
2	L	0.43	0/2231	0.97	8/3009 (0.3%)
2	N	0.47	1/2231 (0.0%)	0.96	11/3009 (0.4%)
2	P	0.43	0/2231	0.95	9/3009 (0.3%)
2	R	0.45	1/2231 (0.0%)	0.98	6/3009 (0.2%)
2	T	0.41	0/2231	0.95	11/3009 (0.4%)
2	V	0.40	0/2231	0.94	7/3009 (0.2%)
2	X	0.38	0/2231	0.93	13/3009 (0.4%)
All	All	0.39	3/113400 (0.0%)	0.97	606/153540 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	142	MET	SD-CE	-6.04	1.64	1.79
2	R	142	MET	SD-CE	-5.89	1.64	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	142	MET	SD-CE	-5.21	1.66	1.79

All (606) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	R	77	VAL	N-CA-C	-9.71	101.29	111.58
1	Q	76	ILE	CA-C-N	9.41	128.75	118.97
1	Q	76	ILE	C-N-CA	9.41	128.75	118.97
1	G	76	ILE	CA-C-N	9.19	128.52	118.97
1	G	76	ILE	C-N-CA	9.19	128.52	118.97
1	W	352	GLY	N-CA-C	-9.14	91.53	113.18
1	G	500	HIS	N-CA-C	9.11	122.18	111.71
1	S	353	GLY	N-CA-C	-9.09	100.07	111.70
1	A	76	ILE	CA-C-N	9.03	128.36	118.97
1	A	76	ILE	C-N-CA	9.03	128.36	118.97
1	A	352	GLY	N-CA-C	-8.98	91.90	113.18
1	U	857	ASN	N-CA-C	8.95	121.85	111.11
1	Q	507	THR	N-CA-C	8.95	123.61	112.87
1	E	353	GLY	N-CA-C	-8.92	101.15	111.85
2	P	77	VAL	N-CA-C	-8.88	101.32	111.00
1	U	507	THR	N-CA-C	8.79	123.42	112.87
1	W	857	ASN	N-CA-C	8.79	121.66	111.11
1	C	352	GLY	N-CA-C	-8.72	92.51	113.18
2	J	77	VAL	N-CA-C	-8.71	102.37	110.82
1	O	352	GLY	N-CA-C	-8.67	92.63	113.18
1	M	352	GLY	N-CA-C	-8.61	92.77	113.18
1	O	353	GLY	N-CA-C	-8.61	100.68	111.70
1	A	857	ASN	N-CA-C	8.60	121.43	111.11
2	D	77	VAL	N-CA-C	-8.60	101.63	111.00
1	Q	352	GLY	N-CA-C	-8.55	92.91	113.18
1	S	507	THR	N-CA-C	8.55	123.13	112.87
1	S	352	GLY	N-CA-C	-8.53	92.96	113.18
1	U	352	GLY	N-CA-C	-8.52	92.99	113.18
1	W	507	THR	N-CA-C	8.48	123.05	112.87
1	W	353	GLY	N-CA-C	-8.41	101.75	111.85
1	I	352	GLY	N-CA-C	-8.40	93.26	113.18
1	S	76	ILE	CA-C-N	8.35	127.65	118.97
1	S	76	ILE	C-N-CA	8.35	127.65	118.97
1	G	352	GLY	N-CA-C	-8.31	93.48	113.18
1	E	352	GLY	N-CA-C	-8.30	93.50	113.18
1	C	353	GLY	N-CA-C	-8.27	100.69	111.52
1	A	407	GLY	N-CA-C	8.25	124.90	115.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	77	VAL	N-CA-C	-8.25	102.82	110.82
1	K	353	GLY	N-CA-C	-8.18	100.81	111.52
1	A	507	THR	N-CA-C	8.11	122.61	112.87
1	G	353	GLY	N-CA-C	-8.11	101.32	111.70
1	K	352	GLY	N-CA-C	-8.09	94.01	113.18
1	M	353	GLY	N-CA-C	-8.06	101.38	111.70
1	C	507	THR	N-CA-C	7.97	122.70	112.34
1	E	507	THR	N-CA-C	7.96	122.42	112.87
1	E	857	ASN	N-CA-C	7.96	120.66	111.11
1	U	353	GLY	N-CA-C	-7.95	101.11	111.52
1	U	261	ASP	N-CA-C	-7.83	103.95	113.97
1	I	353	GLY	N-CA-C	-7.82	101.69	111.70
1	K	730	TYR	CA-C-N	7.81	127.45	119.56
1	K	730	TYR	C-N-CA	7.81	127.45	119.56
2	H	77	VAL	N-CA-C	-7.79	102.51	111.00
1	G	857	ASN	N-CA-C	7.78	120.74	111.33
1	K	76	ILE	CA-C-N	7.77	127.32	118.85
1	K	76	ILE	C-N-CA	7.77	127.32	118.85
1	Q	353	GLY	N-CA-C	-7.73	101.81	111.70
1	E	407	GLY	N-CA-C	7.69	124.23	115.08
1	C	76	ILE	CA-C-N	7.66	127.55	119.05
1	C	76	ILE	C-N-CA	7.66	127.55	119.05
1	O	422	PHE	N-CA-C	7.60	119.21	111.07
2	B	77	VAL	N-CA-C	-7.58	102.74	111.00
1	M	407	GLY	N-CA-C	7.57	124.08	114.25
1	C	857	ASN	N-CA-C	7.56	120.18	111.11
1	G	507	THR	N-CA-C	7.53	121.91	112.87
1	I	401	PHE	CA-C-N	7.51	127.50	119.76
1	I	401	PHE	C-N-CA	7.51	127.50	119.76
2	P	23	CYS	CB-CA-C	-7.48	99.14	110.88
1	W	104	ASP	CA-C-N	7.47	127.01	119.24
1	W	104	ASP	C-N-CA	7.47	127.01	119.24
1	Q	141	PRO	N-CA-C	-7.45	97.12	112.47
1	W	730	TYR	CA-C-N	7.41	127.05	119.56
1	W	730	TYR	C-N-CA	7.41	127.05	119.56
1	M	141	PRO	N-CA-C	-7.38	97.27	112.47
1	A	401	PHE	CA-C-N	7.34	127.32	119.76
1	A	401	PHE	C-N-CA	7.34	127.32	119.76
1	A	353	GLY	N-CA-C	-7.31	101.95	111.52
1	M	76	ILE	CA-C-N	7.29	126.79	118.85
1	M	76	ILE	C-N-CA	7.29	126.79	118.85
1	E	401	PHE	CA-C-N	7.28	127.26	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	401	PHE	C-N-CA	7.28	127.26	119.76
1	G	141	PRO	N-CA-C	-7.27	97.49	112.47
1	U	76	ILE	CA-C-N	7.25	126.88	119.19
1	U	76	ILE	C-N-CA	7.25	126.88	119.19
2	L	77	VAL	N-CA-C	-7.23	103.41	110.72
1	S	403	GLY	N-CA-C	-7.22	101.48	112.89
1	K	401	PHE	CA-C-N	7.19	127.18	119.78
1	K	401	PHE	C-N-CA	7.19	127.18	119.78
2	T	77	VAL	N-CA-C	-7.18	103.78	110.53
1	Q	224	GLY	N-CA-C	-7.18	96.17	113.18
1	Q	403	GLY	N-CA-C	-7.17	101.56	112.89
1	K	261	ASP	N-CA-C	-7.15	104.70	113.50
1	C	401	PHE	CA-C-N	7.12	127.17	119.90
1	C	401	PHE	C-N-CA	7.12	127.17	119.90
1	E	500	HIS	N-CA-C	7.10	120.83	111.75
2	R	23	CYS	CB-CA-C	-7.07	100.08	110.96
1	E	76	ILE	CA-C-N	7.05	126.30	118.97
1	E	76	ILE	C-N-CA	7.05	126.30	118.97
1	U	771	ILE	N-CA-C	7.05	119.21	108.71
1	W	407	GLY	N-CA-C	7.05	123.47	115.08
2	B	23	CYS	CB-CA-C	-7.00	100.18	110.96
1	A	224	GLY	N-CA-C	-6.99	96.62	113.18
1	O	730	TYR	CA-C-N	6.91	126.53	119.56
1	O	730	TYR	C-N-CA	6.91	126.53	119.56
1	E	224	GLY	N-CA-C	-6.90	96.82	113.18
1	U	407	GLY	N-CA-C	6.88	123.27	115.08
2	N	109	CYS	CB-CA-C	-6.88	103.36	110.17
1	A	141	PRO	N-CA-C	-6.88	98.30	112.47
2	X	77	VAL	N-CA-C	-6.85	103.32	113.39
1	S	736	SER	CA-C-N	6.82	128.37	119.84
1	S	736	SER	C-N-CA	6.82	128.37	119.84
1	C	500	HIS	N-CA-C	6.78	120.43	111.75
1	C	296	ASN	N-CA-C	6.77	121.21	112.41
2	T	45	TRP	N-CA-C	-6.76	103.15	111.33
2	N	23	CYS	CB-CA-C	-6.72	100.61	110.96
1	G	224	GLY	N-CA-C	-6.70	97.30	113.18
1	U	730	TYR	CA-C-N	6.70	126.33	119.56
1	U	730	TYR	C-N-CA	6.70	126.33	119.56
1	O	407	GLY	N-CA-C	6.70	123.05	115.08
1	Q	407	GLY	N-CA-C	6.69	123.90	115.21
1	O	141	PRO	N-CA-C	-6.69	98.70	112.47
1	A	730	TYR	CA-C-N	6.65	126.28	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	730	TYR	C-N-CA	6.65	126.28	119.56
1	I	141	PRO	N-CA-C	-6.65	98.77	112.47
1	G	771	ILE	N-CA-C	6.64	118.61	108.71
1	O	76	ILE	CA-C-N	6.64	126.42	119.05
1	O	76	ILE	C-N-CA	6.64	126.42	119.05
1	O	224	GLY	N-CA-C	-6.62	97.48	113.18
1	S	730	TYR	CA-C-N	6.62	126.25	119.56
1	S	730	TYR	C-N-CA	6.62	126.25	119.56
2	F	23	CYS	CB-CA-C	-6.61	100.51	110.88
1	K	858	ASN	N-CA-C	6.59	122.47	113.37
1	K	141	PRO	N-CA-C	-6.59	98.90	112.47
2	F	27	HIS	N-CA-C	6.59	121.98	113.88
1	S	141	PRO	N-CA-C	-6.59	98.90	112.47
1	G	407	GLY	N-CA-C	6.58	122.91	115.08
1	I	176	TRP	N-CA-C	6.57	121.58	113.50
1	Q	771	ILE	N-CA-C	6.55	118.48	108.71
1	S	261	ASP	N-CA-C	-6.55	105.44	113.50
1	M	104	ASP	CA-C-N	6.54	126.05	119.24
1	M	104	ASP	C-N-CA	6.54	126.05	119.24
2	N	77	VAL	N-CA-C	-6.54	103.87	111.00
1	W	224	GLY	N-CA-C	-6.54	97.69	113.18
1	S	401	PHE	CA-C-N	6.53	126.48	119.76
1	S	401	PHE	C-N-CA	6.53	126.48	119.76
1	C	141	PRO	N-CA-C	-6.52	99.03	112.47
1	M	500	HIS	N-CA-C	6.52	120.09	111.75
1	K	224	GLY	N-CA-C	-6.51	97.75	113.18
1	S	857	ASN	N-CA-C	6.50	122.09	111.37
2	H	23	CYS	CB-CA-C	-6.50	100.95	110.96
1	Q	104	ASP	CA-C-N	6.50	125.73	118.97
1	Q	104	ASP	C-N-CA	6.50	125.73	118.97
1	A	261	ASP	N-CA-C	-6.49	105.52	113.50
1	W	261	ASP	N-CA-C	-6.49	105.52	113.50
1	G	858	ASN	N-CA-C	6.47	122.29	113.37
1	K	407	GLY	N-CA-C	6.46	122.76	115.08
1	C	721	GLN	N-CA-C	6.44	118.30	111.28
1	I	500	HIS	N-CA-C	6.44	120.00	111.75
1	K	500	HIS	N-CA-C	6.43	119.98	111.75
1	U	141	PRO	N-CA-C	-6.42	99.24	112.47
1	E	730	TYR	CA-C-N	6.41	126.54	119.87
1	E	730	TYR	C-N-CA	6.41	126.54	119.87
1	M	224	GLY	N-CA-C	-6.40	98.01	113.18
1	U	104	ASP	CA-C-N	6.39	125.89	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	104	ASP	C-N-CA	6.39	125.89	119.24
1	U	143	SER	N-CA-C	6.38	117.90	111.07
1	I	771	ILE	N-CA-C	6.36	118.18	108.71
1	A	500	HIS	N-CA-C	6.33	119.85	111.75
1	W	500	HIS	N-CA-C	6.31	118.97	111.71
1	A	736	SER	CA-C-N	6.30	127.72	119.84
1	A	736	SER	C-N-CA	6.30	127.72	119.84
1	E	824	ASP	CA-C-N	6.30	126.63	119.83
1	E	824	ASP	C-N-CA	6.30	126.63	119.83
2	L	19	CYS	CB-CA-C	-6.29	97.90	110.42
1	M	403	GLY	N-CA-C	-6.29	101.75	112.51
1	A	403	GLY	N-CA-C	-6.29	103.02	113.02
1	E	771	ILE	N-CA-C	6.29	118.08	108.71
1	G	218	ASP	CA-C-N	6.28	126.48	119.32
1	G	218	ASP	C-N-CA	6.28	126.48	119.32
2	H	267	VAL	N-CA-C	6.27	117.50	108.48
1	W	14	GLY	CA-C-N	6.27	126.23	119.78
1	W	14	GLY	C-N-CA	6.27	126.23	119.78
2	R	19	CYS	CB-CA-C	-6.24	98.00	110.42
1	K	200	ASP	N-CA-C	6.24	120.14	111.90
1	C	261	ASP	N-CA-C	-6.24	105.83	113.50
1	K	422	PHE	N-CA-C	6.23	117.74	111.07
1	S	645	ASN	CA-C-N	6.23	127.63	119.84
1	S	645	ASN	C-N-CA	6.23	127.63	119.84
2	N	145	CYS	CB-CA-C	-6.22	101.38	110.96
2	N	19	CYS	CB-CA-C	-6.21	98.06	110.42
1	O	109	TYR	N-CA-C	6.20	119.64	109.85
1	W	400	TYR	N-CA-C	6.20	118.62	108.52
1	I	218	ASP	CA-C-N	6.20	126.38	119.32
1	I	218	ASP	C-N-CA	6.20	126.38	119.32
2	R	27	HIS	N-CA-C	6.19	121.90	113.97
1	W	141	PRO	N-CA-C	-6.18	99.73	112.47
1	C	407	GLY	N-CA-C	6.18	122.44	115.08
1	E	176	TRP	N-CA-C	6.18	121.10	113.50
1	C	771	ILE	N-CA-C	6.17	117.91	108.71
1	G	824	ASP	CA-C-N	6.17	126.12	119.76
1	G	824	ASP	C-N-CA	6.17	126.12	119.76
1	O	149	ASN	N-CA-C	6.17	118.01	111.28
1	U	224	GLY	N-CA-C	-6.17	98.55	113.18
1	E	403	GLY	N-CA-C	-6.16	103.22	113.02
1	M	109	TYR	N-CA-C	6.15	119.72	109.95
1	G	736	SER	CA-C-N	6.14	127.52	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	736	SER	C-N-CA	6.14	127.52	119.84
1	O	261	ASP	N-CA-C	-6.14	105.92	113.41
1	M	771	ILE	N-CA-C	6.12	118.18	108.87
1	W	109	TYR	N-CA-C	6.12	119.52	109.72
1	S	224	GLY	N-CA-C	-6.12	98.67	113.18
2	L	23	CYS	CB-CA-C	-6.12	101.53	110.96
1	I	403	GLY	N-CA-C	-6.12	103.22	112.89
1	U	401	PHE	CA-C-N	6.11	126.05	119.76
1	U	401	PHE	C-N-CA	6.11	126.05	119.76
2	V	267	VAL	N-CA-C	6.10	117.26	108.48
1	A	858	ASN	N-CA-C	6.10	121.78	113.37
2	J	27	HIS	N-CA-C	6.10	121.77	113.97
1	C	645	ASN	CA-C-N	6.09	126.27	119.32
1	C	645	ASN	C-N-CA	6.09	126.27	119.32
1	U	500	HIS	N-CA-C	6.09	120.26	112.34
2	H	109	CYS	CB-CA-C	-6.08	104.15	110.17
2	B	267	VAL	N-CA-C	6.07	117.33	108.53
1	C	224	GLY	N-CA-C	-6.07	98.79	113.18
1	C	109	TYR	N-CA-C	6.07	119.54	110.14
1	O	463	TRP	N-CA-C	6.06	116.09	108.45
1	G	17	PHE	N-CA-C	-6.06	99.36	109.24
1	I	210	GLU	N-CA-C	-6.06	106.87	114.56
1	W	771	ILE	N-CA-C	6.05	117.72	108.71
1	C	730	TYR	CA-C-N	6.04	125.66	119.56
1	C	730	TYR	C-N-CA	6.04	125.66	119.56
2	R	154	TYR	N-CA-C	6.04	119.92	110.32
1	U	400	TYR	N-CA-C	6.04	118.25	108.41
1	A	144	HIS	N-CA-C	6.02	119.47	110.14
1	I	857	ASN	N-CA-C	6.02	121.30	111.37
1	I	224	GLY	N-CA-C	-6.01	98.93	113.18
1	A	647	ASN	N-CA-C	6.01	120.45	113.18
1	M	144	HIS	N-CA-C	6.01	118.97	110.14
1	I	407	GLY	N-CA-C	6.01	123.14	114.67
1	S	422	PHE	N-CA-C	6.00	117.49	111.07
2	T	23	CYS	CB-CA-C	-5.99	101.73	110.96
1	E	141	PRO	N-CA-C	-5.98	100.16	112.47
2	N	232	PHE	N-CA-C	-5.98	105.64	113.17
1	Q	857	ASN	N-CA-C	5.97	121.23	111.37
1	S	793	TYR	N-CA-C	5.97	117.32	108.60
1	O	296	ASN	N-CA-C	5.95	120.56	112.88
1	G	841	ILE	N-CA-C	-5.95	103.47	111.44
1	S	500	HIS	N-CA-C	5.94	119.36	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	17	PHE	N-CA-C	-5.94	99.56	109.24
2	H	45	TRP	N-CA-C	-5.94	104.88	111.71
2	H	37	ALA	N-CA-C	-5.92	102.89	110.53
2	B	27	HIS	N-CA-C	5.91	121.94	114.31
1	C	393	VAL	CA-C-N	5.91	127.23	119.84
1	C	393	VAL	C-N-CA	5.91	127.23	119.84
1	I	730	TYR	CA-C-N	5.91	125.52	119.56
1	I	730	TYR	C-N-CA	5.91	125.52	119.56
2	H	19	CYS	CB-CA-C	-5.90	98.69	110.42
1	M	227	ALA	N-CA-C	5.90	119.78	112.59
1	M	452	ILE	CB-CA-C	-5.89	108.10	113.70
1	K	507	THR	N-CA-C	5.88	123.33	110.80
1	E	109	TYR	N-CA-C	5.87	119.11	109.72
1	M	645	ASN	CA-C-N	5.87	125.56	119.05
1	M	645	ASN	C-N-CA	5.87	125.56	119.05
1	E	144	HIS	N-CA-C	5.86	118.76	110.14
1	S	407	GLY	N-CA-C	5.86	122.83	115.21
2	X	267	VAL	N-CA-C	5.86	117.03	108.53
1	K	325	SER	N-CA-C	5.86	120.71	113.50
2	L	267	VAL	N-CA-C	5.86	116.31	108.11
1	C	210	GLU	N-CA-C	-5.85	106.79	114.04
1	S	176	TRP	N-CA-C	5.85	120.57	113.38
1	O	17	PHE	N-CA-C	-5.84	99.76	109.46
1	I	109	TYR	N-CA-C	5.84	119.19	110.14
1	O	721	GLN	N-CA-C	5.84	117.64	111.28
2	T	154	TYR	N-CA-C	5.84	119.77	109.96
2	B	45	TRP	N-CA-C	-5.83	104.27	111.33
2	J	19	CYS	CB-CA-C	-5.83	98.81	110.42
1	O	500	HIS	N-CA-C	5.83	119.22	111.75
2	R	232	PHE	N-CA-C	-5.82	105.83	113.17
1	M	857	ASN	N-CA-C	5.81	120.96	111.37
1	O	210	GLU	N-CA-C	-5.81	106.83	114.04
2	B	74	ALA	N-CA-C	5.81	119.75	109.58
1	S	822	VAL	N-CA-C	5.79	116.45	107.99
1	I	149	ASN	N-CA-C	5.79	117.67	111.36
1	I	822	VAL	N-CA-C	5.79	116.44	107.99
1	O	857	ASN	N-CA-C	5.79	120.92	111.37
1	G	176	TRP	N-CA-C	5.78	120.61	113.50
1	G	210	GLU	N-CA-C	-5.78	106.87	114.04
2	B	19	CYS	CB-CA-C	-5.78	98.92	110.42
1	Q	422	PHE	N-CA-C	5.78	117.66	111.36
2	J	23	CYS	CB-CA-C	-5.77	102.08	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	507	THR	N-CA-C	5.76	123.08	110.80
1	U	325	SER	N-CA-C	5.76	120.38	113.23
2	P	267	VAL	N-CA-C	5.76	116.77	108.48
1	E	17	PHE	N-CA-C	-5.76	99.86	109.24
1	O	2	GLY	N-CA-C	5.75	118.62	110.74
1	A	109	TYR	N-CA-C	5.74	118.92	109.85
1	Q	218	ASP	CA-C-N	5.74	125.86	119.32
1	Q	218	ASP	C-N-CA	5.74	125.86	119.32
1	W	76	ILE	CA-C-N	5.73	125.27	119.19
1	W	76	ILE	C-N-CA	5.73	125.27	119.19
1	Q	144	HIS	N-CA-C	5.73	118.57	110.14
1	K	771	ILE	N-CA-C	5.72	117.24	108.71
1	K	172	ASN	N-CA-C	-5.72	102.18	110.08
1	I	144	HIS	N-CA-C	5.71	118.53	110.14
2	F	19	CYS	CB-CA-C	-5.71	99.06	110.42
1	I	507	THR	N-CA-C	5.70	122.95	110.80
1	W	197	GLU	N-CA-C	-5.70	103.01	110.53
2	T	19	CYS	CB-CA-C	-5.70	99.08	110.42
1	E	261	ASP	N-CA-C	-5.70	106.17	113.23
1	E	858	ASN	N-CA-C	5.69	121.22	113.37
1	A	422	PHE	N-CA-C	5.68	117.15	111.07
2	H	154	TYR	N-CA-C	5.68	119.36	110.32
1	Q	176	TRP	N-CA-C	5.68	120.37	113.38
1	Q	200	ASP	N-CA-C	5.68	119.40	111.90
2	V	23	CYS	CB-CA-C	-5.67	101.97	110.88
1	I	452	ILE	CB-CA-C	-5.67	108.34	114.35
1	K	822	VAL	N-CA-C	5.67	116.27	107.99
1	A	771	ILE	N-CA-C	5.67	117.16	108.71
1	Q	393	VAL	CA-C-N	5.67	126.93	119.84
1	Q	393	VAL	C-N-CA	5.67	126.93	119.84
1	C	197	GLU	N-CA-C	-5.66	103.06	110.53
2	L	37	ALA	N-CA-C	-5.66	102.54	110.35
1	M	236	GLN	N-CA-C	-5.66	105.19	111.36
1	W	858	ASN	N-CA-C	5.66	121.18	113.37
2	F	267	VAL	N-CA-C	5.65	116.62	108.48
1	G	30	PRO	N-CA-C	-5.65	103.31	111.22
1	M	507	THR	N-CA-C	5.64	122.82	110.80
1	Q	858	ASN	N-CA-C	5.64	121.16	113.37
2	F	154	TYR	N-CA-C	5.64	119.29	110.32
1	U	227	ALA	N-CA-C	5.64	119.70	112.26
1	G	109	TYR	N-CA-C	5.64	118.76	109.85
1	Q	143	SER	N-CA-C	5.63	117.87	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	433	PHE	CA-C-N	5.63	125.61	120.21
1	M	433	PHE	C-N-CA	5.63	125.61	120.21
1	E	793	TYR	N-CA-C	5.63	116.81	108.60
1	I	104	ASP	CA-C-N	5.61	125.07	119.24
1	I	104	ASP	C-N-CA	5.61	125.07	119.24
1	S	296	ASN	N-CA-C	5.60	120.11	112.88
1	C	144	HIS	N-CA-C	5.60	118.75	110.46
1	O	822	VAL	N-CA-C	5.60	116.16	107.99
1	O	143	SER	N-CA-C	5.59	117.05	111.07
1	I	736	SER	CA-C-N	5.59	126.82	119.84
1	I	736	SER	C-N-CA	5.59	126.82	119.84
1	G	645	ASN	CA-C-N	5.58	125.69	119.32
1	G	645	ASN	C-N-CA	5.58	125.69	119.32
1	S	227	ALA	N-CA-C	5.58	119.40	112.59
2	T	74	ALA	CA-C-N	5.57	125.23	119.05
2	T	74	ALA	C-N-CA	5.57	125.23	119.05
2	D	23	CYS	CB-CA-C	-5.57	102.39	110.96
1	K	143	SER	N-CA-C	5.57	117.79	111.11
1	A	210	GLU	N-CA-C	-5.56	107.14	114.31
2	X	19	CYS	CB-CA-C	-5.54	99.39	110.42
1	E	200	ASP	N-CA-C	5.54	119.22	111.90
1	G	400	TYR	N-CA-C	5.54	117.55	108.52
2	H	27	HIS	N-CA-C	5.54	120.69	113.88
1	K	109	TYR	N-CA-C	5.54	118.76	109.95
1	Q	17	PHE	N-CA-C	-5.54	100.22	109.24
1	W	822	VAL	N-CA-C	5.53	116.06	107.99
2	X	23	CYS	CB-CA-C	-5.52	102.21	110.88
1	W	433	PHE	CA-C-N	5.52	125.51	120.21
1	W	433	PHE	C-N-CA	5.52	125.51	120.21
1	K	210	GLU	N-CA-C	-5.51	107.21	114.04
1	S	144	HIS	N-CA-C	5.51	118.24	110.14
1	A	822	VAL	N-CA-C	5.51	116.03	107.99
2	J	267	VAL	N-CA-C	5.51	116.41	108.48
1	W	401	PHE	CA-C-N	5.50	125.44	119.78
1	W	401	PHE	C-N-CA	5.50	125.44	119.78
2	P	27	HIS	N-CA-C	5.50	120.86	114.04
1	E	32	ASP	CA-C-O	-5.49	114.60	120.92
1	Q	500	HIS	N-CA-C	5.49	119.48	112.34
1	M	858	ASN	N-CA-C	5.49	120.95	113.37
1	Q	197	GLU	N-CA-C	-5.49	103.66	110.41
1	S	210	GLU	N-CA-C	-5.49	107.23	114.04
1	M	199	TYR	N-CA-C	5.48	118.02	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	176	TRP	N-CA-C	5.47	120.11	113.38
1	O	227	ALA	N-CA-C	5.47	119.48	112.26
1	O	403	GLY	N-CA-C	-5.47	104.25	112.89
2	X	27	HIS	N-CA-C	5.47	120.44	113.55
1	U	172	ASN	N-CA-C	-5.46	102.33	110.20
2	D	45	TRP	N-CA-C	-5.46	104.76	111.75
2	N	27	HIS	N-CA-C	5.46	120.81	114.04
2	P	154	TYR	N-CA-C	5.45	118.99	110.32
1	E	218	ASP	CA-C-N	5.45	125.54	119.32
1	E	218	ASP	C-N-CA	5.45	125.54	119.32
1	M	691	ILE	N-CA-C	-5.45	98.06	106.72
2	X	177	LYS	CA-C-N	5.45	125.10	119.05
2	X	177	LYS	C-N-CA	5.45	125.10	119.05
1	E	210	GLU	N-CA-C	-5.45	107.64	114.56
2	B	145	CYS	CB-CA-C	-5.44	99.59	110.42
1	I	691	ILE	N-CA-C	-5.44	98.07	106.72
1	I	858	ASN	N-CA-C	5.44	120.88	113.37
1	G	144	HIS	N-CA-C	5.43	118.12	110.14
1	Q	210	GLU	N-CA-C	-5.43	107.31	114.31
2	T	232	PHE	N-CA-C	-5.43	106.24	112.92
2	P	19	CYS	CB-CA-C	-5.42	99.63	110.42
2	F	232	PHE	N-CA-C	-5.42	106.25	112.92
1	U	14	GLY	CA-C-N	5.42	125.33	119.85
1	U	14	GLY	C-N-CA	5.42	125.33	119.85
1	U	645	ASN	CA-C-N	5.42	125.50	119.32
1	U	645	ASN	C-N-CA	5.42	125.50	119.32
1	M	261	ASP	N-CA-C	-5.41	106.52	113.23
1	I	199	TYR	N-CA-C	5.41	118.19	110.24
1	K	227	ALA	N-CA-C	5.41	119.40	112.26
1	K	400	TYR	N-CA-C	5.40	117.32	108.52
1	C	259	VAL	N-CA-C	5.40	117.60	111.88
1	C	858	ASN	N-CA-C	5.39	120.81	113.37
1	G	730	TYR	CA-C-N	5.39	125.86	120.04
1	G	730	TYR	C-N-CA	5.39	125.86	120.04
2	J	154	TYR	N-CA-C	5.39	118.89	110.32
1	U	565	TYR	N-CA-C	-5.39	106.54	113.01
1	K	518	SER	N-CA-C	-5.39	106.21	112.89
1	U	149	ASN	N-CA-C	5.39	116.83	111.07
1	E	442	SER	N-CA-C	5.38	117.15	111.28
2	P	45	TRP	N-CA-C	-5.38	104.82	111.33
1	G	172	ASN	N-CA-C	-5.38	102.38	110.24
2	D	267	VAL	N-CA-C	5.38	116.22	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	254	HIS	N-CA-C	5.38	117.89	111.71
1	A	255	THR	N-CA-C	-5.38	105.50	111.36
1	Q	400	TYR	N-CA-C	5.37	117.27	108.52
1	Q	227	ALA	N-CA-C	5.37	119.35	112.26
1	A	17	PHE	N-CA-C	-5.37	100.49	109.24
1	A	393	VAL	CA-C-N	5.37	126.55	119.84
1	A	393	VAL	C-N-CA	5.37	126.55	119.84
1	Q	149	ASN	N-CA-C	5.37	117.21	111.36
1	K	645	ASN	CA-C-N	5.36	125.43	119.32
1	K	645	ASN	C-N-CA	5.36	125.43	119.32
1	U	403	GLY	N-CA-C	-5.36	102.33	112.51
1	C	172	ASN	N-CA-C	-5.36	102.69	110.08
1	G	273	ALA	N-CA-C	-5.36	105.52	111.36
1	U	793	TYR	N-CA-C	5.36	116.42	108.60
1	E	104	ASP	CA-C-N	5.35	124.80	119.24
1	E	104	ASP	C-N-CA	5.35	124.80	119.24
1	G	691	ILE	N-CA-C	-5.35	98.21	106.72
1	K	857	ASN	N-CA-C	5.35	120.19	111.37
1	Q	261	ASP	N-CA-C	-5.35	105.90	112.90
1	W	53	PRO	N-CA-C	5.34	117.22	110.70
1	G	325	SER	N-CA-C	5.34	120.07	113.50
2	N	37	ALA	N-CA-C	-5.34	103.64	110.53
2	T	267	VAL	N-CA-C	5.34	116.17	108.48
1	C	227	ALA	N-CA-C	5.34	119.31	112.26
2	D	232	PHE	N-CA-C	-5.34	106.36	112.92
1	S	17	PHE	N-CA-C	-5.33	100.56	109.24
1	K	403	GLY	N-CA-C	-5.33	103.40	112.51
1	G	393	VAL	CA-C-N	5.33	126.50	119.84
1	G	393	VAL	C-N-CA	5.33	126.50	119.84
1	E	452	ILE	CB-CA-C	-5.32	108.64	113.70
1	G	200	ASP	N-CA-C	5.32	118.93	111.90
1	I	30	PRO	N-CA-C	-5.32	103.77	111.22
2	V	27	HIS	N-CA-C	5.32	120.78	113.97
1	M	793	TYR	N-CA-C	5.31	117.15	109.07
1	C	793	TYR	N-CA-C	5.31	116.88	108.96
1	W	227	ALA	N-CA-C	5.31	119.27	112.26
1	M	422	PHE	N-CA-C	5.31	117.07	111.28
1	A	841	ILE	N-CA-C	-5.31	104.61	112.04
2	N	267	VAL	N-CA-C	5.31	116.12	108.48
1	M	74	LEU	N-CA-C	-5.30	106.04	112.88
2	T	37	ALA	N-CA-C	-5.30	103.03	110.35
1	U	210	GLU	N-CA-C	-5.30	107.47	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	401	PHE	CA-C-N	5.29	125.21	119.76
1	G	401	PHE	C-N-CA	5.29	125.21	119.76
1	W	192	ARG	N-CA-C	-5.29	105.48	112.94
1	O	325	SER	N-CA-C	5.29	120.00	113.50
1	C	452	ILE	CB-CA-C	-5.28	108.75	114.35
2	B	232	PHE	N-CA-C	-5.27	106.44	112.92
1	S	53	PRO	N-CA-C	5.27	117.13	110.70
1	I	17	PHE	N-CA-C	-5.27	100.65	109.24
2	B	154	TYR	N-CA-C	5.27	118.81	109.96
1	C	422	PHE	N-CA-C	5.26	117.43	111.11
1	M	149	ASN	N-CA-C	5.26	117.02	111.28
1	S	273	ALA	N-CA-C	-5.26	105.22	111.69
2	L	27	HIS	N-CA-C	5.26	121.09	114.31
1	A	400	TYR	N-CA-C	5.26	117.09	108.52
1	A	296	ASN	N-CA-C	5.25	119.65	112.88
1	O	169	ALA	N-CA-C	-5.25	98.11	107.98
1	O	218	ASP	CA-C-N	5.25	124.70	119.24
1	O	218	ASP	C-N-CA	5.25	124.70	119.24
1	W	17	PHE	N-CA-C	-5.25	100.68	109.24
1	M	197	GLU	N-CA-C	-5.25	103.61	110.53
1	M	400	TYR	N-CA-C	5.24	117.05	108.52
1	S	104	ASP	CA-C-N	5.24	124.69	119.24
1	S	104	ASP	C-N-CA	5.24	124.69	119.24
2	L	145	CYS	CB-CA-C	-5.23	102.67	110.88
1	A	208	HIS	N-CA-C	5.23	120.66	113.97
1	Q	841	ILE	N-CA-C	-5.23	104.56	111.09
2	D	154	TYR	N-CA-C	5.22	118.62	110.32
1	I	824	ASP	CA-C-N	5.22	125.14	119.76
1	I	824	ASP	C-N-CA	5.22	125.14	119.76
2	X	95	ASP	CA-C-N	5.22	126.37	119.84
2	X	95	ASP	C-N-CA	5.22	126.37	119.84
1	C	208	HIS	N-CA-C	5.22	121.04	114.31
1	O	255	THR	N-CA-C	-5.22	105.27	111.69
1	U	721	GLN	N-CA-C	5.22	117.71	111.71
2	V	32	TRP	CA-C-N	5.21	126.36	119.84
2	V	32	TRP	C-N-CA	5.21	126.36	119.84
1	Q	109	TYR	N-CA-C	5.21	118.09	109.85
1	I	39	ALA	CA-C-N	5.21	125.14	119.78
1	I	39	ALA	C-N-CA	5.21	125.14	119.78
1	K	863	GLU	N-CA-C	-5.21	101.16	109.23
1	C	433	PHE	CA-C-N	5.21	125.67	120.52
1	C	433	PHE	C-N-CA	5.21	125.67	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	45	TRP	N-CA-C	-5.21	105.03	111.33
1	Q	730	TYR	CA-C-N	5.21	125.28	119.87
1	Q	730	TYR	C-N-CA	5.21	125.28	119.87
1	C	200	ASP	N-CA-C	5.20	118.76	111.90
1	U	109	TYR	N-CA-C	5.20	118.06	109.85
2	V	45	TRP	N-CA-C	-5.20	105.04	111.33
1	C	738	HIS	CA-C-N	5.19	125.44	119.83
1	C	738	HIS	C-N-CA	5.19	125.44	119.83
1	A	363	GLY	N-CA-C	5.19	119.17	112.83
1	W	172	ASN	N-CA-C	-5.19	102.91	110.08
1	W	736	SER	CA-C-N	5.19	126.33	119.84
1	W	736	SER	C-N-CA	5.19	126.33	119.84
1	G	433	PHE	CA-C-N	5.19	125.19	120.21
1	G	433	PHE	C-N-CA	5.19	125.19	120.21
1	Q	691	ILE	N-CA-C	-5.19	98.47	106.72
1	M	433	PHE	N-CA-C	5.18	118.03	109.58
1	O	736	SER	CA-C-N	5.18	126.32	119.84
1	O	736	SER	C-N-CA	5.18	126.32	119.84
1	U	824	ASP	CA-C-N	5.18	125.10	119.76
1	U	824	ASP	C-N-CA	5.18	125.10	119.76
1	O	401	PHE	CA-C-N	5.18	125.10	119.76
1	O	401	PHE	C-N-CA	5.18	125.10	119.76
1	U	30	PRO	N-CA-C	-5.18	103.97	111.22
1	E	227	ALA	N-CA-C	5.18	119.10	112.26
1	S	145	HIS	N-CA-CB	-5.18	103.54	111.56
1	G	143	SER	N-CA-C	5.17	117.32	111.11
1	K	647	ASN	N-CA-C	5.17	119.59	113.28
1	M	463	TRP	N-CA-C	5.17	115.37	108.38
1	U	822	VAL	N-CA-C	5.17	115.54	107.99
1	A	60	ALA	CA-C-N	5.17	124.61	119.24
1	A	60	ALA	C-N-CA	5.17	124.61	119.24
1	M	273	ALA	N-CA-C	-5.17	105.73	111.36
1	O	793	TYR	N-CA-C	5.17	116.66	108.96
1	U	199	TYR	N-CA-C	5.17	117.53	110.24
1	C	498	GLY	CA-C-N	5.16	125.99	120.47
1	C	498	GLY	C-N-CA	5.16	125.99	120.47
1	O	172	ASN	N-CA-C	-5.15	102.97	110.08
1	Q	736	SER	CA-C-N	5.15	126.28	119.84
1	Q	736	SER	C-N-CA	5.15	126.28	119.84
2	D	19	CYS	CB-CA-C	-5.15	100.17	110.42
1	Q	30	PRO	N-CA-C	-5.15	104.01	111.22
1	W	176	TRP	N-CA-C	5.14	119.83	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	793	TYR	N-CA-C	5.14	116.89	109.07
1	A	199	TYR	N-CA-C	5.14	117.55	110.35
2	J	149	CYS	CB-CA-C	-5.14	101.19	109.72
1	W	422	PHE	N-CA-C	5.14	116.57	111.07
1	I	227	ALA	N-CA-C	5.13	119.03	112.26
1	I	645	ASN	CA-C-N	5.13	125.42	119.47
1	I	645	ASN	C-N-CA	5.13	125.42	119.47
1	S	565	TYR	N-CA-C	-5.13	106.86	113.01
1	M	208	HIS	N-CA-C	5.13	120.92	114.31
1	I	793	TYR	N-CA-C	5.12	116.59	108.96
1	K	149	ASN	N-CA-C	5.12	116.86	111.28
2	P	37	ALA	N-CA-C	-5.11	103.30	110.35
1	Q	678	ARG	N-CA-C	5.10	118.47	111.54
1	W	452	ILE	CB-CA-C	-5.10	108.95	114.35
1	S	30	PRO	N-CA-C	-5.09	103.77	111.41
2	D	27	HIS	N-CA-C	5.09	119.84	113.43
1	S	149	ASN	N-CA-C	5.09	116.52	111.07
1	S	199	TYR	N-CA-C	5.09	117.42	110.24
2	X	32	TRP	CA-C-N	5.09	126.20	119.84
2	X	32	TRP	C-N-CA	5.09	126.20	119.84
2	P	128	MET	N-CA-C	-5.08	105.73	112.24
1	I	255	THR	N-CA-C	-5.08	105.83	111.36
2	J	45	TRP	N-CA-C	-5.07	105.19	111.33
1	U	296	ASN	N-CA-C	5.07	119.42	112.88
1	K	145	HIS	N-CA-CB	-5.07	103.70	111.56
2	N	45	TRP	N-CA-C	-5.07	105.19	111.33
2	X	232	PHE	N-CA-C	-5.07	106.68	112.92
1	K	208	HIS	N-CA-C	5.07	120.46	113.97
2	T	224	VAL	N-CA-C	-5.07	108.57	113.53
2	N	154	TYR	N-CA-C	5.06	118.32	110.17
1	M	574	SER	N-CA-C	5.06	117.50	109.50
1	O	540	LEU	CA-C-N	5.06	126.17	119.84
1	O	540	LEU	C-N-CA	5.06	126.17	119.84
1	Q	133	GLY	CA-C-N	5.06	125.09	119.32
1	Q	133	GLY	C-N-CA	5.06	125.09	119.32
1	A	386	MET	N-CA-C	-5.06	100.49	108.73
1	C	400	TYR	N-CA-C	5.06	116.76	108.52
2	L	154	TYR	N-CA-C	5.05	118.35	110.32
1	C	236	GLN	N-CA-C	-5.05	105.86	111.36
1	U	176	TRP	N-CA-C	5.05	119.71	113.50
1	G	261	ASP	N-CA-C	-5.05	107.29	113.50
1	O	145	HIS	N-CA-CB	-5.04	103.74	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	76	ILE	CA-C-N	5.04	126.14	119.84
1	I	76	ILE	C-N-CA	5.04	126.14	119.84
1	W	133	GLY	CA-C-N	5.04	124.82	119.28
1	W	133	GLY	C-N-CA	5.04	124.82	119.28
1	M	611	ASP	N-CA-C	-5.04	103.29	110.59
1	K	74	LEU	N-CA-C	-5.03	106.73	112.92
1	O	858	ASN	N-CA-C	5.03	121.52	110.80
1	A	53	PRO	N-CA-C	5.03	116.84	110.70
1	C	325	SER	N-CA-C	5.03	119.47	113.23
1	Q	645	ASN	CA-C-N	5.03	124.75	119.82
1	Q	645	ASN	C-N-CA	5.03	124.75	119.82
1	O	565	TYR	N-CA-C	-5.03	106.98	113.01
1	E	678	ARG	N-CA-C	5.02	118.13	111.30
1	M	39	ALA	CA-C-N	5.02	125.30	119.92
1	M	39	ALA	C-N-CA	5.02	125.30	119.92
1	S	200	ASP	N-CA-C	5.02	118.53	111.90
1	A	691	ILE	N-CA-C	-5.02	98.74	106.72
1	C	255	THR	N-CA-C	-5.01	105.89	111.36
1	W	218	ASP	CA-C-N	5.01	124.45	119.24
1	W	218	ASP	C-N-CA	5.01	124.45	119.24
1	I	433	PHE	CA-C-N	5.01	125.02	120.21
1	I	433	PHE	C-N-CA	5.01	125.02	120.21
1	U	53	PRO	N-CA-C	5.00	116.80	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6998	0	6632	169	0
1	C	6998	0	6632	193	0
1	E	6998	0	6632	176	0
1	G	6998	0	6632	161	0
1	I	6998	0	6632	178	0
1	K	6998	0	6632	164	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	6998	0	6632	188	0
1	O	6998	0	6632	199	0
1	Q	6998	0	6632	194	0
1	S	6998	0	6632	182	0
1	U	6998	0	6632	197	0
1	W	6998	0	6632	195	0
2	B	2182	0	2077	79	0
2	D	2182	0	2077	92	0
2	F	2182	0	2077	85	0
2	H	2182	0	2077	75	0
2	J	2182	0	2077	81	0
2	L	2182	0	2077	84	0
2	N	2182	0	2077	92	0
2	P	2182	0	2077	93	0
2	R	2182	0	2077	78	0
2	T	2182	0	2077	84	0
2	V	2182	0	2077	68	0
2	X	2182	0	2077	105	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
3	W	1	0	0	0	0
3	X	1	0	0	0	0
4	A	94	0	44	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	94	0	44	13	0
4	E	94	0	44	14	0
4	G	94	0	44	11	0
4	I	94	0	44	12	0
4	K	94	0	44	13	0
4	M	94	0	44	15	0
4	O	94	0	44	12	0
4	Q	94	0	44	10	0
4	S	94	0	44	11	0
4	U	94	0	44	13	0
4	W	94	0	44	12	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
5	M	1	0	0	0	0
5	O	1	0	0	0	0
5	Q	1	0	0	0	0
5	S	1	0	0	0	0
5	U	1	0	0	0	0
5	W	1	0	0	0	0
6	A	9	0	5	1	0
6	C	9	0	5	0	0
6	E	9	0	5	1	0
6	G	9	0	5	0	0
6	I	9	0	5	1	0
6	K	9	0	5	0	0
6	M	9	0	5	1	0
6	O	9	0	5	1	0
6	Q	9	0	5	1	0
6	S	9	0	5	1	0
6	U	9	0	5	1	0
6	W	9	0	5	0	0
7	B	24	0	0	4	0
7	D	24	0	0	4	0
7	F	24	0	0	4	0
7	H	24	0	0	4	0
7	J	24	0	0	4	0
7	L	24	0	0	4	0
7	N	24	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	24	0	0	4	0
7	R	24	0	0	3	0
7	T	24	0	0	4	0
7	V	24	0	0	4	0
7	X	24	0	0	5	0
8	A	681	0	0	10	0
8	B	170	0	0	1	0
8	C	681	0	0	15	0
8	D	166	0	0	2	0
8	E	684	0	0	9	0
8	F	163	0	0	4	0
8	G	683	0	0	9	0
8	H	161	0	0	1	0
8	I	671	0	0	11	0
8	J	163	0	0	2	0
8	K	681	0	0	10	0
8	L	165	0	0	2	0
8	M	684	0	0	11	0
8	N	159	0	0	5	0
8	O	672	0	0	21	0
8	P	164	0	0	4	0
8	Q	690	0	0	14	0
8	R	161	0	0	0	0
8	S	663	0	0	16	0
8	T	163	0	0	1	0
8	U	668	0	0	12	0
8	V	157	0	0	0	0
8	W	675	0	0	20	0
8	X	164	0	0	7	0
All	All	121808	0	105096	3135	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (3135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:CYS:HB2	2:B:126:CYS:HB3	1.36	1.05
2:F:68:CYS:HB2	2:F:126:CYS:HB3	1.40	1.04
1:E:66:PHE:HZ	1:E:146:MET:HE1	1.23	1.03
2:H:68:CYS:HB2	2:H:126:CYS:HB3	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:68:CYS:HB2	2:L:126:CYS:HB3	1.38	1.02
1:G:69:MET:HE2	1:G:754:MET:HE1	1.42	1.01
1:I:66:PHE:HA	1:I:69:MET:HE3	1.43	1.00
1:O:557:CYS:H	1:O:564:ASN:HD21	1.00	1.00
2:R:207:GLY:HA2	1:U:728:VAL:HG12	1.43	1.00
1:S:557:CYS:H	1:S:564:ASN:HD21	1.10	1.00
2:X:68:CYS:HB2	2:X:126:CYS:HB3	1.44	1.00
1:A:557:CYS:H	1:A:564:ASN:HD21	1.10	0.99
2:X:19:CYS:HB3	2:X:145:CYS:HB3	1.42	0.99
1:K:557:CYS:H	1:K:564:ASN:HD21	1.03	0.98
2:J:46:MET:HE1	2:J:66:THR:N	1.79	0.98
1:M:557:CYS:H	1:M:564:ASN:HD21	0.99	0.98
2:P:46:MET:HE1	2:P:66:THR:N	1.79	0.98
1:U:66:PHE:HZ	1:U:146:MET:HE1	1.27	0.98
2:T:68:CYS:HB2	2:T:126:CYS:HB3	1.46	0.97
2:N:68:CYS:HB2	2:N:126:CYS:HB3	1.45	0.96
1:C:66:PHE:HZ	1:C:146:MET:HE1	1.27	0.96
2:J:68:CYS:HB2	2:J:126:CYS:HB3	1.45	0.96
1:K:28:MET:HE1	1:K:66:PHE:HB3	1.49	0.95
2:N:207:GLY:HA2	1:S:728:VAL:HG12	1.44	0.95
2:R:68:CYS:HB2	2:R:126:CYS:HB3	1.48	0.95
1:S:66:PHE:HZ	1:S:146:MET:HE1	1.32	0.95
2:P:2:GLU:HG2	2:P:158:LYS:HG2	1.48	0.94
2:P:68:CYS:HB2	2:P:126:CYS:HB3	1.47	0.94
2:V:68:CYS:HB2	2:V:126:CYS:HB3	1.49	0.94
1:K:66:PHE:HZ	1:K:146:MET:HE1	1.28	0.94
1:A:66:PHE:HZ	1:A:146:MET:HE1	1.32	0.93
2:D:19:CYS:HB3	2:D:145:CYS:HB3	1.47	0.93
1:M:211:MET:HE1	2:N:231:PHE:CZ	2.04	0.93
2:R:46:MET:HE1	2:R:66:THR:N	1.84	0.93
1:G:66:PHE:HA	1:G:69:MET:HE3	1.51	0.93
1:G:557:CYS:H	1:G:564:ASN:HD21	1.14	0.93
1:Q:557:CYS:H	1:Q:564:ASN:HD21	1.02	0.92
2:F:70:HIS:HD2	2:F:92:VAL:H	1.16	0.92
1:C:557:CYS:H	1:C:564:ASN:HD21	1.09	0.92
2:D:23:CYS:HB3	2:D:39:MET:HE1	1.51	0.92
1:E:557:CYS:H	1:E:564:ASN:HD21	1.09	0.92
2:H:105:LEU:HB3	2:H:114:MET:HE1	1.52	0.92
1:Q:426:MET:HA	1:Q:426:MET:HE3	1.52	0.92
1:I:66:PHE:HZ	1:I:146:MET:HE1	1.30	0.91
1:W:557:CYS:H	1:W:564:ASN:HD21	1.12	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:105:LEU:HB3	2:N:114:MET:HE1	1.51	0.91
1:A:66:PHE:HA	1:A:69:MET:HE3	1.51	0.91
1:S:426:MET:HE3	1:S:426:MET:HA	1.52	0.91
2:T:70:HIS:HD2	2:T:92:VAL:H	1.18	0.91
1:A:426:MET:HA	1:A:426:MET:HE3	1.53	0.91
1:E:211:MET:HE1	2:F:231:PHE:CZ	2.05	0.91
1:G:211:MET:HE1	2:H:231:PHE:CZ	2.06	0.91
1:Q:66:PHE:HZ	1:Q:146:MET:HE1	1.35	0.91
1:Q:211:MET:HE1	2:R:231:PHE:CZ	2.05	0.91
2:H:46:MET:HE1	2:H:66:THR:N	1.85	0.91
1:I:557:CYS:H	1:I:564:ASN:HD21	0.91	0.90
1:K:426:MET:HE1	1:K:618:GLN:HG2	1.52	0.90
1:M:426:MET:HA	1:M:426:MET:HE3	1.54	0.90
2:V:46:MET:HE1	2:V:66:THR:N	1.87	0.90
1:M:610:LYS:NZ	1:M:618:GLN:HE22	1.69	0.90
2:T:46:MET:HE1	2:T:66:THR:N	1.87	0.89
1:U:557:CYS:H	1:U:564:ASN:HD21	1.13	0.89
1:Q:66:PHE:CZ	1:Q:146:MET:HE1	2.08	0.89
1:O:426:MET:HA	1:O:426:MET:HE3	1.55	0.89
1:U:66:PHE:CZ	1:U:146:MET:HE1	2.07	0.89
1:E:66:PHE:HA	1:E:69:MET:HE3	1.53	0.89
1:O:100:LEU:HD12	1:O:105:PRO:HG3	1.55	0.89
2:F:68:CYS:HB2	2:F:126:CYS:CB	2.02	0.89
2:L:46:MET:HE1	2:L:66:THR:N	1.88	0.89
1:E:69:MET:HE2	1:E:754:MET:HE1	1.51	0.89
1:K:66:PHE:CZ	1:K:146:MET:HE1	2.07	0.89
2:N:46:MET:HE1	2:N:66:THR:N	1.88	0.88
1:C:360:ALA:HB1	1:C:859:THR:HG23	1.54	0.88
2:D:68:CYS:HB2	2:D:126:CYS:HB3	1.54	0.88
2:H:70:HIS:HD2	2:H:92:VAL:H	1.18	0.88
1:C:66:PHE:HA	1:C:69:MET:HE3	1.54	0.88
1:C:610:LYS:NZ	1:C:618:GLN:HE22	1.69	0.88
1:I:69:MET:HE2	1:I:754:MET:HE1	1.54	0.88
1:A:66:PHE:CZ	1:A:146:MET:HE1	2.09	0.88
2:D:128:MET:HA	7:D:303:SF4:S1	2.14	0.87
2:L:40:GLN:HE22	2:L:118:GLU:H	1.15	0.87
1:W:69:MET:HE2	1:W:754:MET:HE1	1.56	0.87
1:A:69:MET:HE2	1:A:754:MET:CE	2.04	0.87
2:F:46:MET:HE1	2:F:66:THR:N	1.88	0.87
2:N:70:HIS:HD2	2:N:92:VAL:H	1.21	0.87
2:L:142:MET:HE2	2:L:146:ALA:HB1	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:HIS:HD2	2:B:92:VAL:H	1.22	0.87
1:E:66:PHE:CZ	1:E:146:MET:HE1	2.07	0.87
1:Q:211:MET:HE1	2:R:231:PHE:HZ	1.37	0.87
1:C:66:PHE:CZ	1:C:146:MET:HE1	2.08	0.87
1:G:360:ALA:HB1	1:G:859:THR:HG23	1.57	0.87
1:I:66:PHE:CZ	1:I:146:MET:HE1	2.09	0.86
1:I:146:MET:HE3	1:I:545:ASN:OD1	1.75	0.86
1:O:28:MET:HE1	1:O:66:PHE:HB3	1.57	0.86
2:T:68:CYS:HB2	2:T:126:CYS:CB	2.06	0.85
1:O:66:PHE:HZ	1:O:146:MET:HE1	1.40	0.85
2:P:19:CYS:HB3	2:P:145:CYS:HB3	1.57	0.85
1:I:211:MET:HE1	2:J:231:PHE:CZ	2.11	0.85
1:O:146:MET:HE3	1:O:545:ASN:OD1	1.77	0.85
1:O:610:LYS:NZ	1:O:618:GLN:HE22	1.75	0.85
1:O:753:TYR:HB3	2:P:24:MET:HE3	1.59	0.85
1:U:146:MET:HE2	1:U:544:THR:HB	1.58	0.85
2:J:21:MET:HE1	2:J:24:MET:HE3	1.58	0.85
1:A:69:MET:HE2	1:A:754:MET:HE1	1.59	0.85
2:D:46:MET:HE1	2:D:66:THR:N	1.92	0.84
1:A:252:MET:HE3	1:A:263:TRP:CE3	2.12	0.84
2:F:105:LEU:HB3	2:F:114:MET:HE1	1.59	0.84
2:V:23:CYS:HB3	2:V:39:MET:HE1	1.58	0.84
1:O:211:MET:HE1	2:P:231:PHE:CZ	2.12	0.84
2:X:128:MET:HA	7:X:303:SF4:S1	2.16	0.84
2:J:68:CYS:HB2	2:J:126:CYS:CB	2.07	0.84
1:A:211:MET:HE1	2:B:231:PHE:CZ	2.12	0.84
2:R:68:CYS:HB2	2:R:126:CYS:CB	2.06	0.84
1:C:28:MET:HE1	1:C:66:PHE:HB3	1.57	0.84
1:W:610:LYS:NZ	1:W:618:GLN:HE22	1.76	0.84
2:B:68:CYS:HB2	2:B:126:CYS:CB	2.07	0.84
1:I:557:CYS:N	1:I:564:ASN:HD21	1.75	0.84
1:C:146:MET:HE2	1:C:544:THR:HB	1.60	0.84
2:H:76:CYS:HB3	2:H:108:THR:OG1	1.76	0.84
2:P:128:MET:HA	7:P:303:SF4:S1	2.18	0.83
1:M:211:MET:HE1	2:N:231:PHE:HZ	1.43	0.83
1:M:695:LEU:O	1:M:699:GLU:HG2	1.78	0.83
1:O:66:PHE:HA	1:O:69:MET:HE3	1.60	0.83
1:Q:146:MET:HE3	1:Q:545:ASN:OD1	1.78	0.83
1:C:69:MET:HE2	1:C:754:MET:HE1	1.59	0.83
2:P:70:HIS:HD2	2:P:92:VAL:H	1.25	0.83
2:H:68:CYS:HB2	2:H:126:CYS:CB	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:426:MET:CE	1:K:618:GLN:HG2	2.07	0.83
1:Q:426:MET:CE	1:Q:618:GLN:HG2	2.07	0.83
1:S:360:ALA:HB1	1:S:859:THR:HG23	1.58	0.83
2:L:128:MET:HA	7:L:303:SF4:S1	2.17	0.83
2:P:23:CYS:HB3	2:P:39:MET:HE1	1.58	0.83
1:A:426:MET:CE	1:A:618:GLN:HG2	2.09	0.83
2:L:23:CYS:HB3	2:L:39:MET:HE1	1.60	0.83
2:V:128:MET:HA	7:V:303:SF4:S1	2.18	0.83
1:W:66:PHE:HA	1:W:69:MET:HE3	1.60	0.83
2:X:46:MET:HE1	2:X:66:THR:N	1.94	0.83
1:O:426:MET:CE	1:O:618:GLN:HG2	2.08	0.83
1:Q:69:MET:HE2	1:Q:754:MET:CE	2.08	0.83
1:U:426:MET:CE	1:U:618:GLN:HG2	2.09	0.83
1:I:426:MET:HA	1:I:426:MET:HE3	1.59	0.82
2:J:46:MET:HE1	2:J:66:THR:H	1.40	0.82
1:G:610:LYS:NZ	1:G:618:GLN:HE22	1.78	0.82
1:Q:100:LEU:HD21	1:Q:534:PRO:HB2	1.60	0.82
2:L:68:CYS:HB2	2:L:126:CYS:CB	2.08	0.82
1:M:69:MET:HE2	1:M:754:MET:CE	2.09	0.82
1:W:28:MET:HE1	1:W:66:PHE:HB3	1.60	0.82
1:K:69:MET:HE2	1:K:754:MET:CE	2.10	0.82
1:M:28:MET:HE1	1:M:66:PHE:HB3	1.59	0.82
2:R:128:MET:HA	7:R:303:SF4:S1	2.19	0.82
2:D:143:PRO:HB3	7:D:303:SF4:S1	2.18	0.82
1:I:28:MET:HE1	1:I:66:PHE:HB3	1.60	0.82
1:M:610:LYS:HZ3	1:M:618:GLN:HE22	1.27	0.82
2:N:40:GLN:HE22	2:N:118:GLU:H	1.28	0.82
2:B:46:MET:HE1	2:B:66:THR:N	1.94	0.82
1:O:66:PHE:CZ	1:O:146:MET:HE1	2.15	0.82
2:J:128:MET:HA	7:J:302:SF4:S1	2.19	0.81
1:S:69:MET:HE2	1:S:754:MET:HE1	1.61	0.81
1:I:146:MET:HE2	1:I:544:THR:HB	1.61	0.81
1:U:69:MET:HE2	1:U:754:MET:HE1	1.63	0.81
1:U:146:MET:HE3	1:U:545:ASN:OD1	1.80	0.81
2:V:19:CYS:HB3	2:V:145:CYS:HB3	1.60	0.81
1:C:211:MET:HE1	2:D:231:PHE:CZ	2.16	0.81
2:J:70:HIS:HD2	2:J:92:VAL:H	1.26	0.81
2:H:23:CYS:HB3	2:H:39:MET:HE1	1.62	0.81
1:K:146:MET:HE2	1:K:544:THR:HB	1.61	0.81
1:O:146:MET:HE2	1:O:544:THR:HB	1.63	0.81
1:Q:426:MET:HE1	1:Q:618:GLN:HG2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:146:MET:HE3	1:K:545:ASN:OD1	1.80	0.80
1:Q:319:GLU:HG2	1:U:726:LEU:HD13	1.61	0.80
1:A:786:ASN:HD22	1:A:805:VAL:H	1.30	0.80
1:M:557:CYS:N	1:M:564:ASN:HD21	1.80	0.80
1:G:146:MET:HE3	1:G:545:ASN:OD1	1.81	0.80
2:R:70:HIS:HD2	2:R:92:VAL:H	1.29	0.80
2:L:70:HIS:HD2	2:L:92:VAL:H	1.29	0.80
2:N:23:CYS:HB3	2:N:39:MET:HE1	1.62	0.80
2:P:105:LEU:HB3	2:P:114:MET:HE1	1.63	0.80
1:C:141:PRO:HA	1:C:496:TYR:HB3	1.64	0.80
1:A:211:MET:HE1	2:B:231:PHE:HZ	1.47	0.80
1:E:28:MET:HE1	1:E:66:PHE:HB3	1.63	0.80
2:N:21:MET:CE	2:N:24:MET:HE3	2.12	0.80
2:H:68:CYS:CB	2:H:126:CYS:HB3	2.11	0.79
1:C:426:MET:HE3	1:C:426:MET:HA	1.62	0.79
1:Q:66:PHE:HA	1:Q:69:MET:HE3	1.64	0.79
1:I:557:CYS:H	1:I:564:ASN:ND2	1.76	0.79
1:M:360:ALA:HB1	1:M:859:THR:HG23	1.64	0.79
1:E:610:LYS:NZ	1:E:618:GLN:HE22	1.79	0.79
1:A:28:MET:HE1	1:A:66:PHE:HB3	1.62	0.79
1:M:786:ASN:ND2	1:M:804:GLN:HA	1.98	0.79
1:W:146:MET:HE3	1:W:544:THR:HB	1.63	0.79
1:E:69:MET:HE2	1:E:754:MET:CE	2.12	0.79
1:G:629:MET:HE2	1:G:634:PHE:HA	1.65	0.79
1:W:69:MET:HE2	1:W:754:MET:CE	2.13	0.79
2:X:68:CYS:CB	2:X:126:CYS:HB3	2.13	0.79
1:O:786:ASN:ND2	1:O:805:VAL:H	1.81	0.79
1:S:211:MET:HE1	2:T:231:PHE:CZ	2.18	0.79
1:U:695:LEU:O	1:U:699:GLU:HG2	1.82	0.79
1:G:66:PHE:HZ	1:G:146:MET:HE1	1.47	0.78
1:G:823:TYR:CZ	1:G:825:PRO:HG3	2.17	0.78
1:O:823:TYR:CZ	1:O:825:PRO:HG3	2.17	0.78
1:S:66:PHE:CZ	1:S:146:MET:HE1	2.17	0.78
2:T:128:MET:HA	7:T:303:SF4:S1	2.23	0.78
1:U:426:MET:HA	1:U:426:MET:HE3	1.66	0.78
1:S:69:MET:HE2	1:S:754:MET:CE	2.13	0.78
2:F:40:GLN:HE22	2:F:118:GLU:H	1.31	0.78
1:O:610:LYS:HZ3	1:O:618:GLN:HE22	1.29	0.78
2:R:142:MET:HE2	2:R:146:ALA:C	2.08	0.78
1:C:823:TYR:CZ	1:C:825:PRO:HG3	2.19	0.78
1:O:629:MET:HE2	1:O:634:PHE:HA	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:68:CYS:CB	2:V:126:CYS:HB3	2.14	0.78
2:L:166:LYS:O	2:L:170:GLU:HG3	1.84	0.78
1:I:69:MET:HE2	1:I:754:MET:CE	2.13	0.78
1:S:146:MET:HE3	1:S:545:ASN:OD1	1.84	0.78
1:G:69:MET:HE2	1:G:754:MET:CE	2.12	0.78
1:G:146:MET:HE2	1:G:544:THR:HB	1.64	0.78
2:L:68:CYS:CB	2:L:126:CYS:HB3	2.14	0.78
2:N:128:MET:HA	7:N:303:SF4:S1	2.24	0.78
1:U:69:MET:HE2	1:U:754:MET:CE	2.14	0.78
1:U:66:PHE:HA	1:U:69:MET:HE3	1.66	0.77
1:A:146:MET:HE3	1:A:545:ASN:OD1	1.84	0.77
1:E:426:MET:CE	1:E:618:GLN:HG2	2.14	0.77
1:G:28:MET:HE1	1:G:66:PHE:HB3	1.66	0.77
1:I:360:ALA:HB1	1:I:859:THR:HG23	1.64	0.77
1:O:356:GLY:H	4:O:903:MGD:H5'2	1.48	0.77
1:Q:610:LYS:HZ2	1:Q:618:GLN:HE22	1.32	0.77
2:V:70:HIS:HD2	2:V:92:VAL:H	1.32	0.77
1:A:360:ALA:HB1	1:A:859:THR:HG23	1.65	0.77
1:W:252:MET:HE3	1:W:263:TRP:CE3	2.19	0.77
1:E:165:GLY:HA3	1:E:166:PHE:HB3	1.64	0.77
1:K:165:GLY:HA3	1:K:166:PHE:HB3	1.66	0.77
1:A:610:LYS:NZ	1:A:618:GLN:HE22	1.81	0.77
2:T:19:CYS:HB3	2:T:145:CYS:HB3	1.64	0.77
1:U:426:MET:HE1	1:U:618:GLN:HG2	1.64	0.77
1:E:360:ALA:HB1	1:E:859:THR:HG23	1.65	0.77
1:O:557:CYS:N	1:O:564:ASN:HD21	1.81	0.77
2:V:68:CYS:HB2	2:V:126:CYS:CB	2.15	0.77
1:A:503:THR:HG21	4:A:902:MGD:O2A	1.84	0.77
1:K:66:PHE:HA	1:K:69:MET:HE3	1.66	0.77
1:K:610:LYS:NZ	1:K:618:GLN:HE22	1.83	0.77
2:N:21:MET:HE1	2:N:24:MET:HE3	1.64	0.77
1:Q:165:GLY:HA3	1:Q:166:PHE:HB3	1.66	0.77
1:A:426:MET:HE1	1:A:618:GLN:HG2	1.67	0.77
2:L:76:CYS:HB3	2:L:108:THR:OG1	1.85	0.77
1:W:561:ILE:HG22	1:W:564:ASN:HB3	1.66	0.77
1:G:426:MET:HA	1:G:426:MET:HE3	1.67	0.77
1:O:479:GLN:HG2	8:O:1175:HOH:O	1.83	0.76
2:P:68:CYS:HB2	2:P:126:CYS:CB	2.14	0.76
2:L:68:CYS:HB3	2:L:70:HIS:CE1	2.21	0.76
2:D:142:MET:HE2	2:D:146:ALA:HB1	1.65	0.76
1:Q:610:LYS:NZ	1:Q:618:GLN:HE22	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:695:LEU:O	1:S:699:GLU:HG2	1.86	0.76
2:T:68:CYS:CB	2:T:126:CYS:HB3	2.15	0.76
1:O:165:GLY:HA3	1:O:166:PHE:HB3	1.66	0.76
1:I:165:GLY:HA3	1:I:166:PHE:HB3	1.68	0.76
2:J:21:MET:HA	2:J:21:MET:HE3	1.67	0.76
2:H:106:LEU:HD23	2:H:114:MET:HE2	1.68	0.76
2:N:46:MET:HE1	2:N:66:THR:H	1.49	0.76
1:U:211:MET:HE1	2:V:231:PHE:CZ	2.21	0.76
1:K:557:CYS:H	1:K:564:ASN:ND2	1.83	0.76
1:G:141:PRO:HA	1:G:496:TYR:HB3	1.68	0.76
2:H:128:MET:HA	7:H:303:SF4:S1	2.26	0.76
1:S:426:MET:CE	1:S:618:GLN:HG2	2.15	0.76
1:S:753:TYR:HB3	2:T:24:MET:HE3	1.66	0.76
1:W:426:MET:HA	1:W:426:MET:HE3	1.68	0.76
2:X:142:MET:HE2	2:X:146:ALA:HB1	1.67	0.76
2:D:142:MET:HE2	2:D:146:ALA:CB	2.16	0.75
2:F:68:CYS:CB	2:F:126:CYS:HB3	2.16	0.75
2:H:46:MET:HE1	2:H:66:THR:H	1.46	0.75
2:J:23:CYS:HB3	2:J:39:MET:HE1	1.68	0.75
2:T:2:GLU:HG2	2:T:158:LYS:HG2	1.68	0.75
1:A:141:PRO:HA	1:A:496:TYR:HB3	1.68	0.75
1:E:252:MET:HE3	1:E:263:TRP:CE3	2.20	0.75
1:I:823:TYR:CZ	1:I:825:PRO:HG3	2.22	0.75
1:M:823:TYR:CZ	1:M:825:PRO:HG3	2.19	0.75
2:V:76:CYS:HB3	2:V:108:THR:OG1	1.85	0.75
1:C:426:MET:CE	1:C:618:GLN:HG2	2.17	0.75
2:D:68:CYS:CB	2:D:126:CYS:HB3	2.16	0.75
1:G:610:LYS:HZ1	1:G:618:GLN:HE22	1.34	0.75
2:X:23:CYS:HB3	2:X:39:MET:HE1	1.67	0.75
1:I:426:MET:CE	1:I:618:GLN:HG2	2.16	0.75
2:J:40:GLN:NE2	2:J:118:GLU:H	1.84	0.75
1:Q:629:MET:HE2	1:Q:634:PHE:HA	1.68	0.75
1:Q:100:LEU:HD13	1:Q:105:PRO:HG3	1.68	0.75
1:K:426:MET:HE3	1:K:426:MET:HA	1.68	0.75
2:P:76:CYS:HB3	2:P:108:THR:OG1	1.85	0.75
1:Q:69:MET:HE2	1:Q:754:MET:HE1	1.69	0.75
1:W:426:MET:CE	1:W:618:GLN:HG2	2.17	0.75
1:W:645:ASN:ND2	1:W:648:ARG:HB3	2.01	0.75
2:L:59:ASN:HD22	2:L:59:ASN:H	1.35	0.75
2:F:128:MET:HA	7:F:303:SF4:S1	2.27	0.74
1:G:165:GLY:HA3	1:G:166:PHE:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:823:TYR:CZ	1:K:825:PRO:HG3	2.21	0.74
1:M:786:ASN:HD21	1:M:804:GLN:HA	1.49	0.74
2:P:68:CYS:CB	2:P:126:CYS:HB3	2.17	0.74
2:B:68:CYS:CB	2:B:126:CYS:HB3	2.14	0.74
1:U:28:MET:HE1	1:U:66:PHE:HB3	1.69	0.74
2:R:76:CYS:HB3	2:R:108:THR:OG1	1.86	0.74
1:C:146:MET:HE3	1:C:545:ASN:OD1	1.87	0.74
2:R:68:CYS:HB3	2:R:70:HIS:CE1	2.23	0.74
1:M:426:MET:CE	1:M:618:GLN:HG2	2.17	0.73
2:P:46:MET:HE3	2:P:47:ASN:N	2.02	0.73
1:S:100:LEU:HD12	1:S:105:PRO:HG3	1.69	0.73
2:F:106:LEU:HD23	2:F:114:MET:HE2	1.69	0.73
2:J:68:CYS:CB	2:J:126:CYS:HB3	2.18	0.73
2:L:21:MET:HE2	2:L:21:MET:HA	1.68	0.73
2:L:59:ASN:H	2:L:59:ASN:ND2	1.86	0.73
1:K:356:GLY:N	4:K:903:MGD:O2B	2.20	0.73
1:M:141:PRO:HA	1:M:496:TYR:HB3	1.70	0.73
1:O:69:MET:HE2	1:O:754:MET:HE1	1.68	0.73
1:E:426:MET:HA	1:E:426:MET:HE3	1.69	0.73
1:A:356:GLY:N	4:A:903:MGD:O2B	2.20	0.73
1:E:141:PRO:HA	1:E:496:TYR:HB3	1.68	0.73
1:M:165:GLY:HA3	1:M:166:PHE:HB3	1.70	0.73
2:N:142:MET:HE2	2:N:146:ALA:C	2.13	0.73
2:R:68:CYS:CB	2:R:126:CYS:HB3	2.18	0.73
1:S:503:THR:HG21	4:S:902:MGD:O2A	1.88	0.73
1:A:823:TYR:CZ	1:A:825:PRO:HG3	2.23	0.73
2:N:20:PHE:CZ	2:N:24:MET:HE2	2.23	0.73
1:S:610:LYS:NZ	1:S:618:GLN:HE22	1.87	0.73
1:G:394:PRO:HG3	8:G:1319:HOH:O	1.88	0.73
1:G:695:LEU:O	1:G:699:GLU:HG2	1.89	0.73
2:H:21:MET:HE1	2:H:24:MET:HE3	1.68	0.73
1:K:211:MET:HE3	8:K:1447:HOH:O	1.87	0.73
2:F:20:PHE:CZ	2:F:24:MET:HE2	2.24	0.73
1:G:503:THR:HG21	4:G:902:MGD:O2A	1.87	0.73
2:B:128:MET:HA	7:B:303:SF4:S1	2.29	0.72
1:G:66:PHE:CZ	1:G:146:MET:HE1	2.22	0.72
1:S:823:TYR:CZ	1:S:825:PRO:HG3	2.23	0.72
1:I:146:MET:CE	1:I:544:THR:HB	2.19	0.72
2:J:69:MET:HB3	2:J:184:PRO:HB3	1.71	0.72
1:K:360:ALA:HB1	1:K:859:THR:HG23	1.71	0.72
4:A:903:MGD:O2B	4:A:903:MGD:O2A	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:MET:HE2	1:C:754:MET:CE	2.18	0.72
1:I:141:PRO:HA	1:I:496:TYR:HB3	1.71	0.72
1:K:141:PRO:HA	1:K:496:TYR:HB3	1.71	0.72
1:K:629:MET:HE2	1:K:634:PHE:HA	1.70	0.72
1:O:141:PRO:HA	1:O:496:TYR:HB3	1.72	0.72
1:S:211:MET:HE3	8:S:1449:HOH:O	1.89	0.72
2:T:46:MET:HE3	2:T:47:ASN:N	2.04	0.72
1:U:610:LYS:NZ	1:U:618:GLN:HE22	1.86	0.72
1:U:753:TYR:HB3	2:V:24:MET:HE3	1.70	0.72
2:N:68:CYS:CB	2:N:126:CYS:HB3	2.18	0.72
1:A:629:MET:HE2	1:A:634:PHE:HA	1.71	0.72
2:L:19:CYS:HB3	2:L:145:CYS:HB3	1.69	0.72
2:N:2:GLU:HG2	2:N:158:LYS:HG2	1.72	0.72
1:Q:695:LEU:O	1:Q:699:GLU:HG2	1.89	0.72
2:V:142:MET:HE2	2:V:146:ALA:C	2.14	0.72
1:W:356:GLY:H	4:W:903:MGD:H5'2	1.55	0.72
2:J:21:MET:CE	2:J:24:MET:HE3	2.19	0.72
2:N:106:LEU:HD23	2:N:114:MET:HE2	1.71	0.72
1:S:28:MET:HE1	1:S:66:PHE:HB3	1.70	0.72
1:Q:100:LEU:CD2	1:Q:534:PRO:HB2	2.20	0.72
1:S:163:MET:HE1	1:S:606:PHE:HA	1.72	0.72
1:G:100:LEU:HD12	1:G:105:PRO:HG3	1.70	0.72
1:I:610:LYS:NZ	1:I:618:GLN:HE22	1.88	0.72
2:X:143:PRO:HB3	7:X:303:SF4:S1	2.29	0.72
2:H:40:GLN:HE22	2:H:118:GLU:H	1.37	0.71
1:K:211:MET:HE1	2:L:231:PHE:CZ	2.25	0.71
2:T:23:CYS:HB3	2:T:39:MET:HE1	1.72	0.71
1:W:165:GLY:HA3	1:W:166:PHE:HB3	1.71	0.71
1:A:695:LEU:O	1:A:699:GLU:HG2	1.90	0.71
1:G:146:MET:CE	1:G:544:THR:HB	2.20	0.71
1:G:252:MET:HE3	1:G:263:TRP:CE3	2.25	0.71
1:I:695:LEU:O	1:I:699:GLU:HG2	1.90	0.71
1:S:356:GLY:H	4:S:903:MGD:H5'2	1.53	0.71
2:X:100:LYS:HG2	2:X:122:VAL:HB	1.72	0.71
2:B:68:CYS:HB3	2:B:70:HIS:CE1	2.25	0.71
2:N:76:CYS:HB3	2:N:108:THR:OG1	1.90	0.71
2:D:105:LEU:HB3	2:D:114:MET:HE1	1.72	0.71
1:M:100:LEU:HD12	1:M:105:PRO:HG3	1.72	0.71
2:P:40:GLN:HE22	2:P:118:GLU:H	1.37	0.71
1:Q:691:ILE:HD11	1:Q:711:MET:HE3	1.73	0.71
1:Q:823:TYR:CZ	1:Q:825:PRO:HG3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:165:GLY:HA3	1:U:166:PHE:HB3	1.70	0.71
1:C:356:GLY:H	4:C:903:MGD:H5'2	1.56	0.71
1:M:66:PHE:HA	1:M:69:MET:HE3	1.71	0.71
1:W:141:PRO:HA	1:W:496:TYR:HB3	1.72	0.71
2:B:23:CYS:HB3	2:B:39:MET:HE1	1.71	0.71
2:P:59:ASN:H	2:P:59:ASN:HD22	1.37	0.71
2:R:23:CYS:HB3	2:R:39:MET:HE1	1.73	0.71
1:W:557:CYS:N	1:W:564:ASN:HD21	1.88	0.71
1:C:695:LEU:O	1:C:699:GLU:HG2	1.89	0.71
2:D:76:CYS:HB3	2:D:108:THR:OG1	1.90	0.71
1:E:610:LYS:HZ2	1:E:618:GLN:HE22	1.36	0.71
2:N:21:MET:HA	2:N:21:MET:HE3	1.72	0.71
1:Q:218:ASP:OD2	1:Q:253:ASN:HB2	1.90	0.71
1:U:823:TYR:CZ	1:U:825:PRO:HG3	2.26	0.71
1:I:211:MET:HE1	2:J:231:PHE:HZ	1.55	0.71
2:J:71:CYS:HB2	2:J:182:THR:O	1.91	0.71
2:J:142:MET:HE2	2:J:146:ALA:CB	2.20	0.71
1:M:696:LYS:O	1:M:700:GLU:HG3	1.91	0.71
2:X:142:MET:HE2	2:X:146:ALA:CB	2.20	0.71
2:D:75:PRO:HD2	7:D:304:SF4:S4	2.31	0.70
1:K:695:LEU:O	1:K:699:GLU:HG2	1.90	0.70
2:N:21:MET:CE	2:N:21:MET:HA	2.22	0.70
2:V:143:PRO:HB3	7:V:303:SF4:S1	2.31	0.70
2:X:87:ARG:HG3	2:X:91:ILE:O	1.92	0.70
1:M:426:MET:HE1	1:M:618:GLN:HG2	1.73	0.70
2:H:70:HIS:CD2	2:H:92:VAL:H	2.07	0.70
2:N:68:CYS:HB2	2:N:126:CYS:CB	2.19	0.70
2:P:114:MET:HE3	2:P:123:ALA:HB1	1.73	0.70
2:R:143:PRO:HB3	7:R:303:SF4:S1	2.31	0.70
1:S:66:PHE:HA	1:S:69:MET:HE3	1.72	0.70
1:W:360:ALA:HB1	1:W:859:THR:HG23	1.74	0.70
1:I:629:MET:HE2	1:I:634:PHE:HA	1.74	0.70
2:J:20:PHE:CZ	2:J:24:MET:HE2	2.26	0.70
1:O:426:MET:HE2	1:O:618:GLN:HG2	1.74	0.70
1:C:557:CYS:N	1:C:564:ASN:HD21	1.88	0.70
1:K:69:MET:HE2	1:K:754:MET:HE1	1.72	0.70
2:D:71:CYS:HB2	2:D:182:THR:O	1.91	0.70
1:E:146:MET:HE3	1:E:545:ASN:OD1	1.92	0.70
1:A:146:MET:HE2	1:A:544:THR:HB	1.74	0.70
1:C:155:SER:OG	1:C:409:ILE:HG12	1.91	0.70
2:X:68:CYS:HB3	2:X:70:HIS:CE1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:695:LEU:O	1:E:699:GLU:HG2	1.90	0.70
1:S:558:SER:H	1:S:564:ASN:ND2	1.90	0.70
1:O:360:ALA:HB1	1:O:859:THR:HG23	1.73	0.69
2:F:40:GLN:NE2	2:F:118:GLU:H	1.90	0.69
1:U:696:LYS:O	1:U:700:GLU:HG3	1.92	0.69
1:I:786:ASN:ND2	1:I:804:GLN:HA	2.07	0.69
2:L:5:TYR:HB2	2:L:157:LEU:CD1	2.23	0.69
2:X:2:GLU:HG2	2:X:158:LYS:HG2	1.72	0.69
2:F:46:MET:HE1	2:F:66:THR:H	1.55	0.69
2:F:68:CYS:HB3	2:F:70:HIS:CE1	2.28	0.69
2:J:40:GLN:HE22	2:J:118:GLU:H	1.40	0.69
2:T:142:MET:HE2	2:T:146:ALA:HB1	1.74	0.69
1:G:44:ILE:HD11	1:G:394:PRO:HG2	1.73	0.69
1:I:44:ILE:HD11	1:I:394:PRO:HG2	1.73	0.69
1:I:356:GLY:N	4:I:903:MGD:O1B	2.26	0.69
2:P:46:MET:HE1	2:P:66:THR:H	1.54	0.69
1:G:211:MET:HE1	2:H:231:PHE:HZ	1.56	0.69
2:H:21:MET:HA	2:H:21:MET:CE	2.22	0.69
1:O:426:MET:HE1	1:O:618:GLN:HG2	1.74	0.69
1:Q:800:ILE:HD12	1:Q:800:ILE:N	2.08	0.69
2:T:68:CYS:HB3	2:T:70:HIS:CE1	2.27	0.69
2:X:69:MET:HB3	2:X:184:PRO:HB3	1.74	0.69
1:M:69:MET:HE2	1:M:754:MET:HE1	1.74	0.69
1:S:557:CYS:N	1:S:564:ASN:HD21	1.86	0.69
1:C:610:LYS:HZ2	1:C:618:GLN:HE22	1.38	0.69
2:D:73:ASN:HB3	2:D:182:THR:HA	1.73	0.69
2:R:40:GLN:HE22	2:R:118:GLU:H	1.39	0.68
1:G:378:GLY:O	1:G:381:LYS:HG2	1.93	0.68
1:M:35:ASP:OD1	1:M:55:ARG:HD3	1.93	0.68
1:M:146:MET:HE3	1:M:544:THR:HB	1.75	0.68
1:M:163:MET:HE1	1:M:606:PHE:HA	1.76	0.68
1:S:426:MET:HE1	1:S:618:GLN:HG2	1.72	0.68
2:D:40:GLN:NE2	2:D:117:ASN:HA	2.08	0.68
2:T:46:MET:HE1	2:T:66:THR:H	1.56	0.68
1:U:211:MET:HE3	8:U:1453:HOH:O	1.93	0.68
1:C:165:GLY:HA3	1:C:166:PHE:HB3	1.75	0.68
1:Q:141:PRO:HA	1:Q:496:TYR:HB3	1.76	0.68
1:U:141:PRO:HA	1:U:496:TYR:HB3	1.74	0.68
1:E:510:TYR:O	1:E:513:MET:HG2	1.94	0.68
1:G:426:MET:CE	1:G:618:GLN:HG2	2.24	0.68
2:H:143:PRO:HB3	7:H:303:SF4:S1	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:165:GLY:HA3	1:S:166:PHE:HB3	1.75	0.68
2:T:21:MET:HE2	2:T:21:MET:HA	1.76	0.68
2:X:68:CYS:HB2	2:X:126:CYS:CB	2.22	0.68
2:H:20:PHE:CZ	2:H:24:MET:HE2	2.29	0.68
2:J:21:MET:HA	2:J:21:MET:CE	2.22	0.68
2:R:21:MET:HE2	2:R:21:MET:HA	1.74	0.68
2:F:23:CYS:HB3	2:F:39:MET:HE1	1.74	0.68
1:Q:146:MET:HE2	1:Q:544:THR:HB	1.74	0.68
2:B:142:MET:HE2	2:B:147:HIS:N	2.09	0.68
2:T:76:CYS:HB3	2:T:108:THR:OG1	1.94	0.68
1:A:218:ASP:OD2	1:A:253:ASN:HB2	1.95	0.67
1:G:162:ASN:HA	8:G:1362:HOH:O	1.92	0.67
1:I:75:ARG:HH21	1:I:543:CYS:HA	1.58	0.67
1:M:252:MET:HE3	1:M:263:TRP:CE3	2.29	0.67
2:R:142:MET:HE3	2:R:146:ALA:HB1	1.76	0.67
1:M:629:MET:HE2	1:M:634:PHE:HA	1.75	0.67
1:Q:134:PRO:HB2	1:Q:439:LEU:HD11	1.75	0.67
2:R:46:MET:HE1	2:R:66:THR:H	1.54	0.67
1:S:252:MET:HE3	1:S:263:TRP:CE3	2.28	0.67
2:X:46:MET:HE3	2:X:47:ASN:N	2.09	0.67
1:O:69:MET:HE2	1:O:754:MET:CE	2.23	0.67
2:H:68:CYS:HB3	2:H:70:HIS:CE1	2.30	0.67
1:W:75:ARG:HH21	1:W:543:CYS:HA	1.59	0.67
2:L:71:CYS:HB2	2:L:182:THR:O	1.94	0.67
2:H:2:GLU:HG2	2:H:158:LYS:HG2	1.76	0.67
2:X:95:ASP:HB3	2:X:98:LYS:HB2	1.75	0.67
2:J:142:MET:HE2	2:J:146:ALA:HB1	1.77	0.67
1:O:695:LEU:O	1:O:699:GLU:HG2	1.95	0.67
2:X:46:MET:HE1	2:X:66:THR:H	1.59	0.67
1:E:561:ILE:HG22	1:E:564:ASN:HB3	1.76	0.67
2:N:71:CYS:HB2	2:N:182:THR:O	1.94	0.67
1:U:142:SER:OG	4:U:902:MGD:O1A	2.11	0.67
1:W:494:TRP:HE1	1:W:525:GLN:HE21	1.43	0.67
2:D:46:MET:HE3	2:D:47:ASN:N	2.09	0.66
2:F:69:MET:HB3	2:F:184:PRO:HB3	1.78	0.66
2:T:201:ALA:HB2	2:T:269:LEU:HB2	1.77	0.66
1:U:134:PRO:HB2	1:U:439:LEU:HD11	1.76	0.66
1:E:823:TYR:CZ	1:E:825:PRO:HG3	2.30	0.66
1:U:182:GLY:HA3	1:U:364:ILE:HG23	1.76	0.66
1:U:252:MET:HE3	1:U:263:TRP:CE3	2.30	0.66
1:U:617:GLU:HG3	1:U:631:TRP:CG	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:75:PRO:HD2	7:L:304:SF4:S4	2.35	0.66
1:E:100:LEU:HD12	1:E:105:PRO:HG3	1.75	0.66
2:H:21:MET:CE	2:H:24:MET:HE3	2.25	0.66
1:U:163:MET:HE1	1:U:606:PHE:HA	1.78	0.66
1:W:74:LEU:HD12	1:W:750:LYS:HA	1.76	0.66
1:W:426:MET:HE1	1:W:618:GLN:O	1.95	0.66
1:W:610:LYS:HZ2	1:W:618:GLN:HE22	1.43	0.66
1:C:460:LYS:HE3	8:C:1230:HOH:O	1.96	0.66
1:C:753:TYR:HB3	2:D:24:MET:HE3	1.78	0.66
4:K:903:MGD:O2B	4:K:903:MGD:O2A	2.12	0.66
2:L:1:MET:HG3	2:L:88:GLU:HB3	1.76	0.66
2:V:68:CYS:HB3	2:V:70:HIS:CE1	2.30	0.66
1:K:301:GLU:H	1:K:301:GLU:CD	2.04	0.66
1:M:166:PHE:N	1:M:439:LEU:HD12	2.11	0.66
1:M:218:ASP:OD2	1:M:253:ASN:HB2	1.96	0.66
1:W:1:MET:H3	1:W:22:ASP:CG	2.04	0.66
2:H:46:MET:HE3	2:H:47:ASN:N	2.11	0.66
1:G:114:TRP:CZ2	1:G:541:PRO:HD2	2.30	0.65
2:P:143:PRO:HB3	7:P:303:SF4:S1	2.35	0.65
1:C:426:MET:HE1	1:C:618:GLN:O	1.96	0.65
2:J:76:CYS:HB3	2:J:108:THR:OG1	1.96	0.65
1:C:75:ARG:HH21	1:C:543:CYS:HA	1.61	0.65
2:H:71:CYS:HB2	2:H:182:THR:O	1.96	0.65
1:K:630:THR:OG1	1:K:633:GLU:HG3	1.96	0.65
2:T:40:GLN:HE22	2:T:118:GLU:H	1.45	0.65
1:S:311:THR:HG21	8:S:1497:HOH:O	1.96	0.65
1:U:356:GLY:H	4:U:903:MGD:H5'2	1.61	0.65
1:W:426:MET:HE2	1:W:618:GLN:HG2	1.77	0.65
2:B:142:MET:HE2	2:B:146:ALA:C	2.21	0.65
1:C:146:MET:CE	1:C:544:THR:HB	2.26	0.65
1:I:214:PHE:HA	1:I:347:ALA:HB3	1.78	0.65
2:N:68:CYS:HB3	2:N:70:HIS:CE1	2.32	0.65
1:Q:360:ALA:HB1	1:Q:859:THR:HG23	1.79	0.65
1:U:801:LEU:HD11	1:U:839:ILE:HD11	1.78	0.65
1:E:356:GLY:H	4:E:903:MGD:H5'2	1.60	0.65
2:R:142:MET:HE2	2:R:147:HIS:N	2.12	0.65
2:B:76:CYS:HB3	2:B:108:THR:OG1	1.95	0.65
1:M:356:GLY:H	4:M:903:MGD:H5'2	1.62	0.65
1:O:649:LYS:HE3	1:O:651:THR:HG22	1.79	0.65
1:C:561:ILE:HG22	1:C:564:ASN:HB3	1.80	0.64
1:Q:166:PHE:N	1:Q:439:LEU:HD12	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:460:LYS:HE3	8:U:1232:HOH:O	1.97	0.64
1:G:561:ILE:HG22	1:G:564:ASN:HB3	1.78	0.64
1:I:252:MET:HE3	1:I:263:TRP:CE3	2.32	0.64
1:Q:649:LYS:HE3	1:Q:651:THR:CG2	2.27	0.64
1:S:81:LYS:HB2	1:S:112:ILE:HD13	1.79	0.64
2:L:142:MET:HE2	2:L:146:ALA:CB	2.27	0.64
2:P:59:ASN:H	2:P:59:ASN:ND2	1.95	0.64
2:L:143:PRO:HB3	7:L:303:SF4:S1	2.38	0.64
1:M:76:ILE:HG22	1:M:541:PRO:HG3	1.80	0.64
2:T:143:PRO:HB3	7:T:303:SF4:S1	2.37	0.64
2:D:68:CYS:HB2	2:D:126:CYS:CB	2.27	0.64
2:R:104:GLU:CD	2:R:104:GLU:H	2.06	0.64
2:X:19:CYS:CB	2:X:145:CYS:HB3	2.22	0.64
1:C:252:MET:HE3	1:C:263:TRP:CE3	2.33	0.64
2:J:5:TYR:HB2	2:J:157:LEU:CD1	2.28	0.64
1:C:257:ARG:HD3	2:D:61:ILE:HG21	1.79	0.64
1:A:165:GLY:HA3	1:A:166:PHE:HB3	1.78	0.64
1:C:738:HIS:HE2	4:C:902:MGD:H15	1.44	0.64
2:H:142:MET:HE2	2:H:146:ALA:C	2.22	0.64
2:J:46:MET:HE3	2:J:47:ASN:N	2.12	0.64
2:B:40:GLN:NE2	2:B:118:GLU:H	1.96	0.63
1:C:610:LYS:HZ3	1:C:618:GLN:HE22	1.44	0.63
1:O:719:GLU:HG2	1:O:859:THR:O	1.98	0.63
2:B:5:TYR:HB2	2:B:157:LEU:CD1	2.28	0.63
1:C:772:MET:HB2	1:C:801:LEU:HD13	1.81	0.63
2:V:46:MET:HE3	2:V:47:ASN:N	2.12	0.63
1:A:691:ILE:HD11	1:A:711:MET:HE3	1.81	0.63
1:C:696:LYS:O	1:C:700:GLU:HG3	1.99	0.63
2:F:5:TYR:HB2	2:F:157:LEU:CD1	2.28	0.63
1:I:134:PRO:HB2	1:I:439:LEU:HD11	1.80	0.63
1:W:786:ASN:HD21	1:W:804:GLN:HA	1.63	0.63
2:F:201:ALA:HB2	2:F:269:LEU:HB2	1.81	0.63
2:H:21:MET:HA	2:H:21:MET:HE3	1.81	0.63
1:I:630:THR:OG1	1:I:633:GLU:HG3	1.97	0.63
1:S:146:MET:HE2	1:S:544:THR:HB	1.80	0.63
1:S:478:HIS:HD2	8:S:1203:HOH:O	1.82	0.63
1:S:561:ILE:HG22	1:S:564:ASN:HB3	1.80	0.63
2:V:69:MET:HB3	2:V:184:PRO:HB3	1.79	0.63
2:X:70:HIS:HD2	2:X:92:VAL:H	1.46	0.63
1:M:195:ASN:HD21	1:M:354:TRP:CD1	2.16	0.63
1:M:725:PRO:HA	1:S:704:ILE:HG13	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:75:PRO:HD2	7:N:304:SF4:S4	2.39	0.63
1:O:394:PRO:HG3	8:O:1321:HOH:O	1.97	0.63
2:R:105:LEU:HB3	2:R:114:MET:HE1	1.80	0.63
2:R:125:LYS:HD2	2:R:126:CYS:O	1.98	0.63
1:M:32:ASP:HB2	8:M:1657:HOH:O	1.99	0.63
2:F:142:MET:HE2	2:F:146:ALA:C	2.24	0.63
1:G:610:LYS:HB3	1:G:614:ALA:HB3	1.80	0.63
1:O:211:MET:HE1	2:P:231:PHE:HZ	1.62	0.63
2:P:142:MET:HE2	2:P:146:ALA:CB	2.29	0.63
1:G:870:ASP:HB3	1:G:872:TYR:CE1	2.34	0.63
1:E:195:ASN:HD21	1:E:354:TRP:CD1	2.17	0.62
1:G:218:ASP:OD2	1:G:253:ASN:HB2	1.99	0.62
2:F:76:CYS:HB3	2:F:108:THR:OG1	1.99	0.62
1:G:553:GLU:HG2	1:G:556:ASN:HB2	1.81	0.62
2:H:1:MET:HE2	2:H:88:GLU:OE2	1.99	0.62
1:K:786:ASN:ND2	1:K:805:VAL:H	1.97	0.62
1:E:218:ASP:OD2	1:E:253:ASN:HB2	1.98	0.62
2:R:94:ILE:HD11	2:R:114:MET:HE3	1.81	0.62
1:U:76:ILE:HG22	1:U:541:PRO:HG3	1.81	0.62
1:M:823:TYR:CE2	1:M:825:PRO:HG3	2.34	0.62
1:Q:291:GLU:CD	1:Q:291:GLU:H	2.07	0.62
1:W:560:TYR:HB2	8:W:1673:HOH:O	1.98	0.62
2:P:142:MET:HE1	8:P:429:HOH:O	1.99	0.62
2:J:68:CYS:HB3	2:J:70:HIS:CE1	2.34	0.62
1:G:146:MET:HE2	1:G:544:THR:CB	2.30	0.62
2:J:143:PRO:HB3	7:J:302:SF4:S1	2.40	0.62
1:M:197:GLU:OE2	1:M:667:ASP:HB2	1.99	0.62
1:O:469:ALA:HA	8:O:1517:HOH:O	1.99	0.62
1:U:35:ASP:OD1	1:U:55:ARG:HD3	1.99	0.62
1:E:560:TYR:HB2	8:E:1683:HOH:O	1.98	0.62
2:J:46:MET:CE	2:J:66:THR:H	2.13	0.62
1:K:610:LYS:HZ2	1:K:618:GLN:HE22	1.48	0.62
1:K:823:TYR:CE2	1:K:825:PRO:HG3	2.35	0.62
2:R:46:MET:HE3	2:R:47:ASN:N	2.14	0.62
1:A:184:MET:HE2	1:A:190:SER:HA	1.82	0.62
1:U:426:MET:HE2	1:U:618:GLN:HG2	1.80	0.62
2:D:114:MET:HE3	2:D:123:ALA:HB1	1.82	0.62
1:K:557:CYS:N	1:K:564:ASN:HD21	1.87	0.62
1:Q:557:CYS:N	1:Q:564:ASN:HD21	1.85	0.62
1:E:394:PRO:HG3	8:E:1321:HOH:O	1.98	0.61
2:N:207:GLY:HA2	1:S:728:VAL:CG1	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:35:ASP:OD1	1:Q:55:ARG:HD3	2.00	0.61
1:W:146:MET:HE3	1:W:544:THR:CB	2.30	0.61
1:C:726:LEU:HD23	8:C:1193:HOH:O	2.00	0.61
1:K:871:LYS:HG2	8:K:1230:HOH:O	1.99	0.61
1:S:75:ARG:HH21	1:S:543:CYS:HA	1.64	0.61
2:X:40:GLN:NE2	2:X:117:ASN:HA	2.15	0.61
1:O:90:GLU:HB2	8:O:1242:HOH:O	2.00	0.61
2:R:95:ASP:HB3	2:R:98:LYS:HB2	1.80	0.61
2:D:40:GLN:HE22	2:D:118:GLU:H	1.48	0.61
1:I:394:PRO:HG3	8:I:1315:HOH:O	2.00	0.61
1:O:146:MET:CE	1:O:544:THR:HB	2.30	0.61
1:E:629:MET:HE2	1:E:634:PHE:HA	1.83	0.61
2:J:114:MET:HA	2:J:125:LYS:HB3	1.81	0.61
1:M:75:ARG:NH2	1:M:543:CYS:HA	2.14	0.61
2:N:207:GLY:CA	1:S:728:VAL:HG12	2.24	0.61
1:Q:28:MET:HE1	1:Q:66:PHE:HB3	1.82	0.61
1:W:695:LEU:O	1:W:699:GLU:HG2	1.99	0.61
1:C:426:MET:HE1	1:C:618:GLN:HG2	1.82	0.61
1:E:426:MET:HE2	1:E:618:GLN:HG2	1.82	0.61
1:M:557:CYS:H	1:M:564:ASN:ND2	1.84	0.61
1:U:21:LYS:HB3	1:U:26:ILE:HD11	1.82	0.61
1:U:146:MET:CE	1:U:544:THR:HB	2.28	0.61
1:E:673:ASN:HD22	1:E:673:ASN:H	1.48	0.61
1:E:114:TRP:CZ2	1:E:541:PRO:HD2	2.36	0.61
2:F:75:PRO:HD2	7:F:304:SF4:S4	2.41	0.61
2:P:69:MET:HB3	2:P:184:PRO:HB3	1.82	0.61
2:N:143:PRO:HB3	7:N:303:SF4:S1	2.41	0.60
1:U:146:MET:HE2	1:U:544:THR:CB	2.30	0.60
1:A:100:LEU:HD12	1:A:105:PRO:HG3	1.83	0.60
1:C:66:PHE:HA	1:C:69:MET:CE	2.30	0.60
1:M:69:MET:HE2	1:M:754:MET:HE3	1.82	0.60
1:Q:696:LYS:O	1:Q:700:GLU:HG3	2.01	0.60
1:Q:823:TYR:CE2	1:Q:825:PRO:HG3	2.36	0.60
1:W:28:MET:HE1	1:W:66:PHE:CB	2.28	0.60
1:C:146:MET:HE2	1:C:544:THR:CB	2.31	0.60
1:C:696:LYS:HD3	8:C:1677:HOH:O	2.01	0.60
2:H:125:LYS:HD2	2:H:126:CYS:O	2.02	0.60
1:I:426:MET:HE1	1:I:618:GLN:O	2.01	0.60
1:O:311:THR:HG21	8:O:1499:HOH:O	2.00	0.60
1:Q:649:LYS:HE3	1:Q:651:THR:HG22	1.82	0.60
1:S:35:ASP:OD1	1:S:55:ARG:HD3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:71:CYS:HB2	2:T:182:THR:O	2.01	0.60
2:B:143:PRO:HB3	7:B:303:SF4:S1	2.42	0.60
1:C:644:ASP:C	1:C:646:PRO:HD3	2.25	0.60
1:E:426:MET:HE1	1:E:618:GLN:O	2.01	0.60
1:I:610:LYS:HZ2	1:I:618:GLN:HE22	1.48	0.60
1:O:142:SER:HB3	4:O:902:MGD:O1A	2.01	0.60
1:O:738:HIS:HE2	4:O:902:MGD:H15	1.48	0.60
2:P:106:LEU:HD23	2:P:114:MET:HE2	1.82	0.60
1:U:503:THR:HG21	4:U:902:MGD:O2A	2.01	0.60
1:E:630:THR:OG1	1:E:633:GLU:HG3	2.00	0.60
1:G:571:ARG:HB2	1:G:642:VAL:HB	1.84	0.60
1:I:478:HIS:HD2	8:I:1200:HOH:O	1.84	0.60
1:I:565:TYR:C	1:I:567:LEU:H	2.09	0.60
2:L:119:GLU:HB2	8:L:941:HOH:O	2.00	0.60
1:O:35:ASP:OD1	1:O:55:ARG:HD3	2.01	0.60
1:O:44:ILE:HD11	1:O:394:PRO:HG2	1.83	0.60
1:C:700:GLU:HG2	8:C:1568:HOH:O	2.01	0.60
1:Q:333:ARG:NH1	1:U:729:LYS:HE3	2.17	0.60
2:X:1:MET:HG3	2:X:88:GLU:HB3	1.84	0.60
1:O:21:LYS:HB3	1:O:26:ILE:HD11	1.83	0.60
1:O:75:ARG:HH21	1:O:543:CYS:HA	1.64	0.60
2:X:40:GLN:HE22	2:X:118:GLU:H	1.49	0.60
1:A:460:LYS:HE3	8:A:1230:HOH:O	2.02	0.60
2:B:106:LEU:HD23	2:B:114:MET:HG3	1.82	0.60
1:K:356:GLY:H	4:K:903:MGD:H5'2	1.67	0.60
1:Q:708:ARG:HD2	8:Q:1043:HOH:O	2.02	0.60
1:U:44:ILE:HD11	1:U:394:PRO:HG2	1.83	0.60
1:I:146:MET:HE2	1:I:544:THR:CB	2.31	0.60
1:M:826:LEU:HD21	1:M:835:ARG:HD3	1.84	0.60
2:R:87:ARG:HG3	2:R:91:ILE:O	2.01	0.60
2:D:70:HIS:HD2	2:D:92:VAL:H	1.50	0.60
1:I:75:ARG:NH2	1:I:543:CYS:HA	2.17	0.60
1:O:252:MET:HE3	1:O:263:TRP:CE3	2.37	0.60
1:W:786:ASN:ND2	1:W:804:GLN:HA	2.16	0.60
1:A:249:ASP:CG	4:A:903:MGD:H1'	2.27	0.59
1:C:753:TYR:HB3	2:D:24:MET:CE	2.31	0.59
1:I:249:ASP:CG	4:I:903:MGD:H1'	2.27	0.59
2:N:46:MET:HE3	2:N:47:ASN:N	2.17	0.59
2:P:75:PRO:HD2	7:P:304:SF4:S4	2.42	0.59
2:X:75:PRO:HD2	7:X:304:SF4:S4	2.42	0.59
2:F:46:MET:HE1	2:F:65:PRO:C	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:494:TRP:HE1	1:G:525:GLN:HE21	1.50	0.59
2:L:40:GLN:HE22	2:L:118:GLU:N	1.95	0.59
1:O:253:ASN:O	1:O:257:ARG:HG3	2.02	0.59
2:R:56:TYR:HA	2:R:59:ASN:ND2	2.16	0.59
1:W:138:LEU:HB2	1:W:490:ILE:HD12	1.85	0.59
2:F:143:PRO:HB3	7:F:303:SF4:S1	2.41	0.59
2:L:21:MET:HE2	2:L:21:MET:CA	2.32	0.59
1:O:783:GLY:O	1:O:866:LYS:HD2	2.02	0.59
1:S:528:TRP:CD2	1:S:750:LYS:HD3	2.37	0.59
1:U:738:HIS:HE2	4:U:902:MGD:H15	1.51	0.59
2:V:201:ALA:HB2	2:V:269:LEU:HB2	1.84	0.59
1:E:823:TYR:CE2	1:E:825:PRO:HG3	2.38	0.59
1:O:629:MET:HE2	1:O:634:PHE:CA	2.30	0.59
1:O:823:TYR:CE2	1:O:825:PRO:HG3	2.37	0.59
1:Q:171:HIS:HB2	8:Q:1675:HOH:O	2.01	0.59
2:R:114:MET:HE2	2:R:123:ALA:HB1	1.84	0.59
1:U:753:TYR:HB3	2:V:24:MET:CE	2.31	0.59
2:D:106:LEU:HD11	2:D:116:TRP:HB2	1.84	0.59
1:S:738:HIS:HE2	4:S:902:MGD:H15	1.48	0.59
2:X:181:GLY:O	2:X:183:LYS:HE2	2.03	0.59
1:E:557:CYS:N	1:E:564:ASN:HD21	1.89	0.59
2:F:71:CYS:HB2	2:F:182:THR:O	2.03	0.59
1:G:214:PHE:HA	1:G:347:ALA:HB3	1.85	0.59
1:I:426:MET:HA	1:I:426:MET:CE	2.31	0.59
1:M:166:PHE:H	1:M:439:LEU:HD12	1.67	0.59
1:Q:800:ILE:HD11	1:Q:833:ALA:HB1	1.85	0.59
1:W:708:ARG:HD2	8:W:1044:HOH:O	2.02	0.59
1:O:301:GLU:CD	1:O:301:GLU:H	2.11	0.59
2:T:70:HIS:CD2	2:T:92:VAL:H	2.09	0.59
1:U:2:GLY:O	1:U:21:LYS:HE3	2.03	0.59
1:A:557:CYS:N	1:A:564:ASN:HD21	1.93	0.59
2:B:104:GLU:CD	2:B:104:GLU:H	2.10	0.59
1:C:563:ASP:O	1:C:566:GLN:HG2	2.03	0.59
2:F:70:HIS:CD2	2:F:92:VAL:H	2.08	0.59
1:G:629:MET:HE2	1:G:634:PHE:CA	2.32	0.59
1:Q:319:GLU:HG2	1:U:726:LEU:CD1	2.30	0.59
1:C:177:GLU:OE2	1:C:177:GLU:HA	2.03	0.59
1:E:786:ASN:HD22	1:E:805:VAL:H	1.49	0.59
2:H:201:ALA:HB2	2:H:269:LEU:HB2	1.85	0.59
2:L:201:ALA:HB2	2:L:269:LEU:HB2	1.83	0.59
2:P:46:MET:CE	2:P:66:THR:H	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:125:LYS:HD2	2:P:126:CYS:O	2.01	0.59
1:A:753:TYR:HB3	2:B:24:MET:HE3	1.84	0.59
1:G:81:LYS:HB2	1:G:112:ILE:HD13	1.85	0.59
1:G:730:TYR:CE1	1:G:794:ASN:HA	2.38	0.59
1:I:66:PHE:HA	1:I:69:MET:CE	2.26	0.59
1:O:426:MET:HE1	1:O:618:GLN:O	2.03	0.59
1:O:563:ASP:O	1:O:566:GLN:HG2	2.03	0.59
1:Q:630:THR:OG1	1:Q:633:GLU:HG3	2.03	0.59
1:Q:786:ASN:ND2	1:Q:804:GLN:HA	2.17	0.59
1:S:146:MET:HG2	4:S:902:MGD:N7	2.18	0.59
1:W:696:LYS:O	1:W:700:GLU:HG3	2.03	0.59
1:A:610:LYS:HZ2	1:A:618:GLN:HE22	1.50	0.58
2:D:68:CYS:HB3	2:D:70:HIS:CE1	2.38	0.58
1:E:138:LEU:HB2	1:E:490:ILE:HD12	1.83	0.58
1:O:146:MET:HG2	4:O:902:MGD:N7	2.18	0.58
1:U:311:THR:HG21	8:U:1502:HOH:O	2.03	0.58
2:F:166:LYS:O	2:F:170:GLU:HG3	2.03	0.58
2:H:106:LEU:HD22	2:H:114:MET:HB3	1.85	0.58
1:O:610:LYS:HB3	1:O:614:ALA:HB3	1.84	0.58
1:S:214:PHE:HA	1:S:347:ALA:HB3	1.85	0.58
1:A:211:MET:HE2	1:A:246:VAL:HG23	1.85	0.58
1:A:557:CYS:H	1:A:564:ASN:ND2	1.92	0.58
2:B:46:MET:HE1	2:B:66:THR:H	1.65	0.58
1:G:426:MET:HE1	1:G:618:GLN:HG2	1.84	0.58
2:J:104:GLU:CD	2:J:104:GLU:H	2.09	0.58
2:J:211:GLU:HB2	2:J:231:PHE:HA	1.84	0.58
2:R:56:TYR:HA	2:R:59:ASN:HD22	1.68	0.58
1:U:825:PRO:HD2	8:U:1337:HOH:O	2.03	0.58
1:W:855:MET:HB2	1:W:857:ASN:OD1	2.03	0.58
1:K:146:MET:CE	1:K:544:THR:HB	2.31	0.58
2:V:71:CYS:HB2	2:V:182:THR:O	2.03	0.58
1:W:118:THR:O	1:W:122:VAL:HG23	2.03	0.58
1:A:394:PRO:HG3	8:A:1318:HOH:O	2.04	0.58
1:G:174:ASP:OD1	1:G:175:SER:N	2.35	0.58
1:K:28:MET:HE1	1:K:66:PHE:CB	2.27	0.58
2:L:218:LYS:HG2	2:L:223:GLU:HA	1.86	0.58
2:N:87:ARG:HD3	2:N:93:LEU:HD12	1.85	0.58
2:P:105:LEU:HB3	2:P:114:MET:CE	2.34	0.58
2:T:125:LYS:HD2	2:T:126:CYS:O	2.03	0.58
1:U:561:ILE:HG22	1:U:564:ASN:HB3	1.84	0.58
2:F:13:CYS:HB3	2:F:63:TYR:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:MET:HE2	1:K:754:MET:HE3	1.84	0.58
2:B:71:CYS:HB2	2:B:182:THR:O	2.03	0.58
1:I:629:MET:HE2	1:I:634:PHE:CA	2.32	0.58
1:O:587:MET:HE2	1:O:592:ILE:HA	1.85	0.58
1:Q:855:MET:HB2	1:Q:857:ASN:OD1	2.03	0.58
2:L:2:GLU:HG2	2:L:158:LYS:HG2	1.86	0.58
1:Q:738:HIS:HE2	4:Q:902:MGD:H15	1.52	0.58
2:R:5:TYR:HB2	2:R:157:LEU:HD13	1.86	0.58
1:A:426:MET:HE2	1:A:618:GLN:HG2	1.83	0.58
1:K:146:MET:HE2	1:K:544:THR:CB	2.32	0.58
1:M:319:GLU:HG2	1:S:726:LEU:CD1	2.34	0.58
1:Q:786:ASN:ND2	1:Q:805:VAL:H	2.02	0.58
2:R:70:HIS:CD2	2:R:92:VAL:H	2.16	0.58
1:W:426:MET:HE3	1:W:622:ALA:HB2	1.86	0.58
2:X:106:LEU:HD11	2:X:116:TRP:HB2	1.85	0.58
1:A:56:LYS:HG2	1:A:57:THR:O	2.04	0.57
1:C:142:SER:HB3	4:C:902:MGD:O1A	2.04	0.57
1:I:253:ASN:O	1:I:257:ARG:HG3	2.04	0.57
1:A:670:PRO:HG2	1:A:675:GLN:CD	2.29	0.57
2:D:18:ASN:HB2	7:D:302:SF4:S1	2.45	0.57
1:E:426:MET:HE1	1:E:618:GLN:HG2	1.86	0.57
1:O:28:MET:HE1	1:O:66:PHE:CB	2.32	0.57
2:B:46:MET:HE1	2:B:65:PRO:C	2.29	0.57
2:L:46:MET:HE3	2:L:47:ASN:N	2.19	0.57
2:N:87:ARG:HG3	2:N:91:ILE:O	2.05	0.57
1:O:75:ARG:NH2	1:O:543:CYS:HA	2.19	0.57
1:S:630:THR:OG1	1:S:633:GLU:HG3	2.04	0.57
1:M:75:ARG:HH21	1:M:543:CYS:HA	1.69	0.57
1:M:134:PRO:HB2	1:M:439:LEU:HD11	1.85	0.57
1:O:479:GLN:N	8:O:1175:HOH:O	2.37	0.57
1:U:21:LYS:CB	1:U:26:ILE:HD11	2.34	0.57
1:U:360:ALA:HB1	1:U:859:THR:HG23	1.86	0.57
2:X:114:MET:HA	2:X:125:LYS:HB3	1.85	0.57
2:B:20:PHE:CZ	2:B:24:MET:HE2	2.39	0.57
1:C:394:PRO:HG3	8:C:1321:HOH:O	2.03	0.57
1:I:138:LEU:HB2	1:I:490:ILE:HD12	1.86	0.57
2:P:18:ASN:HB2	7:P:302:SF4:S1	2.44	0.57
1:S:476:GLN:OE1	1:S:708:ARG:NH2	2.38	0.57
1:S:746:MET:HE2	4:S:902:MGD:O1B	2.04	0.57
2:T:142:MET:HE2	2:T:146:ALA:CB	2.33	0.57
1:W:400:TYR:CE1	1:W:421:LYS:HD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:75:PRO:HD2	7:H:304:SF4:S4	2.45	0.57
1:M:494:TRP:HE1	1:M:525:GLN:HE21	1.51	0.57
1:Q:319:GLU:CG	1:U:726:LEU:HD13	2.34	0.57
1:W:426:MET:HE1	1:W:618:GLN:HG2	1.86	0.57
1:W:557:CYS:H	1:W:564:ASN:ND2	1.94	0.57
1:C:418:ALA:HB1	1:C:423:ALA:HB2	1.87	0.57
2:L:162:GLU:H	2:L:162:GLU:CD	2.12	0.57
1:O:81:LYS:HB2	1:O:112:ILE:HD13	1.86	0.57
1:A:378:GLY:O	1:A:381:LYS:HG2	2.05	0.57
1:C:138:LEU:HB2	1:C:490:ILE:HD12	1.86	0.57
2:D:59:ASN:H	2:D:59:ASN:ND2	2.01	0.57
1:I:175:SER:HB2	1:I:176:TRP:CE3	2.39	0.57
1:K:85:PHE:CE2	1:K:87:PRO:HG3	2.39	0.57
1:M:426:MET:HA	1:M:426:MET:CE	2.32	0.57
1:S:629:MET:HE2	1:S:634:PHE:HA	1.86	0.57
1:U:510:TYR:O	1:U:513:MET:HG2	2.04	0.57
1:W:142:SER:HB3	4:W:902:MGD:H5'2	1.87	0.57
1:I:426:MET:HE3	1:I:622:ALA:HB2	1.87	0.57
1:I:426:MET:HE1	1:I:618:GLN:HG2	1.86	0.57
1:O:146:MET:HE2	1:O:544:THR:CB	2.33	0.57
1:O:617:GLU:HG3	1:O:631:TRP:CG	2.40	0.57
1:O:647:ASN:HB2	8:O:1442:HOH:O	2.04	0.57
2:P:46:MET:HE1	2:P:65:PRO:C	2.30	0.57
1:Q:494:TRP:HE1	1:Q:525:GLN:HE21	1.52	0.57
1:S:783:GLY:O	1:S:866:LYS:HD2	2.05	0.57
1:U:104:ASP:OD2	1:U:107:SER:HB3	2.05	0.57
2:B:114:MET:HA	2:B:125:LYS:HB3	1.86	0.57
1:C:1:MET:H3	1:C:22:ASP:CG	2.11	0.57
1:C:9:ASN:HA	1:C:576:GLN:HA	1.85	0.57
2:J:75:PRO:HD2	7:J:303:SF4:S4	2.44	0.57
1:K:201:LEU:HD13	1:K:387:TRP:HB2	1.87	0.57
1:Q:75:ARG:HH21	1:Q:543:CYS:HA	1.69	0.57
1:S:505:THR:O	1:S:506:ALA:C	2.47	0.57
1:W:66:PHE:HZ	1:W:146:MET:HE1	1.70	0.57
2:D:26:GLU:HB2	2:D:144:ARG:HH11	1.70	0.56
1:E:565:TYR:C	1:E:567:LEU:H	2.13	0.56
2:F:5:TYR:HB2	2:F:157:LEU:HD11	1.86	0.56
2:H:142:MET:CE	2:H:146:ALA:HB1	2.35	0.56
2:J:19:CYS:O	2:J:22:GLY:N	2.38	0.56
1:K:45:GLU:HG3	8:K:1516:HOH:O	2.04	0.56
1:K:460:LYS:HE3	8:K:1229:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:11:SER:HA	1:M:147:TRP:HB2	1.86	0.56
1:M:66:PHE:HZ	1:M:146:MET:HE1	1.70	0.56
1:M:610:LYS:HZ1	1:M:618:GLN:HE22	1.51	0.56
1:M:797:GLY:HA2	1:M:875:TYR:CE2	2.40	0.56
1:U:85:PHE:CE2	1:U:87:PRO:HG3	2.40	0.56
2:B:205:VAL:HG13	2:B:254:LYS:NZ	2.20	0.56
2:F:21:MET:HA	2:F:21:MET:CE	2.34	0.56
1:G:557:CYS:N	1:G:564:ASN:HD21	1.94	0.56
1:M:319:GLU:HG2	1:S:726:LEU:HD13	1.88	0.56
2:X:157:LEU:HD12	2:X:157:LEU:N	2.20	0.56
1:E:147:TRP:CD1	1:E:552:SER:HG	2.23	0.56
1:G:35:ASP:OD1	1:G:55:ARG:HD3	2.06	0.56
1:O:100:LEU:CD1	1:O:105:PRO:HG3	2.32	0.56
2:R:129:CYS:HB3	2:R:132:LEU:HD12	1.87	0.56
2:R:166:LYS:HG2	2:R:170:GLU:OE2	2.05	0.56
2:T:18:ASN:HB2	7:T:302:SF4:S1	2.46	0.56
2:V:87:ARG:HG3	2:V:91:ILE:O	2.05	0.56
1:A:69:MET:HE2	1:A:754:MET:HE3	1.84	0.56
1:A:730:TYR:CE1	1:A:794:ASN:HA	2.41	0.56
1:C:426:MET:HE2	1:C:618:GLN:HG2	1.86	0.56
1:E:100:LEU:CD1	1:E:105:PRO:HG3	2.36	0.56
1:E:146:MET:HE2	1:E:544:THR:HB	1.88	0.56
2:H:87:ARG:HG3	2:H:91:ILE:O	2.04	0.56
1:I:644:ASP:O	1:I:646:PRO:HD3	2.04	0.56
1:K:561:ILE:HG22	1:K:564:ASN:HB3	1.88	0.56
1:K:786:ASN:ND2	1:K:804:GLN:HA	2.20	0.56
1:M:128:ILE:CD1	1:M:492:MET:HB2	2.35	0.56
1:M:738:HIS:HE2	4:M:902:MGD:H15	1.53	0.56
2:N:201:ALA:HB2	2:N:269:LEU:HB2	1.85	0.56
1:Q:565:TYR:C	1:Q:567:LEU:H	2.12	0.56
2:T:10:VAL:HG13	2:T:63:TYR:O	2.05	0.56
1:U:553:GLU:HG2	1:U:556:ASN:HB2	1.88	0.56
1:C:387:TRP:CE2	1:C:389:THR:HA	2.40	0.56
2:D:40:GLN:HE21	2:D:117:ASN:HA	1.70	0.56
1:G:505:THR:O	1:G:506:ALA:C	2.49	0.56
1:K:387:TRP:CE2	1:K:389:THR:HA	2.40	0.56
2:N:69:MET:HB3	2:N:184:PRO:HB3	1.86	0.56
1:Q:1:MET:H3	1:Q:22:ASP:CG	2.12	0.56
1:Q:153:ARG:O	1:Q:157:TYR:HB3	2.05	0.56
1:S:75:ARG:HH22	1:S:547:GLU:CD	2.13	0.56
1:A:387:TRP:CE2	1:A:389:THR:HA	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:MET:HE1	1:C:66:PHE:CB	2.34	0.56
1:O:1:MET:H2	1:O:22:ASP:CG	2.13	0.56
1:S:617:GLU:HG3	1:S:631:TRP:CG	2.41	0.56
2:D:7:VAL:HB	2:D:155:GLU:HB3	1.86	0.56
1:I:823:TYR:CE2	1:I:825:PRO:HG3	2.40	0.56
2:N:5:TYR:HB2	2:N:157:LEU:CD1	2.36	0.56
2:P:19:CYS:CB	2:P:145:CYS:HB3	2.32	0.56
2:P:104:GLU:H	2:P:104:GLU:CD	2.13	0.56
1:W:660:GLY:HA2	8:W:1205:HOH:O	2.05	0.56
1:A:696:LYS:O	1:A:700:GLU:HG3	2.05	0.56
1:A:823:TYR:CE2	1:A:825:PRO:HG3	2.40	0.56
1:E:146:MET:CE	1:E:544:THR:HB	2.35	0.56
2:H:70:HIS:HD2	2:H:92:VAL:N	1.97	0.56
1:I:195:ASN:HD21	1:I:354:TRP:CD1	2.23	0.56
1:M:333:ARG:NH1	1:S:729:LYS:HE3	2.20	0.56
1:Q:541:PRO:HB2	1:Q:586:SER:HA	1.87	0.56
2:X:59:ASN:ND2	2:X:59:ASN:H	2.04	0.56
1:C:478:HIS:HD2	8:C:1204:HOH:O	1.89	0.56
1:C:870:ASP:HB3	1:C:872:TYR:CE1	2.41	0.56
1:G:195:ASN:HD21	1:G:354:TRP:CD1	2.23	0.56
1:M:146:MET:HE3	1:M:544:THR:CB	2.36	0.56
1:O:645:ASN:ND2	1:O:648:ARG:HB3	2.20	0.56
2:T:104:GLU:CD	2:T:104:GLU:H	2.14	0.56
1:A:291:GLU:CD	1:A:291:GLU:H	2.14	0.56
1:E:142:SER:OG	4:E:902:MGD:O1A	2.24	0.56
2:J:87:ARG:HG3	2:J:91:ILE:O	2.06	0.56
2:L:142:MET:HE1	8:L:929:HOH:O	2.05	0.56
1:M:478:HIS:HD2	8:M:1203:HOH:O	1.88	0.56
2:R:46:MET:CE	2:R:66:THR:H	2.18	0.56
1:W:629:MET:HE2	1:W:634:PHE:HA	1.88	0.56
2:B:69:MET:HB3	2:B:184:PRO:HB3	1.88	0.55
2:F:46:MET:HE1	2:F:65:PRO:CA	2.36	0.55
2:F:87:ARG:HG3	2:F:91:ILE:O	2.05	0.55
1:G:177:GLU:HA	1:G:177:GLU:OE2	2.06	0.55
1:M:400:TYR:CE1	1:M:421:LYS:HD2	2.41	0.55
2:N:142:MET:HE2	2:N:147:HIS:N	2.21	0.55
1:O:476:GLN:OE1	1:O:708:ARG:NH2	2.39	0.55
1:S:146:MET:CE	1:S:544:THR:HB	2.36	0.55
2:T:114:MET:HE3	2:T:123:ALA:HB1	1.87	0.55
1:W:75:ARG:NH2	1:W:543:CYS:HA	2.20	0.55
1:G:426:MET:HE2	1:G:618:GLN:HG2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:74:LEU:HD12	1:I:750:LYS:HA	1.88	0.55
1:W:647:ASN:HB2	8:W:1445:HOH:O	2.05	0.55
2:D:69:MET:HB3	2:D:184:PRO:HB3	1.88	0.55
2:H:46:MET:HE1	2:H:65:PRO:C	2.31	0.55
1:K:100:LEU:CD1	1:K:105:PRO:HG3	2.36	0.55
1:K:195:ASN:HD21	1:K:354:TRP:CD1	2.25	0.55
1:K:478:HIS:HD2	8:K:1202:HOH:O	1.88	0.55
1:O:649:LYS:HE2	8:O:1459:HOH:O	2.07	0.55
2:P:68:CYS:HB3	2:P:70:HIS:CE1	2.42	0.55
1:U:253:ASN:O	1:U:257:ARG:HG3	2.07	0.55
1:U:786:ASN:HD22	1:U:805:VAL:H	1.54	0.55
2:V:75:PRO:HD2	7:V:304:SF4:S4	2.46	0.55
1:W:356:GLY:H	4:W:903:MGD:C5'	2.19	0.55
1:G:617:GLU:HG3	1:G:631:TRP:CG	2.41	0.55
1:I:44:ILE:HD11	1:I:394:PRO:CG	2.37	0.55
1:M:147:TRP:CD1	1:M:552:SER:HG	2.24	0.55
1:M:426:MET:HE1	1:M:618:GLN:O	2.05	0.55
1:M:708:ARG:HD2	8:M:1044:HOH:O	2.04	0.55
2:P:142:MET:HE2	2:P:146:ALA:HB1	1.88	0.55
2:R:46:MET:HE1	2:R:65:PRO:C	2.32	0.55
1:A:175:SER:HB2	1:A:176:TRP:CE3	2.41	0.55
1:A:505:THR:O	1:A:506:ALA:C	2.50	0.55
2:H:40:GLN:NE2	2:H:118:GLU:H	2.02	0.55
1:O:765:ASP:HB2	8:O:1165:HOH:O	2.05	0.55
2:R:20:PHE:CZ	2:R:24:MET:HE2	2.42	0.55
1:S:691:ILE:HD11	1:S:711:MET:HE3	1.89	0.55
1:U:128:ILE:CD1	1:U:492:MET:HB2	2.36	0.55
1:U:184:MET:HE2	1:U:190:SER:HA	1.87	0.55
2:H:69:MET:HB3	2:H:184:PRO:HB3	1.87	0.55
1:I:753:TYR:HB3	2:J:21:MET:HE2	1.88	0.55
2:P:70:HIS:CD2	2:P:92:VAL:H	2.15	0.55
1:A:85:PHE:CE2	1:A:87:PRO:HG3	2.42	0.55
1:C:494:TRP:HE1	1:C:525:GLN:HE21	1.54	0.55
1:E:800:ILE:HD12	1:E:800:ILE:N	2.22	0.55
2:H:46:MET:CE	2:H:66:THR:H	2.19	0.55
2:H:142:MET:HE2	2:H:146:ALA:CB	2.37	0.55
1:I:15:PRO:HD3	1:I:554:PHE:CD1	2.41	0.55
1:I:55:ARG:HD2	8:I:1633:HOH:O	2.05	0.55
2:J:70:HIS:CD2	2:J:92:VAL:H	2.16	0.55
2:L:105:LEU:HB3	2:L:114:MET:CE	2.37	0.55
1:M:187:TRP:CH2	1:M:196:PRO:HB3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:138:LEU:HB2	1:O:490:ILE:HD12	1.89	0.55
1:O:673:ASN:H	1:O:673:ASN:HD22	1.53	0.55
1:Q:426:MET:HE2	1:Q:618:GLN:HG2	1.88	0.55
1:W:610:LYS:HZ3	1:W:618:GLN:HE22	1.54	0.55
1:A:610:LYS:HZ3	1:A:618:GLN:HE22	1.55	0.55
2:D:3:GLN:O	2:D:158:LYS:HA	2.07	0.55
1:I:142:SER:HB3	4:I:902:MGD:O1A	2.06	0.55
1:Q:146:MET:HG2	4:Q:902:MGD:N7	2.22	0.55
1:W:35:ASP:OD1	1:W:55:ARG:HD3	2.07	0.55
2:D:59:ASN:H	2:D:59:ASN:HD22	1.54	0.55
1:E:197:GLU:OE2	1:E:667:ASP:HB2	2.07	0.55
1:E:730:TYR:CZ	1:E:794:ASN:HA	2.42	0.55
2:J:164:MET:O	2:J:168:VAL:HG23	2.06	0.55
2:L:167:LYS:HZ3	2:L:171:GLU:CD	2.15	0.55
1:O:32:ASP:OD1	1:O:56:LYS:HD2	2.07	0.55
1:Q:114:TRP:CZ2	1:Q:541:PRO:HD2	2.41	0.55
2:R:19:CYS:O	2:R:22:GLY:N	2.40	0.55
1:A:81:LYS:HB2	1:A:112:ILE:HD13	1.88	0.55
2:H:166:LYS:O	2:H:170:GLU:HG3	2.07	0.55
1:I:96:ARG:HD2	1:I:514:TYR:O	2.07	0.55
1:K:708:ARG:HD2	8:K:1042:HOH:O	2.07	0.55
2:N:166:LYS:O	2:N:170:GLU:HG3	2.06	0.55
2:P:71:CYS:HB2	2:P:182:THR:O	2.05	0.55
1:Q:166:PHE:H	1:Q:439:LEU:HD12	1.71	0.55
2:R:94:ILE:CD1	2:R:114:MET:HE3	2.37	0.55
2:X:105:LEU:HB3	2:X:114:MET:CE	2.37	0.55
1:E:426:MET:CE	1:E:426:MET:HA	2.37	0.54
1:E:426:MET:HE3	1:E:622:ALA:HB2	1.89	0.54
1:G:691:ILE:HD11	1:G:711:MET:HE3	1.88	0.54
2:H:19:CYS:HB3	2:H:145:CYS:HB3	1.89	0.54
1:M:800:ILE:HD12	1:M:800:ILE:N	2.22	0.54
2:R:75:PRO:HD2	7:R:304:SF4:S4	2.47	0.54
1:W:163:MET:HE1	1:W:606:PHE:HA	1.89	0.54
2:P:21:MET:HE1	2:P:24:MET:CE	2.37	0.54
1:U:176:TRP:O	1:U:177:GLU:C	2.50	0.54
1:A:826:LEU:HD21	1:A:835:ARG:HD3	1.88	0.54
2:J:21:MET:HE3	2:J:21:MET:CA	2.35	0.54
2:L:40:GLN:NE2	2:L:117:ASN:HA	2.22	0.54
2:L:104:GLU:CD	2:L:104:GLU:H	2.15	0.54
1:M:214:PHE:HA	1:M:347:ALA:HB3	1.89	0.54
2:N:46:MET:HE1	2:N:65:PRO:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:177:GLU:OE2	1:Q:177:GLU:HA	2.07	0.54
1:A:142:SER:OG	4:A:902:MGD:O1A	2.12	0.54
1:C:76:ILE:HG22	1:C:541:PRO:HG3	1.88	0.54
1:C:505:THR:O	1:C:506:ALA:C	2.50	0.54
1:E:870:ASP:HB3	1:E:872:TYR:CE1	2.42	0.54
1:I:142:SER:CB	4:I:902:MGD:O1A	2.55	0.54
2:L:46:MET:CE	2:L:66:THR:H	2.20	0.54
2:L:105:LEU:HB3	2:L:114:MET:HE1	1.89	0.54
2:T:106:LEU:HD11	2:T:116:TRP:HB2	1.89	0.54
2:V:46:MET:CE	2:V:66:THR:N	2.67	0.54
1:W:277:ALA:HB2	1:W:321:ALA:HB2	1.88	0.54
1:C:15:PRO:HD3	1:C:554:PHE:CD1	2.42	0.54
1:C:823:TYR:CE2	1:C:825:PRO:HG3	2.42	0.54
1:E:66:PHE:HA	1:E:69:MET:CE	2.34	0.54
2:F:142:MET:CE	2:F:146:ALA:HB1	2.36	0.54
1:G:541:PRO:HB2	1:G:586:SER:HA	1.90	0.54
2:H:3:GLN:O	2:H:158:LYS:HA	2.08	0.54
1:I:114:TRP:CZ2	1:I:541:PRO:HD2	2.41	0.54
1:K:163:MET:HE1	1:K:606:PHE:HA	1.89	0.54
1:M:21:LYS:HB3	1:M:26:ILE:HD11	1.90	0.54
1:O:563:ASP:HA	1:O:565:TYR:CE1	2.42	0.54
1:S:610:LYS:HZ2	1:S:618:GLN:HE22	1.55	0.54
2:T:52:GLU:HG3	2:T:61:ILE:HD12	1.89	0.54
1:W:11:SER:HA	1:W:147:TRP:HB2	1.88	0.54
1:G:142:SER:OG	4:G:902:MGD:O1A	2.25	0.54
1:I:563:ASP:O	1:I:566:GLN:HG2	2.08	0.54
2:R:157:LEU:H	2:R:157:LEU:HD12	1.72	0.54
1:S:647:ASN:O	1:S:648:ARG:O	2.25	0.54
2:V:104:GLU:H	2:V:104:GLU:CD	2.13	0.54
2:X:20:PHE:CZ	2:X:24:MET:HE2	2.43	0.54
1:C:100:LEU:HD12	1:C:105:PRO:HG3	1.90	0.54
2:H:19:CYS:O	2:H:22:GLY:N	2.40	0.54
1:K:610:LYS:HB3	1:K:614:ALA:HB3	1.90	0.54
1:M:353:GLY:O	1:M:354:TRP:HB2	2.08	0.54
1:O:561:ILE:HG22	1:O:564:ASN:HB3	1.88	0.54
1:Q:55:ARG:HD2	8:Q:1631:HOH:O	2.07	0.54
1:Q:214:PHE:HA	1:Q:347:ALA:HB3	1.90	0.54
2:R:40:GLN:NE2	2:R:118:GLU:H	2.04	0.54
1:U:142:SER:CB	4:U:902:MGD:O1A	2.56	0.54
1:W:563:ASP:O	1:W:566:GLN:HG2	2.07	0.54
2:X:76:CYS:HB3	2:X:108:THR:OG1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:541:PRO:HB2	1:M:586:SER:HA	1.89	0.54
1:Q:142:SER:CB	4:Q:902:MGD:O1A	2.56	0.54
1:W:499:PRO:HG3	4:W:902:MGD:O5'	2.08	0.54
2:X:125:LYS:HD2	2:X:126:CYS:O	2.08	0.54
1:A:76:ILE:HG22	1:A:541:PRO:HG3	1.89	0.54
2:B:21:MET:HE2	2:B:24:MET:HE3	1.90	0.54
2:F:2:GLU:HG2	2:F:158:LYS:HG2	1.90	0.54
2:J:105:LEU:HB3	2:J:114:MET:HE1	1.90	0.54
1:K:176:TRP:O	1:K:177:GLU:C	2.50	0.54
1:M:617:GLU:HG3	1:M:631:TRP:CG	2.43	0.54
2:N:21:MET:HE3	2:N:21:MET:CA	2.37	0.54
2:P:201:ALA:HB2	2:P:269:LEU:HB2	1.88	0.54
1:Q:142:SER:HB3	4:Q:902:MGD:O1A	2.07	0.54
1:S:729:LYS:HD2	8:S:1133:HOH:O	2.08	0.54
1:W:214:PHE:HA	1:W:347:ALA:HB3	1.90	0.54
1:W:753:TYR:HB3	2:X:24:MET:HE3	1.89	0.54
2:B:75:PRO:HD2	7:B:304:SF4:S4	2.48	0.54
1:G:175:SER:HB2	1:G:176:TRP:CE3	2.42	0.54
2:H:59:ASN:ND2	2:H:59:ASN:H	2.06	0.54
1:K:211:MET:HE1	1:K:338:GLN:HG2	1.90	0.54
2:L:21:MET:HA	2:L:21:MET:CE	2.38	0.54
2:N:43:HIS:ND1	8:N:403:HOH:O	2.33	0.54
1:O:142:SER:CB	4:O:902:MGD:O1A	2.55	0.54
1:O:257:ARG:HD3	2:P:61:ILE:HG21	1.90	0.54
1:A:100:LEU:CD1	1:A:105:PRO:HG3	2.38	0.53
1:C:142:SER:CB	4:C:902:MGD:O1A	2.56	0.53
2:D:198:TYR:HB3	2:D:238:ASP:HA	1.90	0.53
1:E:673:ASN:H	1:E:673:ASN:ND2	2.06	0.53
1:E:826:LEU:HD21	1:E:835:ARG:HD3	1.90	0.53
1:G:476:GLN:OE1	1:G:708:ARG:NH2	2.40	0.53
2:R:247:VAL:O	2:R:257:SER:HA	2.07	0.53
2:T:87:ARG:HG3	2:T:91:ILE:O	2.07	0.53
1:U:505:THR:O	1:U:506:ALA:C	2.51	0.53
1:W:563:ASP:HA	1:W:565:TYR:CE1	2.43	0.53
1:C:253:ASN:O	1:C:257:ARG:HG3	2.09	0.53
1:E:15:PRO:HD3	1:E:554:PHE:CD1	2.43	0.53
1:G:604:GLU:HB3	8:G:1121:HOH:O	2.08	0.53
1:I:12:THR:O	1:I:226:TYR:HA	2.08	0.53
2:N:5:TYR:CD2	2:N:164:MET:HG2	2.43	0.53
1:O:494:TRP:HE1	1:O:525:GLN:HE21	1.56	0.53
1:Q:44:ILE:HD11	1:Q:394:PRO:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:610:LYS:HZ3	1:S:618:GLN:HE22	1.56	0.53
1:U:610:LYS:HZ3	1:U:618:GLN:HE22	1.54	0.53
1:W:847:TYR:CZ	1:W:853:CYS:HB3	2.44	0.53
2:X:21:MET:HE2	2:X:21:MET:CA	2.38	0.53
1:A:630:THR:OG1	1:A:633:GLU:HG3	2.09	0.53
2:D:121:ASN:CG	1:S:608:GLU:O	2.51	0.53
1:E:557:CYS:H	1:E:564:ASN:ND2	1.91	0.53
2:F:46:MET:CE	2:F:66:THR:H	2.21	0.53
2:F:142:MET:HE2	2:F:146:ALA:CB	2.38	0.53
1:G:15:PRO:HD3	1:G:554:PHE:CD1	2.43	0.53
1:I:426:MET:HE2	1:I:618:GLN:HG2	1.89	0.53
1:M:141:PRO:CA	1:M:496:TYR:HB3	2.38	0.53
1:Q:195:ASN:HD21	1:Q:354:TRP:CD1	2.26	0.53
2:T:40:GLN:NE2	2:T:117:ASN:HA	2.23	0.53
2:T:75:PRO:HD2	7:T:304:SF4:S4	2.49	0.53
2:T:159:THR:OG1	2:T:160:THR:N	2.42	0.53
2:T:218:LYS:HG2	2:T:223:GLU:HA	1.91	0.53
1:G:296:ASN:HB3	1:G:657:PHE:CZ	2.43	0.53
2:H:211:GLU:HB2	2:H:231:PHE:HA	1.90	0.53
2:L:1:MET:HE2	2:L:88:GLU:OE2	2.09	0.53
1:M:476:GLN:OE1	1:M:708:ARG:NH2	2.41	0.53
2:N:106:LEU:CD2	2:N:114:MET:HB3	2.38	0.53
2:P:106:LEU:HD23	2:P:114:MET:CE	2.38	0.53
2:R:5:TYR:O	2:R:157:LEU:HD12	2.08	0.53
2:R:69:MET:HE2	2:R:69:MET:HA	1.89	0.53
1:S:146:MET:HE2	1:S:544:THR:CB	2.38	0.53
1:U:563:ASP:O	1:U:566:GLN:HG2	2.08	0.53
2:X:218:LYS:HA	2:X:222:LYS:O	2.08	0.53
1:A:561:ILE:HG22	1:A:564:ASN:HB3	1.91	0.53
1:C:719:GLU:HG2	1:C:859:THR:O	2.09	0.53
1:E:211:MET:HE3	8:E:1449:HOH:O	2.07	0.53
1:K:767:TYR:HB3	1:K:769:TYR:CE1	2.43	0.53
1:O:140:THR:HB	1:O:169:ALA:HB3	1.91	0.53
1:O:753:TYR:HB3	2:P:24:MET:CE	2.34	0.53
2:P:216:VAL:HG13	2:P:223:GLU:HG3	1.90	0.53
1:W:134:PRO:HD2	8:W:1360:HOH:O	2.09	0.53
1:W:561:ILE:CG2	1:W:564:ASN:HB3	2.37	0.53
1:W:797:GLY:HA2	1:W:875:TYR:CE2	2.43	0.53
2:X:105:LEU:HB3	2:X:114:MET:HE1	1.90	0.53
2:D:2:GLU:HG2	2:D:158:LYS:HG2	1.90	0.53
1:E:730:TYR:CE1	1:E:794:ASN:HA	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:PHE:HA	1:G:69:MET:CE	2.33	0.53
1:O:505:THR:O	1:O:506:ALA:C	2.52	0.53
1:Q:66:PHE:CD1	1:Q:69:MET:HE3	2.44	0.53
1:Q:211:MET:HE2	1:Q:246:VAL:HG23	1.89	0.53
1:Q:505:THR:O	1:Q:506:ALA:C	2.52	0.53
2:X:252:ASP:C	2:X:254:LYS:H	2.17	0.53
1:A:426:MET:HE1	1:A:618:GLN:O	2.09	0.53
1:E:175:SER:HB2	1:E:176:TRP:CE3	2.43	0.53
2:F:46:MET:HE3	2:F:47:ASN:N	2.24	0.53
1:G:146:MET:HG2	4:G:902:MGD:N7	2.24	0.53
1:G:176:TRP:O	1:G:177:GLU:C	2.51	0.53
2:N:40:GLN:NE2	2:N:118:GLU:H	2.00	0.53
2:R:68:CYS:HB2	2:R:126:CYS:HB2	1.89	0.53
1:U:78:TYR:C	1:U:541:PRO:HG2	2.34	0.53
1:W:176:TRP:O	1:W:177:GLU:C	2.52	0.53
1:A:478:HIS:HD2	8:A:1203:HOH:O	1.92	0.53
2:B:210:PHE:HD2	2:B:213:ALA:HB2	1.73	0.53
1:C:786:ASN:ND2	1:C:804:GLN:HA	2.24	0.53
1:E:528:TRP:CG	1:E:750:LYS:HD3	2.43	0.53
1:Q:69:MET:HE2	1:Q:754:MET:HE3	1.88	0.53
1:S:253:ASN:O	1:S:257:ARG:HG3	2.09	0.53
2:V:18:ASN:HB2	7:V:302:SF4:S1	2.48	0.53
1:W:418:ALA:HB1	1:W:423:ALA:HB2	1.89	0.53
1:W:722:LYS:HG2	8:W:1565:HOH:O	2.09	0.53
2:X:73:ASN:HB3	2:X:182:THR:HA	1.90	0.53
1:C:610:LYS:HB3	1:C:614:ALA:HB3	1.91	0.53
2:F:70:HIS:HD2	2:F:92:VAL:N	1.98	0.53
1:I:142:SER:OG	4:I:902:MGD:O1A	2.25	0.53
1:I:147:TRP:CD1	1:I:552:SER:HG	2.26	0.53
1:I:328:PRO:HB2	1:I:331:GLU:HG3	1.90	0.53
2:L:114:MET:HA	2:L:125:LYS:HB3	1.91	0.53
1:M:142:SER:OG	4:M:902:MGD:O1A	2.21	0.53
1:O:499:PRO:HG3	4:O:902:MGD:O5'	2.09	0.53
1:U:478:HIS:HD2	8:U:1205:HOH:O	1.91	0.53
2:V:114:MET:HA	2:V:125:LYS:HB3	1.89	0.53
1:G:356:GLY:HA2	1:G:359:ARG:NH1	2.24	0.53
1:G:400:TYR:CE1	1:G:421:LYS:HD2	2.44	0.53
1:K:786:ASN:HD21	1:K:804:GLN:HA	1.73	0.53
2:P:87:ARG:HG3	2:P:91:ILE:O	2.09	0.53
1:Q:296:ASN:HB3	1:Q:657:PHE:CZ	2.44	0.53
1:U:44:ILE:HD11	1:U:394:PRO:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:56:LYS:HE2	8:W:1468:HOH:O	2.09	0.53
2:X:99:ALA:HA	2:X:102:LYS:HD2	1.90	0.53
2:B:46:MET:HE3	2:B:47:ASN:N	2.24	0.52
2:B:106:LEU:HA	2:B:114:MET:HG3	1.90	0.52
2:J:114:MET:HE3	2:J:123:ALA:HB1	1.89	0.52
1:M:28:MET:HE1	1:M:66:PHE:CB	2.36	0.52
2:X:129:CYS:HB3	2:X:131:HIS:CE1	2.44	0.52
1:A:214:PHE:HA	1:A:347:ALA:HB3	1.91	0.52
1:E:146:MET:HG2	4:E:902:MGD:N7	2.24	0.52
1:I:528:TRP:CG	1:I:750:LYS:HD3	2.43	0.52
2:J:5:TYR:HB2	2:J:157:LEU:HD12	1.91	0.52
1:Q:96:ARG:HD2	1:Q:514:TYR:O	2.09	0.52
1:W:239:LYS:HE2	8:W:1600:HOH:O	2.09	0.52
1:A:249:ASP:OD1	4:A:903:MGD:H1'	2.09	0.52
1:G:452:ILE:HB	1:G:453:PRO:HD3	1.91	0.52
2:J:203:ILE:HD12	2:J:203:ILE:N	2.24	0.52
1:K:629:MET:HE2	1:K:634:PHE:CA	2.36	0.52
1:M:505:THR:O	1:M:506:ALA:C	2.52	0.52
1:M:571:ARG:HB2	1:M:642:VAL:HB	1.91	0.52
1:Q:394:PRO:HG3	8:Q:1315:HOH:O	2.09	0.52
1:S:114:TRP:CZ2	1:S:541:PRO:HD2	2.43	0.52
1:W:505:THR:O	1:W:506:ALA:C	2.52	0.52
1:W:800:ILE:HD12	1:W:800:ILE:N	2.25	0.52
2:X:218:LYS:O	2:X:246:THR:N	2.40	0.52
1:A:253:ASN:O	1:A:257:ARG:HG3	2.09	0.52
2:D:27:HIS:HB2	2:D:39:MET:HE3	1.91	0.52
1:E:587:MET:HE2	1:E:592:ILE:HA	1.89	0.52
1:I:730:TYR:CE1	1:I:794:ASN:HA	2.45	0.52
1:K:656:TRP:CD2	1:K:663:LYS:HA	2.44	0.52
2:N:56:TYR:HA	2:N:59:ASN:HD22	1.74	0.52
1:Q:533:VAL:HB	1:Q:534:PRO:HD3	1.91	0.52
2:V:46:MET:HE1	2:V:65:PRO:C	2.35	0.52
1:W:195:ASN:HD21	1:W:354:TRP:CD1	2.27	0.52
2:X:4:TYR:CE2	2:X:158:LYS:HD2	2.44	0.52
2:F:203:ILE:HD12	2:F:203:ILE:N	2.24	0.52
1:K:253:ASN:O	1:K:257:ARG:HG3	2.10	0.52
1:M:610:LYS:HZ3	1:M:618:GLN:NE2	2.00	0.52
1:S:195:ASN:HD21	1:S:354:TRP:CD1	2.26	0.52
1:U:563:ASP:HA	1:U:565:TYR:CE1	2.44	0.52
1:U:610:LYS:HB3	1:U:614:ALA:HB3	1.90	0.52
2:X:40:GLN:HB3	2:X:43:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:MET:HE2	1:E:544:THR:CB	2.40	0.52
1:E:211:MET:HE1	2:F:231:PHE:HZ	1.65	0.52
1:I:139:SER:OG	1:I:161:MET:HE2	2.09	0.52
1:I:617:GLU:HG3	1:I:631:TRP:CG	2.45	0.52
1:I:786:ASN:HD21	1:I:804:GLN:HA	1.71	0.52
1:O:704:ILE:HG23	8:O:1642:HOH:O	2.09	0.52
2:T:166:LYS:HG2	2:T:170:GLU:OE2	2.09	0.52
1:U:823:TYR:CE2	1:U:825:PRO:HG3	2.44	0.52
2:X:164:MET:O	2:X:168:VAL:HG23	2.10	0.52
1:A:301:GLU:CD	1:A:301:GLU:H	2.17	0.52
2:B:21:MET:HA	2:B:21:MET:CE	2.39	0.52
1:E:75:ARG:HH21	1:E:543:CYS:HA	1.74	0.52
1:I:13:GLY:HA3	1:I:63:THR:OG1	2.10	0.52
1:M:670:PRO:HG2	1:M:675:GLN:CD	2.35	0.52
1:O:478:HIS:HD2	8:O:1204:HOH:O	1.93	0.52
1:Q:452:ILE:HB	1:Q:453:PRO:HD3	1.92	0.52
1:S:153:ARG:O	1:S:157:TYR:HB3	2.09	0.52
2:T:5:TYR:HB2	2:T:157:LEU:HD12	1.92	0.52
1:U:452:ILE:N	1:U:453:PRO:CD	2.72	0.52
1:U:649:LYS:HE3	1:U:651:THR:CG2	2.40	0.52
1:A:144:HIS:HB2	4:A:902:MGD:O1B	2.10	0.52
2:B:46:MET:HE1	2:B:65:PRO:CA	2.40	0.52
2:B:70:HIS:CD2	2:B:92:VAL:H	2.13	0.52
2:B:166:LYS:HG2	2:B:170:GLU:OE2	2.09	0.52
1:C:153:ARG:O	1:C:157:TYR:HB3	2.09	0.52
1:E:153:ARG:O	1:E:157:TYR:HB3	2.10	0.52
1:E:738:HIS:HE2	4:E:902:MGD:H15	1.57	0.52
1:G:426:MET:HE1	1:G:618:GLN:O	2.10	0.52
1:I:47:ARG:HD2	1:I:241:LEU:HD22	1.90	0.52
2:J:46:MET:HE1	2:J:65:PRO:C	2.35	0.52
2:L:18:ASN:HB2	7:L:302:SF4:S1	2.50	0.52
1:O:353:GLY:O	1:O:354:TRP:HB2	2.10	0.52
1:Q:871:LYS:HG2	8:Q:1226:HOH:O	2.10	0.52
1:U:187:TRP:CH2	1:U:196:PRO:HB3	2.45	0.52
2:X:5:TYR:HB2	2:X:157:LEU:HD13	1.91	0.52
2:X:204:LEU:HD23	2:X:209:CYS:HA	1.90	0.52
2:H:21:MET:HE3	2:H:21:MET:CA	2.40	0.52
1:K:75:ARG:NH2	1:K:543:CYS:HA	2.25	0.52
1:K:617:GLU:HG3	1:K:631:TRP:CG	2.45	0.52
1:M:452:ILE:HB	1:M:453:PRO:HD3	1.91	0.52
1:O:55:ARG:HD2	8:O:1634:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:74:LEU:HD12	1:O:750:LYS:HA	1.91	0.52
2:P:19:CYS:HB2	2:P:46:MET:HG2	1.91	0.52
1:Q:2:GLY:O	1:Q:21:LYS:HE3	2.09	0.52
1:Q:767:TYR:HB3	1:Q:769:TYR:CE1	2.44	0.52
1:Q:786:ASN:HD22	1:Q:805:VAL:H	1.57	0.52
1:W:56:LYS:HG2	1:W:57:THR:O	2.09	0.52
1:A:587:MET:HE3	1:A:591:GLU:HB3	1.90	0.52
2:L:46:MET:CE	2:L:66:THR:N	2.65	0.52
1:M:9:ASN:HA	1:M:576:GLN:HA	1.91	0.52
1:M:610:LYS:HB3	1:M:614:ALA:HB3	1.91	0.52
1:O:541:PRO:HB2	1:O:586:SER:HA	1.92	0.52
1:O:628:TYR:CE2	1:O:643:PRO:HG2	2.45	0.52
2:P:46:MET:HE3	2:P:47:ASN:H	1.74	0.52
1:Q:561:ILE:HG22	1:Q:564:ASN:HB3	1.92	0.52
1:U:395:LEU:HD12	1:U:566:GLN:HA	1.92	0.52
1:W:478:HIS:HD2	8:W:1206:HOH:O	1.93	0.52
1:W:738:HIS:HE2	4:W:902:MGD:H15	1.58	0.52
1:A:700:GLU:HG2	8:A:1564:HOH:O	2.09	0.51
2:B:59:ASN:ND2	2:B:59:ASN:H	2.06	0.51
2:D:53:ARG:HB2	2:D:60:ASP:OD1	2.10	0.51
1:E:670:PRO:HG2	1:E:675:GLN:CD	2.35	0.51
1:M:503:THR:HG21	4:M:902:MGD:O2A	2.10	0.51
1:O:746:MET:HE2	4:O:902:MGD:O1B	2.10	0.51
1:Q:252:MET:HE3	1:Q:263:TRP:CE3	2.45	0.51
2:T:46:MET:CE	2:T:66:THR:H	2.23	0.51
1:U:99:GLY:HA2	1:U:102:LYS:HE2	1.91	0.51
1:U:138:LEU:HB2	1:U:490:ILE:HD12	1.92	0.51
1:W:870:ASP:HB3	1:W:872:TYR:CE1	2.45	0.51
1:E:66:PHE:CD1	1:E:69:MET:HE3	2.45	0.51
2:F:56:TYR:HA	2:F:59:ASN:HD22	1.75	0.51
2:F:142:MET:HE1	8:F:431:HOH:O	2.09	0.51
1:K:426:MET:HE2	1:K:618:GLN:HG2	1.90	0.51
2:L:160:THR:HB	2:L:162:GLU:OE1	2.10	0.51
1:Q:356:GLY:H	4:Q:903:MGD:H5'2	1.75	0.51
1:Q:452:ILE:N	1:Q:453:PRO:CD	2.73	0.51
1:U:629:MET:HE2	1:U:634:PHE:HA	1.92	0.51
1:U:729:LYS:HD2	8:U:1135:HOH:O	2.10	0.51
1:W:128:ILE:CD1	1:W:492:MET:HB2	2.40	0.51
2:X:18:ASN:HB2	7:X:302:SF4:S1	2.51	0.51
1:A:139:SER:OG	1:A:161:MET:HE2	2.11	0.51
2:B:203:ILE:HD12	2:B:203:ILE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LYS:HG2	2:D:232:PHE:CE1	2.46	0.51
2:F:1:MET:SD	2:F:88:GLU:HB3	2.50	0.51
2:F:162:GLU:H	2:F:162:GLU:CD	2.19	0.51
1:G:563:ASP:O	1:G:566:GLN:HG2	2.10	0.51
1:I:387:TRP:CE2	1:I:389:THR:HA	2.45	0.51
2:J:70:HIS:HD2	2:J:92:VAL:N	2.02	0.51
2:L:103:LYS:HE2	2:L:116:TRP:NE1	2.25	0.51
1:O:571:ARG:HB2	1:O:642:VAL:HB	1.91	0.51
1:S:187:TRP:CH2	1:S:196:PRO:HB3	2.45	0.51
1:C:75:ARG:NH2	1:C:543:CYS:HA	2.25	0.51
1:E:533:VAL:HB	1:E:534:PRO:HD3	1.92	0.51
1:I:176:TRP:O	1:I:177:GLU:C	2.53	0.51
2:L:216:VAL:HG13	2:L:223:GLU:HG3	1.92	0.51
1:O:323:GLU:HB2	8:O:1568:HOH:O	2.11	0.51
1:O:356:GLY:H	4:O:903:MGD:C5'	2.21	0.51
1:S:696:LYS:O	1:S:700:GLU:HG3	2.10	0.51
1:S:722:LYS:HG2	8:S:1557:HOH:O	2.09	0.51
1:U:28:MET:HE1	1:U:66:PHE:CB	2.40	0.51
1:W:656:TRP:CD2	1:W:663:LYS:HA	2.46	0.51
1:A:21:LYS:HB3	1:A:26:ILE:HD11	1.93	0.51
1:A:75:ARG:NH2	1:A:543:CYS:HA	2.25	0.51
1:A:870:ASP:HB3	1:A:872:TYR:CE1	2.46	0.51
1:I:730:TYR:CZ	1:I:794:ASN:HA	2.46	0.51
2:N:39:MET:HE2	2:N:45:TRP:CD2	2.46	0.51
1:O:558:SER:H	1:O:564:ASN:ND2	2.07	0.51
1:Q:146:MET:CE	1:Q:544:THR:HB	2.41	0.51
2:R:59:ASN:ND2	2:R:59:ASN:H	2.08	0.51
1:S:1:MET:H3	1:S:22:ASP:CG	2.17	0.51
1:S:141:PRO:HA	1:S:496:TYR:HB3	1.92	0.51
1:W:794:ASN:HD22	1:W:862:VAL:HG12	1.75	0.51
1:G:128:ILE:CD1	1:G:492:MET:HB2	2.40	0.51
1:M:13:GLY:HA3	1:M:63:THR:OG1	2.10	0.51
1:M:100:LEU:CD1	1:M:105:PRO:HG3	2.39	0.51
1:M:165:GLY:CA	1:M:166:PHE:HB3	2.40	0.51
1:O:15:PRO:HD3	1:O:554:PHE:CD1	2.46	0.51
2:P:162:GLU:CD	2:P:162:GLU:H	2.18	0.51
2:T:105:LEU:HB3	2:T:114:MET:HE1	1.92	0.51
1:A:147:TRP:CD1	1:A:552:SER:HG	2.29	0.51
1:A:737:PRO:CG	4:A:903:MGD:H2'	2.41	0.51
1:C:757:ILE:HD11	2:D:21:MET:HE3	1.92	0.51
2:D:10:VAL:HG13	2:D:63:TYR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:142:MET:HE1	8:D:429:HOH:O	2.10	0.51
1:K:395:LEU:HD12	1:K:566:GLN:HA	1.93	0.51
1:K:402:PRO:HG2	1:K:422:PHE:CE1	2.45	0.51
2:L:119:GLU:O	2:L:119:GLU:HG2	2.09	0.51
1:O:165:GLY:CA	1:O:166:PHE:HB3	2.36	0.51
2:X:19:CYS:O	2:X:22:GLY:N	2.44	0.51
1:G:630:THR:OG1	1:G:633:GLU:HG3	2.09	0.51
2:N:56:TYR:HA	2:N:59:ASN:ND2	2.26	0.51
1:C:144:HIS:HB2	4:C:902:MGD:O1B	2.11	0.51
1:K:76:ILE:HG22	1:K:541:PRO:HG3	1.93	0.51
1:K:155:SER:OG	1:K:409:ILE:HG12	2.11	0.51
1:K:249:ASP:CG	4:K:903:MGD:H1'	2.36	0.51
1:K:691:ILE:HD11	1:K:711:MET:HE3	1.91	0.51
1:M:197:GLU:OE2	1:M:665:THR:OG1	2.15	0.51
1:O:56:LYS:HE2	8:O:1466:HOH:O	2.11	0.51
1:Q:296:ASN:O	1:Q:687:LYS:HB3	2.11	0.51
1:U:165:GLY:CA	1:U:166:PHE:HB3	2.40	0.51
1:C:176:TRP:O	1:C:177:GLU:C	2.54	0.51
1:C:510:TYR:O	1:C:513:MET:HG2	2.11	0.51
1:E:21:LYS:CB	1:E:26:ILE:HD11	2.41	0.51
2:F:68:CYS:HB2	2:F:126:CYS:HB2	1.90	0.51
1:I:175:SER:HB2	1:I:176:TRP:CZ3	2.46	0.51
1:I:495:LYS:HD3	8:I:1105:HOH:O	2.11	0.51
2:J:18:ASN:HB2	7:J:301:SF4:S1	2.51	0.51
1:M:201:LEU:HD13	1:M:387:TRP:HB2	1.93	0.51
1:U:265:SER:O	1:U:810:GLN:NE2	2.43	0.51
2:X:46:MET:HE1	2:X:65:PRO:C	2.35	0.51
1:C:118:THR:O	1:C:122:VAL:HG23	2.11	0.50
1:C:628:TYR:CE2	1:C:643:PRO:HG2	2.46	0.50
1:E:800:ILE:CD1	1:E:833:ALA:HB1	2.42	0.50
1:G:855:MET:HB2	1:G:857:ASN:OD1	2.11	0.50
1:I:174:ASP:OD1	1:I:175:SER:N	2.40	0.50
1:I:252:MET:HE1	2:J:59:ASN:O	2.11	0.50
1:I:361:SER:OG	1:I:717:ALA:HB1	2.11	0.50
2:L:53:ARG:HB2	2:L:60:ASP:OD1	2.11	0.50
1:M:142:SER:CB	4:M:902:MGD:O1A	2.59	0.50
2:N:19:CYS:O	2:N:22:GLY:N	2.44	0.50
2:N:70:HIS:CD2	2:N:92:VAL:H	2.13	0.50
1:Q:557:CYS:H	1:Q:564:ASN:ND2	1.87	0.50
1:S:100:LEU:CD1	1:S:105:PRO:HG3	2.39	0.50
1:S:855:MET:HB2	1:S:857:ASN:OD1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:76:ILE:HG22	1:W:541:PRO:HG3	1.92	0.50
1:C:786:ASN:HD21	1:C:804:GLN:HA	1.76	0.50
2:D:179:GLU:CD	2:D:179:GLU:H	2.19	0.50
1:E:134:PRO:HB2	1:E:439:LEU:HD11	1.93	0.50
1:K:753:TYR:HB3	2:L:24:MET:HE3	1.93	0.50
2:L:70:HIS:CD2	2:L:92:VAL:H	2.19	0.50
1:Q:142:SER:OG	4:Q:902:MGD:O1A	2.27	0.50
1:S:12:THR:O	1:S:226:TYR:HA	2.11	0.50
1:U:100:LEU:CD1	1:U:105:PRO:HG3	2.40	0.50
2:V:4:TYR:CE2	2:V:158:LYS:HD2	2.46	0.50
1:W:165:GLY:HA3	1:W:166:PHE:CB	2.37	0.50
2:X:73:ASN:O	2:X:75:PRO:HD3	2.11	0.50
1:C:558:SER:H	1:C:564:ASN:ND2	2.08	0.50
2:D:19:CYS:HB2	2:D:46:MET:HG2	1.92	0.50
1:E:21:LYS:HB3	1:E:26:ILE:HD11	1.93	0.50
1:I:35:ASP:OD1	1:I:55:ARG:HD3	2.12	0.50
1:K:165:GLY:CA	1:K:166:PHE:HB3	2.40	0.50
1:K:400:TYR:CE1	1:K:421:LYS:HD2	2.47	0.50
1:K:610:LYS:HZ3	1:K:618:GLN:HE22	1.59	0.50
1:K:730:TYR:CE1	1:K:794:ASN:HA	2.46	0.50
1:M:356:GLY:HA2	1:M:359:ARG:NH1	2.27	0.50
1:M:558:SER:H	1:M:564:ASN:ND2	2.09	0.50
1:S:610:LYS:HB3	1:S:614:ALA:HB3	1.93	0.50
2:T:49:GLU:HG3	2:T:64:ARG:NH2	2.26	0.50
1:U:218:ASP:OD2	1:U:253:ASN:HB2	2.11	0.50
1:W:387:TRP:CE2	1:W:389:THR:HA	2.47	0.50
1:A:855:MET:HB2	1:A:857:ASN:OD1	2.11	0.50
2:H:213:ALA:O	2:H:228:GLU:HA	2.11	0.50
1:I:76:ILE:HG22	1:I:541:PRO:HG3	1.92	0.50
2:L:40:GLN:NE2	2:L:118:GLU:H	1.95	0.50
1:M:825:PRO:HD2	8:M:1334:HOH:O	2.11	0.50
2:R:142:MET:CE	2:R:146:ALA:HB1	2.41	0.50
2:T:71:CYS:HA	2:T:184:PRO:HA	1.92	0.50
2:V:21:MET:HE2	2:V:21:MET:CA	2.42	0.50
2:B:40:GLN:HE22	2:B:118:GLU:H	1.59	0.50
1:E:494:TRP:HE1	1:E:525:GLN:HE21	1.59	0.50
1:G:9:ASN:HA	1:G:576:GLN:HA	1.94	0.50
1:G:696:LYS:O	1:G:700:GLU:HG3	2.12	0.50
2:J:56:TYR:HA	2:J:59:ASN:HD22	1.76	0.50
1:K:378:GLY:O	1:K:381:LYS:HG2	2.11	0.50
1:M:333:ARG:CZ	1:S:729:LYS:HE3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:19:CYS:O	2:T:22:GLY:N	2.43	0.50
1:U:56:LYS:HG2	1:U:57:THR:O	2.11	0.50
1:U:557:CYS:N	1:U:564:ASN:HD21	1.95	0.50
1:W:730:TYR:CE1	1:W:794:ASN:HA	2.46	0.50
1:A:377:GLN:O	1:A:381:LYS:HE2	2.12	0.50
1:C:780:GLU:HB2	8:C:1183:HOH:O	2.10	0.50
1:E:400:TYR:CE1	1:E:421:LYS:HD2	2.46	0.50
1:E:855:MET:HB2	1:E:857:ASN:OD1	2.12	0.50
2:N:46:MET:CE	2:N:66:THR:H	2.19	0.50
1:O:1:MET:N	1:O:22:ASP:OD1	2.42	0.50
1:O:174:ASP:OD1	1:O:175:SER:N	2.40	0.50
1:O:452:ILE:HB	1:O:453:PRO:HD3	1.94	0.50
2:P:5:TYR:HB2	2:P:157:LEU:HD12	1.92	0.50
1:Q:501:LEU:HD13	1:Q:823:TYR:CD2	2.47	0.50
1:Q:725:PRO:HA	1:U:704:ILE:HG13	1.94	0.50
1:S:387:TRP:CE2	1:S:389:THR:HA	2.45	0.50
2:T:68:CYS:HB2	2:T:126:CYS:HB2	1.90	0.50
1:U:855:MET:HB2	1:U:857:ASN:OD1	2.11	0.50
2:V:125:LYS:HD2	2:V:126:CYS:O	2.12	0.50
2:B:19:CYS:O	2:B:22:GLY:N	2.45	0.50
2:D:94:ILE:O	2:D:96:PRO:HD3	2.12	0.50
2:F:56:TYR:HA	2:F:59:ASN:ND2	2.27	0.50
1:G:797:GLY:HA2	1:G:875:TYR:CE2	2.47	0.50
2:J:142:MET:HE1	8:J:429:HOH:O	2.12	0.50
1:K:142:SER:HB3	4:K:902:MGD:O1A	2.12	0.50
1:M:177:GLU:HA	1:M:177:GLU:OE2	2.12	0.50
1:M:501:LEU:HD13	1:M:823:TYR:CD2	2.46	0.50
1:M:855:MET:HB2	1:M:857:ASN:OD1	2.12	0.50
1:O:772:MET:HB2	1:O:801:LEU:HD13	1.94	0.50
1:U:214:PHE:HA	1:U:347:ALA:HB3	1.93	0.50
1:A:176:TRP:O	1:A:177:GLU:C	2.55	0.50
1:C:142:SER:OG	4:C:902:MGD:O1A	2.29	0.50
1:I:21:LYS:HB3	1:I:26:ILE:HD11	1.94	0.50
1:I:85:PHE:CE2	1:I:87:PRO:HG3	2.46	0.50
1:K:118:THR:O	1:K:122:VAL:HG23	2.12	0.50
1:K:177:GLU:HA	1:K:177:GLU:OE2	2.11	0.50
1:M:81:LYS:HB2	1:M:112:ILE:HD13	1.94	0.50
1:M:139:SER:OG	1:M:161:MET:HE2	2.12	0.50
2:R:142:MET:HE3	2:R:146:ALA:CB	2.41	0.50
1:S:361:SER:OG	1:S:717:ALA:HB1	2.11	0.50
1:S:772:MET:HB2	1:S:801:LEU:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:786:ASN:ND2	1:S:804:GLN:HA	2.26	0.50
2:V:19:CYS:HB2	2:V:46:MET:HG2	1.93	0.50
2:X:77:VAL:HG22	2:X:84:VAL:HG12	1.93	0.50
2:B:106:LEU:HD11	2:B:116:TRP:HB2	1.94	0.50
1:C:816:SER:OG	1:C:839:ILE:HG13	2.11	0.50
1:O:141:PRO:CA	1:O:496:TYR:HB3	2.41	0.50
1:O:855:MET:HB2	1:O:857:ASN:OD1	2.11	0.50
1:Q:478:HIS:HD2	8:Q:1199:HOH:O	1.95	0.50
2:R:71:CYS:HB2	2:R:182:THR:O	2.11	0.50
1:S:197:GLU:HG3	1:S:653:ALA:HB1	1.93	0.50
1:S:757:ILE:HD11	8:S:1651:HOH:O	2.10	0.50
2:T:211:GLU:HB2	2:T:231:PHE:HA	1.93	0.50
1:A:146:MET:HG2	4:A:902:MGD:N7	2.26	0.49
1:A:356:GLY:H	4:A:903:MGD:H5'2	1.77	0.49
2:B:142:MET:HE3	2:B:146:ALA:HB1	1.93	0.49
1:C:12:THR:O	1:C:226:TYR:HA	2.12	0.49
1:E:387:TRP:CE2	1:E:389:THR:HA	2.47	0.49
1:I:528:TRP:CD2	1:I:750:LYS:HD3	2.46	0.49
1:K:571:ARG:HB2	1:K:642:VAL:HB	1.94	0.49
1:O:195:ASN:HD21	1:O:354:TRP:CD1	2.30	0.49
1:O:717:ALA:HB3	1:O:720:SER:HB3	1.93	0.49
1:Q:184:MET:HE2	1:Q:190:SER:HA	1.94	0.49
2:T:59:ASN:HD22	2:T:59:ASN:H	1.60	0.49
2:T:105:LEU:HD12	8:T:496:HOH:O	2.11	0.49
1:U:28:MET:HE2	1:U:67:LYS:H	1.77	0.49
1:U:249:ASP:CG	4:U:903:MGD:H1'	2.37	0.49
1:U:670:PRO:HB3	1:U:682:GLN:HB2	1.94	0.49
2:D:114:MET:HA	2:D:125:LYS:HB3	1.95	0.49
1:G:478:HIS:HD2	8:G:1204:HOH:O	1.95	0.49
1:G:786:ASN:ND2	1:G:805:VAL:H	2.09	0.49
1:G:800:ILE:HD12	1:G:800:ILE:N	2.27	0.49
1:K:153:ARG:O	1:K:157:TYR:HB3	2.12	0.49
2:N:142:MET:HE1	8:N:428:HOH:O	2.11	0.49
1:O:730:TYR:CE1	1:O:794:ASN:HA	2.47	0.49
1:S:647:ASN:O	1:S:648:ARG:HG2	2.12	0.49
1:U:74:LEU:HD12	1:U:750:LYS:HA	1.94	0.49
1:U:673:ASN:HD22	1:U:673:ASN:H	1.59	0.49
2:V:21:MET:HE2	2:V:21:MET:N	2.26	0.49
1:A:177:GLU:HA	1:A:177:GLU:OE2	2.12	0.49
1:C:786:ASN:ND2	1:C:805:VAL:H	2.10	0.49
2:D:166:LYS:O	2:D:170:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:503:THR:HG21	4:E:902:MGD:O2A	2.12	0.49
1:G:239:LYS:HE2	8:G:1599:HOH:O	2.12	0.49
1:O:263:TRP:CZ2	1:O:265:SER:HB2	2.46	0.49
1:Q:175:SER:HB2	1:Q:176:TRP:CE3	2.48	0.49
1:S:870:ASP:HB3	1:S:872:TYR:CE1	2.47	0.49
1:A:153:ARG:O	1:A:157:TYR:HB3	2.12	0.49
1:C:141:PRO:CA	1:C:496:TYR:HB3	2.38	0.49
1:C:166:PHE:N	1:C:439:LEU:HD12	2.27	0.49
1:C:563:ASP:HA	1:C:565:TYR:CE1	2.47	0.49
1:G:249:ASP:CG	4:G:903:MGD:H1'	2.36	0.49
2:H:4:TYR:CE2	2:H:158:LYS:HD2	2.46	0.49
1:I:494:TRP:HE1	1:I:525:GLN:HE21	1.60	0.49
1:I:561:ILE:HG22	1:I:564:ASN:HB3	1.94	0.49
1:K:174:ASP:OD1	1:K:175:SER:N	2.45	0.49
1:K:257:ARG:HD3	2:L:61:ILE:HG21	1.93	0.49
1:K:870:ASP:HB3	1:K:872:TYR:CE1	2.47	0.49
2:L:46:MET:HE1	2:L:65:PRO:C	2.36	0.49
1:Q:56:LYS:HG2	1:Q:57:THR:O	2.13	0.49
1:Q:322:GLU:HG3	1:Q:327:VAL:O	2.13	0.49
1:Q:510:TYR:O	1:Q:513:MET:HG2	2.13	0.49
1:U:96:ARG:HD3	1:U:535:PHE:O	2.11	0.49
1:W:451:LYS:HG3	1:W:461:PHE:CE2	2.47	0.49
1:C:452:ILE:HB	1:C:453:PRO:HD3	1.95	0.49
1:C:871:LYS:HG2	8:C:1231:HOH:O	2.13	0.49
1:E:75:ARG:NH2	1:E:543:CYS:HA	2.28	0.49
2:F:177:LYS:N	2:F:178:PRO:HD3	2.28	0.49
1:G:377:GLN:O	1:G:381:LYS:HE2	2.12	0.49
1:G:656:TRP:CD2	1:G:663:LYS:HA	2.48	0.49
2:J:68:CYS:HB2	2:J:126:CYS:HB2	1.94	0.49
1:O:451:LYS:HG3	1:O:461:PHE:CE2	2.47	0.49
2:R:21:MET:HA	2:R:21:MET:CE	2.40	0.49
1:U:387:TRP:CE2	1:U:389:THR:HA	2.47	0.49
1:U:644:ASP:C	1:U:646:PRO:HD3	2.37	0.49
1:A:737:PRO:HG3	4:A:903:MGD:H2'	1.94	0.49
1:C:174:ASP:OD1	1:C:175:SER:N	2.43	0.49
2:D:4:TYR:CE2	2:D:158:LYS:HD2	2.48	0.49
2:D:106:LEU:HD23	2:D:114:MET:HG3	1.95	0.49
1:E:610:LYS:HZ3	1:E:618:GLN:HE22	1.60	0.49
1:I:356:GLY:H	4:I:903:MGD:H5'2	1.77	0.49
1:M:296:ASN:O	1:M:687:LYS:HB3	2.12	0.49
1:O:628:TYR:HE2	1:O:643:PRO:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:533:VAL:HB	1:S:534:PRO:HD3	1.93	0.49
1:S:786:ASN:HD22	1:S:805:VAL:H	1.60	0.49
2:T:23:CYS:O	2:T:27:HIS:N	2.42	0.49
2:T:39:MET:HE2	2:T:45:TRP:CD2	2.48	0.49
2:T:139:ALA:O	2:T:141:LYS:HG3	2.12	0.49
1:W:104:ASP:OD2	1:W:107:SER:HB3	2.13	0.49
1:A:146:MET:HE2	1:A:544:THR:CB	2.41	0.49
1:A:629:MET:HE2	1:A:634:PHE:CA	2.41	0.49
1:E:528:TRP:CD2	1:E:750:LYS:HD3	2.48	0.49
2:F:5:TYR:HB2	2:F:157:LEU:HD12	1.94	0.49
1:G:66:PHE:CD1	1:G:69:MET:HE3	2.48	0.49
1:I:717:ALA:HB3	1:I:720:SER:HB3	1.95	0.49
1:M:870:ASP:HB3	1:M:872:TYR:CE1	2.47	0.49
1:O:700:GLU:HB3	8:O:1199:HOH:O	2.13	0.49
1:Q:163:MET:HE1	1:Q:606:PHE:HA	1.93	0.49
2:R:23:CYS:O	2:R:26:GLU:N	2.45	0.49
2:T:5:TYR:HB2	2:T:157:LEU:CD1	2.43	0.49
1:U:426:MET:HE1	1:U:618:GLN:O	2.12	0.49
1:W:15:PRO:HD3	1:W:554:PHE:CD1	2.47	0.49
1:C:249:ASP:CG	4:C:903:MGD:H1'	2.38	0.49
1:C:801:LEU:HD11	1:C:839:ILE:HD11	1.95	0.49
2:F:59:ASN:ND2	2:F:59:ASN:H	2.11	0.49
1:G:786:ASN:HD22	1:G:805:VAL:H	1.61	0.49
2:L:46:MET:HE1	2:L:66:THR:H	1.71	0.49
2:L:87:ARG:HG3	2:L:91:ILE:O	2.13	0.49
1:Q:146:MET:HE2	1:Q:544:THR:CB	2.40	0.49
1:Q:800:ILE:N	1:Q:800:ILE:CD1	2.76	0.49
1:S:85:PHE:CE2	1:S:87:PRO:HG3	2.48	0.49
1:S:510:TYR:O	1:S:513:MET:HG2	2.12	0.49
1:U:141:PRO:CA	1:U:496:TYR:HB3	2.41	0.49
1:W:218:ASP:OD2	1:W:253:ASN:HB2	2.12	0.49
2:X:198:TYR:HB3	2:X:238:ASP:HA	1.94	0.49
1:A:32:ASP:HB2	8:A:1657:HOH:O	2.13	0.49
2:B:21:MET:HE2	2:B:21:MET:HA	1.95	0.49
1:G:738:HIS:HE2	4:G:902:MGD:H15	1.61	0.49
1:K:510:TYR:O	1:K:513:MET:HG2	2.12	0.49
1:M:175:SER:HB2	1:M:176:TRP:CE3	2.48	0.49
1:M:197:GLU:HG3	1:M:199:TYR:CD1	2.48	0.49
1:M:797:GLY:HA2	1:M:875:TYR:CZ	2.48	0.49
2:N:87:ARG:HD3	2:N:93:LEU:CD1	2.43	0.49
1:O:729:LYS:HD2	8:O:1131:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:249:ASP:CG	4:Q:903:MGD:H1'	2.37	0.49
1:Q:425:ARG:HD3	1:Q:622:ALA:O	2.13	0.49
1:S:138:LEU:HB2	1:S:490:ILE:HD12	1.95	0.49
1:S:554:PHE:HB3	8:S:1028:HOH:O	2.12	0.49
1:U:13:GLY:HA3	1:U:63:THR:OG1	2.13	0.49
2:V:59:ASN:ND2	2:V:59:ASN:H	2.11	0.49
2:X:71:CYS:HA	2:X:184:PRO:HA	1.93	0.49
1:A:791:ARG:NH2	8:A:1580:HOH:O	2.46	0.49
2:B:201:ALA:HB2	2:B:269:LEU:HB2	1.95	0.49
2:D:252:ASP:C	2:D:254:LYS:H	2.20	0.49
1:E:505:THR:O	1:E:506:ALA:C	2.55	0.49
1:G:56:LYS:HG2	1:G:57:THR:O	2.13	0.49
2:H:46:MET:HE1	2:H:65:PRO:CA	2.43	0.49
1:M:211:MET:HE2	1:M:246:VAL:HG23	1.94	0.49
2:N:114:MET:HE3	2:N:123:ALA:HB1	1.95	0.49
1:Q:253:ASN:O	1:Q:257:ARG:HG3	2.12	0.49
1:U:76:ILE:CG2	1:U:541:PRO:HG3	2.41	0.49
1:U:630:THR:OG1	1:U:633:GLU:HG3	2.13	0.49
2:X:157:LEU:HD12	2:X:157:LEU:H	1.78	0.49
2:X:180:LEU:HB2	8:X:520:HOH:O	2.12	0.49
1:C:649:LYS:HE2	1:C:651:THR:HG22	1.95	0.48
1:E:629:MET:HE2	1:E:634:PHE:CA	2.42	0.48
1:G:146:MET:HE2	1:G:544:THR:CA	2.43	0.48
1:G:257:ARG:HD3	2:H:61:ILE:HG21	1.95	0.48
1:K:737:PRO:HG2	4:K:903:MGD:H2'	1.95	0.48
1:K:847:TYR:CZ	1:K:853:CYS:HB3	2.48	0.48
2:N:142:MET:HE3	2:N:146:ALA:HB1	1.94	0.48
2:R:203:ILE:N	2:R:203:ILE:HD12	2.28	0.48
1:S:28:MET:CE	1:S:66:PHE:HB3	2.43	0.48
2:V:96:PRO:O	2:V:100:LYS:HG3	2.13	0.48
1:C:20:VAL:HG13	1:C:24:LYS:O	2.13	0.48
1:C:100:LEU:CD1	1:C:105:PRO:HG3	2.43	0.48
1:C:114:TRP:CZ2	1:C:541:PRO:HD2	2.48	0.48
1:E:56:LYS:HG2	1:E:57:THR:O	2.13	0.48
1:G:356:GLY:H	4:G:903:MGD:H5'2	1.78	0.48
1:I:797:GLY:HA2	1:I:875:TYR:CE2	2.48	0.48
2:J:142:MET:HE2	2:J:146:ALA:HB3	1.95	0.48
1:K:505:THR:O	1:K:506:ALA:C	2.56	0.48
1:K:797:GLY:HA2	1:K:875:TYR:CE2	2.48	0.48
2:N:46:MET:HE1	2:N:65:PRO:CA	2.42	0.48
2:N:106:LEU:HD23	2:N:114:MET:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:56:LYS:HG2	1:O:57:THR:O	2.13	0.48
2:P:167:LYS:HZ3	2:P:171:GLU:CD	2.21	0.48
1:S:426:MET:HE2	1:S:618:GLN:HG2	1.94	0.48
1:U:78:TYR:O	1:U:80:MET:HG3	2.13	0.48
1:A:75:ARG:HH21	1:A:543:CYS:HA	1.78	0.48
1:E:452:ILE:N	1:E:453:PRO:CD	2.76	0.48
1:G:510:TYR:O	1:G:513:MET:HG2	2.13	0.48
1:G:644:ASP:C	1:G:646:PRO:HD3	2.37	0.48
1:Q:250:PRO:HD3	4:Q:903:MGD:C2	2.43	0.48
1:S:66:PHE:CD1	1:S:69:MET:HE3	2.48	0.48
1:S:656:TRP:CD2	1:S:663:LYS:HA	2.48	0.48
1:U:66:PHE:CD1	1:U:69:MET:HE3	2.49	0.48
2:V:94:ILE:O	2:V:96:PRO:HD3	2.14	0.48
1:W:610:LYS:HB3	1:W:614:ALA:HB3	1.94	0.48
1:W:765:ASP:HB2	8:W:1167:HOH:O	2.13	0.48
1:A:195:ASN:HD21	1:A:354:TRP:CD1	2.32	0.48
2:B:18:ASN:HB2	7:B:302:SF4:S1	2.54	0.48
2:J:53:ARG:HB2	2:J:60:ASP:OD1	2.13	0.48
2:J:59:ASN:ND2	2:J:59:ASN:H	2.11	0.48
2:J:106:LEU:HD11	2:J:116:TRP:HB2	1.94	0.48
1:K:644:ASP:C	1:K:646:PRO:HD3	2.38	0.48
1:M:176:TRP:O	1:M:177:GLU:C	2.56	0.48
1:M:249:ASP:CG	4:M:903:MGD:H1'	2.38	0.48
1:M:730:TYR:CZ	1:M:794:ASN:HA	2.48	0.48
2:P:46:MET:CE	2:P:66:THR:N	2.64	0.48
1:U:165:GLY:HA3	1:U:166:PHE:CB	2.37	0.48
1:U:610:LYS:HZ2	1:U:618:GLN:HE22	1.57	0.48
1:W:565:TYR:C	1:W:567:LEU:H	2.21	0.48
1:W:645:ASN:HD21	1:W:648:ARG:HB3	1.75	0.48
2:X:7:VAL:HG21	2:X:167:LYS:HZ2	1.78	0.48
1:A:871:LYS:HE2	8:A:1231:HOH:O	2.12	0.48
1:C:44:ILE:HD11	1:C:394:PRO:HG2	1.95	0.48
1:C:214:PHE:HA	1:C:347:ALA:HB3	1.94	0.48
1:E:142:SER:CB	4:E:902:MGD:O1A	2.61	0.48
1:E:400:TYR:CZ	1:E:421:LYS:HD2	2.48	0.48
1:G:13:GLY:HA3	1:G:63:THR:OG1	2.12	0.48
1:G:103:GLN:N	1:G:103:GLN:CD	2.72	0.48
2:H:166:LYS:HG2	2:H:170:GLU:OE2	2.13	0.48
1:I:565:TYR:C	1:I:567:LEU:N	2.71	0.48
1:K:9:ASN:HA	1:K:576:GLN:HA	1.96	0.48
1:M:250:PRO:HD3	4:M:903:MGD:C2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:786:ASN:ND2	1:O:804:GLN:HA	2.28	0.48
1:U:75:ARG:HH22	1:U:547:GLU:CD	2.20	0.48
1:A:296:ASN:HB3	1:A:657:PHE:CZ	2.49	0.48
1:C:163:MET:HE1	1:C:606:PHE:HA	1.95	0.48
2:F:114:MET:HG2	2:F:125:LYS:HG2	1.94	0.48
1:G:75:ARG:HH22	1:G:547:GLU:CD	2.21	0.48
1:I:155:SER:OG	1:I:409:ILE:HG12	2.14	0.48
1:I:184:MET:HE2	1:I:190:SER:HA	1.95	0.48
1:I:402:PRO:HG2	1:I:422:PHE:CE1	2.49	0.48
1:I:476:GLN:OE1	1:I:708:ARG:NH2	2.47	0.48
1:K:187:TRP:CH2	1:K:196:PRO:HB3	2.48	0.48
1:M:565:TYR:C	1:M:567:LEU:H	2.20	0.48
1:O:2:GLY:N	1:O:22:ASP:OD1	2.47	0.48
2:P:141:LYS:HA	8:P:500:HOH:O	2.14	0.48
1:Q:451:LYS:HG3	1:Q:461:PHE:CE2	2.48	0.48
1:Q:629:MET:HE2	1:Q:634:PHE:CA	2.41	0.48
2:V:90:GLY:HA3	2:V:185:ARG:CZ	2.44	0.48
1:A:494:TRP:HE1	1:A:525:GLN:HE21	1.61	0.48
1:E:34:ASP:HB3	1:E:37:VAL:HG22	1.94	0.48
1:E:561:ILE:CG2	1:E:564:ASN:HB3	2.43	0.48
1:G:165:GLY:CA	1:G:166:PHE:HB3	2.41	0.48
2:H:177:LYS:N	2:H:178:PRO:HD3	2.29	0.48
1:I:263:TRP:CZ2	1:I:265:SER:HB2	2.49	0.48
1:I:505:THR:O	1:I:506:ALA:C	2.56	0.48
1:K:100:LEU:HD12	1:K:105:PRO:HG3	1.95	0.48
1:M:452:ILE:N	1:M:453:PRO:CD	2.76	0.48
1:O:725:PRO:HD2	8:O:1193:HOH:O	2.12	0.48
1:Q:176:TRP:O	1:Q:177:GLU:C	2.56	0.48
1:Q:786:ASN:HD21	1:Q:804:GLN:HA	1.78	0.48
1:U:394:PRO:HG3	8:U:1323:HOH:O	2.13	0.48
1:U:797:GLY:HA2	1:U:875:TYR:CE2	2.48	0.48
1:W:452:ILE:N	1:W:453:PRO:CD	2.77	0.48
2:X:250:ASP:HB2	8:X:433:HOH:O	2.14	0.48
1:A:610:LYS:HB3	1:A:614:ALA:HB3	1.95	0.48
1:A:767:TYR:HB3	1:A:769:TYR:CE1	2.49	0.48
1:C:211:MET:HE3	8:C:1450:HOH:O	2.13	0.48
1:E:184:MET:HE2	1:E:190:SER:HA	1.95	0.48
1:G:146:MET:HE2	1:G:544:THR:HA	1.95	0.48
1:G:730:TYR:CZ	1:G:794:ASN:HA	2.49	0.48
1:I:218:ASP:OD2	1:I:253:ASN:HB2	2.14	0.48
2:L:58:ARG:HD2	2:L:268:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:73:ASN:OD1	2:P:183:LYS:HE3	2.13	0.48
1:U:147:TRP:CD1	1:U:552:SER:HG	2.31	0.48
1:W:177:GLU:HA	1:W:177:GLU:OE2	2.14	0.48
1:A:730:TYR:CZ	1:A:794:ASN:HA	2.49	0.48
1:C:436:PRO:HG3	8:C:1445:HOH:O	2.12	0.48
1:E:165:GLY:HA3	1:E:166:PHE:CB	2.35	0.48
2:F:166:LYS:HG2	2:F:170:GLU:OE2	2.14	0.48
1:G:28:MET:HE1	1:G:66:PHE:CB	2.40	0.48
1:I:224:GLY:O	1:I:225:ILE:HB	2.14	0.48
1:M:144:HIS:HB2	4:M:902:MGD:O1B	2.13	0.48
2:P:53:ARG:HB2	2:P:60:ASP:OD1	2.14	0.48
1:S:55:ARG:HD2	8:S:1627:HOH:O	2.14	0.48
1:S:730:TYR:CE1	1:S:794:ASN:HA	2.48	0.48
2:T:21:MET:HE2	2:T:21:MET:CA	2.41	0.48
1:U:571:ARG:HB2	1:U:642:VAL:HB	1.94	0.48
1:W:263:TRP:CZ2	1:W:265:SER:HB2	2.49	0.48
2:X:1:MET:HE2	2:X:88:GLU:HG2	1.96	0.48
1:A:847:TYR:CZ	1:A:853:CYS:HB3	2.49	0.48
2:B:60:ASP:C	2:B:60:ASP:OD1	2.57	0.48
1:E:772:MET:HB2	1:E:801:LEU:HD13	1.96	0.48
2:F:256:TYR:HB2	2:F:274:LEU:HD21	1.95	0.48
1:G:141:PRO:CA	1:G:496:TYR:HB3	2.40	0.48
2:J:40:GLN:HB3	2:J:43:HIS:CE1	2.49	0.48
1:K:362:HIS:HB3	1:K:717:ALA:HB2	1.95	0.48
2:L:162:GLU:CD	2:L:162:GLU:N	2.72	0.48
2:N:247:VAL:O	2:N:257:SER:HA	2.14	0.48
1:O:94:GLN:HE21	1:O:95:LEU:HG	1.78	0.48
1:O:140:THR:OG1	1:O:171:HIS:HE1	1.97	0.48
1:Q:114:TRP:CZ2	1:Q:587:MET:HG2	2.49	0.48
1:S:165:GLY:CA	1:S:166:PHE:HB3	2.44	0.48
1:U:146:MET:HG2	4:U:902:MGD:N7	2.29	0.48
1:U:871:LYS:HE2	8:U:1233:HOH:O	2.14	0.48
2:V:19:CYS:O	2:V:22:GLY:N	2.47	0.48
1:A:96:ARG:HD2	1:A:514:TYR:O	2.14	0.47
1:C:35:ASP:OD1	1:C:55:ARG:HD3	2.14	0.47
1:C:571:ARG:HB2	1:C:642:VAL:HB	1.95	0.47
2:D:19:CYS:CB	2:D:145:CYS:HB3	2.34	0.47
1:E:249:ASP:CG	4:E:903:MGD:H1'	2.38	0.47
1:K:146:MET:HG2	4:K:902:MGD:N7	2.29	0.47
2:N:142:MET:CE	2:N:146:ALA:HB1	2.43	0.47
1:Q:75:ARG:NH2	1:Q:543:CYS:HA	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:563:ASP:HA	1:S:565:TYR:CE1	2.49	0.47
2:T:21:MET:CA	2:T:21:MET:CE	2.92	0.47
1:U:12:THR:O	1:U:226:TYR:HA	2.14	0.47
2:X:59:ASN:H	2:X:59:ASN:HD22	1.62	0.47
2:X:142:MET:HE1	8:X:431:HOH:O	2.15	0.47
1:A:197:GLU:HG3	1:A:653:ALA:HB1	1.96	0.47
1:C:395:LEU:HD12	1:C:566:GLN:HA	1.96	0.47
1:C:459:GLY:O	1:C:489:LYS:HE2	2.13	0.47
1:C:797:GLY:HA2	1:C:875:TYR:CD2	2.49	0.47
2:D:114:MET:HB3	2:D:125:LYS:HB3	1.96	0.47
2:D:216:VAL:HG13	2:D:223:GLU:HG3	1.95	0.47
1:G:12:THR:HB	1:G:743:MET:HG3	1.96	0.47
1:I:165:GLY:CA	1:I:166:PHE:HB3	2.41	0.47
1:I:258:LEU:HG	1:I:259:VAL:HG13	1.95	0.47
1:I:558:SER:H	1:I:564:ASN:ND2	2.12	0.47
1:K:296:ASN:HB3	1:K:657:PHE:CZ	2.49	0.47
1:K:744:HIS:HA	1:K:819:SER:CB	2.44	0.47
1:M:15:PRO:HD3	1:M:554:PHE:CD1	2.49	0.47
1:O:258:LEU:HG	1:O:259:VAL:HG13	1.95	0.47
1:O:825:PRO:HD2	8:O:1334:HOH:O	2.13	0.47
2:P:114:MET:HA	2:P:125:LYS:HB3	1.95	0.47
2:P:142:MET:HE2	2:P:146:ALA:C	2.39	0.47
2:P:164:MET:O	2:P:168:VAL:HG23	2.13	0.47
1:Q:800:ILE:CD1	1:Q:833:ALA:HB1	2.42	0.47
2:R:210:PHE:HD2	2:R:213:ALA:HB2	1.79	0.47
1:S:649:LYS:HE2	8:S:1458:HOH:O	2.13	0.47
2:T:69:MET:HB3	2:T:184:PRO:HB3	1.96	0.47
1:U:521:PHE:CE2	1:U:523:VAL:CG2	2.97	0.47
1:W:100:LEU:HD12	1:W:105:PRO:HG3	1.96	0.47
1:W:253:ASN:O	1:W:257:ARG:HG3	2.13	0.47
1:W:780:GLU:CD	1:W:780:GLU:C	2.83	0.47
1:A:146:MET:CE	1:A:544:THR:HB	2.42	0.47
1:A:786:ASN:ND2	1:A:805:VAL:H	2.06	0.47
1:E:144:HIS:HB2	4:E:902:MGD:O1B	2.13	0.47
1:G:144:HIS:HB2	4:G:902:MGD:O1B	2.15	0.47
1:K:670:PRO:HG2	1:K:675:GLN:CD	2.39	0.47
1:M:322:GLU:HG3	1:M:327:VAL:O	2.14	0.47
1:U:772:MET:HB2	1:U:801:LEU:HD13	1.96	0.47
1:W:78:TYR:O	1:W:80:MET:HG3	2.14	0.47
2:X:201:ALA:HB2	2:X:269:LEU:HB2	1.95	0.47
1:A:28:MET:HE1	1:A:66:PHE:CB	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:GLY:N	1:E:22:ASP:OD1	2.46	0.47
2:F:94:ILE:O	2:F:96:PRO:HD3	2.15	0.47
1:I:696:LYS:O	1:I:700:GLU:HG3	2.14	0.47
1:K:494:TRP:HE1	1:K:525:GLN:HE21	1.62	0.47
1:M:55:ARG:HD2	8:M:1639:HOH:O	2.14	0.47
1:O:85:PHE:CE2	1:O:87:PRO:HG3	2.49	0.47
1:O:177:GLU:HA	1:O:177:GLU:OE2	2.14	0.47
1:O:847:TYR:CZ	1:O:853:CYS:HB3	2.49	0.47
2:P:86:GLN:NE2	8:P:475:HOH:O	2.45	0.47
1:Q:265:SER:O	1:Q:810:GLN:NE2	2.46	0.47
2:T:59:ASN:H	2:T:59:ASN:ND2	2.12	0.47
1:U:9:ASN:HA	1:U:576:GLN:HA	1.96	0.47
1:W:15:PRO:HD3	1:W:554:PHE:CE1	2.48	0.47
2:X:97:GLU:OE2	2:X:100:LYS:HE2	2.14	0.47
1:A:575:LEU:HD22	1:A:635:PHE:HA	1.97	0.47
1:A:797:GLY:HA2	1:A:875:TYR:CE2	2.49	0.47
1:C:797:GLY:HA2	1:C:875:TYR:CE2	2.49	0.47
1:E:138:LEU:HD12	1:E:167:THR:O	2.14	0.47
1:E:176:TRP:O	1:E:177:GLU:C	2.57	0.47
2:F:19:CYS:HB2	2:F:46:MET:HG2	1.96	0.47
1:K:65:GLY:HA3	2:L:21:MET:HG3	1.97	0.47
1:M:155:SER:OG	1:M:409:ILE:HG12	2.14	0.47
1:M:296:ASN:HB3	1:M:657:PHE:CZ	2.49	0.47
1:M:401:PHE:CD1	1:M:573:ILE:HD13	2.50	0.47
2:N:2:GLU:HB3	2:N:158:LYS:HE2	1.96	0.47
1:O:176:TRP:O	1:O:177:GLU:C	2.57	0.47
1:O:387:TRP:CE2	1:O:389:THR:HA	2.49	0.47
1:Q:201:LEU:HD13	1:Q:387:TRP:HB2	1.96	0.47
1:U:100:LEU:HD12	1:U:105:PRO:HG3	1.97	0.47
1:U:744:HIS:HA	1:U:819:SER:CB	2.45	0.47
1:W:174:ASP:OD1	1:W:175:SER:N	2.40	0.47
2:D:5:TYR:HB2	2:D:157:LEU:CD1	2.44	0.47
2:F:138:TRP:HB3	8:F:503:HOH:O	2.14	0.47
1:I:501:LEU:HD13	1:I:823:TYR:CD2	2.48	0.47
1:I:756:TYR:HB2	2:J:24:MET:HE1	1.96	0.47
1:I:871:LYS:HE2	8:I:1228:HOH:O	2.14	0.47
2:L:1:MET:HE2	2:L:88:GLU:CD	2.40	0.47
2:N:18:ASN:HB2	7:N:302:SF4:S1	2.55	0.47
1:Q:501:LEU:HD13	1:Q:823:TYR:CG	2.49	0.47
1:Q:677:CYS:C	1:Q:678:ARG:HG2	2.39	0.47
1:S:144:HIS:HB2	4:S:902:MGD:O1B	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:296:ASN:HB3	1:S:657:PHE:CZ	2.49	0.47
1:S:823:TYR:CE2	1:S:825:PRO:HG3	2.49	0.47
1:U:737:PRO:HG3	4:U:903:MGD:H2'	1.95	0.47
2:X:1:MET:HE2	2:X:88:GLU:CG	2.45	0.47
2:X:203:ILE:HD12	2:X:203:ILE:N	2.29	0.47
1:A:356:GLY:HA2	1:A:359:ARG:NH1	2.30	0.47
1:C:656:TRP:CD2	1:C:663:LYS:HA	2.50	0.47
1:E:9:ASN:HA	1:E:576:GLN:HA	1.97	0.47
1:E:696:LYS:O	1:E:700:GLU:HG3	2.15	0.47
1:G:56:LYS:HE2	8:G:1466:HOH:O	2.14	0.47
1:I:81:LYS:HB2	1:I:112:ILE:HD13	1.95	0.47
1:I:165:GLY:HA3	1:I:166:PHE:CB	2.37	0.47
1:I:700:GLU:HG2	8:I:1563:HOH:O	2.14	0.47
1:K:75:ARG:HH21	1:K:543:CYS:HA	1.79	0.47
1:K:775:ASN:HA	1:K:806:THR:O	2.15	0.47
2:L:5:TYR:HB2	2:L:157:LEU:HD12	1.96	0.47
1:M:610:LYS:NZ	1:M:618:GLN:NE2	2.50	0.47
2:N:94:ILE:O	2:N:96:PRO:HD3	2.15	0.47
1:O:426:MET:HE3	1:O:622:ALA:HB2	1.95	0.47
1:S:177:GLU:HA	1:S:177:GLU:OE2	2.15	0.47
1:S:645:ASN:HB3	8:S:1038:HOH:O	2.14	0.47
1:U:11:SER:HA	1:U:147:TRP:HB2	1.97	0.47
1:U:75:ARG:HH21	1:U:543:CYS:HA	1.80	0.47
1:U:105:PRO:HB2	1:U:529:PHE:HE2	1.80	0.47
1:U:744:HIS:HA	1:U:819:SER:HB3	1.96	0.47
1:U:767:TYR:HB3	1:U:769:TYR:CE1	2.50	0.47
1:W:100:LEU:CD1	1:W:105:PRO:HG3	2.44	0.47
1:W:139:SER:OG	1:W:161:MET:HE2	2.14	0.47
1:W:630:THR:OG1	1:W:633:GLU:HG3	2.14	0.47
2:X:21:MET:HE2	2:X:21:MET:HA	1.96	0.47
1:C:96:ARG:HD3	1:C:535:PHE:O	2.15	0.47
1:C:476:GLN:OE1	1:C:708:ARG:NH2	2.48	0.47
2:J:52:GLU:HG3	2:J:61:ILE:HD12	1.97	0.47
2:L:21:MET:CA	2:L:21:MET:CE	2.93	0.47
2:L:103:LYS:HG2	2:L:116:TRP:CD2	2.50	0.47
1:M:630:THR:OG1	1:M:633:GLU:HG3	2.14	0.47
2:N:127:THR:HG22	8:N:519:HOH:O	2.15	0.47
1:O:657:PHE:CE1	1:O:681:LEU:HG	2.49	0.47
1:Q:141:PRO:HA	1:Q:496:TYR:O	2.15	0.47
1:U:28:MET:CE	1:U:67:LYS:H	2.28	0.47
1:U:177:GLU:HA	1:U:177:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:857:ASN:HB3	4:U:902:MGD:N19	2.30	0.47
1:W:528:TRP:CG	1:W:750:LYS:HD3	2.50	0.47
1:W:756:TYR:OH	2:X:41:ARG:HD3	2.15	0.47
2:D:166:LYS:HG2	2:D:170:GLU:OE2	2.15	0.47
1:G:540:LEU:HA	1:G:541:PRO:HD3	1.80	0.47
1:I:610:LYS:HB3	1:I:614:ALA:HB3	1.96	0.47
1:K:56:LYS:HG2	1:K:57:THR:O	2.15	0.47
1:K:628:TYR:CE2	1:K:643:PRO:HG2	2.49	0.47
2:L:16:CYS:O	2:L:17:ASN:HB2	2.15	0.47
1:M:142:SER:HB3	4:M:902:MGD:O1A	2.14	0.47
2:N:5:TYR:HB2	2:N:157:LEU:HD12	1.97	0.47
1:O:66:PHE:CD1	1:O:69:MET:HE3	2.50	0.47
1:O:96:ARG:HD2	1:O:514:TYR:O	2.15	0.47
1:O:365:GLU:OE1	1:O:365:GLU:HA	2.14	0.47
1:Q:103:GLN:CD	1:Q:103:GLN:N	2.73	0.47
8:Q:1676:HOH:O	1:S:871:LYS:HG2	2.15	0.47
1:S:176:TRP:O	1:S:177:GLU:C	2.57	0.47
1:U:175:SER:HB2	1:U:176:TRP:CE3	2.50	0.47
1:U:211:MET:HE1	1:U:338:GLN:HG2	1.97	0.47
2:X:19:CYS:HB2	2:X:46:MET:HG2	1.97	0.47
1:A:175:SER:HB2	1:A:176:TRP:CZ3	2.50	0.47
1:C:162:ASN:HA	8:C:1363:HOH:O	2.14	0.47
1:C:717:ALA:HB3	1:C:720:SER:HB3	1.97	0.47
1:E:530:GLU:CD	1:E:750:LYS:HZ2	2.23	0.47
1:G:11:SER:HA	1:G:147:TRP:HB2	1.97	0.47
1:G:100:LEU:CD1	1:G:105:PRO:HG3	2.43	0.47
2:H:157:LEU:HD12	2:H:157:LEU:N	2.29	0.47
1:I:182:GLY:HA3	1:I:364:ILE:HG23	1.97	0.47
1:I:571:ARG:HB2	1:I:642:VAL:HB	1.97	0.47
2:J:13:CYS:HB3	2:J:63:TYR:HB2	1.97	0.47
1:M:28:MET:HE2	8:M:1398:HOH:O	2.15	0.47
2:N:23:CYS:O	2:N:26:GLU:N	2.48	0.47
1:O:610:LYS:HZ1	1:O:618:GLN:HE22	1.59	0.47
2:P:203:ILE:HD12	2:P:203:ILE:N	2.30	0.47
1:Q:387:TRP:CE2	1:Q:389:THR:HA	2.50	0.47
2:R:157:LEU:HD12	2:R:157:LEU:N	2.30	0.47
1:S:696:LYS:HD3	8:S:1659:HOH:O	2.15	0.47
1:S:737:PRO:HG3	4:S:903:MGD:H2'	1.97	0.47
1:U:296:ASN:HB3	1:U:657:PHE:CZ	2.50	0.47
1:U:476:GLN:OE1	1:U:708:ARG:NH2	2.48	0.47
2:V:142:MET:HE2	2:V:147:HIS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:PHE:N	1:E:439:LEU:HD12	2.30	0.46
2:F:112:GLY:HA2	8:F:520:HOH:O	2.15	0.46
1:K:452:ILE:HB	1:K:453:PRO:HD3	1.97	0.46
1:M:282:TRP:HA	1:M:287:SER:OG	2.16	0.46
1:O:249:ASP:CG	4:O:903:MGD:H1'	2.40	0.46
2:P:87:ARG:HD3	2:P:93:LEU:HD12	1.97	0.46
2:P:94:ILE:O	2:P:96:PRO:HD3	2.15	0.46
1:E:296:ASN:O	1:E:687:LYS:HB3	2.16	0.46
1:I:644:ASP:C	1:I:646:PRO:HD3	2.39	0.46
1:O:426:MET:HA	1:O:426:MET:CE	2.37	0.46
1:O:498:GLY:N	1:O:499:PRO:HD3	2.30	0.46
2:T:21:MET:HA	2:T:21:MET:CE	2.43	0.46
1:U:166:PHE:N	1:U:439:LEU:HD12	2.30	0.46
1:U:269:GLY:HA2	1:U:362:HIS:CE1	2.50	0.46
1:U:322:GLU:HG3	1:U:327:VAL:O	2.16	0.46
2:X:46:MET:HE1	2:X:65:PRO:CA	2.45	0.46
1:A:114:TRP:CZ2	1:A:541:PRO:HD2	2.49	0.46
2:B:142:MET:HE3	2:B:146:ALA:CB	2.45	0.46
1:E:187:TRP:CH2	1:E:196:PRO:HB3	2.50	0.46
2:J:2:GLU:HG2	2:J:158:LYS:HG2	1.98	0.46
2:J:125:LYS:HD2	2:J:126:CYS:O	2.14	0.46
1:O:656:TRP:CD2	1:O:663:LYS:HA	2.50	0.46
2:P:102:LYS:HB3	2:P:104:GLU:OE2	2.15	0.46
1:Q:670:PRO:HB3	1:Q:682:GLN:HB2	1.97	0.46
1:Q:753:TYR:HB3	2:R:24:MET:HE3	1.96	0.46
1:S:140:THR:HB	1:S:169:ALA:HB3	1.98	0.46
1:S:400:TYR:CE1	1:S:421:LYS:HD2	2.50	0.46
2:V:177:LYS:N	2:V:178:PRO:HD3	2.31	0.46
2:V:256:TYR:HB2	2:V:274:LEU:HD21	1.97	0.46
1:A:128:ILE:CD1	1:A:492:MET:HB2	2.45	0.46
1:A:563:ASP:O	1:A:566:GLN:HG2	2.16	0.46
2:B:10:VAL:HG13	2:B:63:TYR:O	2.15	0.46
2:B:213:ALA:O	2:B:228:GLU:HA	2.16	0.46
1:C:173:PRO:HG3	1:C:180:HIS:CG	2.50	0.46
1:C:503:THR:HG21	4:C:902:MGD:O2A	2.15	0.46
1:E:96:ARG:HD2	1:E:514:TYR:O	2.15	0.46
1:E:737:PRO:CG	4:E:903:MGD:H2'	2.45	0.46
1:G:565:TYR:C	1:G:567:LEU:H	2.23	0.46
2:H:5:TYR:CD2	2:H:164:MET:HG2	2.50	0.46
2:J:2:GLU:HG3	2:J:159:THR:C	2.40	0.46
1:K:28:MET:HE2	8:K:1394:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:101:GLY:HA2	2:L:121:ASN:ND2	2.30	0.46
2:L:247:VAL:O	2:L:257:SER:HA	2.15	0.46
1:M:15:PRO:HD2	8:M:1003:HOH:O	2.15	0.46
1:M:77:PRO:HB2	1:M:78:TYR:CD2	2.50	0.46
1:O:9:ASN:HA	1:O:576:GLN:HA	1.97	0.46
1:O:78:TYR:C	1:O:541:PRO:HG2	2.40	0.46
1:O:735:LEU:H	1:O:735:LEU:HD23	1.80	0.46
2:T:72:GLU:HB2	2:T:183:LYS:HE3	1.97	0.46
1:U:387:TRP:CZ2	1:U:389:THR:HA	2.51	0.46
1:A:565:TYR:C	1:A:567:LEU:H	2.24	0.46
2:B:112:GLY:HA2	8:B:521:HOH:O	2.14	0.46
2:B:249:ILE:O	2:B:255:SER:HA	2.15	0.46
1:C:81:LYS:HB2	1:C:112:ILE:HD13	1.97	0.46
2:D:94:ILE:HG13	2:D:125:LYS:HE3	1.98	0.46
1:E:521:PHE:CE2	1:E:523:VAL:HG22	2.50	0.46
1:E:691:ILE:HD11	1:E:711:MET:CE	2.45	0.46
1:I:353:GLY:O	1:I:354:TRP:HB2	2.16	0.46
1:I:656:TRP:CD2	1:I:663:LYS:HA	2.51	0.46
1:I:776:SER:HA	1:I:805:VAL:HG13	1.98	0.46
2:J:60:ASP:OD1	2:J:60:ASP:C	2.59	0.46
2:J:210:PHE:CE2	2:J:251:ALA:HB1	2.51	0.46
1:U:257:ARG:HD3	2:V:61:ILE:HG21	1.96	0.46
1:W:28:MET:HE2	8:X:480:HOH:O	2.16	0.46
1:A:35:ASP:OD1	1:A:55:ARG:HD3	2.16	0.46
1:A:141:PRO:CA	1:A:496:TYR:HB3	2.43	0.46
1:E:671:ARG:HD2	8:E:1098:HOH:O	2.16	0.46
1:I:451:LYS:HG3	1:I:461:PHE:CE2	2.50	0.46
1:I:452:ILE:N	1:I:453:PRO:CD	2.79	0.46
1:I:510:TYR:O	1:I:513:MET:HG2	2.16	0.46
1:K:855:MET:HB2	1:K:857:ASN:OD1	2.16	0.46
2:L:9:ASP:HA	2:L:189:LYS:HB3	1.97	0.46
1:O:662:GLU:N	1:O:662:GLU:OE1	2.49	0.46
2:P:16:CYS:O	2:P:17:ASN:HB2	2.16	0.46
1:Q:396:ASP:OD2	1:Q:398:GLU:HB2	2.16	0.46
2:R:129:CYS:CB	2:R:132:LEU:HD12	2.45	0.46
1:S:452:ILE:HB	1:S:453:PRO:HD3	1.97	0.46
1:S:528:TRP:CG	1:S:750:LYS:HD3	2.51	0.46
1:U:81:LYS:HB2	1:U:112:ILE:HD13	1.98	0.46
2:V:40:GLN:HE22	2:V:118:GLU:H	1.61	0.46
1:W:499:PRO:CB	1:W:745:THR:HG21	2.46	0.46
2:X:16:CYS:O	2:X:17:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:736:SER:OG	4:C:902:MGD:N19	2.42	0.46
2:D:9:ASP:HA	2:D:189:LYS:HB3	1.98	0.46
2:D:26:GLU:HB2	2:D:144:ARG:NH1	2.31	0.46
2:D:58:ARG:HD2	2:D:268:ASP:OD1	2.16	0.46
1:E:165:GLY:CA	1:E:166:PHE:HB3	2.39	0.46
1:G:44:ILE:HD11	1:G:394:PRO:CG	2.42	0.46
1:G:387:TRP:CE2	1:G:389:THR:HA	2.51	0.46
1:G:498:GLY:N	1:G:499:PRO:HD3	2.31	0.46
1:I:629:MET:HE2	1:I:634:PHE:N	2.30	0.46
2:J:23:CYS:O	2:J:27:HIS:N	2.35	0.46
2:R:40:GLN:HB3	2:R:43:HIS:CE1	2.51	0.46
1:S:249:ASP:CG	4:S:903:MGD:H1'	2.39	0.46
2:T:191:LEU:HG	2:T:195:GLU:HG3	1.98	0.46
1:A:265:SER:O	1:A:810:GLN:NE2	2.49	0.46
2:B:216:VAL:HG13	2:B:223:GLU:HG3	1.96	0.46
2:D:87:ARG:HG3	2:D:91:ILE:O	2.15	0.46
1:E:6:ARG:HD2	8:E:1012:HOH:O	2.16	0.46
1:E:81:LYS:HB2	1:E:112:ILE:HD13	1.97	0.46
1:E:214:PHE:HA	1:E:347:ALA:HB3	1.98	0.46
1:E:452:ILE:HB	1:E:453:PRO:HD3	1.96	0.46
1:G:452:ILE:N	1:G:453:PRO:CD	2.79	0.46
1:M:1:MET:H3	1:M:22:ASP:CG	2.23	0.46
2:N:103:LYS:HG2	2:N:116:TRP:CD2	2.50	0.46
1:Q:258:LEU:HG	1:Q:259:VAL:HG13	1.98	0.46
1:Q:395:LEU:HD12	1:Q:566:GLN:HA	1.97	0.46
2:R:201:ALA:HB2	2:R:269:LEU:HB2	1.98	0.46
1:S:426:MET:HE3	1:S:622:ALA:HB2	1.97	0.46
1:A:395:LEU:HD13	1:A:571:ARG:HG3	1.98	0.46
2:B:72:GLU:HG2	2:B:185:ARG:NH2	2.30	0.46
2:B:87:ARG:HD3	2:B:93:LEU:HD12	1.97	0.46
1:C:730:TYR:CE1	1:C:794:ASN:HA	2.51	0.46
2:D:142:MET:CE	2:D:146:ALA:HB1	2.39	0.46
1:E:12:THR:O	1:E:226:TYR:HA	2.15	0.46
1:E:177:GLU:HA	1:E:177:GLU:OE2	2.14	0.46
1:E:498:GLY:N	1:E:499:PRO:HD3	2.31	0.46
1:I:296:ASN:HB3	1:I:657:PHE:CZ	2.51	0.46
1:K:11:SER:HA	1:K:147:TRP:HB2	1.96	0.46
1:K:418:ALA:HB1	1:K:423:ALA:HB2	1.97	0.46
1:K:563:ASP:HA	1:K:565:TYR:CE1	2.51	0.46
1:M:139:SER:CB	1:M:161:MET:HE2	2.46	0.46
1:M:730:TYR:CE1	1:M:794:ASN:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:59:ASN:ND2	2:N:59:ASN:H	2.12	0.46
2:N:198:TYR:HB3	2:N:238:ASP:HA	1.98	0.46
1:Q:364:ILE:HD13	1:Q:708:ARG:HG3	1.98	0.46
2:T:9:ASP:HA	2:T:189:LYS:HB3	1.98	0.46
1:U:250:PRO:HD3	4:U:903:MGD:C2	2.46	0.46
2:V:106:LEU:HD23	2:V:114:MET:HE2	1.98	0.46
1:W:116:GLU:O	1:W:120:ILE:HG13	2.16	0.46
1:W:165:GLY:CA	1:W:166:PHE:HB3	2.41	0.46
2:X:255:SER:HB2	8:X:538:HOH:O	2.14	0.46
1:A:138:LEU:HB2	1:A:490:ILE:HD12	1.98	0.46
1:A:174:ASP:OD1	1:A:175:SER:N	2.43	0.46
2:B:205:VAL:HG13	2:B:254:LYS:HZ1	1.81	0.46
1:C:587:MET:HE3	1:C:591:GLU:HB3	1.97	0.46
2:D:46:MET:HE1	2:D:66:THR:H	1.79	0.46
1:E:142:SER:HB3	4:E:902:MGD:O1A	2.15	0.46
1:I:177:GLU:HA	1:I:177:GLU:OE2	2.16	0.46
1:I:498:GLY:N	1:I:499:PRO:HD3	2.31	0.46
1:K:173:PRO:HA	1:K:468:PHE:CE1	2.50	0.46
1:K:452:ILE:N	1:K:453:PRO:CD	2.79	0.46
1:K:565:TYR:C	1:K:567:LEU:H	2.24	0.46
1:M:656:TRP:CD2	1:M:663:LYS:HA	2.51	0.46
1:O:786:ASN:HD21	1:O:805:VAL:H	1.62	0.46
2:P:27:HIS:HB2	2:P:39:MET:HE3	1.97	0.46
1:Q:128:ILE:CD1	1:Q:492:MET:HB2	2.46	0.46
1:Q:353:GLY:O	1:Q:354:TRP:HB2	2.15	0.46
1:S:452:ILE:N	1:S:453:PRO:CD	2.79	0.46
1:W:378:GLY:O	1:W:381:LYS:HG2	2.16	0.46
1:A:452:ILE:N	1:A:453:PRO:CD	2.80	0.45
1:C:361:SER:N	1:C:856:ALA:HB1	2.31	0.45
1:C:561:ILE:N	1:C:562:PRO:HD3	2.32	0.45
1:C:670:PRO:HG2	1:C:675:GLN:CD	2.41	0.45
2:D:201:ALA:HB2	2:D:269:LEU:HB2	1.97	0.45
1:E:15:PRO:HD3	1:E:554:PHE:CE1	2.51	0.45
1:E:565:TYR:C	1:E:567:LEU:N	2.74	0.45
2:F:21:MET:CA	2:F:21:MET:HE3	2.46	0.45
1:I:404:TYR:CD1	1:I:405:ALA:N	2.84	0.45
1:K:141:PRO:CA	1:K:496:TYR:HB3	2.45	0.45
1:O:247:PHE:CZ	1:O:255:THR:HG22	2.51	0.45
1:O:395:LEU:HD12	1:O:566:GLN:HA	1.97	0.45
1:O:649:LYS:HE3	1:O:651:THR:CG2	2.45	0.45
1:Q:565:TYR:C	1:Q:567:LEU:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:216:VAL:HG13	2:R:223:GLU:HG3	1.99	0.45
1:W:673:ASN:H	1:W:673:ASN:HD22	1.64	0.45
2:B:46:MET:CE	2:B:66:THR:H	2.29	0.45
1:C:134:PRO:HB2	1:C:439:LEU:HD11	1.98	0.45
1:C:140:THR:HB	1:C:169:ALA:HB3	1.98	0.45
1:C:146:MET:HG2	4:C:902:MGD:N7	2.31	0.45
1:C:644:ASP:OD1	1:C:646:PRO:HG3	2.16	0.45
2:D:176:ILE:HG22	2:D:177:LYS:HG3	1.99	0.45
1:I:517:ASP:HB3	8:I:1201:HOH:O	2.15	0.45
1:K:722:LYS:HG2	8:K:1560:HOH:O	2.16	0.45
1:M:174:ASP:OD1	1:M:175:SER:N	2.48	0.45
2:N:166:LYS:HE2	2:N:170:GLU:OE2	2.16	0.45
2:P:40:GLN:NE2	2:P:117:ASN:HA	2.31	0.45
1:S:670:PRO:HG2	1:S:675:GLN:CD	2.41	0.45
1:S:708:ARG:HD2	8:S:1045:HOH:O	2.14	0.45
2:T:19:CYS:HB2	2:T:46:MET:HG2	1.98	0.45
1:U:34:ASP:HB3	1:U:37:VAL:HG22	1.99	0.45
1:U:141:PRO:HA	1:U:496:TYR:O	2.16	0.45
1:U:144:HIS:HB2	4:U:902:MGD:O1B	2.16	0.45
1:U:301:GLU:H	1:U:301:GLU:CD	2.24	0.45
1:W:744:HIS:HA	1:W:819:SER:CB	2.47	0.45
2:X:60:ASP:C	2:X:60:ASP:OD1	2.59	0.45
1:C:734:MET:HB2	1:C:814:VAL:HG23	1.98	0.45
2:D:177:LYS:N	2:D:178:PRO:HD3	2.31	0.45
1:G:147:TRP:CD1	1:G:552:SER:HG	2.34	0.45
1:G:730:TYR:HB3	1:G:862:VAL:C	2.41	0.45
2:H:245:TYR:HB2	2:H:260:VAL:CG1	2.47	0.45
1:I:521:PHE:CE2	1:I:523:VAL:HG22	2.52	0.45
1:I:610:LYS:HZ3	1:I:618:GLN:HE22	1.61	0.45
1:K:144:HIS:HB2	4:K:902:MGD:O1B	2.17	0.45
2:L:106:LEU:HD11	2:L:116:TRP:HB2	1.96	0.45
1:M:211:MET:CE	2:N:231:PHE:CZ	2.89	0.45
1:M:387:TRP:CE2	1:M:389:THR:HA	2.51	0.45
1:Q:736:SER:O	4:Q:902:MGD:N18	2.49	0.45
1:S:134:PRO:HB2	1:S:439:LEU:HD11	1.99	0.45
1:S:558:SER:H	1:S:564:ASN:HD22	1.58	0.45
2:V:5:TYR:HB2	2:V:157:LEU:CD1	2.46	0.45
2:X:70:HIS:CD2	2:X:92:VAL:H	2.31	0.45
2:X:99:ALA:O	2:X:100:LYS:C	2.59	0.45
2:B:19:CYS:HB2	2:B:46:MET:HG2	1.97	0.45
1:C:165:GLY:CA	1:C:166:PHE:HB3	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:TRP:HZ3	2:D:59:ASN:HD21	1.64	0.45
1:C:565:TYR:C	1:C:567:LEU:H	2.24	0.45
1:E:141:PRO:CA	1:E:496:TYR:HB3	2.42	0.45
1:I:11:SER:HA	1:I:147:TRP:HB2	1.97	0.45
1:K:142:SER:CB	4:K:902:MGD:O1A	2.65	0.45
1:K:263:TRP:CZ2	1:K:265:SER:HB2	2.51	0.45
1:K:353:GLY:O	1:K:354:TRP:HB2	2.16	0.45
2:L:213:ALA:O	2:L:228:GLU:HA	2.17	0.45
1:M:847:TYR:CZ	1:M:853:CYS:HB3	2.52	0.45
2:N:203:ILE:HD12	2:N:203:ILE:N	2.30	0.45
1:O:134:PRO:HB2	1:O:439:LEU:HD11	1.97	0.45
2:R:69:MET:HB3	2:R:184:PRO:HB3	1.98	0.45
1:U:142:SER:HB3	4:U:902:MGD:O1A	2.16	0.45
1:C:378:GLY:O	1:C:381:LYS:HG2	2.17	0.45
1:C:452:ILE:N	1:C:453:PRO:CD	2.79	0.45
1:C:767:TYR:HB3	1:C:769:TYR:CE1	2.51	0.45
1:C:847:TYR:CZ	1:C:853:CYS:HB3	2.52	0.45
1:E:451:LYS:HG3	1:E:461:PHE:CE2	2.52	0.45
2:F:247:VAL:O	2:F:257:SER:HA	2.17	0.45
1:G:173:PRO:HA	1:G:468:PHE:CE1	2.52	0.45
1:G:353:GLY:O	1:G:354:TRP:HB2	2.16	0.45
1:G:482:TYR:HA	1:G:483:PRO:C	2.41	0.45
1:G:823:TYR:CE2	1:G:825:PRO:HG3	2.52	0.45
1:K:75:ARG:HH22	1:K:547:GLU:CD	2.24	0.45
1:K:738:HIS:HE2	4:K:902:MGD:H15	1.64	0.45
1:M:426:MET:HE2	1:M:618:GLN:HG2	1.97	0.45
1:M:719:GLU:O	1:M:859:THR:HB	2.16	0.45
1:M:776:SER:HA	1:M:805:VAL:HG13	1.98	0.45
1:Q:670:PRO:HG2	1:Q:675:GLN:CD	2.41	0.45
1:Q:782:ARG:HH11	1:Q:782:ARG:HG3	1.82	0.45
1:S:322:GLU:HG3	1:S:327:VAL:O	2.15	0.45
1:S:786:ASN:ND2	1:S:805:VAL:H	2.15	0.45
2:T:114:MET:HA	2:T:125:LYS:HB3	1.99	0.45
2:T:198:TYR:HB3	2:T:238:ASP:HA	1.99	0.45
1:U:677:CYS:O	1:U:679:LYS:HG3	2.17	0.45
1:W:17:PHE:CE2	1:W:31:MET:HE3	2.52	0.45
2:X:143:PRO:HD3	2:X:156:PHE:CE2	2.52	0.45
2:X:177:LYS:N	2:X:178:PRO:HD3	2.31	0.45
2:B:7:VAL:HB	2:B:155:GLU:HB3	1.99	0.45
1:G:96:ARG:HD2	1:G:514:TYR:O	2.17	0.45
1:G:356:GLY:N	4:G:903:MGD:O1B	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:CYS:O	2:H:17:ASN:HB2	2.16	0.45
2:H:164:MET:O	2:H:168:VAL:HG23	2.16	0.45
2:L:94:ILE:O	2:L:96:PRO:HD3	2.16	0.45
1:M:501:LEU:HD13	1:M:823:TYR:CG	2.52	0.45
1:O:165:GLY:HA3	1:O:166:PHE:CB	2.34	0.45
1:Q:15:PRO:HD2	8:Q:1003:HOH:O	2.15	0.45
1:Q:571:ARG:HB2	1:Q:642:VAL:HB	1.99	0.45
2:R:159:THR:OG1	2:R:160:THR:N	2.50	0.45
1:S:826:LEU:HD21	1:S:835:ARG:HD3	1.98	0.45
2:T:16:CYS:O	2:T:17:ASN:HB2	2.17	0.45
1:U:494:TRP:HE1	1:U:525:GLN:HE21	1.64	0.45
2:X:69:MET:HB2	7:X:304:SF4:S2	2.57	0.45
1:C:195:ASN:HD21	1:C:354:TRP:CD1	2.34	0.45
1:C:402:PRO:CD	1:C:623:THR:HG22	2.47	0.45
1:E:140:THR:OG1	1:E:171:HIS:HE1	2.00	0.45
1:E:797:GLY:HA2	1:E:875:TYR:CE2	2.51	0.45
2:H:129:CYS:HB3	2:H:132:LEU:HD12	1.99	0.45
2:H:142:MET:HE2	2:H:146:ALA:HB1	1.96	0.45
1:K:165:GLY:HA3	1:K:166:PHE:CB	2.35	0.45
2:L:106:LEU:HD23	2:L:114:MET:HE2	1.98	0.45
2:N:23:CYS:O	2:N:27:HIS:N	2.47	0.45
1:S:770:TRP:HB3	1:S:801:LEU:HD23	1.98	0.45
1:W:146:MET:HG2	4:W:902:MGD:N7	2.31	0.45
1:W:782:ARG:HD3	1:W:864:ILE:O	2.17	0.45
2:F:179:GLU:OE1	2:F:179:GLU:N	2.44	0.45
1:G:211:MET:HE3	1:G:244:ASP:HB2	1.99	0.45
2:H:18:ASN:HB2	7:H:302:SF4:S1	2.56	0.45
1:I:32:ASP:HB2	8:I:1650:HOH:O	2.15	0.45
1:M:184:MET:HE2	1:M:190:SER:HA	1.99	0.45
2:N:5:TYR:HB2	2:N:157:LEU:HD11	1.98	0.45
2:N:27:HIS:HB2	2:N:39:MET:HE3	1.99	0.45
1:O:402:PRO:HG2	1:O:422:PHE:CE1	2.51	0.45
2:T:5:TYR:CD2	2:T:164:MET:HG2	2.52	0.45
1:U:734:MET:HB2	1:U:814:VAL:HG23	1.99	0.45
1:W:201:LEU:HD13	1:W:387:TRP:HB2	1.99	0.45
1:W:249:ASP:CG	4:W:903:MGD:H1'	2.42	0.45
1:A:510:TYR:O	1:A:513:MET:HG2	2.17	0.45
2:B:5:TYR:CD2	2:B:164:MET:HG2	2.52	0.45
1:C:501:LEU:HD13	1:C:823:TYR:CD2	2.52	0.45
2:D:23:CYS:O	2:D:27:HIS:N	2.44	0.45
2:D:46:MET:HE1	2:D:65:PRO:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:GLU:HG3	1:E:199:TYR:CD1	2.51	0.45
1:E:482:TYR:HA	1:E:483:PRO:C	2.42	0.45
1:K:15:PRO:HD3	1:K:554:PHE:CD1	2.52	0.45
1:K:134:PRO:HB2	1:K:439:LEU:HD11	1.99	0.45
1:K:560:TYR:HB2	8:K:1677:HOH:O	2.16	0.45
2:L:19:CYS:HA	2:L:145:CYS:HA	1.99	0.45
1:M:48:GLY:HA3	2:R:252:ASP:O	2.17	0.45
1:Q:74:LEU:HD12	1:Q:750:LYS:HA	1.99	0.45
1:Q:141:PRO:CA	1:Q:496:TYR:HB3	2.43	0.45
1:U:195:ASN:HD21	1:U:354:TRP:CD1	2.35	0.45
1:W:343:ASN:ND2	8:W:1430:HOH:O	2.50	0.45
1:W:510:TYR:O	1:W:513:MET:HG2	2.16	0.45
1:W:644:ASP:O	1:W:646:PRO:HD3	2.17	0.45
1:A:426:MET:HE3	1:A:426:MET:CA	2.37	0.45
1:C:521:PHE:CE2	1:C:523:VAL:CG2	3.00	0.45
1:E:848:ILE:HG12	1:E:856:ALA:HB2	1.99	0.45
2:F:40:GLN:HB3	2:F:43:HIS:CE1	2.52	0.45
1:G:670:PRO:HG2	1:G:675:GLN:CD	2.41	0.45
1:K:696:LYS:O	1:K:700:GLU:HG3	2.17	0.45
1:M:153:ARG:O	1:M:157:TYR:HB3	2.17	0.45
1:M:394:PRO:HG3	8:M:1320:HOH:O	2.17	0.45
1:O:76:ILE:HG22	1:O:541:PRO:HG3	1.98	0.45
1:O:265:SER:O	1:O:810:GLN:NE2	2.50	0.45
1:Q:257:ARG:HD3	2:R:61:ILE:HG21	1.98	0.45
1:S:277:ALA:HA	1:S:316:LYS:O	2.16	0.45
1:S:571:ARG:HB2	1:S:642:VAL:HB	1.99	0.45
1:S:847:TYR:CZ	1:S:853:CYS:HB3	2.52	0.45
1:U:174:ASP:OD1	1:U:175:SER:N	2.47	0.45
1:U:735:LEU:HD23	1:U:735:LEU:H	1.81	0.45
1:W:85:PHE:CE2	1:W:87:PRO:HG3	2.52	0.45
2:X:21:MET:HE2	2:X:21:MET:N	2.32	0.45
2:X:122:VAL:HG22	2:X:123:ALA:N	2.31	0.45
1:A:9:ASN:HA	1:A:576:GLN:HA	1.98	0.44
2:B:142:MET:CE	2:B:146:ALA:HB1	2.46	0.44
1:C:134:PRO:HD2	8:C:1359:HOH:O	2.17	0.44
1:C:426:MET:HE3	1:C:622:ALA:HB2	1.99	0.44
1:C:786:ASN:HD22	1:C:786:ASN:HA	1.57	0.44
2:D:46:MET:HE3	2:D:47:ASN:H	1.82	0.44
2:F:46:MET:HE1	2:F:65:PRO:HA	1.97	0.44
2:F:60:ASP:C	2:F:60:ASP:OD1	2.60	0.44
2:F:142:MET:HE2	2:F:146:ALA:HB1	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:77:PRO:HB2	1:I:78:TYR:CD2	2.52	0.44
1:I:211:MET:HE2	1:I:246:VAL:HG23	1.98	0.44
1:K:277:ALA:HA	1:K:316:LYS:O	2.17	0.44
1:K:744:HIS:HA	1:K:819:SER:HB3	1.99	0.44
1:M:146:MET:HG2	4:M:902:MGD:N7	2.32	0.44
1:O:786:ASN:ND2	1:O:805:VAL:N	2.59	0.44
1:Q:378:GLY:O	1:Q:381:LYS:HG2	2.17	0.44
1:S:716:PRO:HB3	1:S:723:HIS:CD2	2.52	0.44
1:W:449:ARG:HD2	8:W:1037:HOH:O	2.17	0.44
2:X:40:GLN:NE2	8:X:443:HOH:O	2.49	0.44
1:A:498:GLY:N	1:A:499:PRO:HD3	2.32	0.44
2:B:21:MET:CE	2:B:24:MET:HE3	2.47	0.44
2:B:40:GLN:HB3	2:B:43:HIS:CE1	2.53	0.44
1:C:296:ASN:HB3	1:C:657:PHE:CZ	2.52	0.44
1:I:269:GLY:HA2	1:I:362:HIS:CE1	2.52	0.44
2:J:166:LYS:O	2:J:170:GLU:HG3	2.17	0.44
1:K:691:ILE:HD11	1:K:711:MET:CE	2.47	0.44
1:M:141:PRO:HA	1:M:496:TYR:O	2.17	0.44
1:M:253:ASN:O	1:M:257:ARG:HG3	2.17	0.44
1:O:114:TRP:CZ2	1:O:541:PRO:HD2	2.52	0.44
1:Q:277:ALA:HA	1:Q:316:LYS:O	2.17	0.44
1:Q:558:SER:H	1:Q:564:ASN:ND2	2.15	0.44
1:Q:847:TYR:CZ	1:Q:853:CYS:HB3	2.52	0.44
2:T:203:ILE:N	2:T:203:ILE:HD12	2.31	0.44
2:V:40:GLN:NE2	2:V:118:GLU:H	2.16	0.44
1:W:187:TRP:CH2	1:W:196:PRO:HB3	2.52	0.44
1:W:794:ASN:HD21	1:W:842:LEU:HB3	1.82	0.44
2:X:235:PHE:CD1	2:X:235:PHE:C	2.95	0.44
1:A:15:PRO:HD2	8:A:1003:HOH:O	2.17	0.44
1:A:76:ILE:HA	1:A:77:PRO:HD3	1.76	0.44
2:D:103:LYS:HG2	2:D:116:TRP:CD2	2.53	0.44
1:E:253:ASN:O	1:E:257:ARG:HG3	2.17	0.44
1:G:153:ARG:O	1:G:157:TYR:HB3	2.18	0.44
1:G:756:TYR:HB2	2:H:24:MET:HE1	1.98	0.44
2:J:112:GLY:HA2	8:J:518:HOH:O	2.17	0.44
1:M:328:PRO:HB2	1:M:331:GLU:HG3	1.98	0.44
1:O:670:PRO:HG2	1:O:675:GLN:CD	2.42	0.44
1:W:134:PRO:HB2	1:W:439:LEU:HD11	1.99	0.44
1:W:184:MET:HE2	1:W:190:SER:HA	1.98	0.44
1:W:647:ASN:O	1:W:648:ARG:C	2.60	0.44
1:A:250:PRO:HD3	4:A:903:MGD:C2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ARG:HD2	8:A:1044:HOH:O	2.16	0.44
2:B:142:MET:CE	2:B:146:ALA:CB	2.95	0.44
1:C:218:ASP:OD2	1:C:253:ASN:HB2	2.16	0.44
1:C:252:MET:HB3	1:C:808:CYS:HB3	1.99	0.44
1:C:785:LYS:NZ	8:C:1622:HOH:O	2.48	0.44
2:D:129:CYS:CB	2:D:132:LEU:HD12	2.48	0.44
2:F:64:ARG:NH1	8:F:419:HOH:O	2.48	0.44
2:F:106:LEU:HD11	2:F:116:TRP:HB2	1.99	0.44
1:I:433:PHE:HA	1:I:434:PRO:HD3	1.83	0.44
2:J:56:TYR:HA	2:J:59:ASN:ND2	2.32	0.44
1:K:737:PRO:CG	4:K:903:MGD:H2'	2.47	0.44
1:M:629:MET:HE2	1:M:634:PHE:CA	2.45	0.44
2:N:210:PHE:HD2	2:N:213:ALA:HB2	1.82	0.44
2:P:247:VAL:O	2:P:257:SER:HA	2.17	0.44
1:S:801:LEU:HD11	1:S:839:ILE:HD11	1.99	0.44
1:U:263:TRP:CZ2	1:U:265:SER:HB2	2.51	0.44
1:U:452:ILE:HB	1:U:453:PRO:HD3	2.00	0.44
1:W:114:TRP:CZ2	1:W:541:PRO:HD2	2.52	0.44
1:W:677:CYS:C	1:W:678:ARG:HG2	2.42	0.44
1:A:521:PHE:CE2	1:A:523:VAL:HG22	2.53	0.44
1:E:647:ASN:O	1:E:648:ARG:C	2.59	0.44
2:H:114:MET:HA	2:H:125:LYS:HB3	2.00	0.44
1:M:76:ILE:HA	1:M:77:PRO:HD3	1.78	0.44
1:Q:426:MET:HE3	1:Q:426:MET:CA	2.36	0.44
1:Q:656:TRP:CD2	1:Q:663:LYS:HA	2.52	0.44
1:Q:716:PRO:HB3	1:Q:723:HIS:CG	2.53	0.44
1:Q:730:TYR:CE1	1:Q:794:ASN:HA	2.52	0.44
2:R:39:MET:HE2	2:R:45:TRP:CD2	2.53	0.44
2:R:177:LYS:N	2:R:178:PRO:HD3	2.32	0.44
1:S:540:LEU:HA	1:S:541:PRO:HD3	1.78	0.44
2:X:46:MET:HE2	2:X:48:ILE:HG12	2.00	0.44
2:X:210:PHE:CE2	2:X:251:ALA:HB1	2.53	0.44
1:A:797:GLY:HA2	1:A:875:TYR:CZ	2.53	0.44
2:B:247:VAL:O	2:B:257:SER:HA	2.17	0.44
1:C:162:ASN:HD22	1:C:166:PHE:HE2	1.64	0.44
1:C:222:ASN:HA	4:C:903:MGD:H22	1.83	0.44
1:C:670:PRO:HB3	1:C:682:GLN:HB2	1.98	0.44
1:C:785:LYS:NZ	1:C:785:LYS:HB2	2.32	0.44
2:D:19:CYS:HA	2:D:145:CYS:HA	1.99	0.44
1:E:75:ARG:HH22	1:E:547:GLU:CD	2.26	0.44
2:F:139:ALA:HB3	2:F:140:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:175:SER:HB2	1:G:176:TRP:CZ3	2.52	0.44
1:G:501:LEU:HA	1:G:507:THR:HB	2.00	0.44
1:G:610:LYS:HZ3	1:G:618:GLN:HE22	1.60	0.44
1:G:786:ASN:ND2	1:G:804:GLN:HA	2.32	0.44
1:I:673:ASN:H	1:I:673:ASN:HD22	1.65	0.44
1:K:533:VAL:HB	1:K:534:PRO:HD3	1.99	0.44
2:L:114:MET:HE3	2:L:123:ALA:HB1	1.99	0.44
1:M:587:MET:HG3	1:M:592:ILE:CG1	2.48	0.44
1:O:144:HIS:NE2	6:O:905:PYG:O1	2.48	0.44
1:Q:28:MET:CE	1:Q:67:LYS:H	2.30	0.44
1:S:730:TYR:CZ	1:S:794:ASN:HA	2.52	0.44
2:V:102:LYS:HB3	2:V:104:GLU:OE2	2.17	0.44
1:W:296:ASN:HB3	1:W:657:PHE:CZ	2.52	0.44
1:W:730:TYR:CZ	1:W:794:ASN:HA	2.52	0.44
2:B:4:TYR:CE2	2:B:158:LYS:HD2	2.53	0.44
1:C:165:GLY:HA3	1:C:166:PHE:CB	2.39	0.44
1:C:533:VAL:HB	1:C:534:PRO:HD3	1.99	0.44
1:E:265:SER:O	1:E:810:GLN:NE2	2.51	0.44
1:E:501:LEU:HB2	8:E:1360:HOH:O	2.18	0.44
1:E:857:ASN:HB3	4:E:902:MGD:N19	2.33	0.44
2:L:75:PRO:O	2:L:79:LYS:HG3	2.17	0.44
1:M:96:ARG:HD2	1:M:514:TYR:O	2.17	0.44
1:O:673:ASN:H	1:O:673:ASN:ND2	2.14	0.44
2:P:70:HIS:HD2	2:P:92:VAL:N	2.04	0.44
1:Q:717:ALA:HB3	1:Q:720:SER:HB3	2.00	0.44
2:R:21:MET:CE	2:R:21:MET:CA	2.95	0.44
2:T:251:ALA:HB3	2:T:274:LEU:HD12	2.00	0.44
1:W:124:GLU:HG3	1:W:521:PHE:CD2	2.53	0.44
1:W:337:ARG:O	1:W:341:LYS:HG2	2.18	0.44
2:X:23:CYS:O	2:X:27:HIS:N	2.40	0.44
2:X:249:ILE:HG22	2:X:250:ASP:N	2.32	0.44
1:A:187:TRP:CH2	1:A:196:PRO:HB3	2.52	0.44
1:C:201:LEU:HD13	1:C:387:TRP:HB2	1.98	0.44
2:H:60:ASP:C	2:H:60:ASP:OD1	2.61	0.44
1:I:855:MET:HB2	1:I:857:ASN:OD1	2.18	0.44
1:K:13:GLY:HA3	1:K:63:THR:OG1	2.17	0.44
1:K:649:LYS:O	1:K:649:LYS:HG3	2.16	0.44
1:M:784:ILE:HD13	1:M:790:ILE:HG21	2.00	0.44
1:O:404:TYR:CD1	1:O:405:ALA:N	2.85	0.44
1:O:499:PRO:CB	1:O:745:THR:HG21	2.48	0.44
1:O:857:ASN:HB3	4:O:902:MGD:N19	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:159:THR:HG23	2:P:160:THR:N	2.33	0.44
1:Q:426:MET:HA	1:Q:426:MET:CE	2.36	0.44
2:R:5:TYR:CD2	2:R:164:MET:HG2	2.52	0.44
2:T:174:GLU:OE1	2:T:191:LEU:HB3	2.18	0.44
1:U:74:LEU:HD23	1:U:74:LEU:HA	1.85	0.44
1:U:528:TRP:CD2	1:U:750:LYS:HD3	2.53	0.44
2:V:3:GLN:O	2:V:158:LYS:HA	2.18	0.44
2:V:46:MET:HE3	2:V:47:ASN:H	1.82	0.44
1:W:353:GLY:O	1:W:354:TRP:HB2	2.18	0.44
2:X:94:ILE:O	2:X:96:PRO:HD3	2.16	0.44
1:A:55:ARG:HD2	8:A:1636:HOH:O	2.17	0.44
1:C:121:VAL:O	1:C:125:ILE:HG13	2.17	0.44
1:C:498:GLY:N	1:C:499:PRO:HD3	2.33	0.44
2:D:166:LYS:HE2	2:D:170:GLU:OE2	2.18	0.44
1:G:138:LEU:HB2	1:G:490:ILE:HD12	2.00	0.44
1:G:561:ILE:CG2	1:G:564:ASN:HB3	2.44	0.44
1:I:141:PRO:CA	1:I:496:TYR:HB3	2.44	0.44
1:I:870:ASP:HB3	1:I:872:TYR:CE1	2.52	0.44
1:M:211:MET:CE	2:N:231:PHE:HZ	2.23	0.44
1:M:433:PHE:CD1	1:M:433:PHE:N	2.86	0.44
1:O:533:VAL:HB	1:O:534:PRO:HD3	2.00	0.44
1:Q:498:GLY:N	1:Q:499:PRO:HD3	2.32	0.44
2:R:19:CYS:HB2	2:R:46:MET:HG2	2.00	0.44
1:S:353:GLY:O	1:S:354:TRP:HB2	2.18	0.44
1:S:717:ALA:HB3	1:S:720:SER:HB3	2.00	0.44
2:V:13:CYS:HB3	2:V:63:TYR:HB2	2.00	0.44
2:V:166:LYS:O	2:V:170:GLU:HG3	2.17	0.44
1:A:800:ILE:HD12	1:A:800:ILE:N	2.33	0.43
2:B:23:CYS:O	2:B:27:HIS:N	2.47	0.43
1:C:855:MET:HB2	1:C:857:ASN:OD1	2.18	0.43
1:E:17:PHE:CE2	1:E:31:MET:HE3	2.54	0.43
1:E:401:PHE:HA	1:E:402:PRO:HD3	1.78	0.43
1:E:426:MET:HE1	1:E:618:GLN:C	2.42	0.43
1:E:782:ARG:HH11	1:E:782:ARG:HG3	1.83	0.43
1:G:211:MET:HE1	2:H:231:PHE:CE1	2.53	0.43
1:G:282:TRP:HA	1:G:287:SER:OG	2.18	0.43
1:K:66:PHE:CD1	1:K:69:MET:HE3	2.53	0.43
1:K:451:LYS:HG3	1:K:461:PHE:CE2	2.53	0.43
1:K:521:PHE:CE2	1:K:523:VAL:CG2	3.01	0.43
1:K:598:LYS:HA	1:K:603:GLU:HB2	1.98	0.43
2:L:203:ILE:N	2:L:203:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:217:LEU:HB2	2:L:237:PHE:CD1	2.53	0.43
1:M:408:GLY:HA2	1:M:619:TYR:HE1	1.81	0.43
1:M:753:TYR:HB3	2:N:21:MET:HE2	1.99	0.43
2:N:164:MET:O	2:N:168:VAL:HG23	2.18	0.43
1:Q:187:TRP:CH2	1:Q:196:PRO:HB3	2.53	0.43
2:R:106:LEU:HD22	2:R:114:MET:HB3	2.00	0.43
1:U:356:GLY:H	4:U:903:MGD:C5'	2.30	0.43
1:A:44:ILE:HD11	1:A:394:PRO:HG2	1.99	0.43
1:A:776:SER:HA	1:A:805:VAL:HG13	2.00	0.43
1:E:174:ASP:OD1	1:E:175:SER:N	2.46	0.43
2:F:20:PHE:CE2	2:F:24:MET:HE2	2.52	0.43
2:F:21:MET:HA	2:F:21:MET:HE3	1.98	0.43
1:G:15:PRO:HD2	8:G:1003:HOH:O	2.16	0.43
1:G:134:PRO:HB2	1:G:439:LEU:HD11	1.99	0.43
1:I:401:PHE:HA	1:I:402:PRO:HD3	1.77	0.43
1:K:730:TYR:CZ	1:K:794:ASN:HA	2.52	0.43
1:M:15:PRO:HD3	1:M:554:PHE:CE1	2.53	0.43
2:P:142:MET:CE	2:P:146:ALA:HB1	2.48	0.43
1:Q:563:ASP:HA	1:Q:565:TYR:CE1	2.53	0.43
1:S:521:PHE:CE2	1:S:523:VAL:CG2	3.01	0.43
2:T:94:ILE:O	2:T:96:PRO:HD3	2.17	0.43
2:X:83:ALA:HB1	2:X:99:ALA:HB2	2.00	0.43
1:A:155:SER:OG	1:A:409:ILE:HG12	2.18	0.43
1:A:165:GLY:CA	1:A:166:PHE:HB3	2.48	0.43
2:B:19:CYS:HA	2:B:145:CYS:HA	2.00	0.43
2:D:203:ILE:N	2:D:203:ILE:HD12	2.33	0.43
1:I:166:PHE:N	1:I:439:LEU:HD12	2.34	0.43
2:L:3:GLN:O	2:L:158:LYS:HA	2.19	0.43
1:M:78:TYR:C	1:M:541:PRO:HG2	2.43	0.43
2:P:73:ASN:ND2	2:P:182:THR:HA	2.33	0.43
8:Q:1676:HOH:O	1:S:871:LYS:HE2	2.17	0.43
2:R:68:CYS:HB3	2:R:70:HIS:ND1	2.33	0.43
1:S:32:ASP:HB2	8:S:1642:HOH:O	2.17	0.43
1:S:550:ASP:OD1	1:S:551:ILE:N	2.42	0.43
2:T:76:CYS:O	2:T:80:GLY:N	2.51	0.43
2:T:247:VAL:O	2:T:257:SER:HA	2.18	0.43
2:V:58:ARG:HD2	2:V:268:ASP:OD1	2.17	0.43
2:V:106:LEU:HD22	2:V:114:MET:HG3	2.00	0.43
1:W:673:ASN:H	1:W:673:ASN:ND2	2.15	0.43
1:W:800:ILE:CD1	1:W:833:ALA:HB1	2.48	0.43
1:A:503:THR:CG2	4:A:902:MGD:O2A	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:TYR:CE2	2:F:158:LYS:HD2	2.54	0.43
1:G:393:VAL:HA	1:G:394:PRO:HD3	1.82	0.43
2:J:146:ALA:HA	2:J:154:TYR:CD1	2.53	0.43
1:K:214:PHE:HA	1:K:347:ALA:HB3	1.99	0.43
1:M:356:GLY:H	4:M:903:MGD:C5'	2.30	0.43
1:Q:644:ASP:OD1	1:Q:646:PRO:HG3	2.18	0.43
1:S:716:PRO:HB3	1:S:723:HIS:CG	2.52	0.43
2:T:4:TYR:CE2	2:T:158:LYS:HD2	2.52	0.43
2:T:122:VAL:HG22	2:T:123:ALA:N	2.32	0.43
1:U:528:TRP:CG	1:U:750:LYS:HD3	2.54	0.43
1:W:449:ARG:NH1	8:W:1037:HOH:O	2.50	0.43
1:A:13:GLY:HA3	1:A:63:THR:OG1	2.19	0.43
1:A:476:GLN:OE1	1:A:708:ARG:NH2	2.50	0.43
2:B:245:TYR:HB2	2:B:260:VAL:CG1	2.48	0.43
1:G:75:ARG:NH2	1:G:543:CYS:HA	2.34	0.43
1:M:265:SER:O	1:M:810:GLN:NE2	2.50	0.43
1:O:364:ILE:HD13	1:O:708:ARG:HG3	2.01	0.43
2:P:40:GLN:HB3	2:P:43:HIS:CE1	2.52	0.43
1:Q:28:MET:HE2	1:Q:67:LYS:HB2	2.00	0.43
1:Q:499:PRO:CB	1:Q:745:THR:HG21	2.48	0.43
1:S:61:PRO:HB3	8:S:1651:HOH:O	2.18	0.43
1:S:75:ARG:NH2	1:S:543:CYS:HA	2.30	0.43
1:S:644:ASP:O	1:S:646:PRO:HD3	2.17	0.43
1:W:426:MET:HE1	1:W:618:GLN:C	2.42	0.43
2:X:174:GLU:HB3	8:X:454:HOH:O	2.18	0.43
1:A:291:GLU:CD	1:A:291:GLU:N	2.75	0.43
1:A:393:VAL:HA	1:A:394:PRO:HD3	1.79	0.43
1:C:732:LEU:CD1	1:C:864:ILE:HG12	2.47	0.43
2:D:129:CYS:HB3	2:D:132:LEU:HD12	2.00	0.43
1:E:753:TYR:HB3	2:F:24:MET:HE3	2.00	0.43
1:E:786:ASN:ND2	1:E:805:VAL:H	2.14	0.43
1:G:265:SER:O	1:G:810:GLN:NE2	2.52	0.43
1:G:826:LEU:HD21	1:G:835:ARG:HD3	1.99	0.43
2:J:128:MET:O	2:J:129:CYS:C	2.61	0.43
1:K:21:LYS:HB3	1:K:26:ILE:HD11	2.00	0.43
1:K:114:TRP:CZ2	1:K:541:PRO:HD2	2.53	0.43
2:N:16:CYS:O	2:N:17:ASN:HB2	2.18	0.43
2:N:60:ASP:C	2:N:60:ASP:OD1	2.62	0.43
2:N:219:SER:C	2:N:221:GLY:H	2.27	0.43
1:O:39:ALA:HA	1:O:40:PRO:HD3	1.92	0.43
1:S:395:LEU:HD12	1:S:566:GLN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:677:CYS:C	1:S:678:ARG:HG2	2.42	0.43
1:U:269:GLY:HA2	1:U:362:HIS:CG	2.52	0.43
1:U:649:LYS:O	1:U:649:LYS:HG3	2.18	0.43
1:U:786:ASN:ND2	1:U:805:VAL:H	2.14	0.43
1:W:65:GLY:HA3	2:X:21:MET:HG3	1.99	0.43
1:W:530:GLU:CD	1:W:750:LYS:HZ2	2.25	0.43
1:A:175:SER:OG	6:A:905:PYG:C1	2.66	0.43
1:E:395:LEU:HD13	1:E:571:ARG:HG3	2.01	0.43
1:E:629:MET:HE2	1:E:634:PHE:N	2.34	0.43
1:E:800:ILE:N	1:E:800:ILE:CD1	2.81	0.43
1:G:797:GLY:HA2	1:G:875:TYR:CZ	2.53	0.43
2:H:59:ASN:H	2:H:59:ASN:HD22	1.66	0.43
1:I:673:ASN:H	1:I:673:ASN:ND2	2.17	0.43
1:K:12:THR:O	1:K:226:TYR:HA	2.18	0.43
1:K:387:TRP:CZ2	1:K:389:THR:HA	2.54	0.43
1:K:501:LEU:HD13	1:K:823:TYR:CD2	2.54	0.43
1:M:737:PRO:CG	4:M:903:MGD:H2'	2.48	0.43
2:N:5:TYR:CE2	2:N:164:MET:HG2	2.54	0.43
1:O:627:LYS:HD3	8:O:1215:HOH:O	2.18	0.43
1:O:737:PRO:CG	4:O:903:MGD:H2'	2.49	0.43
1:S:139:SER:OG	1:S:161:MET:HE2	2.18	0.43
1:S:140:THR:OG1	1:S:171:HIS:HE1	2.01	0.43
1:U:197:GLU:HG3	1:U:653:ALA:HB1	1.99	0.43
1:U:267:LYS:HB3	1:U:721:GLN:NE2	2.34	0.43
1:U:370:MET:HE2	1:U:370:MET:HA	1.99	0.43
1:U:549:TRP:HB3	1:U:613:LEU:HD13	2.01	0.43
2:V:5:TYR:HB2	2:V:157:LEU:HD11	2.01	0.43
1:W:364:ILE:HD13	1:W:708:ARG:HG3	2.01	0.43
1:A:10:SER:HA	1:A:15:PRO:HA	2.01	0.43
1:A:364:ILE:HD13	1:A:708:ARG:HG3	2.00	0.43
1:C:15:PRO:HD3	1:C:554:PHE:CE1	2.54	0.43
2:D:213:ALA:O	2:D:228:GLU:HA	2.19	0.43
2:H:210:PHE:HD2	2:H:213:ALA:HB2	1.84	0.43
1:I:176:TRP:CD1	1:I:193:LEU:HB2	2.54	0.43
2:J:5:TYR:HB2	2:J:157:LEU:HD11	2.01	0.43
1:K:249:ASP:OD1	4:K:903:MGD:H1'	2.18	0.43
1:M:12:THR:O	1:M:226:TYR:HA	2.19	0.43
2:N:124:GLN:O	2:N:125:LYS:HB3	2.19	0.43
1:O:15:PRO:HD2	8:O:1003:HOH:O	2.17	0.43
2:P:210:PHE:CE2	2:P:251:ALA:HB1	2.54	0.43
2:R:142:MET:CE	2:R:146:ALA:CB	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:21:LYS:HB3	1:S:26:ILE:HD11	2.01	0.43
1:U:378:GLY:O	1:U:381:LYS:HG2	2.19	0.43
2:V:128:MET:O	2:V:129:CYS:C	2.61	0.43
1:W:28:MET:CE	1:W:66:PHE:HB3	2.41	0.43
1:W:498:GLY:N	1:W:499:PRO:HD3	2.33	0.43
1:W:767:TYR:HB3	1:W:769:TYR:CE1	2.54	0.43
2:X:39:MET:HE2	2:X:45:TRP:CD2	2.54	0.43
1:A:274:LEU:O	1:A:278:ILE:HG13	2.19	0.43
1:A:433:PHE:HA	1:A:434:PRO:HD3	1.83	0.43
1:C:454:GLU:CD	1:C:454:GLU:H	2.27	0.43
1:C:630:THR:OG1	1:C:633:GLU:HG3	2.18	0.43
2:F:125:LYS:HD2	2:F:126:CYS:O	2.19	0.43
2:F:210:PHE:HD2	2:F:213:ALA:HB2	1.83	0.43
1:G:75:ARG:HH21	1:G:543:CYS:HA	1.84	0.43
1:I:563:ASP:HA	1:I:565:TYR:CE1	2.54	0.43
1:M:756:TYR:HB2	2:N:24:MET:HE1	2.01	0.43
8:N:545:HOH:O	1:S:729:LYS:HE2	2.19	0.43
1:O:142:SER:HB3	4:O:902:MGD:H5'2	2.01	0.43
1:O:296:ASN:O	1:O:687:LYS:HB3	2.19	0.43
1:Q:175:SER:OG	6:Q:905:PYG:C1	2.67	0.43
1:Q:468:PHE:HB2	8:Q:1671:HOH:O	2.17	0.43
1:S:144:HIS:NE2	6:S:905:PYG:O1	2.48	0.43
1:U:155:SER:OG	1:U:409:ILE:HG12	2.19	0.43
1:U:561:ILE:CG2	1:U:564:ASN:HB3	2.49	0.43
1:W:2:GLY:N	1:W:22:ASP:OD1	2.52	0.43
1:W:362:HIS:HB3	1:W:717:ALA:HB2	2.00	0.43
2:X:273:LYS:O	2:X:274:LEU:HD23	2.19	0.43
1:A:571:ARG:HB2	1:A:642:VAL:HB	2.01	0.43
2:D:125:LYS:HD2	2:D:126:CYS:O	2.19	0.43
2:F:166:LYS:HE2	2:F:170:GLU:OE2	2.18	0.43
1:G:818:GLU:O	1:G:819:SER:HB2	2.19	0.43
2:H:46:MET:HE1	2:H:65:PRO:HA	2.01	0.43
1:I:144:HIS:HB2	4:I:902:MGD:O1B	2.19	0.43
1:I:825:PRO:HD2	8:I:1329:HOH:O	2.18	0.43
1:K:100:LEU:HD13	1:K:105:PRO:HG3	2.01	0.43
1:O:1:MET:N	1:O:22:ASP:CG	2.76	0.43
1:O:175:SER:HB2	1:O:176:TRP:CE3	2.54	0.43
1:Q:138:LEU:HB2	1:Q:490:ILE:HD12	2.01	0.43
1:Q:540:LEU:HA	1:Q:541:PRO:HD3	1.78	0.43
1:S:69:MET:HE2	1:S:754:MET:HE3	1.97	0.43
1:S:141:PRO:HA	1:S:496:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:176:ILE:HG22	2:T:177:LYS:HG3	2.01	0.43
1:U:281:THR:O	1:U:285:GLU:HG3	2.19	0.43
1:U:604:GLU:HB3	1:U:605:MET:HE3	1.99	0.43
1:U:670:PRO:HG2	1:U:675:GLN:CD	2.44	0.43
1:W:175:SER:HB2	1:W:176:TRP:CE3	2.54	0.43
2:X:46:MET:HE1	2:X:65:PRO:HA	2.00	0.43
1:C:800:ILE:N	1:C:800:ILE:HD12	2.33	0.42
1:G:649:LYS:HE3	1:G:651:THR:CG2	2.49	0.42
1:I:15:PRO:HD3	1:I:554:PHE:CE1	2.54	0.42
1:I:175:SER:OG	6:I:905:PYG:C1	2.65	0.42
2:J:3:GLN:O	2:J:158:LYS:HA	2.18	0.42
2:N:114:MET:HA	2:N:125:LYS:HB3	2.01	0.42
2:R:16:CYS:O	2:R:17:ASN:HB2	2.19	0.42
1:S:251:HIS:HA	1:S:809:LEU:HD23	2.00	0.42
1:S:587:MET:HE2	1:S:592:ILE:HA	2.01	0.42
1:U:69:MET:HE2	1:U:754:MET:HE3	1.99	0.42
1:U:451:LYS:HG3	1:U:461:PHE:CE2	2.54	0.42
1:W:182:GLY:HA3	1:W:364:ILE:HG23	2.01	0.42
1:W:433:PHE:HA	1:W:434:PRO:HD3	1.82	0.42
2:B:69:MET:O	2:B:70:HIS:C	2.62	0.42
2:D:70:HIS:CD2	2:D:92:VAL:H	2.31	0.42
1:E:175:SER:OG	6:E:905:PYG:C1	2.67	0.42
1:E:366:TRP:O	1:E:370:MET:HG2	2.19	0.42
2:F:95:ASP:HB3	2:F:98:LYS:HB2	2.01	0.42
1:I:2:GLY:O	1:I:21:LYS:HE3	2.19	0.42
1:I:708:ARG:HD2	8:I:1043:HOH:O	2.18	0.42
1:K:426:MET:HE2	1:K:618:GLN:OE1	2.19	0.42
1:K:495:LYS:HD2	1:K:514:TYR:OH	2.19	0.42
1:O:173:PRO:HA	1:O:468:PHE:CE1	2.55	0.42
2:P:159:THR:OG1	2:P:160:THR:N	2.52	0.42
1:Q:77:PRO:HB2	1:Q:78:TYR:CE2	2.53	0.42
1:Q:219:PRO:HD2	1:Q:255:THR:OG1	2.19	0.42
1:Q:521:PHE:CE2	1:Q:523:VAL:HG22	2.54	0.42
1:Q:610:LYS:HB3	1:Q:614:ALA:HB3	2.00	0.42
1:U:79:PRO:HB2	1:U:112:ILE:O	2.19	0.42
1:U:144:HIS:NE2	6:U:905:PYG:O1	2.48	0.42
2:V:87:ARG:HB2	2:V:89:ASP:OD2	2.19	0.42
1:W:66:PHE:CD1	1:W:69:MET:HE3	2.54	0.42
1:W:103:GLN:N	1:W:103:GLN:CD	2.77	0.42
1:W:810:GLN:O	1:W:811:PRO:C	2.62	0.42
2:X:81:ASN:OD1	2:X:81:ASN:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:TYR:HB2	2:B:157:LEU:HD13	2.02	0.42
1:C:166:PHE:H	1:C:439:LEU:HD12	1.84	0.42
1:E:736:SER:OG	4:E:902:MGD:N19	2.48	0.42
1:G:756:TYR:CZ	2:H:41:ARG:HB3	2.54	0.42
2:L:23:CYS:O	2:L:27:HIS:N	2.45	0.42
1:M:737:PRO:HG3	4:M:903:MGD:H2'	2.01	0.42
1:O:272:HIS:ND1	1:O:272:HIS:N	2.68	0.42
2:P:5:TYR:CE2	2:P:164:MET:HG2	2.54	0.42
1:S:269:GLY:HA2	1:S:362:HIS:CE1	2.55	0.42
1:S:565:TYR:C	1:S:567:LEU:H	2.27	0.42
2:V:10:VAL:HG13	2:V:63:TYR:O	2.20	0.42
1:W:162:ASN:CG	1:W:437:SER:HB2	2.45	0.42
1:W:402:PRO:HG2	1:W:422:PHE:CE1	2.54	0.42
2:X:244:GLU:HG3	2:X:261:VAL:HG22	2.00	0.42
1:A:258:LEU:HG	1:A:259:VAL:HG13	2.00	0.42
1:A:533:VAL:HG12	1:A:539:ILE:HD13	2.02	0.42
1:E:103:GLN:CD	1:E:103:GLN:N	2.77	0.42
1:E:404:TYR:CD1	1:E:405:ALA:N	2.87	0.42
1:E:433:PHE:CD1	1:E:433:PHE:N	2.87	0.42
1:I:647:ASN:O	1:I:648:ARG:C	2.60	0.42
1:I:736:SER:O	4:I:902:MGD:N18	2.52	0.42
2:J:4:TYR:CE2	2:J:158:LYS:HD2	2.55	0.42
1:M:540:LEU:HA	1:M:541:PRO:HD3	1.81	0.42
1:M:800:ILE:CD1	1:M:833:ALA:HB1	2.49	0.42
1:O:44:ILE:HG23	1:O:203:GLU:HG3	2.01	0.42
2:P:5:TYR:CD2	2:P:164:MET:HG2	2.54	0.42
1:S:411:GLY:HA3	1:S:434:PRO:HB3	2.01	0.42
1:S:561:ILE:CG2	1:S:564:ASN:HB3	2.47	0.42
2:T:27:HIS:HB2	2:T:39:MET:HE3	2.01	0.42
1:A:211:MET:HE3	1:A:244:ASP:HB2	2.01	0.42
2:B:5:TYR:O	2:B:157:LEU:HD12	2.20	0.42
2:B:105:LEU:HB3	2:B:114:MET:HE1	2.01	0.42
1:E:563:ASP:HA	1:E:565:TYR:CE1	2.54	0.42
1:G:396:ASP:OD2	1:G:398:GLU:HB2	2.20	0.42
1:G:744:HIS:HA	1:G:819:SER:HB3	2.02	0.42
1:I:735:LEU:HD23	1:I:735:LEU:H	1.85	0.42
2:J:46:MET:HE3	2:J:46:MET:C	2.43	0.42
2:J:142:MET:CE	2:J:146:ALA:HB1	2.47	0.42
1:K:720:SER:O	1:K:724:SER:HB3	2.18	0.42
2:N:3:GLN:O	2:N:158:LYS:HA	2.20	0.42
1:O:15:PRO:HB2	1:O:31:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:66:PHE:HA	1:O:69:MET:CE	2.41	0.42
1:O:387:TRP:CZ2	1:O:389:THR:HA	2.55	0.42
1:O:452:ILE:N	1:O:453:PRO:CD	2.81	0.42
1:S:700:GLU:HG2	8:S:1563:HOH:O	2.19	0.42
1:S:737:PRO:CG	4:S:903:MGD:H2'	2.50	0.42
1:S:816:SER:OG	1:S:839:ILE:HG13	2.18	0.42
1:U:10:SER:HA	1:U:15:PRO:HA	2.01	0.42
1:U:162:ASN:HD22	1:U:166:PHE:HE2	1.67	0.42
2:V:168:VAL:HG13	2:V:173:LEU:HB2	2.01	0.42
1:W:142:SER:CB	4:W:902:MGD:O1A	2.67	0.42
1:W:839:ILE:HD13	1:W:839:ILE:HA	1.92	0.42
1:A:418:ALA:HB1	1:A:423:ALA:HB2	2.00	0.42
1:A:452:ILE:HB	1:A:453:PRO:HD3	2.01	0.42
2:B:9:ASP:HA	2:B:189:LYS:HB3	2.00	0.42
1:E:610:LYS:NZ	1:E:618:GLN:NE2	2.57	0.42
1:G:249:ASP:OD2	4:G:903:MGD:H1'	2.19	0.42
1:G:277:ALA:HB2	1:G:321:ALA:HB2	2.01	0.42
1:G:387:TRP:CZ2	1:G:389:THR:HA	2.55	0.42
1:I:378:GLY:O	1:I:381:LYS:HG2	2.20	0.42
1:I:540:LEU:HA	1:I:541:PRO:HD3	1.76	0.42
1:I:782:ARG:HH11	1:I:782:ARG:HG3	1.85	0.42
2:J:71:CYS:HA	2:J:184:PRO:HA	2.01	0.42
2:J:166:LYS:HG2	2:J:170:GLU:OE2	2.20	0.42
1:M:426:MET:HE3	1:M:622:ALA:HB2	2.01	0.42
1:O:13:GLY:HA3	1:O:63:THR:OG1	2.19	0.42
2:P:10:VAL:HG13	2:P:63:TYR:O	2.19	0.42
1:S:651:THR:HB	1:S:665:THR:HG22	2.01	0.42
1:S:735:LEU:HD23	1:S:735:LEU:H	1.84	0.42
1:U:797:GLY:HA2	1:U:875:TYR:CD2	2.54	0.42
2:X:1:MET:HE2	2:X:88:GLU:CB	2.49	0.42
2:B:164:MET:O	2:B:168:VAL:HG23	2.19	0.42
1:C:395:LEU:HD13	1:C:571:ARG:HG2	2.02	0.42
1:I:56:LYS:HG2	1:I:57:THR:O	2.19	0.42
1:I:250:PRO:HD3	4:I:903:MGD:C2	2.50	0.42
1:I:262:LYS:HG2	2:J:232:PHE:CE1	2.54	0.42
1:I:521:PHE:CE2	1:I:523:VAL:CG2	3.02	0.42
1:I:670:PRO:HG2	1:I:675:GLN:CD	2.45	0.42
2:J:177:LYS:N	2:J:178:PRO:HD3	2.34	0.42
1:K:269:GLY:HA2	1:K:362:HIS:CG	2.54	0.42
1:M:364:ILE:HD13	1:M:708:ARG:HG3	2.01	0.42
2:N:126:CYS:HB2	8:N:466:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:239:LYS:HE2	8:O:1595:HOH:O	2.20	0.42
1:Q:730:TYR:CZ	1:Q:794:ASN:HA	2.54	0.42
1:S:250:PRO:HD3	4:S:903:MGD:C2	2.49	0.42
1:S:301:GLU:H	1:S:301:GLU:CD	2.28	0.42
1:U:554:PHE:HB3	8:U:1031:HOH:O	2.20	0.42
1:W:427:PHE:HB3	8:W:1027:HOH:O	2.20	0.42
1:W:744:HIS:HA	1:W:819:SER:HB3	2.02	0.42
1:A:211:MET:HE2	1:A:246:VAL:CG2	2.49	0.42
1:A:328:PRO:HB2	1:A:331:GLU:HG3	2.02	0.42
1:A:521:PHE:CE2	1:A:523:VAL:CG2	3.02	0.42
2:B:124:GLN:O	2:B:125:LYS:HB3	2.20	0.42
1:C:76:ILE:HA	1:C:77:PRO:HD3	1.77	0.42
1:E:68:SER:HB3	1:E:753:TYR:CE2	2.55	0.42
1:E:756:TYR:CD1	2:F:24:MET:HE1	2.54	0.42
1:G:66:PHE:CD1	1:G:69:MET:CE	3.03	0.42
1:G:730:TYR:HB3	1:G:862:VAL:CA	2.50	0.42
2:J:44:ARG:O	2:J:45:TRP:C	2.63	0.42
1:K:76:ILE:HA	1:K:77:PRO:HD3	1.73	0.42
1:K:250:PRO:HD3	4:K:903:MGD:C2	2.50	0.42
1:M:677:CYS:C	1:M:678:ARG:HG2	2.44	0.42
2:N:20:PHE:CE1	2:N:24:MET:HE2	2.55	0.42
2:N:166:LYS:HG2	2:N:170:GLU:OE2	2.20	0.42
1:O:510:TYR:O	1:O:513:MET:HG2	2.20	0.42
2:P:69:MET:O	2:P:70:HIS:C	2.62	0.42
1:Q:625:MET:N	1:Q:626:PRO:CD	2.83	0.42
2:T:70:HIS:HD2	2:T:92:VAL:N	2.00	0.42
1:U:673:ASN:H	1:U:673:ASN:ND2	2.18	0.42
2:V:191:LEU:HG	2:V:195:GLU:HG3	2.01	0.42
1:W:528:TRP:CD2	1:W:750:LYS:HD3	2.55	0.42
1:W:729:LYS:HD2	8:W:1132:HOH:O	2.18	0.42
1:C:737:PRO:CG	4:C:903:MGD:H2'	2.50	0.42
1:E:571:ARG:HA	8:E:1026:HOH:O	2.20	0.42
2:F:69:MET:O	2:F:70:HIS:C	2.63	0.42
2:F:114:MET:HE3	2:F:123:ALA:HB1	2.01	0.42
1:G:736:SER:O	4:G:902:MGD:N18	2.53	0.42
1:I:501:LEU:HD13	1:I:823:TYR:CG	2.55	0.42
1:I:847:TYR:CZ	1:I:853:CYS:HB3	2.55	0.42
1:K:505:THR:HB	1:K:845:ASP:HA	2.01	0.42
1:M:763:GLU:HA	1:M:768:LYS:HA	2.01	0.42
1:O:114:TRP:CZ2	1:O:587:MET:HG2	2.54	0.42
1:O:162:ASN:HD22	1:O:166:PHE:HE2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:401:PHE:HA	1:O:402:PRO:HD3	1.86	0.42
1:O:770:TRP:HB3	1:O:801:LEU:HD23	2.02	0.42
2:P:81:ASN:OD1	2:P:81:ASN:O	2.36	0.42
2:P:166:LYS:HE2	2:P:170:GLU:OE2	2.20	0.42
1:Q:620:PHE:CZ	1:Q:625:MET:HB3	2.55	0.42
2:R:122:VAL:HG22	2:R:123:ALA:N	2.35	0.42
2:R:164:MET:O	2:R:168:VAL:HG23	2.20	0.42
1:S:56:LYS:HG2	1:S:57:THR:O	2.20	0.42
1:S:563:ASP:O	1:S:566:GLN:HG2	2.19	0.42
2:T:53:ARG:HB2	2:T:60:ASP:OD1	2.20	0.42
1:U:173:PRO:HG3	1:U:180:HIS:CG	2.55	0.42
1:U:396:ASP:OD2	1:U:398:GLU:HB2	2.20	0.42
1:U:498:GLY:N	1:U:499:PRO:HD3	2.35	0.42
1:U:786:ASN:HD22	1:U:805:VAL:N	2.16	0.42
2:V:198:TYR:CD1	2:V:198:TYR:C	2.98	0.42
1:W:338:GLN:OE1	1:W:341:LYS:HE3	2.19	0.42
1:W:387:TRP:CZ2	1:W:389:THR:HA	2.54	0.42
2:X:139:ALA:O	2:X:141:LYS:HG3	2.19	0.42
1:A:12:THR:HB	1:A:743:MET:HG3	2.01	0.42
1:A:604:GLU:HB3	1:A:605:MET:HE3	2.02	0.42
2:B:59:ASN:H	2:B:59:ASN:HD22	1.67	0.42
1:C:540:LEU:HA	1:C:541:PRO:HD3	1.83	0.42
1:C:557:CYS:H	1:C:564:ASN:ND2	1.94	0.42
1:C:691:ILE:HD11	1:C:711:MET:CE	2.50	0.42
2:D:46:MET:CE	2:D:66:THR:N	2.74	0.42
1:E:288:TYR:HB2	1:E:376:MET:O	2.20	0.42
1:G:76:ILE:HG22	1:G:541:PRO:HG3	2.02	0.42
1:I:452:ILE:HB	1:I:453:PRO:HD3	2.02	0.42
1:I:605:MET:SD	1:I:605:MET:N	2.91	0.42
1:K:498:GLY:N	1:K:499:PRO:HD3	2.35	0.42
2:L:60:ASP:OD1	2:L:60:ASP:C	2.62	0.42
1:O:56:LYS:HG2	1:O:57:THR:N	2.35	0.42
1:O:262:LYS:HG2	2:P:232:PHE:CE1	2.55	0.42
1:O:404:TYR:CD1	1:O:404:TYR:C	2.98	0.42
1:O:605:MET:SD	1:O:605:MET:N	2.90	0.42
1:Q:74:LEU:HD23	1:Q:74:LEU:HA	1.90	0.42
1:Q:782:ARG:HD3	1:Q:864:ILE:O	2.20	0.42
1:S:401:PHE:HA	1:S:402:PRO:HD3	1.79	0.42
2:T:40:GLN:NE2	2:T:118:GLU:H	2.14	0.42
2:V:74:ALA:HA	2:V:75:PRO:HD3	1.93	0.42
1:W:13:GLY:HA3	1:W:63:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:495:LYS:HD2	1:W:514:TYR:OH	2.20	0.42
1:W:782:ARG:HG3	1:W:782:ARG:HH11	1.85	0.42
1:C:744:HIS:HA	1:C:819:SER:HB3	2.02	0.41
2:D:270:GLY:HA2	8:D:534:HOH:O	2.20	0.41
1:E:521:PHE:CE2	1:E:523:VAL:CG2	3.03	0.41
1:E:748:ASP:O	1:E:750:LYS:HG3	2.20	0.41
2:F:94:ILE:HG13	2:F:125:LYS:HE3	2.02	0.41
2:F:114:MET:HA	2:F:125:LYS:HB3	2.01	0.41
1:G:404:TYR:CD1	1:G:405:ALA:N	2.88	0.41
1:G:746:MET:HE2	4:G:902:MGD:O1B	2.20	0.41
1:I:176:TRP:NE1	1:I:354:TRP:HE1	2.17	0.41
1:K:35:ASP:OD1	1:K:55:ARG:HD3	2.20	0.41
1:K:563:ASP:O	1:K:566:GLN:HG2	2.20	0.41
1:M:460:LYS:HG3	8:M:1230:HOH:O	2.18	0.41
1:O:15:PRO:HD3	1:O:554:PHE:CE1	2.55	0.41
1:O:218:ASP:OD2	1:O:253:ASN:HB2	2.20	0.41
2:P:1:MET:HE2	2:P:88:GLU:HG2	2.02	0.41
2:P:40:GLN:NE2	8:P:441:HOH:O	2.52	0.41
2:P:62:ASN:CG	2:P:193:ARG:HB3	2.45	0.41
1:S:296:ASN:O	1:S:687:LYS:HB3	2.20	0.41
1:S:387:TRP:CZ2	1:S:389:THR:HA	2.55	0.41
2:T:19:CYS:HA	2:T:145:CYS:HA	2.02	0.41
1:U:565:TYR:C	1:U:567:LEU:H	2.27	0.41
2:V:219:SER:C	2:V:221:GLY:H	2.28	0.41
1:W:489:LYS:HG3	8:W:1212:HOH:O	2.19	0.41
1:A:553:GLU:HG2	1:A:556:ASN:HB2	2.02	0.41
1:C:55:ARG:HG3	8:C:1548:HOH:O	2.19	0.41
1:C:404:TYR:CD1	1:C:405:ALA:N	2.88	0.41
1:C:776:SER:HA	1:C:805:VAL:HG13	2.01	0.41
1:C:868:ASP:OD1	1:C:870:ASP:HB2	2.20	0.41
1:E:249:ASP:OD2	4:E:903:MGD:H1'	2.19	0.41
1:I:737:PRO:CG	4:I:903:MGD:H2'	2.50	0.41
1:K:269:GLY:HA2	1:K:362:HIS:CE1	2.55	0.41
2:L:20:PHE:CZ	2:L:24:MET:HE2	2.55	0.41
1:M:76:ILE:CG2	1:M:541:PRO:HG3	2.50	0.41
1:Q:76:ILE:HA	1:Q:77:PRO:HD3	1.75	0.41
1:Q:649:LYS:HE2	8:Q:1454:HOH:O	2.20	0.41
1:U:107:SER:HB3	8:U:1624:HOH:O	2.20	0.41
2:X:120:GLU:O	2:X:121:ASN:C	2.62	0.41
1:A:103:GLN:CD	1:A:103:GLN:N	2.78	0.41
1:A:289:ASP:CG	1:A:292:TYR:HB2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:177:LYS:C	2:D:179:GLU:OE1	2.63	0.41
1:E:13:GLY:HA3	1:E:63:THR:OG1	2.20	0.41
1:G:296:ASN:O	1:G:687:LYS:HB3	2.21	0.41
1:I:39:ALA:HA	1:I:40:PRO:HD3	1.87	0.41
1:M:269:GLY:HA2	1:M:362:HIS:CE1	2.55	0.41
1:M:402:PRO:HG2	1:M:422:PHE:CE1	2.55	0.41
2:P:19:CYS:O	2:P:22:GLY:N	2.53	0.41
2:P:162:GLU:CD	2:P:162:GLU:N	2.78	0.41
1:Q:56:LYS:HE2	8:Q:1461:HOH:O	2.20	0.41
1:Q:165:GLY:C	1:Q:439:LEU:HD12	2.45	0.41
1:Q:716:PRO:HB3	1:Q:723:HIS:CD2	2.55	0.41
1:Q:724:SER:HA	1:Q:725:PRO:HD3	1.91	0.41
2:T:46:MET:HE1	2:T:65:PRO:C	2.43	0.41
2:V:213:ALA:O	2:V:228:GLU:HA	2.20	0.41
1:W:9:ASN:HA	1:W:576:GLN:HA	2.01	0.41
1:W:770:TRP:HB3	1:W:801:LEU:HD23	2.01	0.41
2:X:135:ASP:OD1	2:X:137:SER:HB2	2.19	0.41
1:A:735:LEU:HD23	1:A:735:LEU:H	1.84	0.41
1:A:770:TRP:HB3	1:A:801:LEU:HD23	2.02	0.41
1:C:224:GLY:O	1:C:225:ILE:HB	2.20	0.41
1:E:35:ASP:OD1	1:E:55:ARG:HD3	2.20	0.41
1:E:233:ILE:HD11	8:E:1179:HOH:O	2.19	0.41
1:G:12:THR:HG23	8:G:1326:HOH:O	2.20	0.41
1:I:656:TRP:CG	1:I:663:LYS:HA	2.54	0.41
1:K:128:ILE:CD1	1:K:492:MET:HB2	2.50	0.41
1:K:323:GLU:HB2	8:K:1567:HOH:O	2.20	0.41
1:M:257:ARG:HD3	2:N:61:ILE:HG21	2.01	0.41
1:M:482:TYR:HA	1:M:483:PRO:C	2.46	0.41
2:N:162:GLU:H	2:N:162:GLU:CD	2.27	0.41
1:O:561:ILE:CG2	1:O:564:ASN:HB3	2.51	0.41
1:Q:587:MET:HG3	1:Q:592:ILE:CG1	2.51	0.41
2:R:46:MET:HE3	2:R:46:MET:C	2.46	0.41
1:S:74:LEU:HD12	1:S:750:LYS:HA	2.02	0.41
1:S:175:SER:HB2	1:S:176:TRP:CE3	2.55	0.41
1:S:426:MET:HA	1:S:426:MET:CE	2.35	0.41
2:T:69:MET:O	2:T:70:HIS:C	2.63	0.41
1:U:549:TRP:CG	1:U:613:LEU:HD13	2.55	0.41
1:U:708:ARG:HD2	8:U:1049:HOH:O	2.19	0.41
1:W:96:ARG:HD2	1:W:514:TYR:O	2.20	0.41
1:W:250:PRO:HD3	4:W:903:MGD:C2	2.51	0.41
1:W:722:LYS:HB2	1:W:722:LYS:HE3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:753:TYR:HB3	2:X:24:MET:CE	2.50	0.41
2:X:23:CYS:CB	2:X:39:MET:HE1	2.44	0.41
2:X:124:GLN:O	2:X:125:LYS:HB3	2.19	0.41
1:A:21:LYS:CB	1:A:26:ILE:HD11	2.50	0.41
1:E:347:ALA:CB	1:E:388:SER:HA	2.51	0.41
1:G:610:LYS:NZ	1:G:618:GLN:NE2	2.57	0.41
2:H:46:MET:HE3	2:H:46:MET:C	2.46	0.41
1:I:457:MET:HE3	8:I:1504:HOH:O	2.19	0.41
1:I:625:MET:N	1:I:626:PRO:CD	2.84	0.41
2:J:204:LEU:HD23	2:J:209:CYS:HA	2.01	0.41
1:K:301:GLU:CD	1:K:301:GLU:N	2.76	0.41
1:M:249:ASP:OD2	4:M:903:MGD:H1'	2.21	0.41
1:M:625:MET:N	1:M:626:PRO:CD	2.83	0.41
1:Q:13:GLY:O	1:Q:59:ILE:HA	2.20	0.41
1:Q:277:ALA:HB2	1:Q:321:ALA:HB2	2.01	0.41
1:Q:613:LEU:HD12	1:Q:613:LEU:HA	1.94	0.41
1:S:166:PHE:N	1:S:439:LEU:HD12	2.36	0.41
1:S:724:SER:HA	1:S:725:PRO:HD3	1.94	0.41
1:U:201:LEU:HD13	1:U:387:TRP:HB2	2.02	0.41
1:W:75:ARG:HH22	1:W:547:GLU:CD	2.28	0.41
1:W:142:SER:HB3	4:W:902:MGD:O1A	2.20	0.41
1:W:143:SER:N	4:W:902:MGD:O1A	2.53	0.41
1:W:173:PRO:HG3	1:W:180:HIS:CG	2.56	0.41
1:W:476:GLN:OE1	1:W:708:ARG:NH2	2.54	0.41
2:X:5:TYR:CD2	2:X:164:MET:HG2	2.55	0.41
1:A:396:ASP:OD2	1:A:398:GLU:HB2	2.21	0.41
1:C:56:LYS:HG2	1:C:57:THR:O	2.20	0.41
1:C:402:PRO:HG2	1:C:422:PHE:CE1	2.55	0.41
1:E:114:TRP:CZ2	1:E:587:MET:HG2	2.56	0.41
1:K:225:ILE:HG12	1:K:226:TYR:CD1	2.55	0.41
2:L:210:PHE:HD2	2:L:213:ALA:HB2	1.86	0.41
1:M:66:PHE:CD1	1:M:69:MET:HE3	2.55	0.41
1:M:647:ASN:O	1:M:648:ARG:C	2.61	0.41
1:M:736:SER:O	4:M:902:MGD:N18	2.53	0.41
2:N:154:TYR:CE1	7:N:302:SF4:S4	3.13	0.41
1:O:95:LEU:HD23	1:O:95:LEU:HA	1.89	0.41
1:O:269:GLY:HA2	1:O:362:HIS:ND1	2.36	0.41
2:P:218:LYS:HG2	2:P:223:GLU:N	2.36	0.41
1:Q:44:ILE:HD11	1:Q:394:PRO:CG	2.50	0.41
1:Q:66:PHE:CD1	1:Q:69:MET:CE	3.03	0.41
1:S:786:ASN:HD21	1:S:804:GLN:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:40:GLN:HB3	2:T:43:HIS:CE1	2.56	0.41
1:U:105:PRO:HD2	8:U:1425:HOH:O	2.21	0.41
1:W:162:ASN:HD22	1:W:166:PHE:HE2	1.69	0.41
1:W:554:PHE:HB3	8:W:1025:HOH:O	2.20	0.41
2:X:173:LEU:HB3	2:X:187:TYR:HB3	2.03	0.41
1:A:404:TYR:CD1	1:A:405:ALA:N	2.88	0.41
2:B:125:LYS:HD2	2:B:126:CYS:O	2.20	0.41
1:C:76:ILE:CG2	1:C:541:PRO:HG3	2.50	0.41
1:E:617:GLU:HG3	1:E:631:TRP:CG	2.55	0.41
2:F:210:PHE:CE2	2:F:251:ALA:HB1	2.55	0.41
1:G:176:TRP:CD1	1:G:193:LEU:HB2	2.55	0.41
1:M:21:LYS:CB	1:M:26:ILE:HD11	2.50	0.41
1:M:175:SER:OG	6:M:905:PYG:C1	2.68	0.41
1:M:597:ALA:HB1	1:M:603:GLU:HA	2.03	0.41
1:O:734:MET:HB2	1:O:814:VAL:HG23	2.03	0.41
2:P:124:GLN:O	2:P:125:LYS:HB3	2.20	0.41
1:Q:426:MET:HE1	1:Q:618:GLN:O	2.21	0.41
2:R:13:CYS:HB3	2:R:63:TYR:HB2	2.02	0.41
1:S:289:ASP:OD2	1:S:381:LYS:NZ	2.44	0.41
1:W:11:SER:C	1:W:13:GLY:H	2.27	0.41
1:A:263:TRP:CZ2	1:A:265:SER:HB2	2.55	0.41
1:C:138:LEU:HB2	1:C:490:ILE:CD1	2.50	0.41
1:C:191:TRP:HE1	1:C:667:ASP:CG	2.29	0.41
1:C:272:HIS:ND1	1:C:272:HIS:N	2.67	0.41
1:E:10:SER:HA	1:E:15:PRO:HA	2.03	0.41
1:E:211:MET:HE1	2:F:231:PHE:CE1	2.54	0.41
2:F:39:MET:HE2	2:F:45:TRP:CD2	2.56	0.41
2:F:106:LEU:HD22	2:F:114:MET:HB3	2.02	0.41
2:H:166:LYS:HE2	2:H:170:GLU:OE2	2.19	0.41
1:I:155:SER:HA	1:I:407:GLY:O	2.21	0.41
2:J:106:LEU:HA	2:J:114:MET:HG3	2.02	0.41
2:J:198:TYR:HB3	2:J:238:ASP:HA	2.03	0.41
2:L:128:MET:O	2:L:129:CYS:C	2.63	0.41
1:M:501:LEU:HB2	8:M:1360:HOH:O	2.20	0.41
2:N:26:GLU:HB2	2:N:144:ARG:HH11	1.84	0.41
1:O:11:SER:HA	1:O:147:TRP:HB2	2.02	0.41
1:O:153:ARG:O	1:O:157:TYR:HB3	2.20	0.41
1:O:391:GLN:HG2	1:O:567:LEU:CD2	2.50	0.41
1:O:870:ASP:HB3	1:O:872:TYR:CE1	2.55	0.41
2:P:166:LYS:HE2	2:P:170:GLU:CD	2.46	0.41
1:Q:28:MET:HE1	1:Q:67:LYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:647:ASN:O	1:Q:648:ARG:C	2.64	0.41
1:U:99:GLY:HA2	1:U:102:LYS:HG2	2.01	0.41
1:U:867:TRP:CE2	1:U:869:GLY:HA2	2.55	0.41
1:W:21:LYS:HB3	1:W:26:ILE:HD11	2.02	0.41
1:A:425:ARG:HD3	1:A:622:ALA:O	2.20	0.41
1:C:356:GLY:H	4:C:903:MGD:C5'	2.26	0.41
1:C:433:PHE:HA	1:C:434:PRO:HD3	1.81	0.41
1:C:739:PRO:HG2	1:C:742:SER:O	2.21	0.41
2:D:13:CYS:HB3	2:D:63:TYR:HB2	2.03	0.41
1:E:187:TRP:HB2	1:E:681:LEU:HD13	2.03	0.41
1:E:501:LEU:HA	1:E:507:THR:HB	2.02	0.41
2:F:19:CYS:O	2:F:22:GLY:N	2.53	0.41
2:F:77:VAL:HG22	2:F:84:VAL:HG12	2.02	0.41
1:G:277:ALA:HA	1:G:316:LYS:O	2.21	0.41
1:G:301:GLU:H	1:G:301:GLU:CD	2.29	0.41
2:H:106:LEU:CD2	2:H:114:MET:HB3	2.50	0.41
2:H:142:MET:HE1	8:H:926:HOH:O	2.21	0.41
2:H:216:VAL:HG13	2:H:223:GLU:HG3	2.03	0.41
2:H:254:LYS:HD2	2:H:274:LEU:OXT	2.21	0.41
1:I:28:MET:HE1	1:I:66:PHE:CB	2.41	0.41
1:I:100:LEU:HD12	1:I:105:PRO:HG3	2.02	0.41
1:I:301:GLU:H	1:I:301:GLU:CD	2.29	0.41
2:J:245:TYR:HB2	2:J:260:VAL:CG1	2.51	0.41
1:K:328:PRO:HB2	1:K:331:GLU:HG3	2.02	0.41
1:K:561:ILE:N	1:K:562:PRO:HD3	2.36	0.41
1:O:356:GLY:HA2	1:O:359:ARG:NH1	2.36	0.41
2:P:1:MET:HG3	2:P:88:GLU:HB3	2.02	0.41
1:Q:39:ALA:HA	1:Q:40:PRO:HD3	1.91	0.41
1:Q:165:GLY:CA	1:Q:166:PHE:HB3	2.43	0.41
1:Q:249:ASP:OD2	4:Q:903:MGD:H1'	2.21	0.41
1:Q:287:SER:HB2	1:Q:340:ALA:HB1	2.02	0.41
1:S:39:ALA:HA	1:S:40:PRO:HD3	1.90	0.41
1:S:96:ARG:HD2	1:S:514:TYR:O	2.21	0.41
1:S:263:TRP:CZ2	1:S:265:SER:HB2	2.55	0.41
1:S:737:PRO:HB3	4:S:903:MGD:H3'	2.03	0.41
1:U:719:GLU:HG2	1:U:859:THR:O	2.21	0.41
2:V:204:LEU:HD23	2:V:209:CYS:HA	2.02	0.41
1:W:144:HIS:HB2	4:W:902:MGD:O1B	2.21	0.41
1:W:171:HIS:HD2	8:W:1457:HOH:O	2.04	0.41
1:W:645:ASN:HD22	1:W:648:ARG:HB3	1.84	0.41
2:B:105:LEU:HB3	2:B:114:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:TYR:C	1:C:541:PRO:HG2	2.46	0.41
1:C:100:LEU:HD22	1:C:534:PRO:HB2	2.02	0.41
2:D:106:LEU:HD23	2:D:114:MET:CE	2.51	0.41
2:D:118:GLU:O	2:D:121:ASN:ND2	2.54	0.41
2:D:178:PRO:C	2:D:180:LEU:H	2.28	0.41
1:E:162:ASN:HD22	1:E:166:PHE:HE2	1.68	0.41
1:E:175:SER:HB2	1:E:176:TRP:CZ3	2.56	0.41
1:E:828:THR:HG21	1:E:831:LYS:HD2	2.03	0.41
1:G:165:GLY:HA3	1:G:166:PHE:CB	2.37	0.41
1:I:146:MET:HG2	4:I:902:MGD:N7	2.36	0.41
1:M:263:TRP:CZ2	1:M:265:SER:HB2	2.56	0.41
1:M:498:GLY:N	1:M:499:PRO:HD3	2.36	0.41
1:M:644:ASP:C	1:M:646:PRO:HD3	2.46	0.41
1:O:274:LEU:O	1:O:278:ILE:HG13	2.21	0.41
2:P:44:ARG:O	2:P:45:TRP:C	2.64	0.41
2:P:218:LYS:HG2	2:P:222:LYS:C	2.46	0.41
1:Q:61:PRO:HG3	2:R:16:CYS:HB2	2.03	0.41
1:Q:140:THR:HB	1:Q:169:ALA:HB3	2.02	0.41
1:S:107:SER:HB3	8:S:1619:HOH:O	2.20	0.41
1:S:211:MET:HE1	2:T:231:PHE:CE1	2.54	0.41
1:W:439:LEU:HD21	1:W:487:TYR:CE2	2.56	0.41
1:W:587:MET:HE2	1:W:592:ILE:HA	2.02	0.41
1:W:704:ILE:HG23	8:W:1646:HOH:O	2.21	0.41
2:X:216:VAL:HG13	2:X:223:GLU:HG3	2.03	0.41
1:A:347:ALA:CB	1:A:388:SER:HA	2.51	0.40
1:A:395:LEU:HD13	1:A:571:ARG:CG	2.51	0.40
1:C:274:LEU:O	1:C:278:ILE:HG13	2.20	0.40
1:C:387:TRP:CZ2	1:C:389:THR:HA	2.56	0.40
2:F:18:ASN:HB2	7:F:302:SF4:S1	2.61	0.40
1:G:476:GLN:HG2	8:G:1279:HOH:O	2.20	0.40
1:K:100:LEU:HD22	1:K:534:PRO:HB2	2.03	0.40
2:L:1:MET:CG	2:L:88:GLU:HB3	2.49	0.40
2:L:164:MET:HE3	2:L:168:VAL:HG23	2.03	0.40
1:M:128:ILE:HD12	1:M:492:MET:HB2	2.01	0.40
1:M:695:LEU:HD22	1:M:708:ARG:HD3	2.03	0.40
1:O:610:LYS:NZ	1:O:618:GLN:NE2	2.57	0.40
1:Q:95:LEU:HD23	1:Q:95:LEU:HA	1.90	0.40
1:Q:647:ASN:HB2	8:Q:1437:HOH:O	2.20	0.40
1:S:347:ALA:CB	1:S:388:SER:HA	2.51	0.40
1:U:393:VAL:HA	1:U:394:PRO:HD3	1.86	0.40
1:U:482:TYR:HA	1:U:483:PRO:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:29:LEU:HD23	2:V:29:LEU:HA	1.91	0.40
2:V:139:ALA:HB3	2:V:140:PRO:HD3	2.03	0.40
1:A:404:TYR:CD1	1:A:404:TYR:C	2.99	0.40
1:A:426:MET:HA	1:A:426:MET:CE	2.37	0.40
1:A:604:GLU:HB3	1:A:605:MET:CE	2.52	0.40
1:C:13:GLY:HA3	1:C:63:THR:OG1	2.21	0.40
1:C:393:VAL:HA	1:C:394:PRO:HD3	1.78	0.40
1:E:540:LEU:HA	1:E:541:PRO:HD3	1.83	0.40
1:G:28:MET:HE3	1:G:28:MET:HB2	1.93	0.40
1:I:1:MET:H3	1:I:22:ASP:CG	2.28	0.40
1:I:192:ARG:CZ	1:I:562:PRO:HD2	2.51	0.40
1:K:786:ASN:HD22	1:K:805:VAL:H	1.66	0.40
1:M:378:GLY:O	1:M:381:LYS:HG2	2.21	0.40
1:M:782:ARG:HH11	1:M:782:ARG:HG3	1.85	0.40
1:O:630:THR:OG1	1:O:633:GLU:HG3	2.20	0.40
1:O:670:PRO:HB3	1:O:682:GLN:HB2	2.03	0.40
1:O:767:TYR:HB3	1:O:769:TYR:CE1	2.57	0.40
2:P:210:PHE:HD2	2:P:213:ALA:HB2	1.87	0.40
1:U:499:PRO:CB	1:U:745:THR:HG21	2.51	0.40
1:W:155:SER:OG	1:W:409:ILE:HG12	2.20	0.40
1:W:258:LEU:HG	1:W:259:VAL:HG13	2.02	0.40
1:W:354:TRP:HB3	1:W:355:GLY:H	1.76	0.40
2:B:139:ALA:HB3	2:B:140:PRO:HD3	2.03	0.40
1:C:62:TYR:HB3	1:C:742:SER:HA	2.03	0.40
1:C:541:PRO:HB2	1:C:586:SER:HA	2.03	0.40
1:C:724:SER:HA	1:C:725:PRO:HD3	1.94	0.40
2:D:104:GLU:CD	2:D:104:GLU:H	2.28	0.40
2:D:106:LEU:HA	2:D:114:MET:HE2	2.02	0.40
2:D:210:PHE:O	2:D:233:GLY:HA2	2.21	0.40
1:E:66:PHE:CD1	1:E:69:MET:CE	3.05	0.40
1:E:92:ASN:N	1:E:93:PRO:HD3	2.36	0.40
1:E:642:VAL:HA	1:E:643:PRO:HD3	1.96	0.40
1:E:738:HIS:ND1	4:E:903:MGD:N15	2.70	0.40
1:G:714:TYR:O	1:G:716:PRO:HD3	2.22	0.40
1:I:249:ASP:OD2	4:I:903:MGD:H1'	2.21	0.40
1:K:716:PRO:HB3	1:K:723:HIS:CG	2.56	0.40
2:N:95:ASP:HB3	2:N:98:LYS:HB2	2.04	0.40
1:Q:165:GLY:HA3	1:Q:166:PHE:CB	2.36	0.40
1:Q:200:ASP:HB3	8:Q:1055:HOH:O	2.21	0.40
1:Q:826:LEU:HD21	1:Q:835:ARG:HD3	2.04	0.40
2:T:46:MET:HE3	2:T:46:MET:C	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:52:GLU:CG	2:T:61:ILE:HD12	2.52	0.40
1:U:138:LEU:HB2	1:U:490:ILE:CD1	2.51	0.40
1:W:452:ILE:HB	1:W:453:PRO:HD3	2.04	0.40
1:A:433:PHE:CD1	1:A:433:PHE:N	2.88	0.40
1:A:505:THR:HG22	1:A:857:ASN:ND2	2.36	0.40
1:C:187:TRP:CH2	1:C:196:PRO:HB3	2.56	0.40
1:C:211:MET:HE1	2:D:231:PHE:HZ	1.77	0.40
1:C:396:ASP:OD2	1:C:398:GLU:HB2	2.21	0.40
1:C:729:LYS:HD2	8:C:1131:HOH:O	2.21	0.40
2:D:55:THR:O	2:D:56:TYR:C	2.64	0.40
1:E:15:PRO:HD2	8:E:1003:HOH:O	2.20	0.40
2:H:52:GLU:CG	2:H:61:ILE:HD12	2.52	0.40
1:I:2:GLY:N	1:I:22:ASP:OD1	2.55	0.40
1:K:328:PRO:O	1:K:332:ILE:HG13	2.21	0.40
1:M:491:LYS:HD3	8:M:1557:HOH:O	2.21	0.40
2:N:19:CYS:HA	2:N:145:CYS:HA	2.04	0.40
1:O:201:LEU:HD13	1:O:387:TRP:HB2	2.03	0.40
1:O:786:ASN:HD21	1:O:805:VAL:N	2.19	0.40
1:Q:10:SER:HA	1:Q:15:PRO:HA	2.04	0.40
1:S:362:HIS:HB3	1:S:717:ALA:HB2	2.03	0.40
1:S:378:GLY:O	1:S:381:LYS:HG2	2.22	0.40
1:S:722:LYS:HE3	1:S:722:LYS:HB2	1.87	0.40
2:T:60:ASP:OD1	2:T:60:ASP:C	2.64	0.40
1:U:227:ALA:O	1:U:228:GLY:C	2.64	0.40
1:U:353:GLY:O	1:U:354:TRP:HB2	2.21	0.40
1:W:141:PRO:CA	1:W:496:TYR:HB3	2.47	0.40
1:W:301:GLU:CD	1:W:301:GLU:H	2.29	0.40
1:W:426:MET:HA	1:W:426:MET:CE	2.46	0.40
1:W:460:LYS:HE3	8:W:1232:HOH:O	2.22	0.40
1:W:542:ALA:HA	1:W:587:MET:O	2.21	0.40
2:X:142:MET:CE	2:X:146:ALA:HB1	2.45	0.40
2:B:74:ALA:HA	2:B:75:PRO:HD3	1.85	0.40
1:C:356:GLY:HA2	1:C:359:ARG:NH1	2.36	0.40
2:D:251:ALA:O	2:D:254:LYS:HB2	2.22	0.40
1:G:867:TRP:CE2	1:G:869:GLY:HA2	2.56	0.40
1:K:67:LYS:NZ	2:L:25:ASP:O	2.48	0.40
1:K:274:LEU:O	1:K:278:ILE:HG13	2.21	0.40
1:K:528:TRP:CD2	1:K:750:LYS:HD3	2.57	0.40
1:M:176:TRP:CD1	1:M:193:LEU:HB2	2.57	0.40
1:M:180:HIS:HD2	1:M:193:LEU:HD22	1.86	0.40
1:O:77:PRO:HB2	1:O:78:TYR:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:347:ALA:CB	1:O:388:SER:HA	2.52	0.40
2:P:9:ASP:HA	2:P:189:LYS:HB3	2.04	0.40
2:P:23:CYS:O	2:P:27:HIS:N	2.47	0.40
1:Q:147:TRP:CD1	1:Q:552:SER:HG	2.39	0.40
1:Q:347:ALA:CB	1:Q:388:SER:HA	2.52	0.40
1:Q:628:TYR:CE2	1:Q:643:PRO:HG2	2.56	0.40
1:Q:691:ILE:CD1	1:Q:711:MET:HE3	2.44	0.40
2:R:207:GLY:CA	1:U:728:VAL:HG12	2.31	0.40
2:V:46:MET:CE	2:V:66:THR:H	2.33	0.40
2:V:60:ASP:C	2:V:60:ASP:OD1	2.64	0.40
2:V:62:ASN:CG	2:V:193:ARG:HB3	2.47	0.40
2:V:106:LEU:CD2	2:V:114:MET:HG3	2.51	0.40
1:W:404:TYR:CD1	1:W:405:ALA:N	2.90	0.40
1:W:499:PRO:HB2	1:W:745:THR:HG21	2.04	0.40
1:W:598:LYS:HA	1:W:603:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	873/875 (100%)	815 (93%)	54 (6%)	4 (0%)	24	27
1	C	873/875 (100%)	822 (94%)	46 (5%)	5 (1%)	21	23
1	E	873/875 (100%)	820 (94%)	50 (6%)	3 (0%)	36	42
1	G	873/875 (100%)	823 (94%)	46 (5%)	4 (0%)	24	27
1	I	873/875 (100%)	821 (94%)	49 (6%)	3 (0%)	36	42
1	K	873/875 (100%)	822 (94%)	48 (6%)	3 (0%)	36	42
1	M	873/875 (100%)	825 (94%)	45 (5%)	3 (0%)	36	42
1	O	873/875 (100%)	816 (94%)	51 (6%)	6 (1%)	18	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	873/875 (100%)	821 (94%)	48 (6%)	4 (0%)	24	27
1	S	873/875 (100%)	814 (93%)	52 (6%)	7 (1%)	16	16
1	U	873/875 (100%)	820 (94%)	49 (6%)	4 (0%)	24	27
1	W	873/875 (100%)	815 (93%)	55 (6%)	3 (0%)	36	42
2	B	272/274 (99%)	261 (96%)	10 (4%)	1 (0%)	30	34
2	D	272/274 (99%)	256 (94%)	14 (5%)	2 (1%)	18	19
2	F	272/274 (99%)	257 (94%)	14 (5%)	1 (0%)	30	34
2	H	272/274 (99%)	258 (95%)	11 (4%)	3 (1%)	11	10
2	J	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	34
2	L	272/274 (99%)	259 (95%)	11 (4%)	2 (1%)	18	19
2	N	272/274 (99%)	260 (96%)	11 (4%)	1 (0%)	30	34
2	P	272/274 (99%)	256 (94%)	15 (6%)	1 (0%)	30	34
2	R	272/274 (99%)	258 (95%)	13 (5%)	1 (0%)	30	34
2	T	272/274 (99%)	259 (95%)	12 (4%)	1 (0%)	30	34
2	V	272/274 (99%)	258 (95%)	12 (4%)	2 (1%)	18	19
2	X	272/274 (99%)	245 (90%)	25 (9%)	2 (1%)	18	19
All	All	13740/13788 (100%)	12921 (94%)	752 (6%)	67 (0%)	24	27

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	C	177	GLU
1	E	177	GLU
1	G	177	GLU
1	I	177	GLU
1	I	225	ILE
1	K	177	GLU
1	M	177	GLU
1	O	177	GLU
1	Q	177	GLU
1	S	141	PRO
1	S	177	GLU
1	U	177	GLU
1	W	177	GLU
1	A	141	PRO

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

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Mol	Chain	Res	Type
1	E	225	ILE
2	L	67	PRO
1	W	225	ILE
2	L	221	GLY
1	C	394	PRO
1	G	225	ILE
2	H	221	GLY
1	Q	225	ILE
1	Q	394	PRO
1	S	182	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	729/729 (100%)	720 (99%)	9 (1%)	63	78
1	C	729/729 (100%)	717 (98%)	12 (2%)	55	71
1	E	729/729 (100%)	722 (99%)	7 (1%)	68	81
1	G	729/729 (100%)	722 (99%)	7 (1%)	68	81
1	I	729/729 (100%)	719 (99%)	10 (1%)	59	75
1	K	729/729 (100%)	723 (99%)	6 (1%)	73	85
1	M	729/729 (100%)	721 (99%)	8 (1%)	65	79
1	O	729/729 (100%)	718 (98%)	11 (2%)	57	73
1	Q	729/729 (100%)	718 (98%)	11 (2%)	57	73
1	S	729/729 (100%)	720 (99%)	9 (1%)	63	78
1	U	729/729 (100%)	723 (99%)	6 (1%)	73	85
1	W	729/729 (100%)	719 (99%)	10 (1%)	59	75
2	B	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	D	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	F	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	H	235/235 (100%)	223 (95%)	12 (5%)	21	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	L	235/235 (100%)	224 (95%)	11 (5%)	23	31
2	N	235/235 (100%)	224 (95%)	11 (5%)	23	31
2	P	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	R	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	T	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	V	235/235 (100%)	223 (95%)	12 (5%)	21	27
2	X	235/235 (100%)	226 (96%)	9 (4%)	29	40
All	All	11568/11568 (100%)	11323 (98%)	245 (2%)	47	63

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASP
1	A	142	SER
1	A	373	LEU
1	A	499	PRO
1	A	564	ASN
1	A	605	MET
1	A	726	LEU
1	A	743	MET
1	A	818	GLU
2	B	13	CYS
2	B	19	CYS
2	B	21	MET
2	B	24	MET
2	B	71	CYS
2	B	76	CYS
2	B	104	GLU
2	B	109	CYS
2	B	129	CYS
2	B	145	CYS
2	B	149	CYS
2	B	157	LEU
1	C	78	TYR
1	C	119	ASP
1	C	142	SER
1	C	373	LEU
1	C	426	MET

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Mol	Chain	Res	Type
1	C	499	PRO
1	C	564	ASN
1	C	605	MET
1	C	743	MET
1	C	786	ASN
1	C	818	GLU
1	C	870	ASP
2	D	13	CYS
2	D	19	CYS
2	D	21	MET
2	D	71	CYS
2	D	73	ASN
2	D	76	CYS
2	D	109	CYS
2	D	129	CYS
2	D	145	CYS
2	D	149	CYS
2	D	157	LEU
2	D	179	GLU
1	E	142	SER
1	E	373	LEU
1	E	426	MET
1	E	499	PRO
1	E	564	ASN
1	E	673	ASN
1	E	743	MET
2	F	13	CYS
2	F	19	CYS
2	F	21	MET
2	F	24	MET
2	F	29	LEU
2	F	71	CYS
2	F	76	CYS
2	F	109	CYS
2	F	129	CYS
2	F	145	CYS
2	F	149	CYS
2	F	157	LEU
1	G	100	LEU
1	G	142	SER
1	G	373	LEU
1	G	426	MET

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Mol	Chain	Res	Type
1	G	564	ASN
1	G	726	LEU
1	G	743	MET
2	H	13	CYS
2	H	19	CYS
2	H	21	MET
2	H	24	MET
2	H	57	PRO
2	H	71	CYS
2	H	76	CYS
2	H	109	CYS
2	H	129	CYS
2	H	145	CYS
2	H	149	CYS
2	H	157	LEU
1	I	142	SER
1	I	373	LEU
1	I	426	MET
1	I	492	MET
1	I	499	PRO
1	I	564	ASN
1	I	605	MET
1	I	726	LEU
1	I	743	MET
1	I	801	LEU
2	J	13	CYS
2	J	19	CYS
2	J	21	MET
2	J	24	MET
2	J	71	CYS
2	J	76	CYS
2	J	104	GLU
2	J	109	CYS
2	J	129	CYS
2	J	145	CYS
2	J	149	CYS
2	J	157	LEU
1	K	142	SER
1	K	274	LEU
1	K	499	PRO
1	K	564	ASN
1	K	726	LEU

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Mol	Chain	Res	Type
1	K	786	ASN
2	L	13	CYS
2	L	19	CYS
2	L	21	MET
2	L	59	ASN
2	L	71	CYS
2	L	76	CYS
2	L	109	CYS
2	L	129	CYS
2	L	145	CYS
2	L	149	CYS
2	L	157	LEU
1	M	142	SER
1	M	426	MET
1	M	499	PRO
1	M	564	ASN
1	M	605	MET
1	M	726	LEU
1	M	743	MET
1	M	786	ASN
2	N	2	GLU
2	N	13	CYS
2	N	19	CYS
2	N	21	MET
2	N	24	MET
2	N	71	CYS
2	N	76	CYS
2	N	109	CYS
2	N	129	CYS
2	N	145	CYS
2	N	149	CYS
1	O	100	LEU
1	O	142	SER
1	O	373	LEU
1	O	426	MET
1	O	499	PRO
1	O	564	ASN
1	O	605	MET
1	O	673	ASN
1	O	726	LEU
1	O	743	MET
1	O	786	ASN

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Mol	Chain	Res	Type
2	P	13	CYS
2	P	19	CYS
2	P	59	ASN
2	P	71	CYS
2	P	73	ASN
2	P	76	CYS
2	P	104	GLU
2	P	109	CYS
2	P	129	CYS
2	P	145	CYS
2	P	149	CYS
2	P	157	LEU
1	Q	100	LEU
1	Q	142	SER
1	Q	373	LEU
1	Q	426	MET
1	Q	499	PRO
1	Q	564	ASN
1	Q	605	MET
1	Q	726	LEU
1	Q	743	MET
1	Q	786	ASN
1	Q	800	ILE
2	R	13	CYS
2	R	19	CYS
2	R	21	MET
2	R	24	MET
2	R	29	LEU
2	R	71	CYS
2	R	76	CYS
2	R	109	CYS
2	R	129	CYS
2	R	145	CYS
2	R	149	CYS
2	R	157	LEU
1	S	142	SER
1	S	274	LEU
1	S	373	LEU
1	S	426	MET
1	S	499	PRO
1	S	605	MET
1	S	699	GLU

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Mol	Chain	Res	Type
1	S	726	LEU
1	S	743	MET
2	T	13	CYS
2	T	19	CYS
2	T	21	MET
2	T	24	MET
2	T	71	CYS
2	T	76	CYS
2	T	104	GLU
2	T	109	CYS
2	T	129	CYS
2	T	145	CYS
2	T	149	CYS
2	T	157	LEU
1	U	142	SER
1	U	499	PRO
1	U	564	ASN
1	U	605	MET
1	U	726	LEU
1	U	743	MET
2	V	13	CYS
2	V	19	CYS
2	V	21	MET
2	V	57	PRO
2	V	71	CYS
2	V	73	ASN
2	V	76	CYS
2	V	104	GLU
2	V	109	CYS
2	V	129	CYS
2	V	145	CYS
2	V	149	CYS
1	W	142	SER
1	W	373	LEU
1	W	426	MET
1	W	499	PRO
1	W	564	ASN
1	W	587	MET
1	W	605	MET
1	W	743	MET
1	W	786	ASN
1	W	801	LEU

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Mol	Chain	Res	Type
2	X	13	CYS
2	X	19	CYS
2	X	21	MET
2	X	71	CYS
2	X	109	CYS
2	X	129	CYS
2	X	145	CYS
2	X	149	CYS
2	X	157	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (267) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	162	ASN
1	A	171	HIS
1	A	222	ASN
1	A	232	ASN
1	A	391	GLN
1	A	478	HIS
1	A	525	GLN
1	A	564	ASN
1	A	576	GLN
1	A	618	GLN
1	A	647	ASN
1	A	673	ASN
1	A	674	ASN
1	A	697	ASN
1	A	701	GLN
1	A	786	ASN
2	B	18	ASN
2	B	27	HIS
2	B	59	ASN
2	B	70	HIS
2	B	73	ASN
2	B	81	ASN
1	C	162	ASN
1	C	171	HIS
1	C	222	ASN
1	C	232	ASN
1	C	391	GLN
1	C	415	ASN

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Mol	Chain	Res	Type
1	C	440	ASN
1	C	462	GLN
1	C	478	HIS
1	C	525	GLN
1	C	564	ASN
1	C	576	GLN
1	C	618	GLN
1	C	673	ASN
1	C	674	ASN
1	C	697	ASN
1	C	701	GLN
1	C	786	ASN
2	D	17	ASN
2	D	18	ASN
2	D	40	GLN
2	D	59	ASN
2	D	70	HIS
2	D	73	ASN
2	D	81	ASN
2	D	121	ASN
1	E	88	ASN
1	E	162	ASN
1	E	171	HIS
1	E	222	ASN
1	E	440	ASN
1	E	462	GLN
1	E	478	HIS
1	E	525	GLN
1	E	564	ASN
1	E	576	GLN
1	E	618	GLN
1	E	647	ASN
1	E	673	ASN
1	E	674	ASN
1	E	697	ASN
1	E	701	GLN
1	E	786	ASN
2	F	18	ASN
2	F	40	GLN
2	F	59	ASN
2	F	70	HIS
2	F	73	ASN

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Mol	Chain	Res	Type
2	F	190	ASN
1	G	162	ASN
1	G	171	HIS
1	G	222	ASN
1	G	232	ASN
1	G	440	ASN
1	G	462	GLN
1	G	478	HIS
1	G	525	GLN
1	G	564	ASN
1	G	618	GLN
1	G	673	ASN
1	G	674	ASN
1	G	697	ASN
1	G	701	GLN
1	G	786	ASN
2	H	27	HIS
2	H	40	GLN
2	H	59	ASN
2	H	70	HIS
2	H	73	ASN
2	H	81	ASN
1	I	162	ASN
1	I	171	HIS
1	I	222	ASN
1	I	232	ASN
1	I	462	GLN
1	I	478	HIS
1	I	525	GLN
1	I	564	ASN
1	I	576	GLN
1	I	618	GLN
1	I	673	ASN
1	I	674	ASN
1	I	697	ASN
1	I	701	GLN
1	I	786	ASN
2	J	40	GLN
2	J	59	ASN
2	J	70	HIS
2	J	73	ASN
2	J	81	ASN

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Mol	Chain	Res	Type
1	K	162	ASN
1	K	171	HIS
1	K	222	ASN
1	K	232	ASN
1	K	478	HIS
1	K	525	GLN
1	K	564	ASN
1	K	576	GLN
1	K	618	GLN
1	K	647	ASN
1	K	673	ASN
1	K	674	ASN
1	K	697	ASN
1	K	701	GLN
1	K	786	ASN
2	L	18	ASN
2	L	27	HIS
2	L	40	GLN
2	L	59	ASN
2	L	70	HIS
2	L	73	ASN
2	L	81	ASN
1	M	162	ASN
1	M	171	HIS
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	576	GLN
1	M	618	GLN
1	M	673	ASN
1	M	674	ASN
1	M	697	ASN
1	M	701	GLN
1	M	721	GLN
1	M	786	ASN
2	N	18	ASN
2	N	27	HIS
2	N	40	GLN
2	N	59	ASN

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Mol	Chain	Res	Type
2	N	70	HIS
2	N	73	ASN
1	O	162	ASN
1	O	171	HIS
1	O	222	ASN
1	O	232	ASN
1	O	478	HIS
1	O	525	GLN
1	O	564	ASN
1	O	576	GLN
1	O	618	GLN
1	O	645	ASN
1	O	673	ASN
1	O	674	ASN
1	O	697	ASN
1	O	701	GLN
1	O	786	ASN
1	O	804	GLN
2	P	30	ASN
2	P	40	GLN
2	P	59	ASN
2	P	70	HIS
2	P	81	ASN
2	P	86	GLN
1	Q	88	ASN
1	Q	162	ASN
1	Q	171	HIS
1	Q	222	ASN
1	Q	440	ASN
1	Q	462	GLN
1	Q	478	HIS
1	Q	525	GLN
1	Q	564	ASN
1	Q	576	GLN
1	Q	618	GLN
1	Q	621	ASN
1	Q	673	ASN
1	Q	674	ASN
1	Q	697	ASN
1	Q	701	GLN
1	Q	786	ASN
2	R	27	HIS

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Mol	Chain	Res	Type
2	R	40	GLN
2	R	59	ASN
2	R	70	HIS
2	R	73	ASN
1	S	88	ASN
1	S	162	ASN
1	S	171	HIS
1	S	222	ASN
1	S	462	GLN
1	S	478	HIS
1	S	525	GLN
1	S	564	ASN
1	S	576	GLN
1	S	618	GLN
1	S	673	ASN
1	S	674	ASN
1	S	697	ASN
1	S	701	GLN
1	S	786	ASN
2	T	17	ASN
2	T	18	ASN
2	T	40	GLN
2	T	59	ASN
2	T	70	HIS
2	T	73	ASN
1	U	162	ASN
1	U	171	HIS
1	U	478	HIS
1	U	479	GLN
1	U	525	GLN
1	U	564	ASN
1	U	576	GLN
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	59	ASN
2	V	70	HIS
2	V	73	ASN

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Mol	Chain	Res	Type
2	V	81	ASN
1	W	88	ASN
1	W	162	ASN
1	W	171	HIS
1	W	222	ASN
1	W	232	ASN
1	W	415	ASN
1	W	462	GLN
1	W	478	HIS
1	W	525	GLN
1	W	564	ASN
1	W	576	GLN
1	W	618	GLN
1	W	621	ASN
1	W	645	ASN
1	W	673	ASN
1	W	674	ASN
1	W	697	ASN
1	W	701	GLN
1	W	721	GLN
1	W	786	ASN
1	W	810	GLN
2	X	18	ASN
2	X	40	GLN
2	X	59	ASN
2	X	70	HIS
2	X	73	ASN
2	X	121	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 107 ligands modelled in this entry, 35 are monoatomic - leaving 72 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PYG	Q	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.11	4 (33%)
4	MGD	Q	903	5	47,52,52	2.23	12 (25%)	58,81,81	1.47	3 (5%)
4	MGD	G	903	5	47,52,52	2.29	17 (36%)	58,81,81	1.52	2 (3%)
4	MGD	G	902	5	47,52,52	2.25	12 (25%)	58,81,81	2.18	7 (12%)
6	PYG	M	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.12	5 (41%)
7	SF4	L	304	2	0,12,12	-	-	-		
4	MGD	K	903	5	47,52,52	2.35	15 (31%)	58,81,81	2.16	9 (15%)
6	PYG	O	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.17	5 (41%)
7	SF4	P	303	2	0,12,12	-	-	-		
4	MGD	Q	902	5	47,52,52	2.06	13 (27%)	58,81,81	2.02	7 (12%)
7	SF4	P	304	2	0,12,12	-	-	-		
7	SF4	R	302	2	0,12,12	-	-	-		
7	SF4	T	304	2	0,12,12	-	-	-		
7	SF4	V	302	2	0,12,12	-	-	-		
7	SF4	V	303	2	0,12,12	-	-	-		
7	SF4	X	302	2	0,12,12	-	-	-		
7	SF4	X	303	2	0,12,12	-	-	-		
4	MGD	M	902	5	47,52,52	2.03	14 (29%)	58,81,81	2.04	9 (15%)
4	MGD	O	903	5	47,52,52	2.46	16 (34%)	58,81,81	1.32	4 (6%)
7	SF4	H	304	2	0,12,12	-	-	-		
4	MGD	C	902	5	47,52,52	2.22	13 (27%)	58,81,81	2.05	9 (15%)
7	SF4	D	302	2	0,12,12	-	-	-		
6	PYG	A	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.09	4 (33%)
7	SF4	J	302	2	0,12,12	-	-	-		
7	SF4	V	304	2	0,12,12	-	-	-		
7	SF4	R	304	2	0,12,12	-	-	-		
4	MGD	I	902	5	47,52,52	2.03	12 (25%)	58,81,81	1.99	8 (13%)
7	SF4	F	303	2	0,12,12	-	-	-		
4	MGD	A	903	5	47,52,52	2.31	14 (29%)	58,81,81	2.26	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SF4	N	302	2	0,12,12	-	-	-		
7	SF4	H	302	2	0,12,12	-	-	-		
4	MGD	S	902	5	47,52,52	2.12	14 (29%)	58,81,81	2.13	8 (13%)
7	SF4	J	301	2	0,12,12	-	-	-		
6	PYG	U	905	5	9,9,9	4.64	9 (100%)	12,12,12	3.13	4 (33%)
6	PYG	C	905	5	9,9,9	4.63	9 (100%)	12,12,12	3.15	5 (41%)
7	SF4	X	304	2	0,12,12	-	-	-		
4	MGD	E	903	5	47,52,52	2.37	15 (31%)	58,81,81	1.40	4 (6%)
4	MGD	U	903	5	47,52,52	2.46	12 (25%)	58,81,81	1.32	4 (6%)
7	SF4	N	303	2	0,12,12	-	-	-		
4	MGD	I	903	5	47,52,52	2.31	14 (29%)	58,81,81	1.55	4 (6%)
7	SF4	B	302	2	0,12,12	-	-	-		
4	MGD	U	902	5	47,52,52	2.17	16 (34%)	58,81,81	2.10	8 (13%)
7	SF4	D	304	2	0,12,12	-	-	-		
6	PYG	W	905	5	9,9,9	4.68	9 (100%)	12,12,12	3.21	5 (41%)
7	SF4	R	303	2	0,12,12	-	-	-		
7	SF4	B	303	2	0,12,12	-	-	-		
6	PYG	I	905	5	9,9,9	4.67	9 (100%)	12,12,12	3.13	5 (41%)
6	PYG	K	905	5	9,9,9	4.71	9 (100%)	12,12,12	3.16	4 (33%)
6	PYG	S	905	5	9,9,9	4.72	9 (100%)	12,12,12	3.10	4 (33%)
7	SF4	F	304	2	0,12,12	-	-	-		
4	MGD	W	903	5	47,52,52	2.66	13 (27%)	58,81,81	1.20	3 (5%)
6	PYG	E	905	5	9,9,9	4.69	9 (100%)	12,12,12	3.12	4 (33%)
7	SF4	B	304	2	0,12,12	-	-	-		
4	MGD	O	902	5	47,52,52	2.11	12 (25%)	58,81,81	2.03	9 (15%)
4	MGD	C	903	5	47,52,52	2.60	18 (38%)	58,81,81	1.30	3 (5%)
7	SF4	N	304	2	0,12,12	-	-	-		
7	SF4	T	302	2	0,12,12	-	-	-		
4	MGD	K	902	5	47,52,52	2.08	12 (25%)	58,81,81	1.98	8 (13%)
7	SF4	J	303	2	0,12,12	-	-	-		
6	PYG	G	905	5	9,9,9	4.64	9 (100%)	12,12,12	3.12	4 (33%)
4	MGD	M	903	5	47,52,52	2.42	16 (34%)	58,81,81	1.43	5 (8%)
7	SF4	L	302	2	0,12,12	-	-	-		
4	MGD	A	902	5	47,52,52	2.21	13 (27%)	58,81,81	2.24	9 (15%)
7	SF4	T	303	2	0,12,12	-	-	-		
4	MGD	S	903	5	47,52,52	2.34	14 (29%)	58,81,81	1.38	3 (5%)
7	SF4	F	302	2	0,12,12	-	-	-		
4	MGD	W	902	5	47,52,52	2.12	13 (27%)	58,81,81	2.01	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SF4	L	303	2	0,12,12	-	-	-		
7	SF4	D	303	2	0,12,12	-	-	-		
7	SF4	P	302	2	0,12,12	-	-	-		
7	SF4	H	303	2	0,12,12	-	-	-		
4	MGD	E	902	5	47,52,52	2.12	13 (27%)	58,81,81	2.08	8 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PYG	Q	905	5	-	-	0/1/1/1
4	MGD	Q	903	5	-	4/22/66/66	0/6/6/6
4	MGD	G	903	5	-	3/22/66/66	0/6/6/6
4	MGD	G	902	5	-	10/22/66/66	0/6/6/6
6	PYG	M	905	5	-	-	0/1/1/1
7	SF4	L	304	2	-	-	0/6/5/5
4	MGD	K	903	5	-	4/22/66/66	0/6/6/6
6	PYG	O	905	5	-	-	0/1/1/1
7	SF4	P	303	2	-	-	0/6/5/5
4	MGD	Q	902	5	-	7/22/66/66	0/6/6/6
7	SF4	P	304	2	-	-	0/6/5/5
7	SF4	R	302	2	-	-	0/6/5/5
7	SF4	T	304	2	-	-	0/6/5/5
7	SF4	V	302	2	-	-	0/6/5/5
7	SF4	V	303	2	-	-	0/6/5/5
7	SF4	X	302	2	-	-	0/6/5/5
7	SF4	X	303	2	-	-	0/6/5/5
4	MGD	M	902	5	-	7/22/66/66	0/6/6/6
4	MGD	O	903	5	-	4/22/66/66	0/6/6/6
7	SF4	H	304	2	-	-	0/6/5/5
4	MGD	C	902	5	-	7/22/66/66	0/6/6/6
7	SF4	D	302	2	-	-	0/6/5/5
6	PYG	A	905	5	-	-	0/1/1/1
7	SF4	J	302	2	-	-	0/6/5/5
7	SF4	V	304	2	-	-	0/6/5/5
7	SF4	R	304	2	-	-	0/6/5/5
4	MGD	I	902	5	-	8/22/66/66	0/6/6/6
7	SF4	F	303	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MGD	A	903	5	-	5/22/66/66	0/6/6/6
7	SF4	N	302	2	-	-	0/6/5/5
7	SF4	H	302	2	-	-	0/6/5/5
4	MGD	S	902	5	-	9/22/66/66	0/6/6/6
7	SF4	J	301	2	-	-	0/6/5/5
6	PYG	U	905	5	-	-	0/1/1/1
6	PYG	C	905	5	-	-	0/1/1/1
7	SF4	X	304	2	-	-	0/6/5/5
4	MGD	E	903	5	-	4/22/66/66	0/6/6/6
4	MGD	U	903	5	-	4/22/66/66	0/6/6/6
7	SF4	N	303	2	-	-	0/6/5/5
4	MGD	I	903	5	-	6/22/66/66	0/6/6/6
7	SF4	B	302	2	-	-	0/6/5/5
4	MGD	U	902	5	-	7/22/66/66	0/6/6/6
7	SF4	D	304	2	-	-	0/6/5/5
6	PYG	W	905	5	-	-	0/1/1/1
7	SF4	R	303	2	-	-	0/6/5/5
7	SF4	B	303	2	-	-	0/6/5/5
6	PYG	I	905	5	-	-	0/1/1/1
6	PYG	K	905	5	-	-	0/1/1/1
6	PYG	S	905	5	-	-	0/1/1/1
7	SF4	F	304	2	-	-	0/6/5/5
4	MGD	W	903	5	-	5/22/66/66	0/6/6/6
6	PYG	E	905	5	-	-	0/1/1/1
7	SF4	B	304	2	-	-	0/6/5/5
4	MGD	O	902	5	-	8/22/66/66	0/6/6/6
4	MGD	C	903	5	-	4/22/66/66	0/6/6/6
7	SF4	N	304	2	-	-	0/6/5/5
7	SF4	T	302	2	-	-	0/6/5/5
4	MGD	K	902	5	-	8/22/66/66	0/6/6/6
7	SF4	J	303	2	-	-	0/6/5/5
6	PYG	G	905	5	-	-	0/1/1/1
4	MGD	M	903	5	-	4/22/66/66	0/6/6/6
7	SF4	L	302	2	-	-	0/6/5/5
4	MGD	A	902	5	-	9/22/66/66	0/6/6/6
7	SF4	T	303	2	-	-	0/6/5/5
4	MGD	S	903	5	-	4/22/66/66	0/6/6/6
7	SF4	F	302	2	-	-	0/6/5/5
4	MGD	W	902	5	-	8/22/66/66	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	L	303	2	-	-	0/6/5/5
7	SF4	D	303	2	-	-	0/6/5/5
7	SF4	P	302	2	-	-	0/6/5/5
7	SF4	H	303	2	-	-	0/6/5/5
4	MGD	E	902	5	-	8/22/66/66	0/6/6/6

All (441) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	905	PYG	C1-C2	8.07	1.49	1.40
6	I	905	PYG	C1-C2	8.04	1.49	1.40
6	E	905	PYG	C1-C2	8.01	1.49	1.40
6	U	905	PYG	C1-C2	7.99	1.49	1.40
6	C	905	PYG	C1-C2	7.98	1.49	1.40
6	O	905	PYG	C1-C2	7.97	1.49	1.40
4	W	903	MGD	PA-O3B	7.94	1.68	1.59
6	K	905	PYG	C1-C2	7.91	1.49	1.40
6	S	905	PYG	C1-C2	7.91	1.49	1.40
4	S	903	MGD	C14-N15	7.88	1.55	1.46
6	M	905	PYG	C1-C2	7.85	1.49	1.40
6	G	905	PYG	C1-C2	7.82	1.49	1.40
6	A	905	PYG	C1-C2	7.79	1.49	1.40
4	U	903	MGD	C14-N15	7.71	1.55	1.46
4	K	903	MGD	C14-N15	7.52	1.55	1.46
6	W	905	PYG	C1-C2	7.51	1.48	1.40
4	A	903	MGD	C14-N15	7.38	1.54	1.46
4	E	903	MGD	C14-N15	7.29	1.54	1.46
4	Q	903	MGD	C14-N15	7.19	1.54	1.46
4	C	903	MGD	C14-N15	7.06	1.54	1.46
4	I	903	MGD	C14-N15	7.05	1.54	1.46
4	W	903	MGD	C14-N15	7.00	1.54	1.46
4	M	903	MGD	C14-N15	6.98	1.54	1.46
4	O	903	MGD	C14-N15	6.96	1.54	1.46
4	G	903	MGD	C14-N15	6.78	1.54	1.46
4	K	902	MGD	C23-C14	6.55	1.58	1.53
4	W	902	MGD	C23-C14	6.46	1.58	1.53
4	C	903	MGD	C23-C14	6.44	1.58	1.53
4	W	903	MGD	C21-N22	6.31	1.42	1.35
4	C	903	MGD	PA-O3B	6.26	1.66	1.59
4	U	903	MGD	C21-N22	6.22	1.42	1.35
4	Q	902	MGD	C23-C14	6.17	1.58	1.53
4	O	903	MGD	C23-C14	6.13	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	902	MGD	C23-C14	6.12	1.58	1.53
4	C	903	MGD	C21-N22	6.11	1.41	1.35
4	M	903	MGD	PA-O3B	6.11	1.66	1.59
6	W	905	PYG	C3-C2	6.08	1.47	1.40
6	S	905	PYG	C3-C2	5.97	1.46	1.40
4	U	903	MGD	C23-C14	5.96	1.58	1.53
4	I	902	MGD	C23-C14	5.90	1.58	1.53
4	K	903	MGD	C23-C14	5.90	1.58	1.53
6	K	905	PYG	C3-C2	5.87	1.46	1.40
6	M	905	PYG	C3-C2	5.82	1.46	1.40
4	O	902	MGD	C23-C14	5.80	1.58	1.53
4	A	903	MGD	C23-C14	5.79	1.58	1.53
6	O	905	PYG	C3-C2	5.77	1.46	1.40
6	W	905	PYG	O3-C3	5.75	1.47	1.36
6	U	905	PYG	C3-C2	5.73	1.46	1.40
4	W	903	MGD	C23-C14	5.70	1.58	1.53
4	O	903	MGD	C21-N22	5.68	1.41	1.35
6	C	905	PYG	O3-C3	5.66	1.47	1.36
6	A	905	PYG	C3-C2	5.65	1.46	1.40
6	K	905	PYG	O3-C3	5.65	1.47	1.36
6	A	905	PYG	O3-C3	5.64	1.47	1.36
6	S	905	PYG	O3-C3	5.64	1.47	1.36
4	G	902	MGD	C23-C14	5.63	1.58	1.53
6	G	905	PYG	C3-C2	5.63	1.46	1.40
4	A	902	MGD	C23-C14	5.62	1.58	1.53
6	I	905	PYG	O3-C3	5.57	1.47	1.36
6	Q	905	PYG	O3-C3	5.56	1.47	1.36
6	O	905	PYG	O3-C3	5.56	1.47	1.36
6	E	905	PYG	C3-C2	5.56	1.46	1.40
6	C	905	PYG	C3-C2	5.54	1.46	1.40
6	M	905	PYG	O3-C3	5.51	1.47	1.36
4	U	902	MGD	C23-C14	5.50	1.58	1.53
6	U	905	PYG	O3-C3	5.50	1.47	1.36
6	G	905	PYG	O3-C3	5.50	1.47	1.36
6	E	905	PYG	O3-C3	5.48	1.47	1.36
6	Q	905	PYG	C3-C2	5.45	1.46	1.40
4	S	902	MGD	C21-N22	5.45	1.41	1.35
6	I	905	PYG	C3-C2	5.44	1.46	1.40
4	S	903	MGD	C23-C14	5.42	1.57	1.53
4	O	903	MGD	PA-O3B	5.37	1.65	1.59
4	E	903	MGD	C21-N22	5.37	1.41	1.35
4	K	903	MGD	PA-O3B	5.35	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	902	MGD	C23-C14	5.33	1.57	1.53
4	G	902	MGD	C21-N22	5.29	1.41	1.35
4	E	902	MGD	C23-C14	5.29	1.57	1.53
4	I	903	MGD	C21-N22	5.28	1.41	1.35
4	K	903	MGD	C21-N22	5.28	1.41	1.35
4	G	903	MGD	C21-N22	5.26	1.41	1.35
4	Q	903	MGD	C23-C14	5.25	1.57	1.53
4	G	903	MGD	C23-C14	5.23	1.57	1.53
4	I	903	MGD	C23-C14	5.20	1.57	1.53
4	O	902	MGD	C21-N22	5.20	1.41	1.35
4	W	902	MGD	C21-N22	5.19	1.40	1.35
4	M	903	MGD	C23-C14	5.17	1.57	1.53
4	G	902	MGD	C14-N15	5.11	1.52	1.46
4	E	903	MGD	C23-C14	5.11	1.57	1.53
4	M	902	MGD	C23-C14	5.06	1.57	1.53
6	S	905	PYG	C6-C1	5.05	1.48	1.39
4	A	903	MGD	C21-N22	5.03	1.40	1.35
6	E	905	PYG	C6-C1	5.00	1.48	1.39
6	K	905	PYG	C6-C1	5.00	1.48	1.39
4	M	903	MGD	C21-N22	5.00	1.40	1.35
6	W	905	PYG	C6-C1	5.00	1.48	1.39
4	S	903	MGD	C21-N22	4.99	1.40	1.35
6	A	905	PYG	C6-C1	4.97	1.48	1.39
6	O	905	PYG	C6-C1	4.91	1.48	1.39
4	E	902	MGD	C21-N22	4.90	1.40	1.35
6	Q	905	PYG	C6-C1	4.88	1.48	1.39
4	U	903	MGD	PA-O3B	4.88	1.64	1.59
4	A	902	MGD	C21-N22	4.87	1.40	1.35
6	M	905	PYG	C6-C1	4.86	1.47	1.39
6	I	905	PYG	C6-C1	4.85	1.47	1.39
6	C	905	PYG	C6-C1	4.82	1.47	1.39
4	E	902	MGD	C14-N15	4.81	1.51	1.46
6	G	905	PYG	C6-C1	4.80	1.47	1.39
4	C	902	MGD	C14-N15	4.79	1.51	1.46
4	U	902	MGD	C21-N22	4.79	1.40	1.35
4	O	902	MGD	C14-N15	4.77	1.51	1.46
4	W	903	MGD	O11-C23	4.76	1.50	1.43
4	Q	903	MGD	C21-N22	4.73	1.40	1.35
4	Q	902	MGD	C21-N22	4.68	1.40	1.35
4	I	903	MGD	C16-N15	4.68	1.48	1.37
4	A	902	MGD	C16-N15	4.67	1.48	1.37
6	U	905	PYG	C6-C1	4.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	902	MGD	C21-N22	4.65	1.40	1.35
4	I	903	MGD	PA-O3B	4.61	1.64	1.59
4	A	902	MGD	C14-N15	4.61	1.51	1.46
4	Q	903	MGD	C16-N15	4.59	1.48	1.37
4	C	902	MGD	C21-N22	4.59	1.40	1.35
4	A	903	MGD	C16-N15	4.57	1.48	1.37
4	U	902	MGD	C14-N15	4.57	1.51	1.46
4	A	903	MGD	PA-O3B	4.53	1.64	1.59
4	G	902	MGD	PA-O3B	4.51	1.64	1.59
4	C	902	MGD	PA-O3B	4.50	1.64	1.59
4	U	902	MGD	C16-N15	4.47	1.48	1.37
4	S	902	MGD	C14-N15	4.47	1.51	1.46
4	M	902	MGD	C14-N15	4.40	1.51	1.46
4	G	902	MGD	O11-C11	4.39	1.52	1.43
4	E	903	MGD	PA-O3B	4.39	1.64	1.59
4	C	902	MGD	C16-N15	4.38	1.48	1.37
4	K	902	MGD	C16-N15	4.37	1.48	1.37
4	S	903	MGD	C16-N15	4.37	1.48	1.37
4	U	902	MGD	O11-C11	4.36	1.52	1.43
4	M	903	MGD	C16-N15	4.36	1.48	1.37
4	G	902	MGD	C16-N15	4.36	1.48	1.37
4	S	902	MGD	C16-N15	4.33	1.48	1.37
4	I	902	MGD	C21-N22	4.32	1.40	1.35
4	E	903	MGD	C16-N15	4.31	1.48	1.37
4	S	903	MGD	PA-O3B	4.28	1.64	1.59
4	A	902	MGD	O11-C11	4.26	1.51	1.43
4	C	903	MGD	O11-C11	4.26	1.51	1.43
4	K	903	MGD	C16-N15	4.24	1.47	1.37
4	M	902	MGD	C21-N22	4.23	1.40	1.35
4	K	902	MGD	C14-N15	4.22	1.51	1.46
4	G	903	MGD	C16-N15	4.22	1.47	1.37
4	C	903	MGD	C16-N15	4.21	1.47	1.37
4	W	902	MGD	C16-N15	4.20	1.47	1.37
4	W	903	MGD	C16-N15	4.20	1.47	1.37
4	G	903	MGD	PA-O3B	4.18	1.64	1.59
4	O	903	MGD	C16-N15	4.16	1.47	1.37
4	I	902	MGD	C14-N15	4.16	1.51	1.46
4	W	903	MGD	O11-C11	4.15	1.51	1.43
4	C	902	MGD	O11-C11	4.13	1.51	1.43
4	S	903	MGD	O11-C23	4.12	1.49	1.43
4	W	902	MGD	C14-N15	4.12	1.51	1.46
4	U	903	MGD	C16-N15	4.10	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	902	MGD	O11-C11	4.08	1.51	1.43
4	Q	902	MGD	C16-N15	4.08	1.47	1.37
4	M	902	MGD	C16-N15	4.07	1.47	1.37
4	O	902	MGD	C16-N15	4.07	1.47	1.37
4	Q	902	MGD	C14-N15	4.05	1.51	1.46
4	U	903	MGD	O11-C11	4.02	1.51	1.43
6	M	905	PYG	C5-C6	4.02	1.45	1.38
4	I	902	MGD	C16-N15	4.00	1.47	1.37
4	O	902	MGD	O11-C11	3.98	1.51	1.43
4	C	903	MGD	O11-C23	3.98	1.49	1.43
4	E	902	MGD	C16-N15	3.96	1.47	1.37
6	I	905	PYG	C5-C6	3.95	1.45	1.38
6	W	905	PYG	C5-C6	3.94	1.45	1.38
4	S	902	MGD	O11-C11	3.94	1.51	1.43
6	K	905	PYG	C5-C6	3.94	1.45	1.38
4	G	903	MGD	O11-C11	3.93	1.51	1.43
6	A	905	PYG	C5-C6	3.92	1.45	1.38
4	E	903	MGD	O11-C11	3.91	1.51	1.43
6	G	905	PYG	C5-C6	3.89	1.45	1.38
6	O	905	PYG	C5-C6	3.89	1.45	1.38
6	U	905	PYG	C5-C6	3.88	1.45	1.38
6	E	905	PYG	C5-C6	3.88	1.45	1.38
4	O	903	MGD	O11-C11	3.87	1.51	1.43
6	Q	905	PYG	C5-C6	3.86	1.45	1.38
6	C	905	PYG	C5-C6	3.83	1.45	1.38
4	E	902	MGD	PA-O3B	3.83	1.63	1.59
4	E	902	MGD	O11-C11	3.83	1.50	1.43
4	S	902	MGD	C21-N20	3.80	1.42	1.36
6	S	905	PYG	C5-C6	3.80	1.45	1.38
4	U	903	MGD	O11-C23	3.77	1.49	1.43
4	C	902	MGD	C21-N20	3.76	1.42	1.36
4	W	902	MGD	O11-C11	3.76	1.50	1.43
4	Q	903	MGD	O11-C11	3.74	1.50	1.43
4	O	903	MGD	O11-C23	3.71	1.49	1.43
4	W	903	MGD	C21-N20	3.71	1.41	1.36
4	A	902	MGD	C21-N20	3.70	1.41	1.36
4	I	902	MGD	O11-C11	3.69	1.50	1.43
4	M	903	MGD	O11-C23	3.66	1.49	1.43
4	I	903	MGD	C21-N20	3.56	1.41	1.36
4	U	903	MGD	C21-N20	3.54	1.41	1.36
4	C	903	MGD	C21-N20	3.54	1.41	1.36
4	I	903	MGD	O11-C11	3.54	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	902	MGD	C21-N20	3.51	1.41	1.36
4	M	903	MGD	O11-C11	3.50	1.50	1.43
4	E	903	MGD	C21-N20	3.50	1.41	1.36
4	S	903	MGD	O11-C11	3.48	1.50	1.43
4	E	903	MGD	O11-C23	3.47	1.48	1.43
4	M	903	MGD	C17-N18	3.46	1.45	1.38
4	A	903	MGD	C21-N20	3.46	1.41	1.36
6	E	905	PYG	O1-C1	3.45	1.43	1.36
4	Q	903	MGD	C17-N18	3.44	1.45	1.38
4	K	902	MGD	O11-C11	3.44	1.50	1.43
6	M	905	PYG	O1-C1	3.42	1.43	1.36
4	M	902	MGD	PA-O3B	3.41	1.63	1.59
6	G	905	PYG	O1-C1	3.39	1.43	1.36
4	G	903	MGD	O11-C23	3.39	1.48	1.43
4	K	902	MGD	C17-N18	3.35	1.45	1.38
4	U	902	MGD	C17-N18	3.32	1.45	1.38
4	Q	902	MGD	O11-C11	3.32	1.50	1.43
4	U	902	MGD	C21-N20	3.31	1.41	1.36
4	G	903	MGD	C21-N20	3.30	1.41	1.36
4	Q	903	MGD	C21-N20	3.29	1.41	1.36
4	A	902	MGD	PA-O3B	3.28	1.63	1.59
4	Q	902	MGD	C17-N18	3.26	1.45	1.38
4	G	903	MGD	C17-N18	3.26	1.45	1.38
4	K	903	MGD	C21-N20	3.26	1.41	1.36
4	A	903	MGD	C17-N18	3.24	1.44	1.38
4	Q	902	MGD	C21-N20	3.24	1.41	1.36
4	K	902	MGD	C21-N20	3.23	1.41	1.36
4	I	903	MGD	C17-N18	3.23	1.44	1.38
6	I	905	PYG	O1-C1	3.22	1.42	1.36
4	W	902	MGD	C21-N20	3.21	1.41	1.36
4	W	903	MGD	C23-N22	3.20	1.50	1.45
4	O	902	MGD	C21-N20	3.20	1.41	1.36
4	S	903	MGD	C21-N20	3.20	1.41	1.36
4	C	902	MGD	C17-N18	3.17	1.44	1.38
4	I	902	MGD	C21-N20	3.17	1.41	1.36
4	W	903	MGD	C17-N18	3.15	1.44	1.38
4	S	903	MGD	C17-N18	3.13	1.44	1.38
4	I	902	MGD	PA-O3B	3.12	1.62	1.59
4	C	903	MGD	C23-N22	3.11	1.50	1.45
6	A	905	PYG	O1-C1	3.10	1.42	1.36
6	Q	905	PYG	O1-C1	3.09	1.42	1.36
4	S	902	MGD	C17-N18	3.07	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	902	MGD	C17-N18	3.07	1.44	1.38
4	O	902	MGD	PA-O3B	3.05	1.62	1.59
4	Q	903	MGD	O11-C23	3.01	1.48	1.43
4	C	903	MGD	C17-N18	3.01	1.44	1.38
4	U	903	MGD	C17-N18	3.01	1.44	1.38
4	M	902	MGD	C21-N20	3.01	1.40	1.36
4	A	902	MGD	C17-N18	2.99	1.44	1.38
6	O	905	PYG	C5-C4	2.99	1.44	1.38
6	W	905	PYG	C5-C4	2.99	1.44	1.38
4	M	903	MGD	C21-N20	2.99	1.40	1.36
6	Q	905	PYG	C5-C4	2.98	1.44	1.38
4	E	903	MGD	C17-N18	2.97	1.44	1.38
4	U	902	MGD	C23-N22	2.97	1.50	1.45
6	C	905	PYG	C5-C4	2.96	1.44	1.38
4	E	902	MGD	C21-N20	2.96	1.40	1.36
6	U	905	PYG	C5-C4	2.96	1.44	1.38
4	E	902	MGD	C17-N18	2.93	1.44	1.38
6	U	905	PYG	O2-C2	2.93	1.43	1.36
6	S	905	PYG	C5-C4	2.93	1.43	1.38
4	K	902	MGD	PA-O3B	2.93	1.62	1.59
4	G	902	MGD	C23-N22	2.92	1.50	1.45
4	W	902	MGD	PA-O3B	2.92	1.62	1.59
4	E	902	MGD	C6-N1	2.92	1.44	1.38
4	O	903	MGD	C21-N20	2.91	1.40	1.36
4	I	902	MGD	C17-N18	2.91	1.44	1.38
6	I	905	PYG	C5-C4	2.90	1.43	1.38
6	K	905	PYG	C5-C4	2.90	1.43	1.38
6	A	905	PYG	C5-C4	2.89	1.43	1.38
4	U	902	MGD	PA-O3B	2.89	1.62	1.59
4	A	902	MGD	C6-N1	2.88	1.44	1.38
4	O	902	MGD	C17-N18	2.87	1.44	1.38
4	O	903	MGD	C17-N18	2.86	1.44	1.38
4	W	902	MGD	C17-N18	2.86	1.44	1.38
6	K	905	PYG	O2-C2	2.86	1.43	1.36
4	O	903	MGD	C23-N22	2.85	1.49	1.45
6	Q	905	PYG	O2-C2	2.84	1.43	1.36
4	I	902	MGD	C6-N1	2.84	1.44	1.38
4	Q	903	MGD	C16-C21	2.84	1.43	1.38
6	G	905	PYG	O2-C2	2.84	1.43	1.36
6	S	905	PYG	O2-C2	2.83	1.43	1.36
4	Q	902	MGD	PA-O3B	2.83	1.62	1.59
6	A	905	PYG	O2-C2	2.83	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	902	MGD	C6-N1	2.83	1.44	1.38
6	S	905	PYG	O1-C1	2.83	1.42	1.36
4	W	902	MGD	C23-N22	2.82	1.49	1.45
4	A	902	MGD	C23-N22	2.82	1.49	1.45
4	Q	902	MGD	C6-N1	2.82	1.44	1.38
4	S	903	MGD	C16-C21	2.82	1.43	1.38
6	W	905	PYG	O1-C1	2.81	1.42	1.36
6	K	905	PYG	O1-C1	2.81	1.42	1.36
4	A	903	MGD	C16-C21	2.80	1.43	1.38
6	O	905	PYG	O2-C2	2.79	1.43	1.36
6	M	905	PYG	C5-C4	2.79	1.43	1.38
4	K	903	MGD	C17-N18	2.78	1.44	1.38
4	S	902	MGD	C23-N22	2.77	1.49	1.45
4	E	902	MGD	C23-N22	2.77	1.49	1.45
6	W	905	PYG	O2-C2	2.76	1.43	1.36
6	I	905	PYG	O2-C2	2.74	1.43	1.36
4	M	902	MGD	C6-N1	2.74	1.44	1.38
4	M	902	MGD	C23-N22	2.74	1.49	1.45
4	U	902	MGD	C6-N1	2.73	1.44	1.38
6	O	905	PYG	O1-C1	2.73	1.41	1.36
4	M	903	MGD	C16-C21	2.72	1.43	1.38
4	K	903	MGD	C16-C21	2.72	1.43	1.38
4	U	903	MGD	C16-C21	2.71	1.43	1.38
4	K	903	MGD	O6-C6	2.71	1.28	1.23
4	O	902	MGD	C6-N1	2.71	1.43	1.38
6	E	905	PYG	C5-C4	2.71	1.43	1.38
4	M	902	MGD	C17-N18	2.70	1.43	1.38
4	G	902	MGD	C6-N1	2.70	1.43	1.38
4	C	903	MGD	C16-C21	2.69	1.43	1.38
6	E	905	PYG	O2-C2	2.69	1.43	1.36
4	E	903	MGD	C3'-C4'	2.68	1.59	1.53
4	I	903	MGD	C16-C21	2.67	1.43	1.38
4	E	903	MGD	C16-C21	2.66	1.43	1.38
4	G	903	MGD	C16-C21	2.66	1.43	1.38
6	C	905	PYG	O2-C2	2.65	1.42	1.36
6	G	905	PYG	C5-C4	2.65	1.43	1.38
6	M	905	PYG	O2-C2	2.64	1.42	1.36
6	C	905	PYG	O1-C1	2.61	1.41	1.36
4	I	902	MGD	C23-N22	2.61	1.49	1.45
4	A	903	MGD	C2'-C3'	2.61	1.60	1.53
4	A	902	MGD	C16-C21	2.60	1.43	1.38
4	Q	902	MGD	C23-N22	2.59	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	903	MGD	C16-C21	2.59	1.43	1.38
4	W	903	MGD	C16-C21	2.58	1.43	1.38
4	W	902	MGD	C6-N1	2.58	1.43	1.38
6	E	905	PYG	C4-C3	2.58	1.44	1.39
4	I	903	MGD	O11-C23	2.56	1.47	1.43
4	A	903	MGD	O6-C6	2.56	1.28	1.23
6	U	905	PYG	O1-C1	2.55	1.41	1.36
6	A	905	PYG	C4-C3	2.54	1.43	1.39
6	S	905	PYG	C4-C3	2.54	1.43	1.39
4	C	902	MGD	C23-N22	2.54	1.49	1.45
4	O	903	MGD	C3'-C4'	2.53	1.59	1.53
4	U	903	MGD	C23-N22	2.52	1.49	1.45
4	A	903	MGD	O11-C11	2.52	1.48	1.43
4	O	903	MGD	O6-C6	2.51	1.28	1.23
4	E	903	MGD	C23-N22	2.51	1.49	1.45
4	I	903	MGD	C23-N22	2.49	1.49	1.45
6	W	905	PYG	C4-C3	2.49	1.43	1.39
6	U	905	PYG	C4-C3	2.48	1.43	1.39
6	O	905	PYG	C4-C3	2.48	1.43	1.39
4	O	902	MGD	C23-N22	2.48	1.49	1.45
4	G	902	MGD	C16-C21	2.48	1.42	1.38
4	C	902	MGD	C16-C21	2.47	1.42	1.38
4	C	903	MGD	O17-C17	2.47	1.28	1.23
4	K	903	MGD	C2'-C3'	2.47	1.60	1.53
4	Q	903	MGD	PA-O3B	2.47	1.62	1.59
4	Q	903	MGD	O17-C17	2.46	1.28	1.23
6	Q	905	PYG	C4-C3	2.46	1.43	1.39
4	E	902	MGD	C16-C21	2.46	1.42	1.38
4	W	903	MGD	O17-C17	2.45	1.28	1.23
4	G	903	MGD	C4-N3	2.44	1.39	1.34
6	C	905	PYG	C4-C3	2.43	1.43	1.39
4	G	903	MGD	C23-N22	2.43	1.49	1.45
4	K	903	MGD	O11-C11	2.41	1.48	1.43
4	S	903	MGD	C23-N22	2.39	1.49	1.45
6	I	905	PYG	C4-C3	2.39	1.43	1.39
4	I	903	MGD	O17-C17	2.38	1.28	1.23
4	K	902	MGD	C6-N1	2.38	1.43	1.38
6	K	905	PYG	C4-C3	2.38	1.43	1.39
6	G	905	PYG	C4-C3	2.37	1.43	1.39
4	E	903	MGD	O6-C6	2.35	1.28	1.23
4	U	902	MGD	O17-C17	2.34	1.28	1.23
4	Q	902	MGD	O17-C17	2.34	1.28	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	903	MGD	O6-C6	2.33	1.28	1.23
4	E	902	MGD	C4-N3	2.33	1.39	1.34
4	I	903	MGD	C2-N1	2.33	1.43	1.37
6	M	905	PYG	C4-C3	2.33	1.43	1.39
4	K	902	MGD	O4'-C1'	2.32	1.47	1.42
4	A	902	MGD	O11-C23	2.32	1.47	1.43
4	G	903	MGD	O6-C6	2.31	1.27	1.23
4	M	903	MGD	C2-N1	2.31	1.43	1.37
4	U	902	MGD	C10-C11	2.31	1.55	1.51
4	Q	902	MGD	C16-C21	2.31	1.42	1.38
4	O	902	MGD	C4-N3	2.30	1.39	1.34
4	S	902	MGD	PA-O3B	2.30	1.62	1.59
4	S	902	MGD	O17-C17	2.30	1.27	1.23
4	U	902	MGD	O3'-C3'	2.28	1.48	1.43
4	M	903	MGD	C4-N3	2.28	1.39	1.34
4	I	902	MGD	C4-N3	2.27	1.39	1.34
4	S	902	MGD	C4-N3	2.27	1.39	1.34
4	S	902	MGD	C16-C21	2.26	1.42	1.38
4	S	902	MGD	C6-N1	2.26	1.43	1.38
4	C	902	MGD	O4'-C1'	2.26	1.47	1.42
4	I	903	MGD	O6-C6	2.26	1.27	1.23
4	K	903	MGD	C2-N1	2.25	1.43	1.37
4	M	903	MGD	O6-C6	2.25	1.27	1.23
4	O	903	MGD	O17-C17	2.25	1.27	1.23
4	W	902	MGD	C16-C21	2.23	1.42	1.38
4	A	903	MGD	O17-C17	2.23	1.27	1.23
4	G	903	MGD	O17-C17	2.23	1.27	1.23
4	C	903	MGD	PB-O3B	2.22	1.61	1.59
4	K	903	MGD	C23-N22	2.21	1.48	1.45
4	C	903	MGD	O6-C6	2.21	1.27	1.23
4	A	902	MGD	C4-N3	2.21	1.39	1.34
4	M	902	MGD	C16-C21	2.21	1.42	1.38
4	M	903	MGD	C3'-C4'	2.21	1.58	1.53
4	Q	903	MGD	C23-N22	2.21	1.48	1.45
4	S	902	MGD	O3'-C3'	2.20	1.48	1.43
4	O	902	MGD	O4'-C1'	2.20	1.47	1.42
4	U	902	MGD	C16-C21	2.20	1.42	1.38
4	M	903	MGD	C6-N1	2.19	1.43	1.38
4	O	903	MGD	PB-O3B	2.19	1.61	1.59
4	M	902	MGD	O17-C17	2.19	1.27	1.23
4	G	903	MGD	C6-N1	2.18	1.42	1.38
4	K	903	MGD	C6-N1	2.18	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	902	MGD	O17-C17	2.18	1.27	1.23
4	U	903	MGD	O17-C17	2.17	1.27	1.23
4	C	902	MGD	O17-C17	2.16	1.27	1.23
4	K	902	MGD	C23-N22	2.16	1.48	1.45
4	E	903	MGD	C2-N1	2.15	1.42	1.37
4	A	903	MGD	C2-N1	2.15	1.42	1.37
4	E	903	MGD	O17-C17	2.15	1.27	1.23
4	O	903	MGD	C2-N1	2.15	1.42	1.37
4	K	903	MGD	O17-C17	2.14	1.27	1.23
4	M	902	MGD	C4-N3	2.12	1.39	1.34
4	S	903	MGD	C2-N1	2.11	1.42	1.37
4	E	902	MGD	O4'-C1'	2.11	1.46	1.42
4	C	903	MGD	C4-N3	2.11	1.39	1.34
4	C	903	MGD	C2-N1	2.10	1.42	1.37
4	C	903	MGD	C6-N1	2.10	1.42	1.38
4	G	903	MGD	C2-N2	2.09	1.39	1.34
4	W	902	MGD	O17-C17	2.09	1.27	1.23
4	I	902	MGD	O4'-C1'	2.09	1.46	1.42
4	S	903	MGD	O17-C17	2.07	1.27	1.23
4	M	903	MGD	PB-O3B	2.07	1.61	1.59
4	W	902	MGD	O4'-C1'	2.06	1.46	1.42
4	G	903	MGD	C2-N1	2.05	1.42	1.37
4	K	902	MGD	C16-C21	2.04	1.42	1.38
4	C	903	MGD	C8-N9	2.04	1.42	1.37
4	A	903	MGD	C6-N1	2.03	1.42	1.38
4	Q	902	MGD	C4-N3	2.03	1.38	1.34
4	W	903	MGD	C4-N3	2.02	1.38	1.34
4	U	902	MGD	C4-N3	2.02	1.38	1.34
4	U	902	MGD	O4'-C1'	2.02	1.46	1.42
4	M	902	MGD	O4'-C1'	2.01	1.46	1.42

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	902	MGD	O2A-PA-O3B	-11.71	75.62	107.27
4	G	902	MGD	O2A-PA-O3B	-11.59	75.95	107.27
4	S	902	MGD	O2A-PA-O3B	-11.18	77.06	107.27
4	Q	902	MGD	O2A-PA-O3B	-10.63	78.54	107.27
4	W	902	MGD	O2A-PA-O3B	-10.63	78.55	107.27
4	E	902	MGD	O2A-PA-O3B	-10.61	78.61	107.27
4	O	902	MGD	O2A-PA-O3B	-10.51	78.88	107.27
4	A	903	MGD	O11-C23-C14	-10.46	101.98	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	902	MGD	O2A-PA-O3B	-10.27	79.51	107.27
4	U	902	MGD	O2A-PA-O3B	-10.23	79.63	107.27
4	M	902	MGD	O2A-PA-O3B	-10.17	79.78	107.27
4	K	902	MGD	O2A-PA-O3B	-10.16	79.82	107.27
4	I	902	MGD	O2A-PA-O3B	-10.01	80.23	107.27
4	K	903	MGD	O11-C23-C14	-9.78	102.44	108.96
6	W	905	PYG	O1-C1-C2	-7.69	98.12	117.90
4	I	903	MGD	O11-C23-C14	-7.56	103.92	108.96
6	K	905	PYG	O1-C1-C2	-7.55	98.48	117.90
6	C	905	PYG	O1-C1-C2	-7.53	98.54	117.90
6	O	905	PYG	O1-C1-C2	-7.51	98.60	117.90
6	U	905	PYG	O1-C1-C2	-7.45	98.75	117.90
6	A	905	PYG	O1-C1-C2	-7.40	98.87	117.90
6	S	905	PYG	O1-C1-C2	-7.33	99.05	117.90
6	I	905	PYG	O1-C1-C2	-7.29	99.16	117.90
6	G	905	PYG	O1-C1-C2	-7.27	99.22	117.90
6	E	905	PYG	O1-C1-C2	-7.26	99.23	117.90
4	A	903	MGD	O4'-C4'-C5'	-7.25	86.10	109.33
6	Q	905	PYG	O1-C1-C2	-7.23	99.30	117.90
6	M	905	PYG	O1-C1-C2	-7.17	99.47	117.90
4	G	903	MGD	O11-C23-C14	-7.12	104.21	108.96
4	K	903	MGD	O4'-C4'-C5'	-6.95	87.06	109.33
4	Q	903	MGD	O11-C23-C14	-6.21	104.82	108.96
4	M	903	MGD	O11-C23-C14	-5.89	105.03	108.96
4	C	902	MGD	O2A-PA-O3A	-5.60	82.20	107.57
4	Q	903	MGD	O4'-C4'-C5'	-5.57	91.50	109.33
4	M	902	MGD	O2A-PA-O3A	-5.55	82.40	107.57
4	A	902	MGD	O2A-PA-O3A	-5.51	82.57	107.57
4	G	903	MGD	O4'-C4'-C5'	-5.46	91.84	109.33
4	I	902	MGD	O2A-PA-O3A	-5.43	82.96	107.57
4	E	903	MGD	O4'-C4'-C5'	-5.39	92.08	109.33
4	U	902	MGD	O2A-PA-O3A	-5.35	83.30	107.57
4	S	903	MGD	O11-C23-C14	-5.29	105.44	108.96
4	W	902	MGD	O2A-PA-O3A	-5.26	83.75	107.57
4	Q	902	MGD	O2A-PA-O3A	-5.24	83.82	107.57
4	S	903	MGD	O4'-C4'-C5'	-5.20	92.69	109.33
4	E	902	MGD	O2A-PA-O3A	-5.18	84.08	107.57
4	K	902	MGD	O2A-PA-O3A	-5.16	84.18	107.57
4	I	903	MGD	O4'-C4'-C5'	-5.15	92.84	109.33
4	U	902	MGD	C23-C14-N15	5.15	112.92	107.87
4	S	902	MGD	O2A-PA-O1A	-5.14	88.52	112.44
4	G	902	MGD	O2A-PA-O3A	-5.12	84.36	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	U	903	MGD	O11-C23-C14	-5.12	105.55	108.96
4	A	902	MGD	C23-C14-N15	5.07	112.85	107.87
4	O	902	MGD	O2A-PA-O3A	-5.05	84.69	107.57
4	U	902	MGD	O2A-PA-O1A	-5.05	88.97	112.44
4	E	903	MGD	O11-C23-C14	-5.04	105.60	108.96
4	C	902	MGD	C23-C14-N15	4.98	112.76	107.87
4	S	902	MGD	O2A-PA-O3A	-4.92	85.24	107.57
4	E	902	MGD	O2A-PA-O1A	-4.92	89.55	112.44
4	K	903	MGD	O11-C23-N22	-4.92	104.14	108.61
4	S	902	MGD	C23-C14-N15	4.86	112.65	107.87
4	A	903	MGD	O11-C23-N22	-4.84	104.21	108.61
6	O	905	PYG	O3-C3-C2	4.82	130.29	117.90
6	W	905	PYG	O3-C3-C2	4.82	130.29	117.90
4	M	902	MGD	O2A-PA-O1A	-4.81	90.06	112.44
4	W	902	MGD	C23-C14-N15	4.79	112.57	107.87
6	I	905	PYG	O3-C3-C2	4.79	130.22	117.90
4	K	902	MGD	C23-C14-N15	4.78	112.57	107.87
4	G	902	MGD	C23-C14-N15	4.78	112.56	107.87
4	E	902	MGD	C23-C14-N15	4.78	112.56	107.87
4	O	903	MGD	O4'-C4'-C5'	-4.77	94.06	109.33
6	M	905	PYG	O3-C3-C2	4.76	130.15	117.90
6	U	905	PYG	O3-C3-C2	4.76	130.15	117.90
6	C	905	PYG	O3-C3-C2	4.76	130.13	117.90
6	E	905	PYG	O3-C3-C2	4.75	130.12	117.90
6	K	905	PYG	O3-C3-C2	4.75	130.11	117.90
6	S	905	PYG	O3-C3-C2	4.74	130.10	117.90
6	G	905	PYG	O3-C3-C2	4.74	130.08	117.90
6	Q	905	PYG	O3-C3-C2	4.73	130.07	117.90
4	G	902	MGD	O2A-PA-O1A	-4.73	90.43	112.44
6	A	905	PYG	O3-C3-C2	4.73	130.05	117.90
4	O	902	MGD	C23-C14-N15	4.72	112.51	107.87
4	A	902	MGD	O2A-PA-O1A	-4.71	90.53	112.44
4	M	903	MGD	O4'-C4'-C5'	-4.66	94.40	109.33
4	O	903	MGD	O11-C23-C14	-4.60	105.89	108.96
4	Q	902	MGD	C23-C14-N15	4.59	112.38	107.87
4	I	902	MGD	C23-C14-N15	4.56	112.34	107.87
4	U	903	MGD	O4'-C4'-C5'	-4.55	94.75	109.33
4	C	902	MGD	O2A-PA-O1A	-4.55	91.28	112.44
4	C	903	MGD	O4'-C4'-C5'	-4.54	94.81	109.33
4	C	903	MGD	O11-C23-C14	-4.40	106.03	108.96
4	I	902	MGD	O2A-PA-O1A	-4.39	92.02	112.44
4	M	902	MGD	C23-C14-N15	4.38	112.17	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	902	MGD	O2A-PA-O1A	-4.34	92.24	112.44
4	W	903	MGD	O4'-C4'-C5'	-4.31	95.54	109.33
4	K	902	MGD	O2A-PA-O1A	-4.19	92.97	112.44
6	M	905	PYG	C6-C1-C2	-4.14	115.80	120.09
4	Q	902	MGD	O2A-PA-O1A	-4.08	93.48	112.44
6	E	905	PYG	C6-C1-C2	-4.07	115.87	120.09
4	W	902	MGD	O2A-PA-O1A	-4.05	93.59	112.44
6	G	905	PYG	C6-C1-C2	-4.05	115.89	120.09
4	K	903	MGD	O2B-PB-O3B	-4.03	96.38	107.27
6	I	905	PYG	C6-C1-C2	-4.03	115.91	120.09
6	Q	905	PYG	C6-C1-C2	-4.00	115.94	120.09
6	W	905	PYG	C6-C1-C2	-3.99	115.95	120.09
6	K	905	PYG	C6-C1-C2	-3.99	115.95	120.09
6	M	905	PYG	O3-C3-C4	-3.98	108.69	119.36
4	G	902	MGD	O3B-PA-O1A	3.98	122.67	110.70
4	A	903	MGD	O2B-PB-O3B	-3.98	96.52	107.27
6	O	905	PYG	C6-C1-C2	-3.97	115.97	120.09
6	E	905	PYG	O3-C3-C4	-3.97	108.71	119.36
6	I	905	PYG	O3-C3-C4	-3.97	108.72	119.36
6	G	905	PYG	O3-C3-C4	-3.97	108.73	119.36
4	S	902	MGD	O3B-PA-O1A	3.96	122.62	110.70
6	O	905	PYG	O3-C3-C4	-3.94	108.79	119.36
6	W	905	PYG	O3-C3-C4	-3.94	108.80	119.36
6	Q	905	PYG	O3-C3-C4	-3.94	108.80	119.36
6	S	905	PYG	O3-C3-C4	-3.92	108.84	119.36
6	K	905	PYG	O3-C3-C4	-3.92	108.86	119.36
6	U	905	PYG	C6-C1-C2	-3.91	116.03	120.09
6	C	905	PYG	C6-C1-C2	-3.90	116.04	120.09
6	U	905	PYG	O3-C3-C4	-3.90	108.92	119.36
6	S	905	PYG	C6-C1-C2	-3.89	116.05	120.09
6	C	905	PYG	O3-C3-C4	-3.89	108.94	119.36
6	A	905	PYG	O3-C3-C4	-3.88	108.95	119.36
6	A	905	PYG	C6-C1-C2	-3.77	116.17	120.09
4	A	902	MGD	O11-C23-C14	3.76	111.47	108.96
4	A	903	MGD	O5'-C5'-C4'	3.70	121.59	108.99
4	K	903	MGD	O5'-C5'-C4'	3.54	121.04	108.99
4	W	903	MGD	O11-C23-C14	-3.51	106.63	108.96
4	A	902	MGD	O3B-PA-O1A	3.38	120.88	110.70
4	G	902	MGD	O11-C23-C14	3.31	111.17	108.96
4	K	903	MGD	PB-O5'-C5'	-3.18	103.14	121.35
4	U	902	MGD	O11-C23-C14	3.11	111.04	108.96
4	O	902	MGD	O11-C23-C14	3.07	111.01	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	902	MGD	O4'-C4'-C5'	-3.03	99.62	109.33
4	O	902	MGD	O3B-PA-O1A	2.99	119.71	110.70
4	G	902	MGD	O4'-C4'-C5'	-2.98	99.80	109.33
4	E	902	MGD	O3B-PA-O1A	2.94	119.56	110.70
4	U	902	MGD	O4'-C4'-C5'	-2.92	99.97	109.33
4	A	903	MGD	PB-O5'-C5'	-2.86	104.96	121.35
4	Q	902	MGD	O3A-C10-C11	-2.82	101.61	108.58
4	I	902	MGD	O11-C23-C14	2.80	110.83	108.96
4	S	902	MGD	O11-C23-C14	2.80	110.83	108.96
4	E	902	MGD	O11-C23-C14	2.76	110.81	108.96
4	C	902	MGD	O11-C23-C14	2.74	110.79	108.96
4	U	902	MGD	O3B-PA-O1A	2.73	118.91	110.70
4	I	902	MGD	O4'-C4'-C5'	-2.70	100.69	109.33
4	M	902	MGD	O11-C23-C14	2.69	110.76	108.96
4	I	903	MGD	O11-C23-N22	-2.68	106.17	108.61
4	K	902	MGD	O3B-PA-O1A	2.67	118.73	110.70
4	C	902	MGD	O3B-PA-O1A	2.65	118.66	110.70
4	A	902	MGD	O3A-C10-C11	-2.63	102.10	108.58
4	A	903	MGD	O4'-C1'-N9	-2.62	102.43	108.36
4	E	902	MGD	O4'-C4'-C5'	-2.57	101.11	109.33
4	C	903	MGD	O3A-C10-C11	2.50	114.76	108.58
4	U	903	MGD	O3A-C10-C11	2.48	114.71	108.58
4	M	902	MGD	O3B-PA-O1A	2.48	118.16	110.70
4	K	902	MGD	O11-C23-C14	2.47	110.61	108.96
4	A	903	MGD	C4'-O4'-C1'	2.46	114.89	109.47
4	A	902	MGD	O4'-C4'-C5'	-2.46	101.47	109.33
4	Q	902	MGD	O3B-PA-O1A	2.45	118.08	110.70
4	M	902	MGD	O3A-C10-C11	-2.45	102.54	108.58
4	Q	902	MGD	O4'-C4'-C5'	-2.44	101.52	109.33
4	M	903	MGD	O3A-C10-C11	2.43	114.59	108.58
4	W	902	MGD	O3B-PA-O1A	2.43	118.00	110.70
4	O	903	MGD	O3A-C10-C11	2.42	114.56	108.58
4	S	902	MGD	O3A-C10-C11	-2.40	102.64	108.58
4	W	902	MGD	O4'-C4'-C5'	-2.37	101.74	109.33
4	O	902	MGD	O4'-C4'-C5'	-2.35	101.79	109.33
4	A	903	MGD	C2'-C1'-N9	2.35	119.79	113.25
4	E	902	MGD	O3A-C10-C11	-2.33	102.83	108.58
4	S	903	MGD	O11-C23-N22	-2.29	106.53	108.61
4	I	903	MGD	O4'-C4'-C3'	2.29	109.69	105.15
4	M	902	MGD	O4'-C4'-C5'	-2.28	102.02	109.33
4	E	903	MGD	O4'-C1'-N9	-2.28	103.19	108.36
4	C	902	MGD	O3A-C10-C11	-2.27	102.98	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	902	MGD	O4'-C4'-C5'	-2.27	102.08	109.33
4	K	903	MGD	C4'-O4'-C1'	2.25	114.44	109.47
4	I	902	MGD	O3A-C10-C11	-2.22	103.09	108.58
4	E	903	MGD	O3B-PB-O1B	2.22	117.39	110.70
4	M	903	MGD	O4'-C1'-N9	-2.22	103.33	108.36
4	O	903	MGD	O4'-C1'-N9	-2.21	103.36	108.36
4	I	902	MGD	O3B-PA-O1A	2.19	117.31	110.70
4	M	903	MGD	C23-C14-N15	2.18	110.01	107.87
4	K	903	MGD	O3B-PA-O1A	-2.18	104.15	110.70
4	W	902	MGD	O5'-C5'-C4'	-2.18	101.58	108.99
6	W	905	PYG	C3-C2-C1	2.17	120.88	119.53
4	U	902	MGD	O3A-C10-C11	-2.16	103.24	108.58
4	A	902	MGD	O2B-PB-O3B	-2.12	101.54	107.27
4	K	903	MGD	O2B-PB-O5'	-2.11	97.98	107.57
6	O	905	PYG	C3-C2-C1	2.11	120.84	119.53
4	Q	903	MGD	O4'-C1'-N9	-2.09	103.61	108.36
6	I	905	PYG	C3-C2-C1	2.09	120.83	119.53
4	K	902	MGD	O3A-C10-C11	-2.08	103.44	108.58
4	O	902	MGD	O3A-C10-C11	-2.08	103.45	108.58
4	W	903	MGD	O4'-C1'-N9	-2.07	103.66	108.36
4	C	902	MGD	C3'-C2'-C1'	2.06	105.36	101.46
6	C	905	PYG	C3-C2-C1	2.06	120.81	119.53
4	C	902	MGD	O5'-C5'-C4'	-2.05	102.00	108.99
4	W	902	MGD	O11-C23-C14	2.04	110.32	108.96
4	O	902	MGD	O5'-C5'-C4'	-2.03	102.07	108.99
4	M	902	MGD	O5'-C5'-C4'	-2.03	102.07	108.99
6	M	905	PYG	C3-C2-C1	2.02	120.79	119.53
4	A	903	MGD	O2B-PB-O5'	-2.02	98.41	107.57
4	U	903	MGD	O4'-C1'-N9	-2.01	103.80	108.36

There are no chirality outliers.

All (147) torsion outliers are listed below:

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

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

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

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Mol	Chain	Res	Type	Atoms
4	W	902	MGD	O3A-C10-C11-O11
4	W	902	MGD	O3A-C10-C11-C12
4	W	903	MGD	PA-O3B-PB-O5'
4	W	903	MGD	C5'-O5'-PB-O1B
4	W	903	MGD	C5'-O5'-PB-O3B
4	A	903	MGD	C4'-C5'-O5'-PB
4	K	903	MGD	C4'-C5'-O5'-PB
4	A	902	MGD	PA-O3B-PB-O5'
4	G	902	MGD	PA-O3B-PB-O5'
4	S	902	MGD	PA-O3B-PB-O5'
4	A	902	MGD	O3A-C10-C11-C12
4	A	902	MGD	C10-O3A-PA-O3B
4	C	902	MGD	C10-O3A-PA-O3B
4	C	903	MGD	C5'-O5'-PB-O2B
4	E	902	MGD	C10-O3A-PA-O3B
4	E	903	MGD	C5'-O5'-PB-O2B
4	G	902	MGD	C10-O3A-PA-O3B
4	G	903	MGD	C5'-O5'-PB-O2B
4	I	902	MGD	C10-O3A-PA-O3B
4	K	902	MGD	C10-O3A-PA-O3B
4	M	902	MGD	C10-O3A-PA-O3B
4	M	903	MGD	C5'-O5'-PB-O2B
4	O	902	MGD	C10-O3A-PA-O3B
4	O	903	MGD	C5'-O5'-PB-O2B
4	Q	902	MGD	C10-O3A-PA-O3B
4	Q	903	MGD	C5'-O5'-PB-O2B
4	S	902	MGD	C10-O3A-PA-O3B
4	S	903	MGD	C5'-O5'-PB-O2B
4	U	902	MGD	C10-O3A-PA-O3B
4	U	903	MGD	C5'-O5'-PB-O2B
4	W	902	MGD	C10-O3A-PA-O3B
4	W	903	MGD	C5'-O5'-PB-O2B
4	A	903	MGD	O3A-C10-C11-O11
4	G	902	MGD	O3A-C10-C11-O11
4	O	903	MGD	O4'-C4'-C5'-O5'
4	A	902	MGD	PB-O3B-PA-O2A
4	E	902	MGD	PB-O3B-PA-O2A
4	G	902	MGD	PA-O3B-PB-O1B
4	G	902	MGD	PB-O3B-PA-O1A
4	I	903	MGD	PA-O3B-PB-O1B
4	O	902	MGD	PB-O3B-PA-O2A
4	S	902	MGD	PA-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
4	E	903	MGD	O4'-C4'-C5'-O5'
4	M	903	MGD	O4'-C4'-C5'-O5'
4	U	903	MGD	O4'-C4'-C5'-O5'
4	W	903	MGD	O4'-C4'-C5'-O5'
4	C	903	MGD	O4'-C4'-C5'-O5'
4	S	903	MGD	O4'-C4'-C5'-O5'
4	G	902	MGD	O3A-C10-C11-C12
4	I	902	MGD	PB-O3B-PA-O2A
4	I	903	MGD	PA-O3B-PB-O2B
4	I	903	MGD	PB-O3B-PA-O1A
4	K	902	MGD	PB-O3B-PA-O2A
4	W	902	MGD	PB-O3B-PA-O2A
4	Q	903	MGD	O4'-C4'-C5'-O5'

There are no ring outliers.

67 monomers are involved in 206 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	905	PYG	1	0
4	Q	903	MGD	4	0
4	G	903	MGD	4	0
4	G	902	MGD	7	0
6	M	905	PYG	1	0
7	L	304	SF4	1	0
4	K	903	MGD	8	0
6	O	905	PYG	1	0
7	P	303	SF4	2	0
4	Q	902	MGD	6	0
7	P	304	SF4	1	0
7	T	304	SF4	1	0
7	V	302	SF4	1	0
7	V	303	SF4	2	0
7	X	302	SF4	1	0
7	X	303	SF4	2	0
4	M	902	MGD	8	0
4	O	903	MGD	4	0
7	H	304	SF4	1	0
4	C	902	MGD	8	0
7	D	302	SF4	1	0
6	A	905	PYG	1	0
7	J	302	SF4	2	0
7	V	304	SF4	1	0

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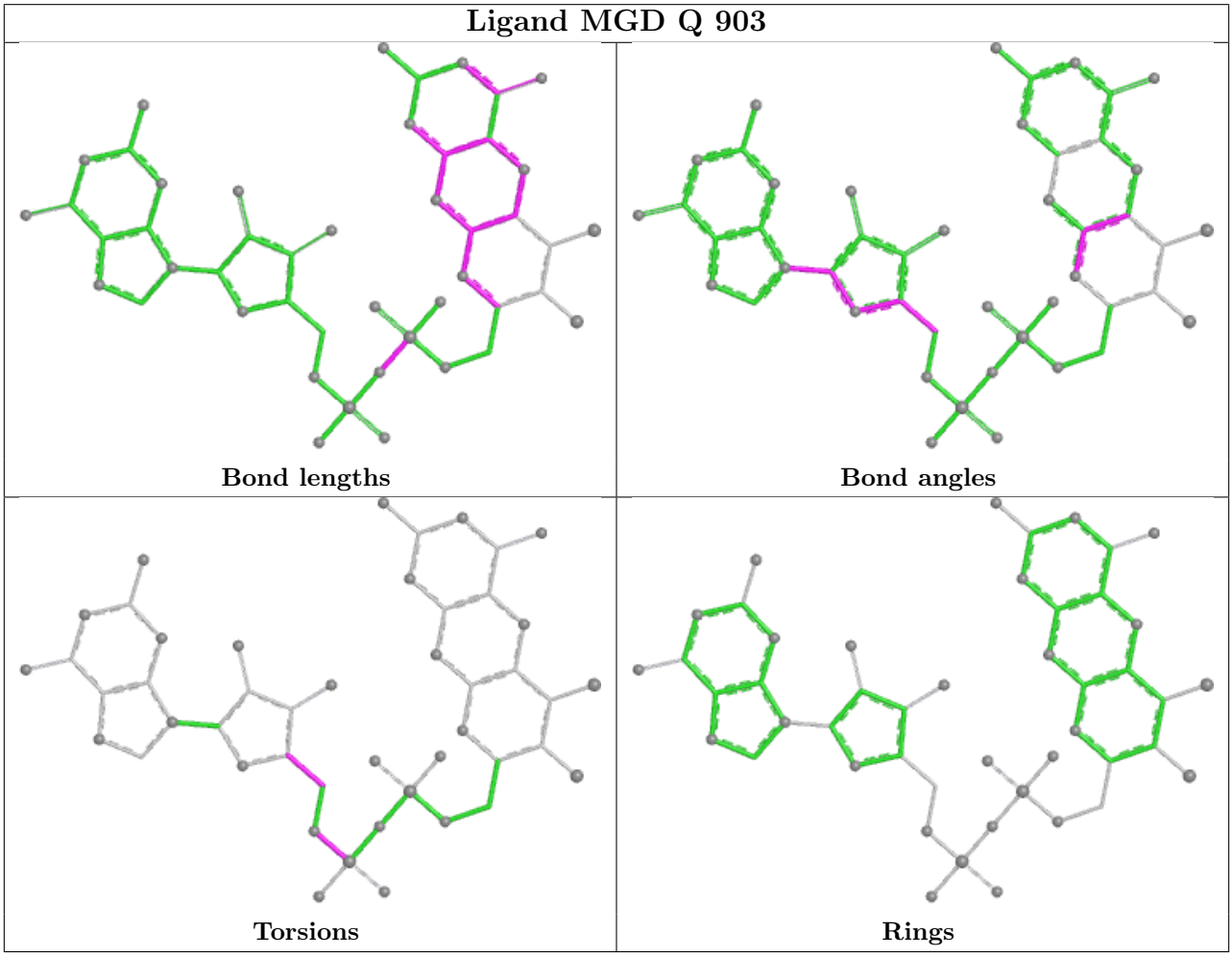
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	304	SF4	1	0
4	I	902	MGD	6	0
7	F	303	SF4	2	0
4	A	903	MGD	8	0
7	N	302	SF4	2	0
7	H	302	SF4	1	0
4	S	902	MGD	5	0
7	J	301	SF4	1	0
6	U	905	PYG	1	0
7	X	304	SF4	2	0
4	E	903	MGD	5	0
4	U	903	MGD	5	0
7	N	303	SF4	2	0
4	I	903	MGD	6	0
7	B	302	SF4	1	0
4	U	902	MGD	8	0
7	D	304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

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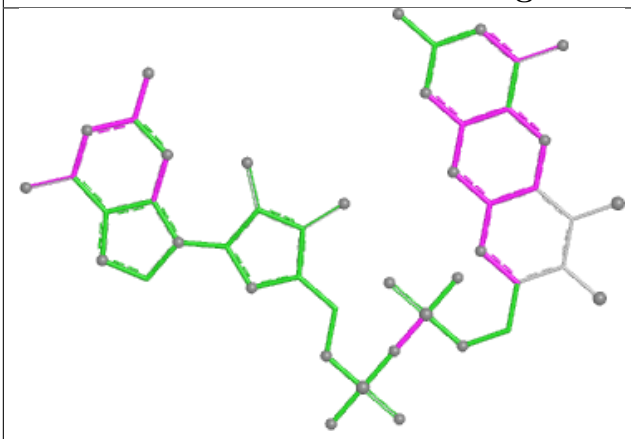
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	902	MGD	9	0

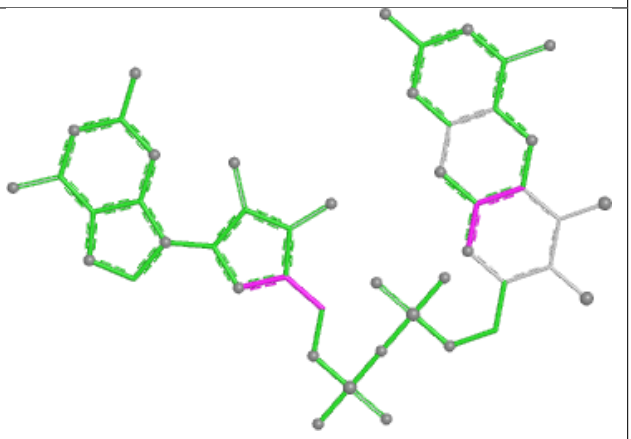
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



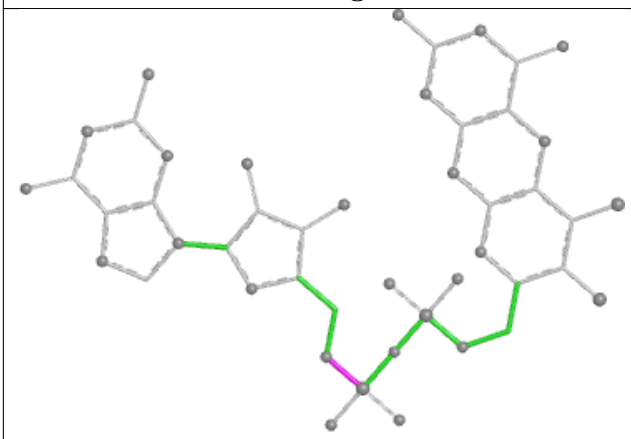
Ligand MGD G 903



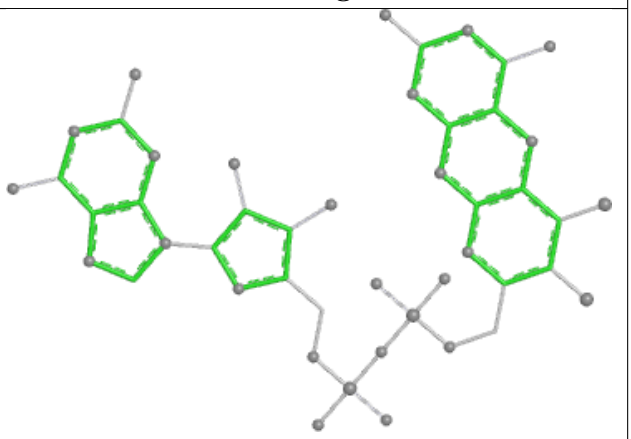
Bond lengths



Bond angles

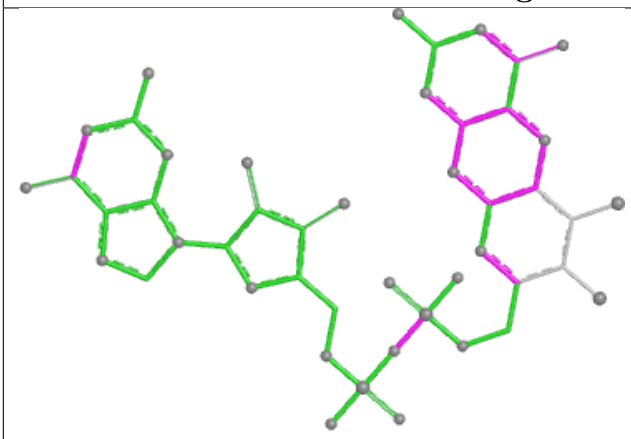


Torsions

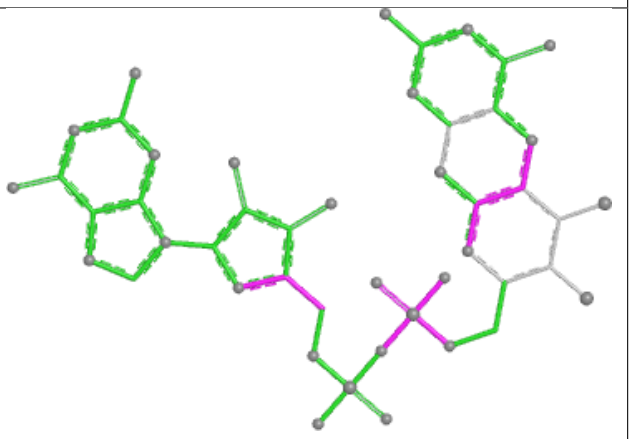


Rings

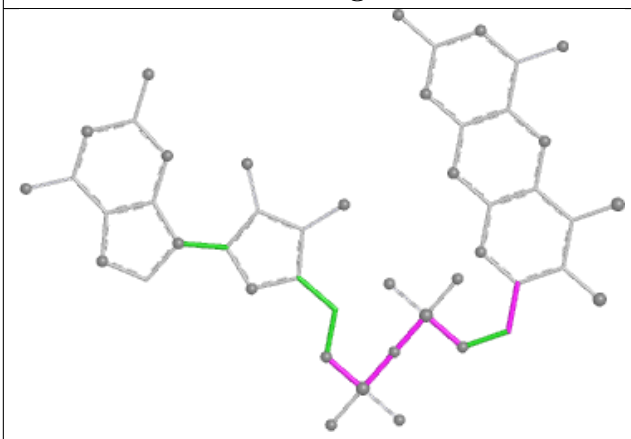
Ligand MGD G 902



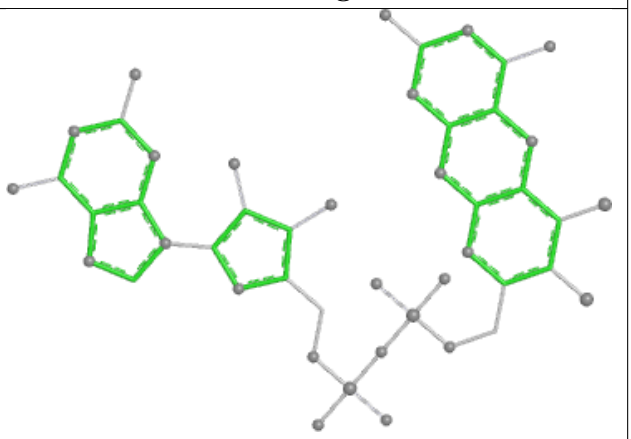
Bond lengths



Bond angles

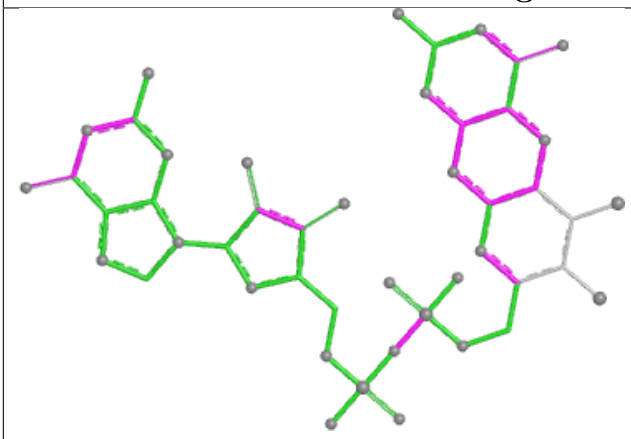


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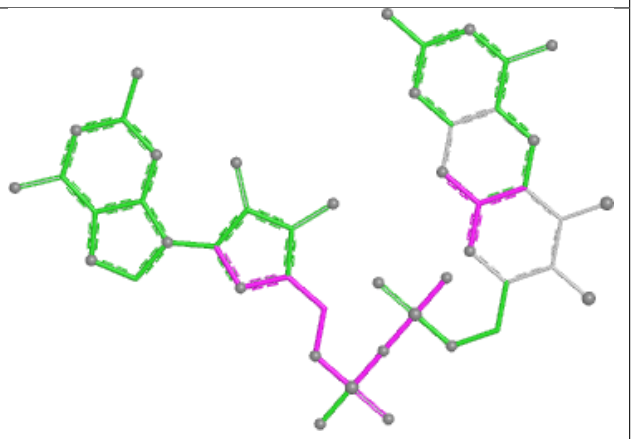


Rings

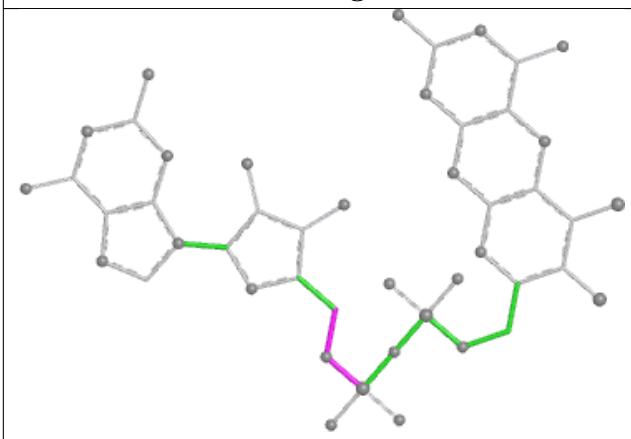
Ligand MGD K 903



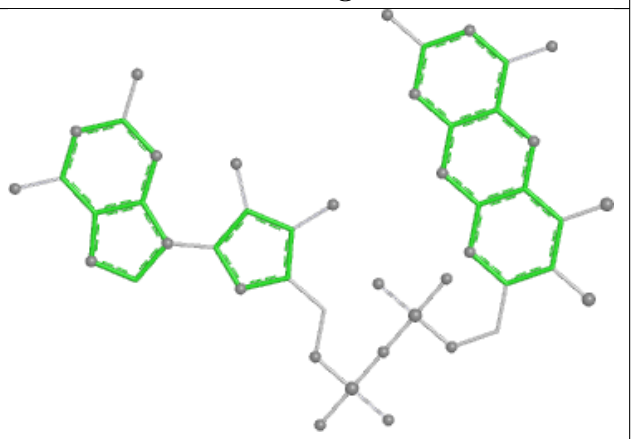
Bond lengths



Bond angles

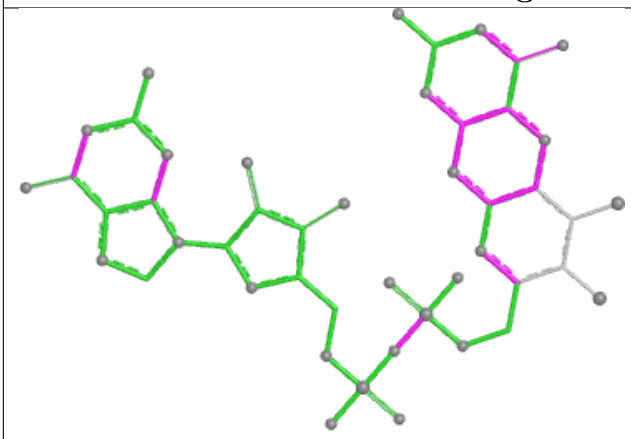


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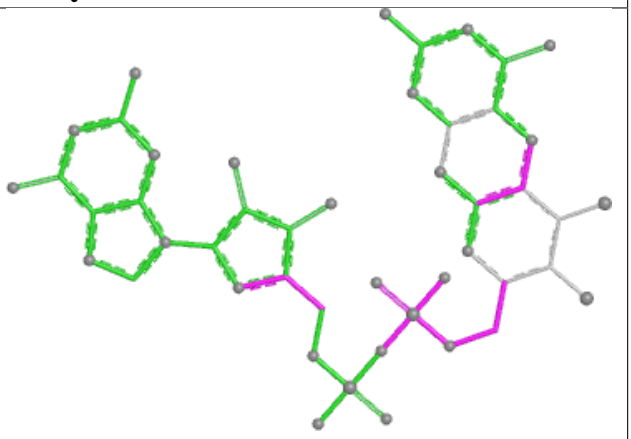


Rings

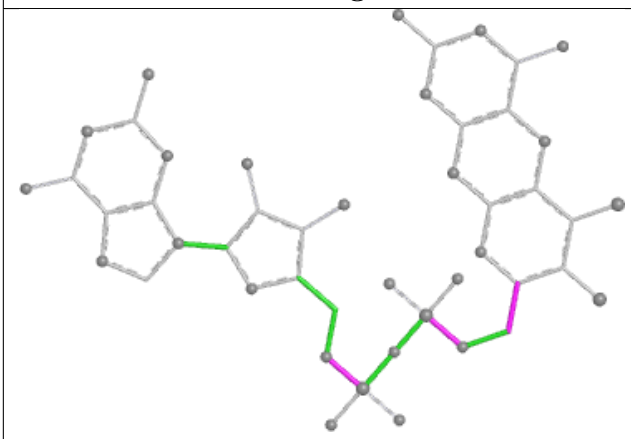
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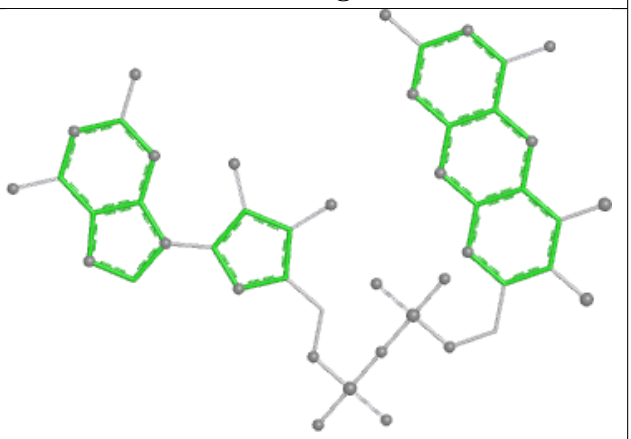
Bond lengths



Bond angles

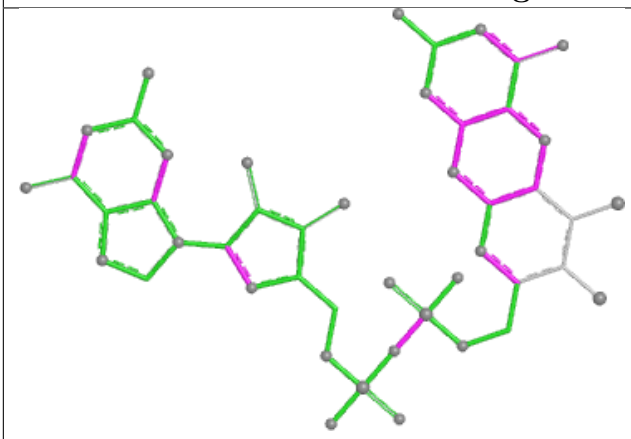


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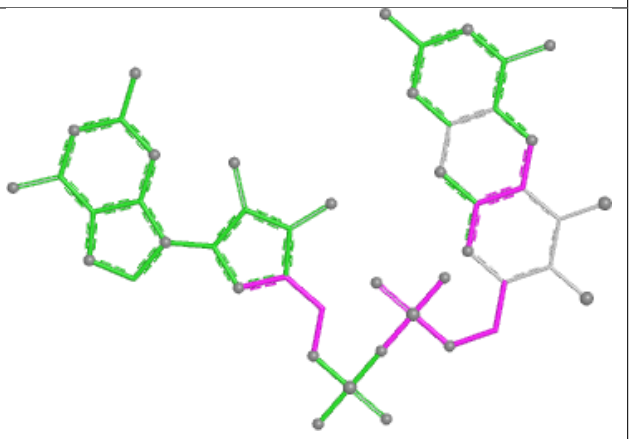


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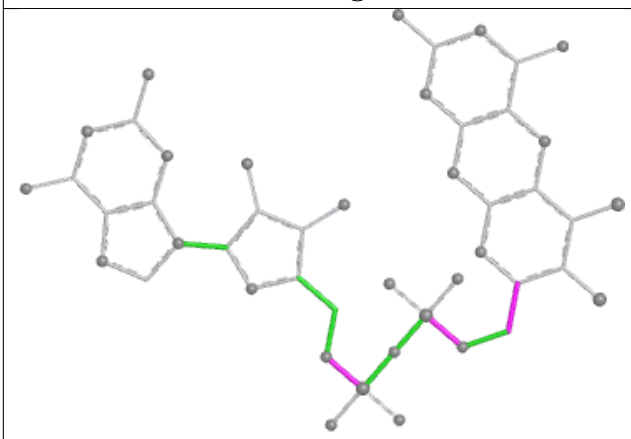
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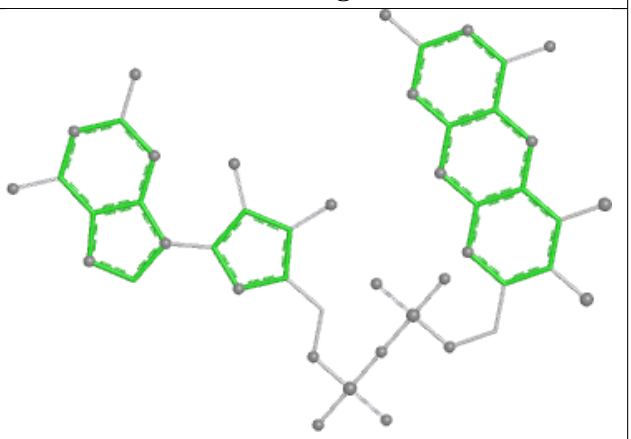
Bond lengths



Bond angles

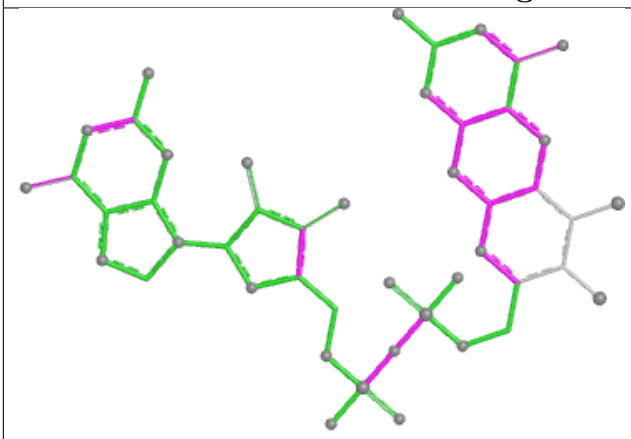


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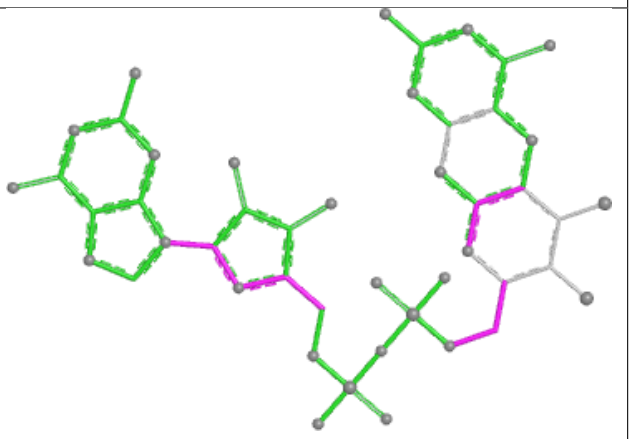


Rings

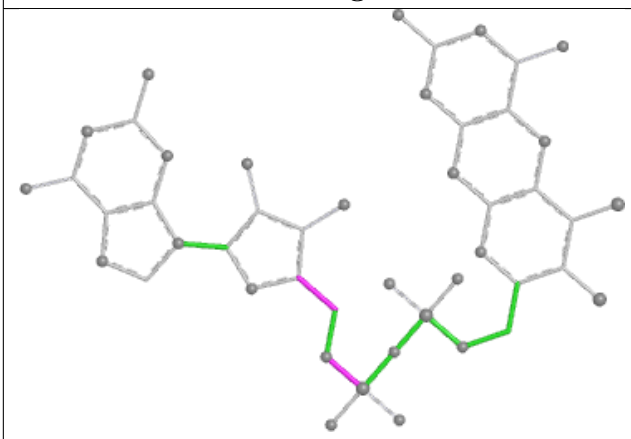
Ligand MGD O 903



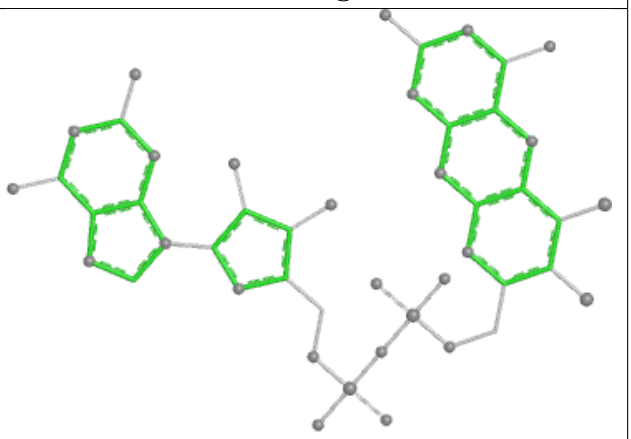
Bond lengths



Bond angles

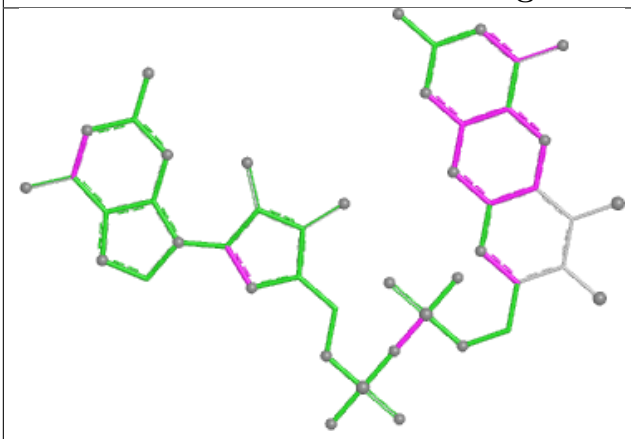


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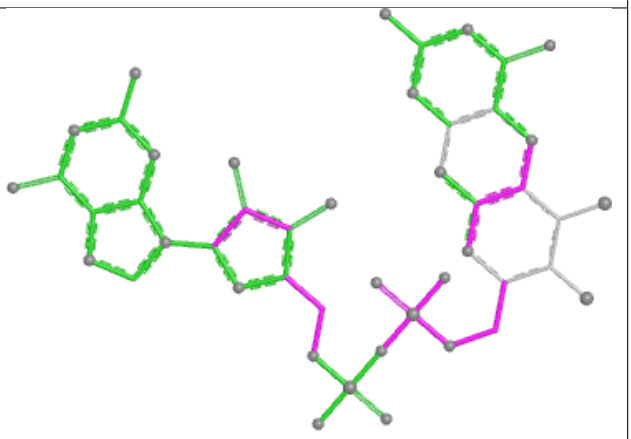


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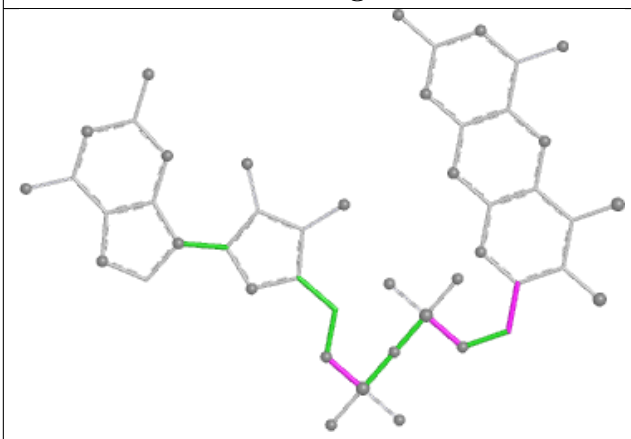
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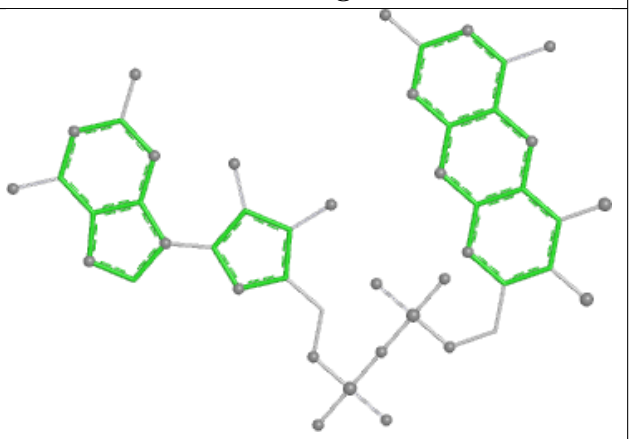
Bond lengths



Bond angles

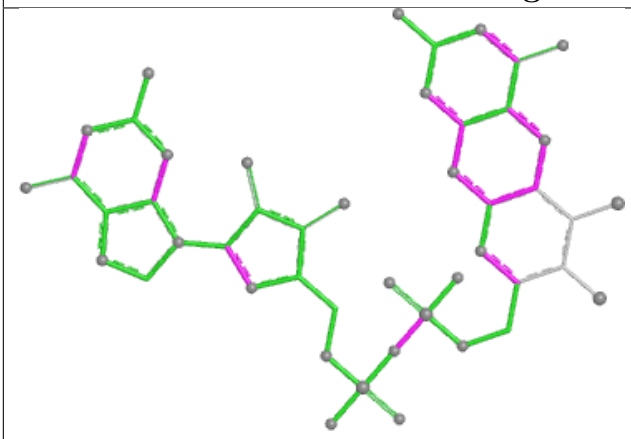


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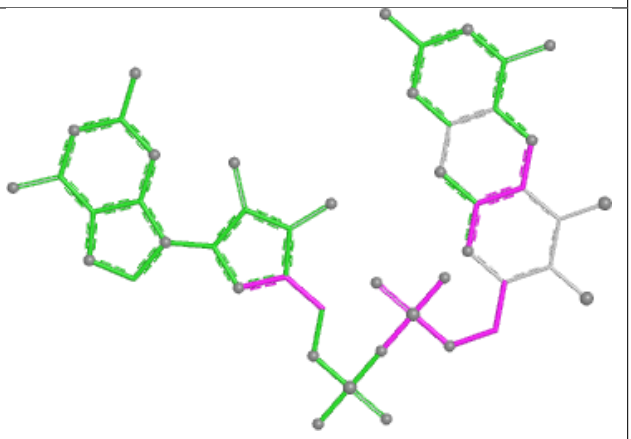


Rings

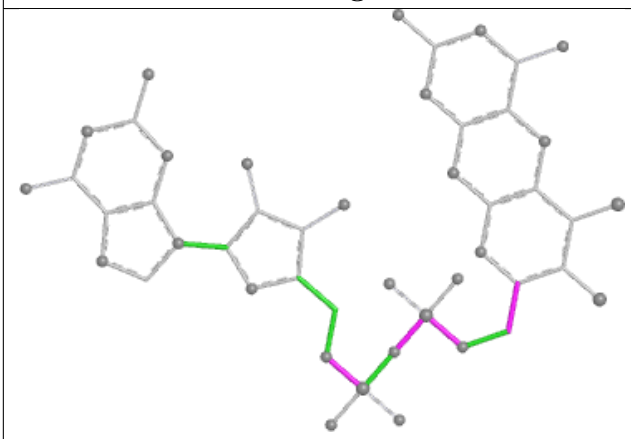
Ligand MGD I 902



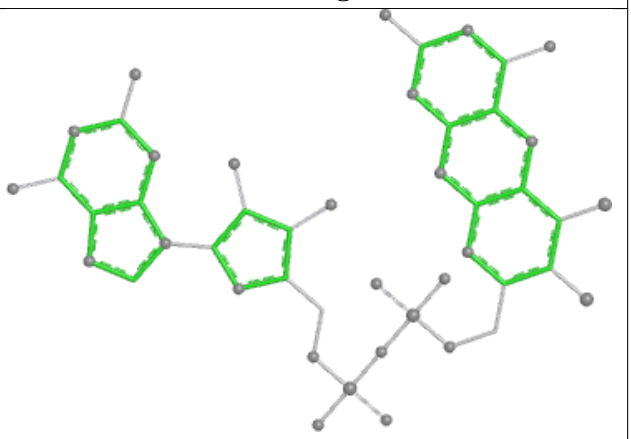
Bond lengths



Bond angles

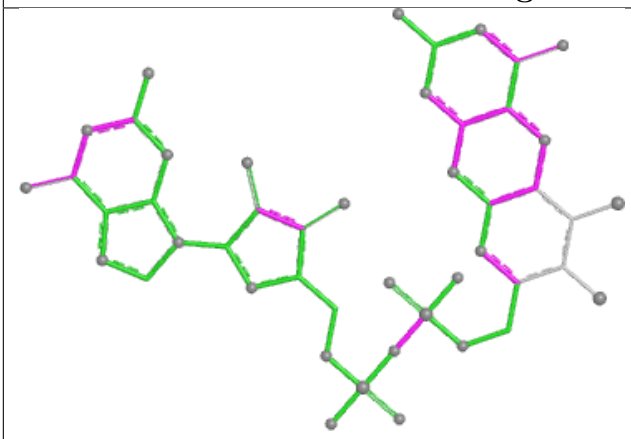


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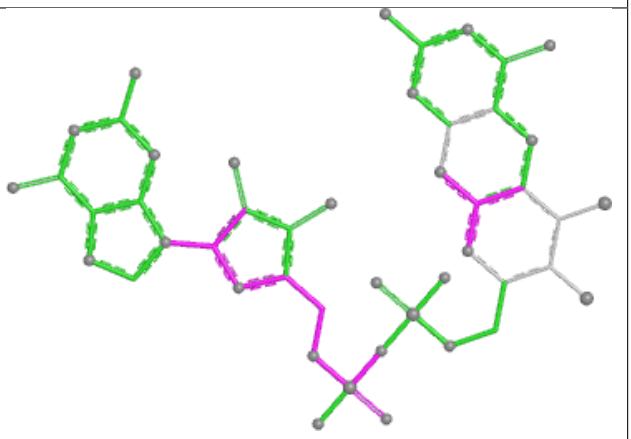


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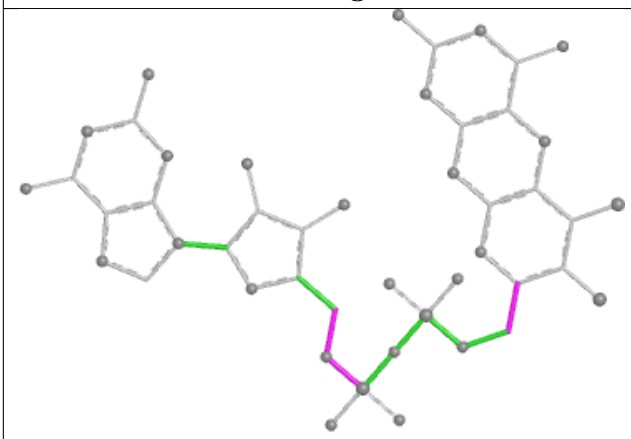
Ligand MGD A 903



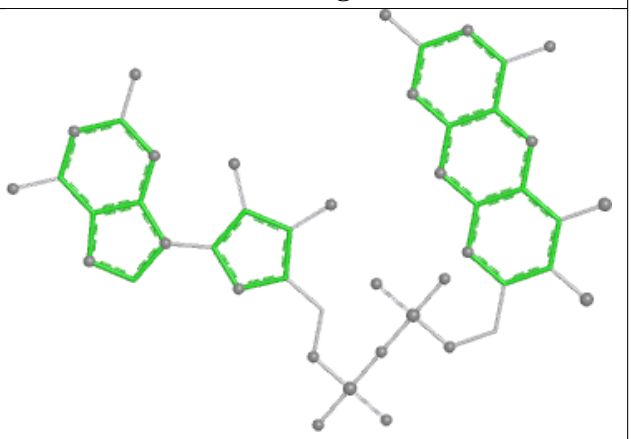
Bond lengths



Bond angles

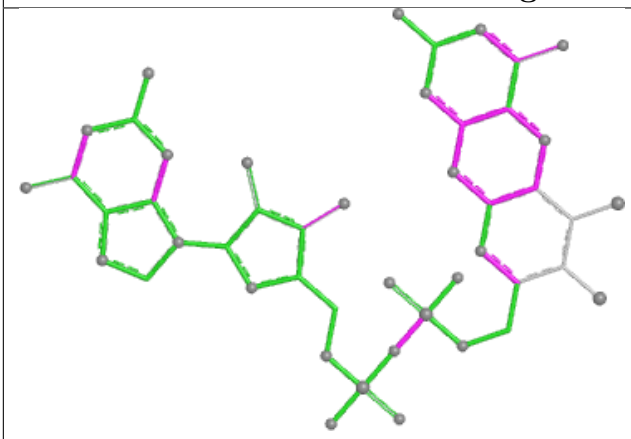


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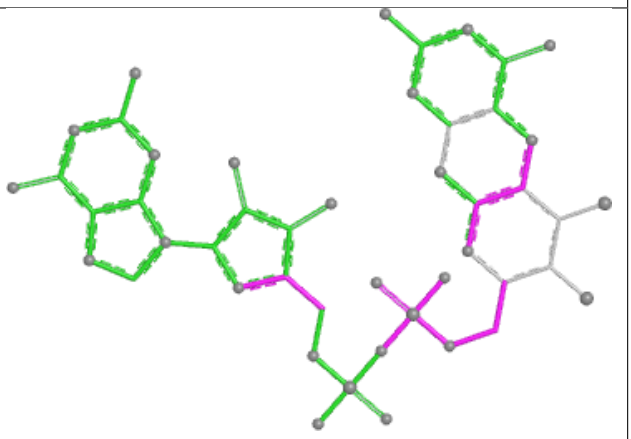


Rings

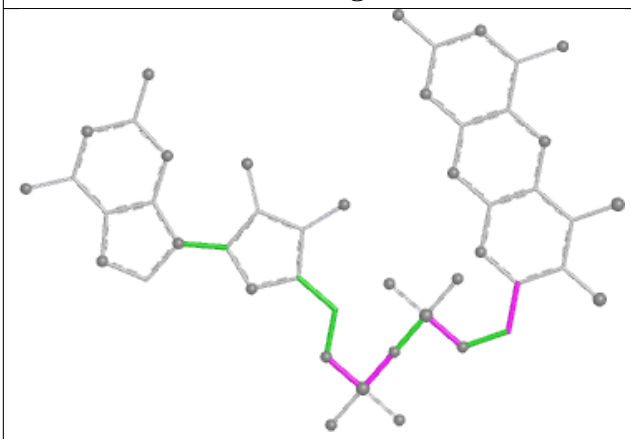
Ligand MGD S 902



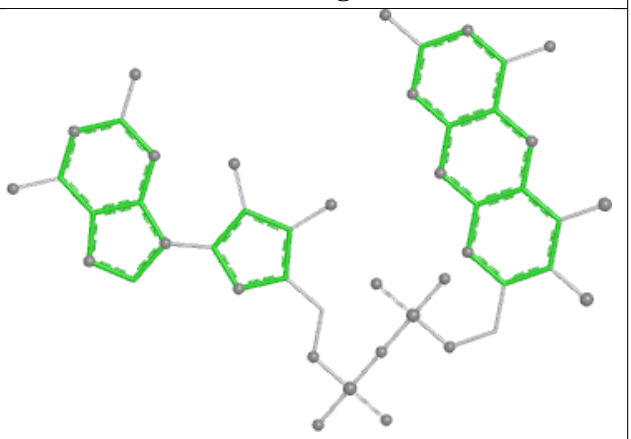
Bond lengths



Bond angles

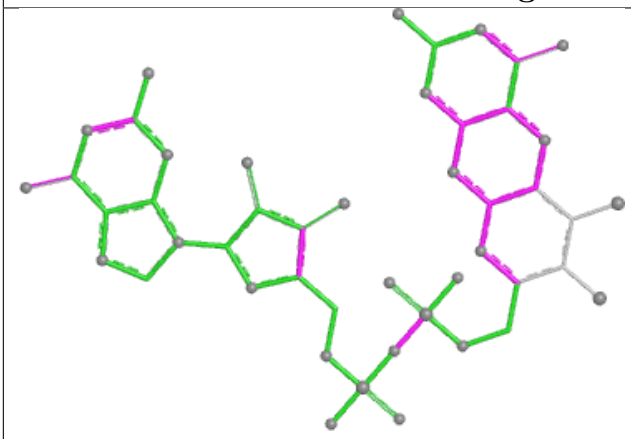


Torsions

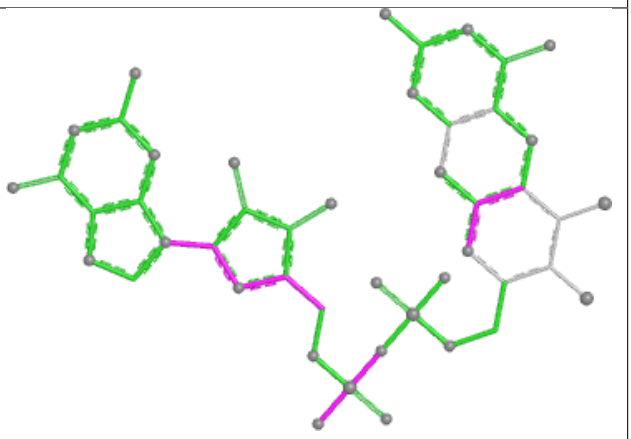


Rings

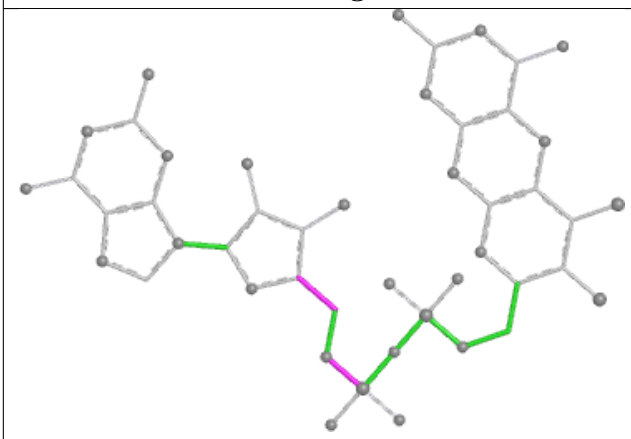
Ligand MGD E 903



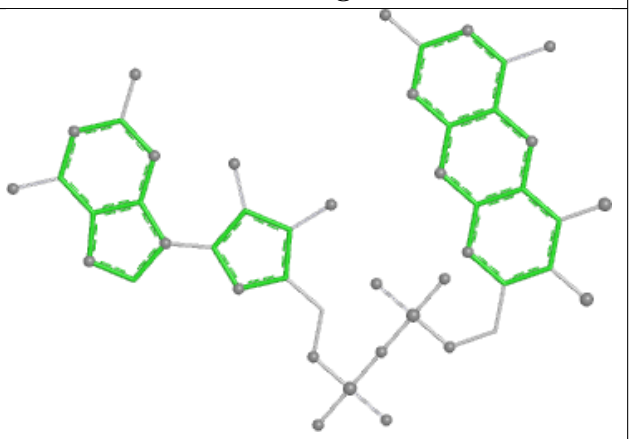
Bond lengths



Bond angles

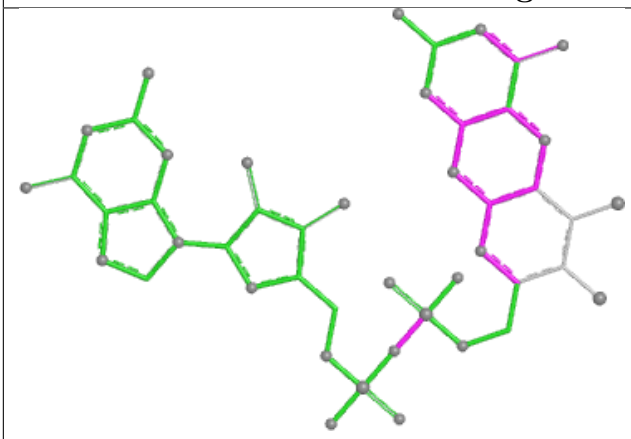


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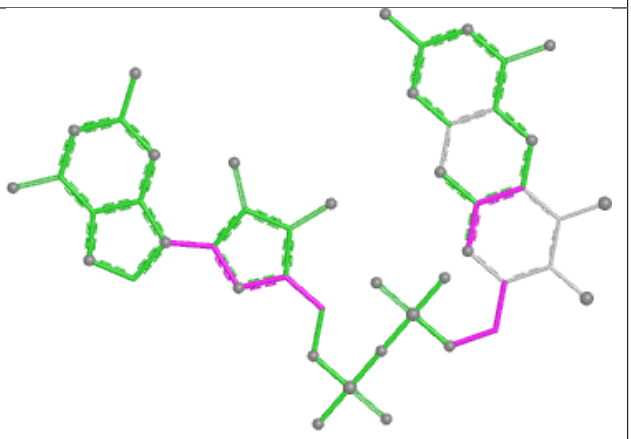


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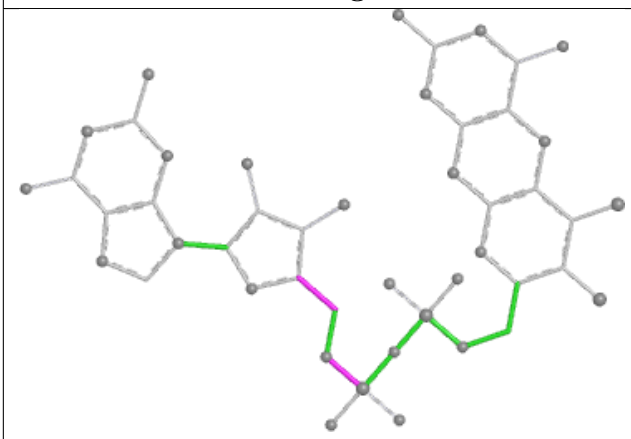
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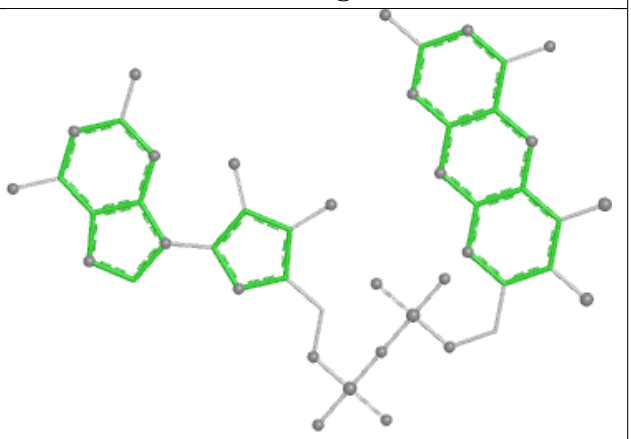
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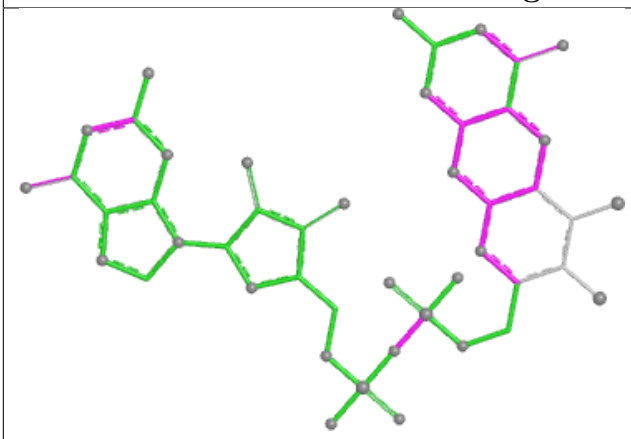


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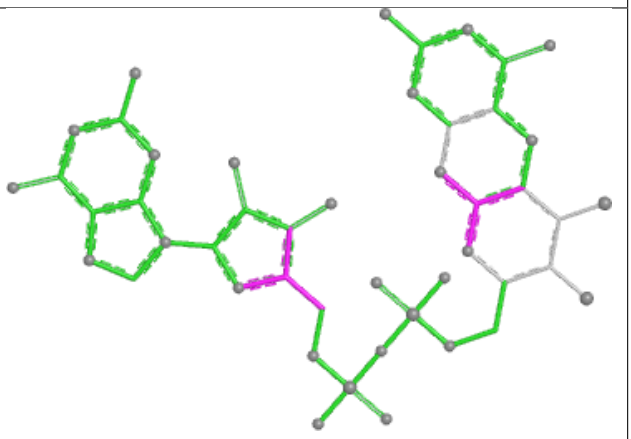


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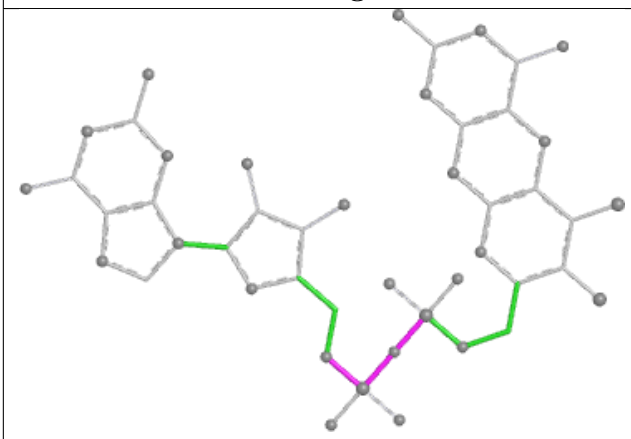
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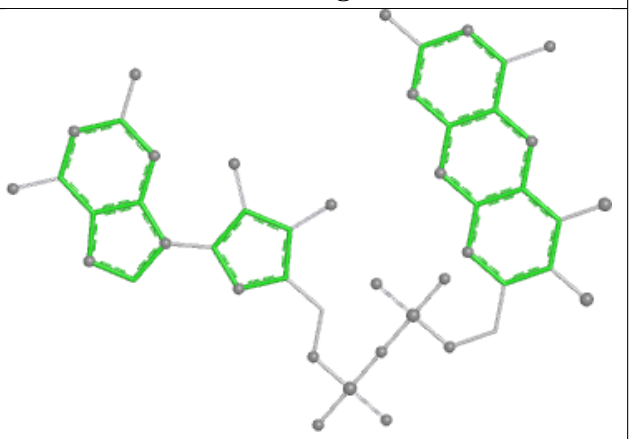
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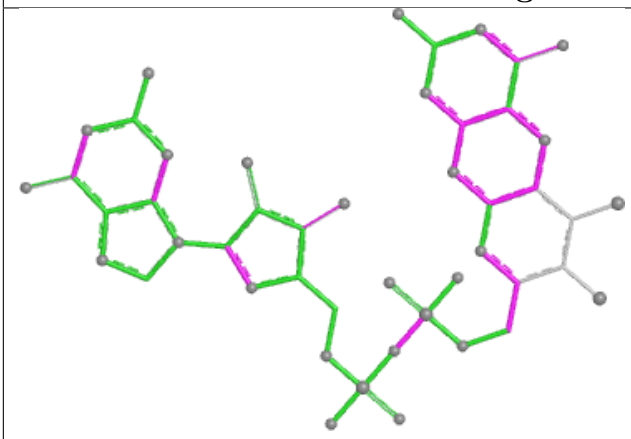


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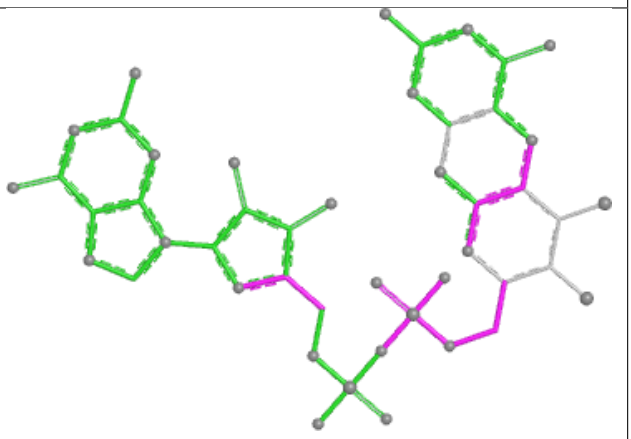


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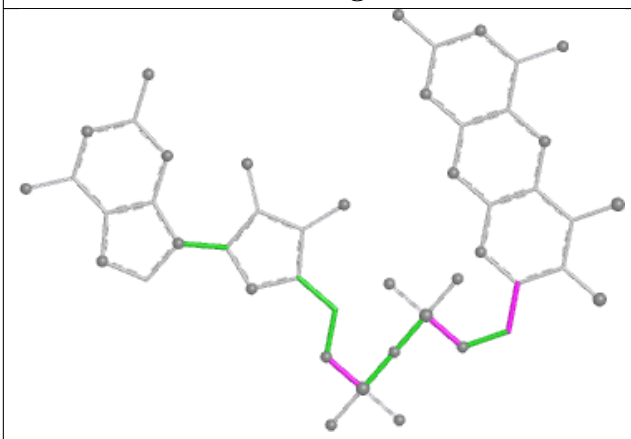
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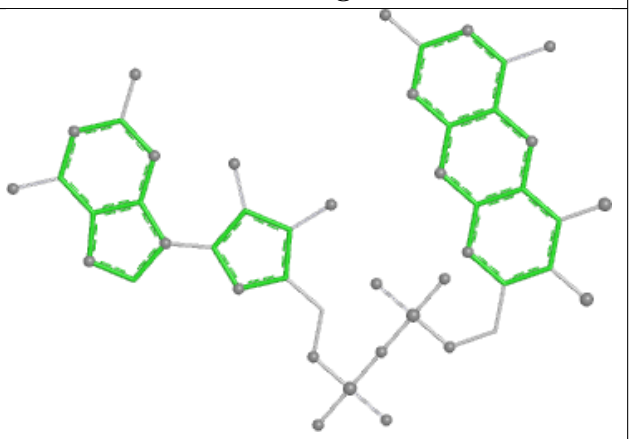
Bond lengths



Bond angles

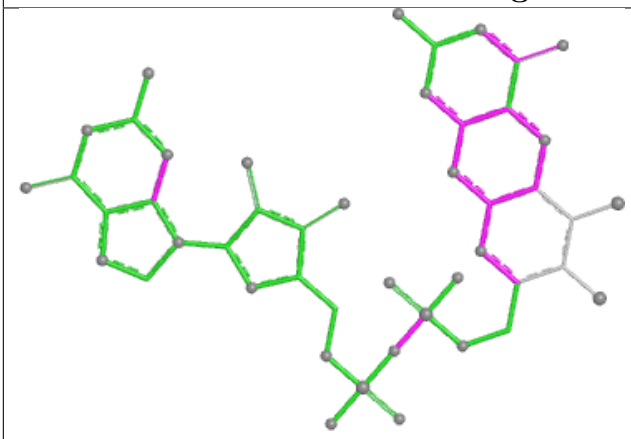


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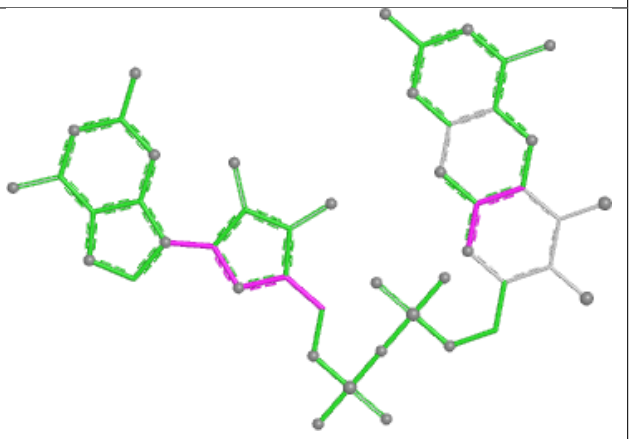


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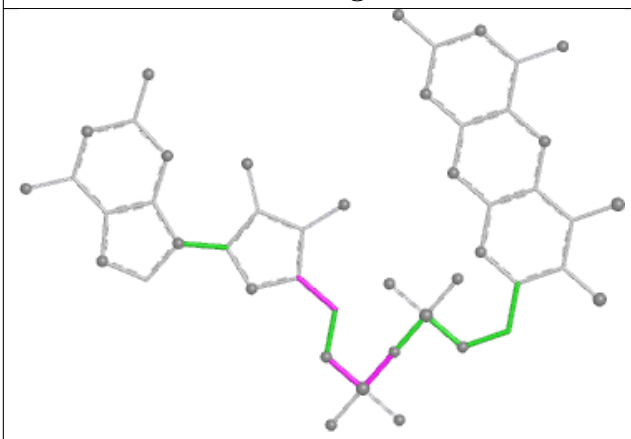
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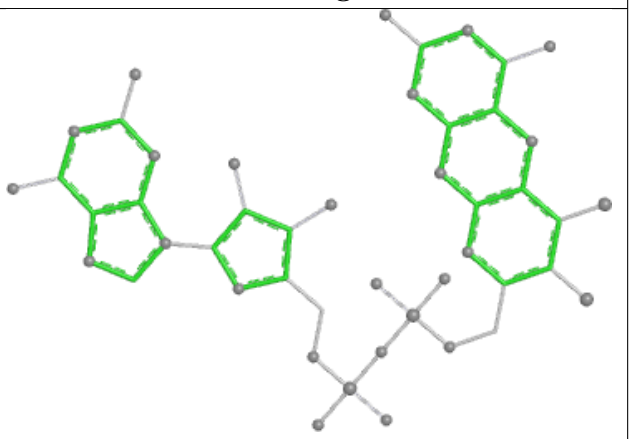
Bond lengths



Bond angles

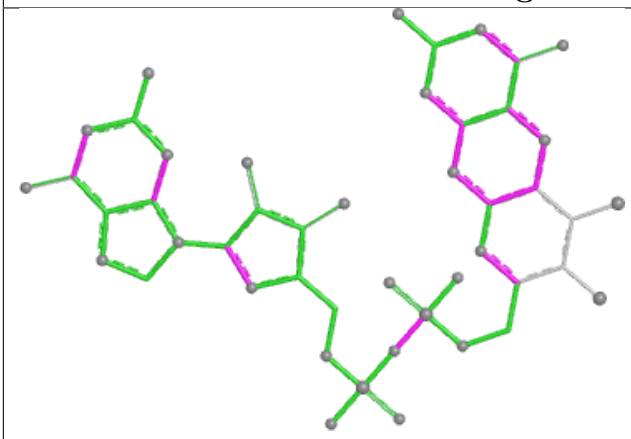


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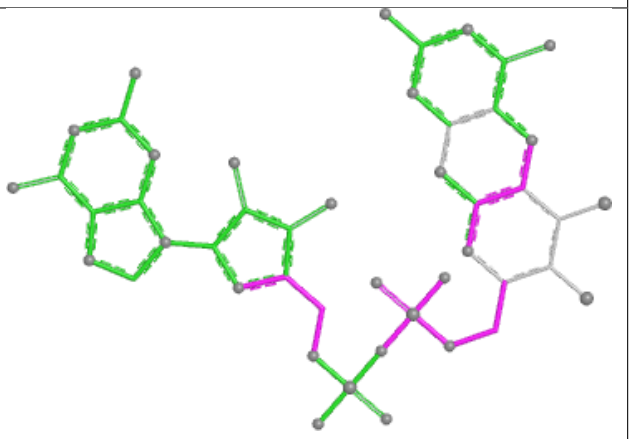


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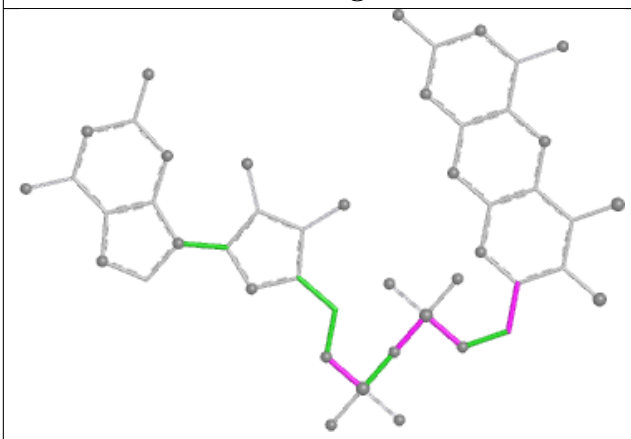
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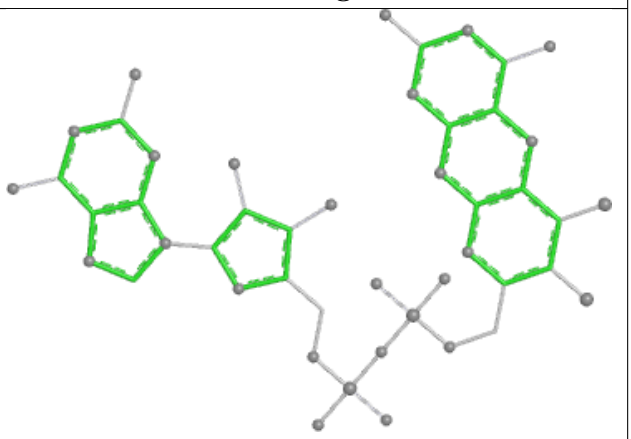
Bond lengths



Bond angles

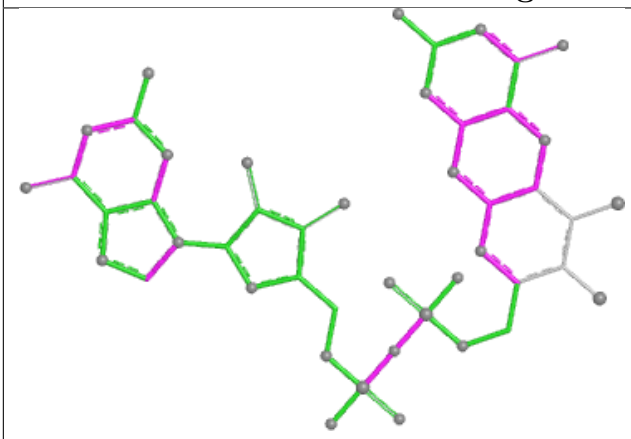


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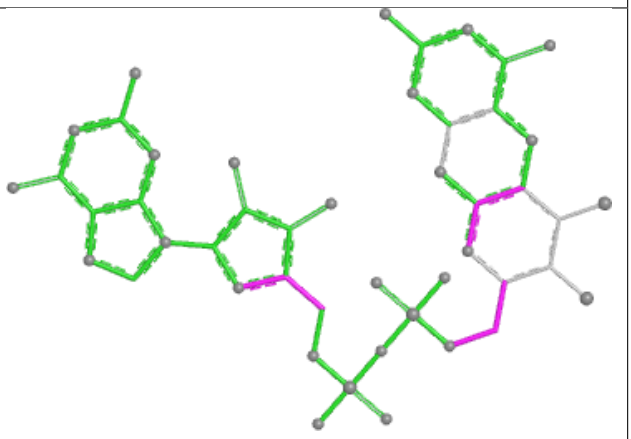


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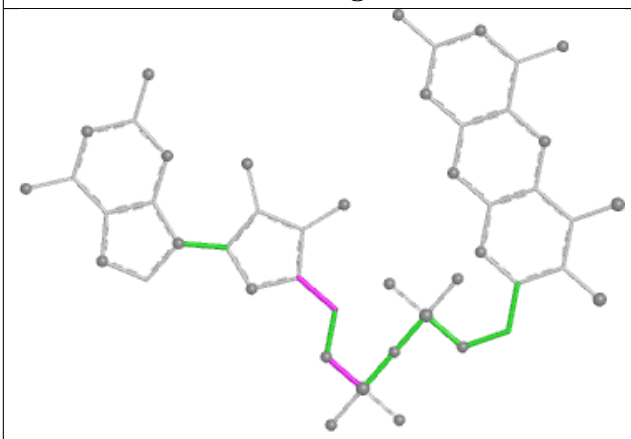
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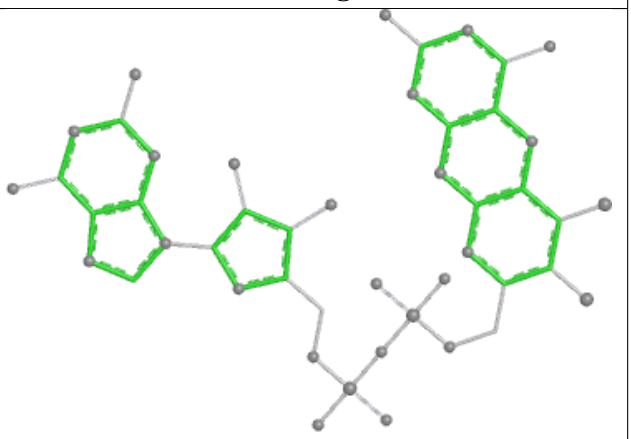
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Bond angles

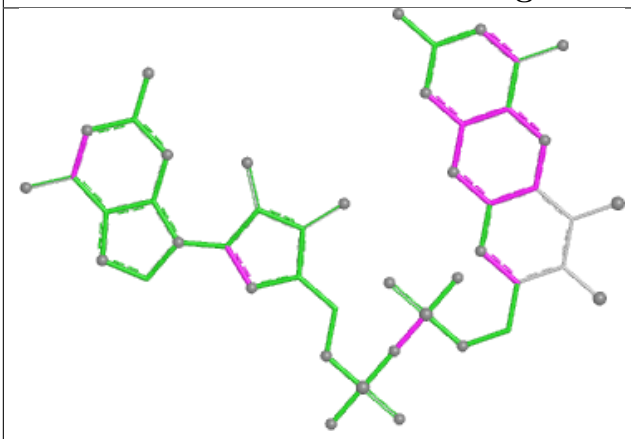


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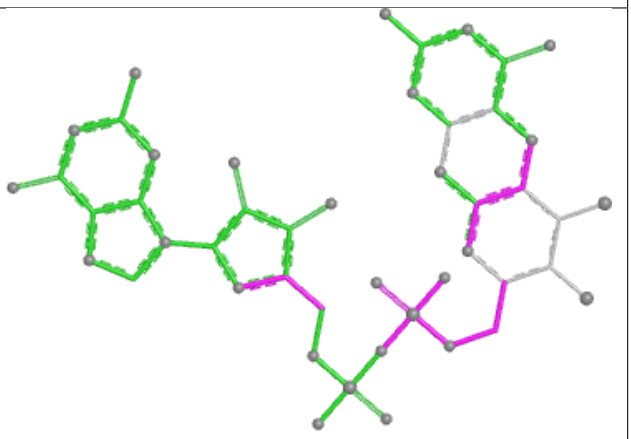


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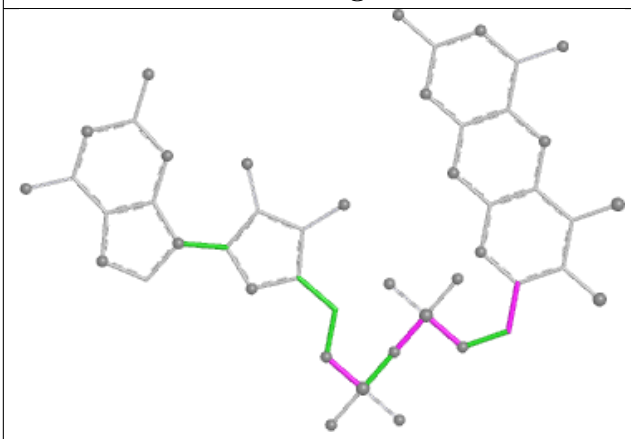
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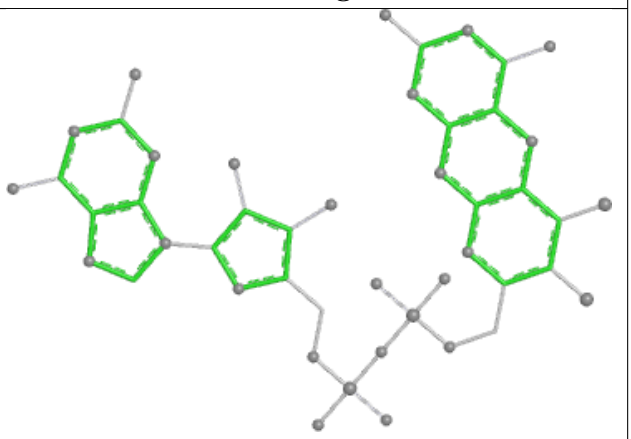
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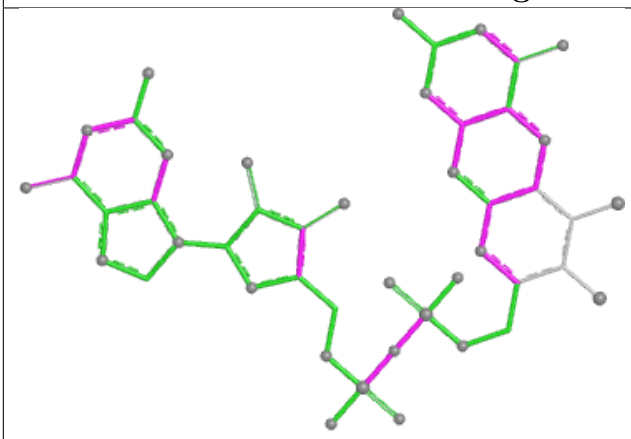


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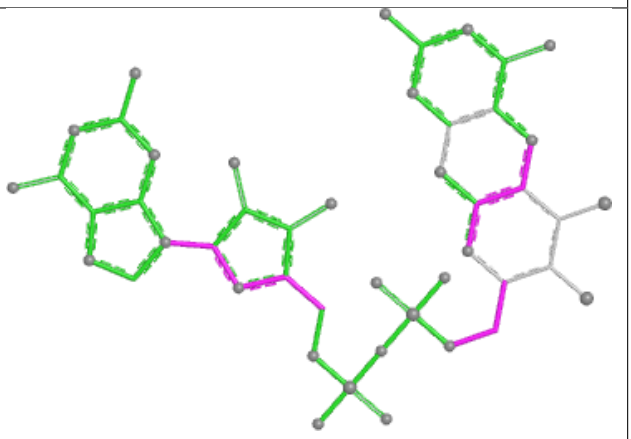


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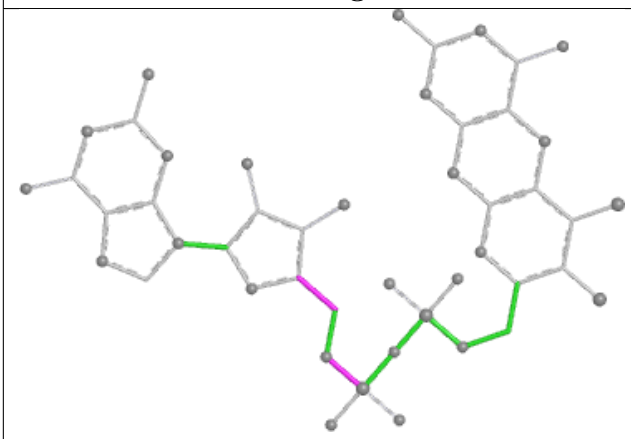
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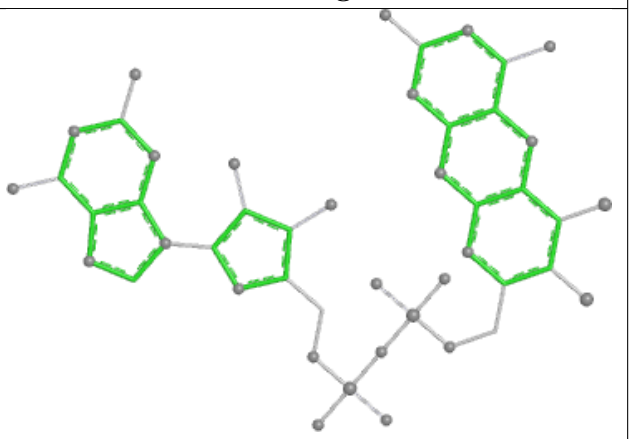
Bond lengths



Bond angles

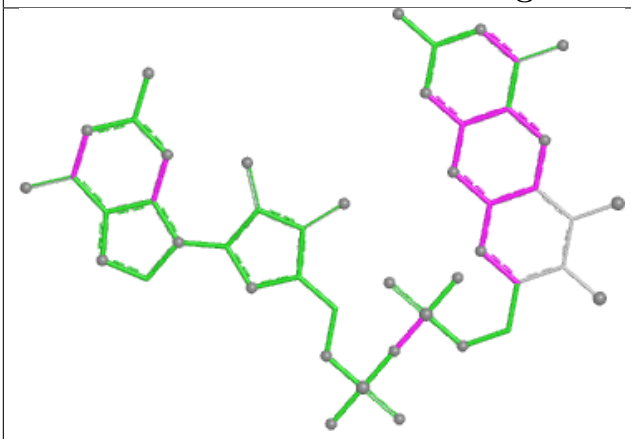


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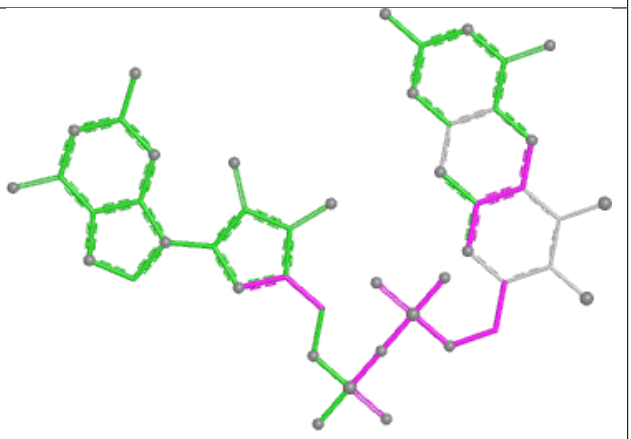


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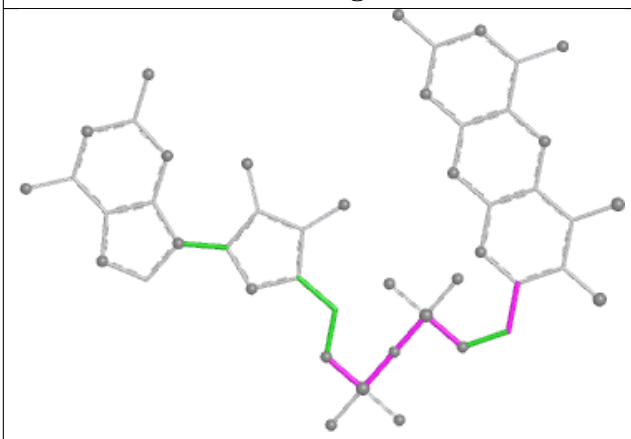
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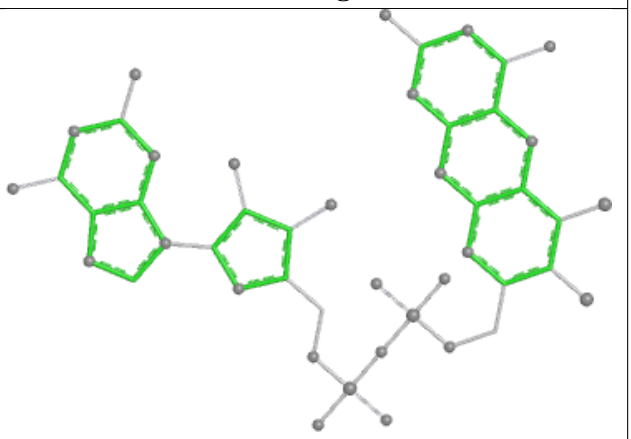
Bond lengths



Bond angles

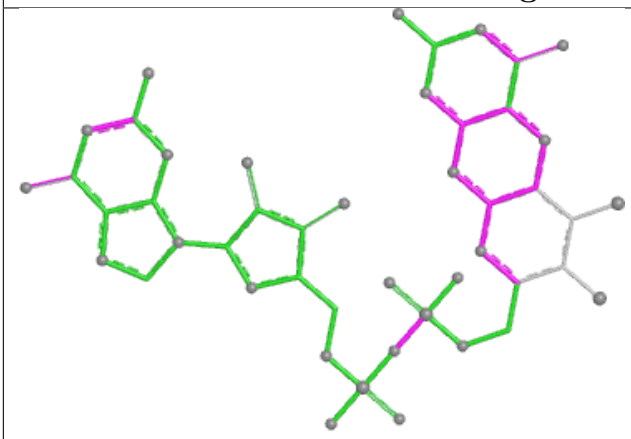


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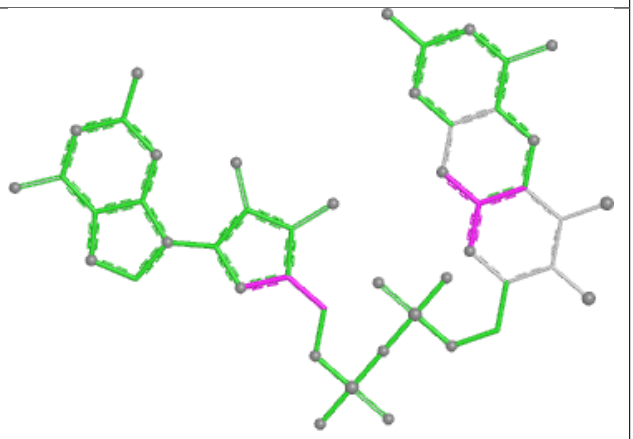


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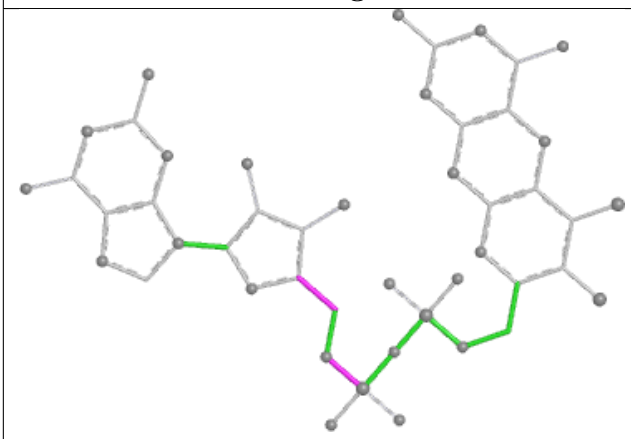
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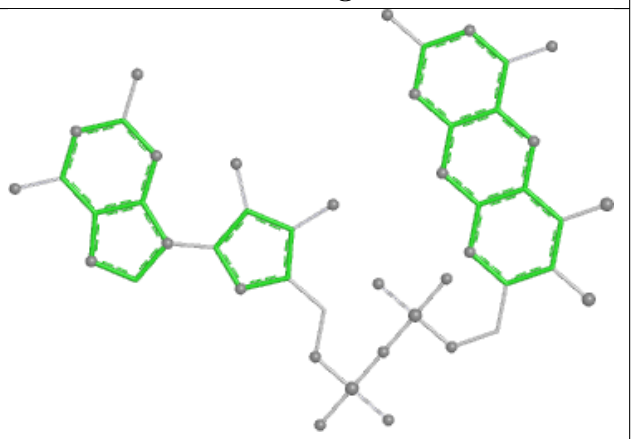
Bond lengths



Bond angles

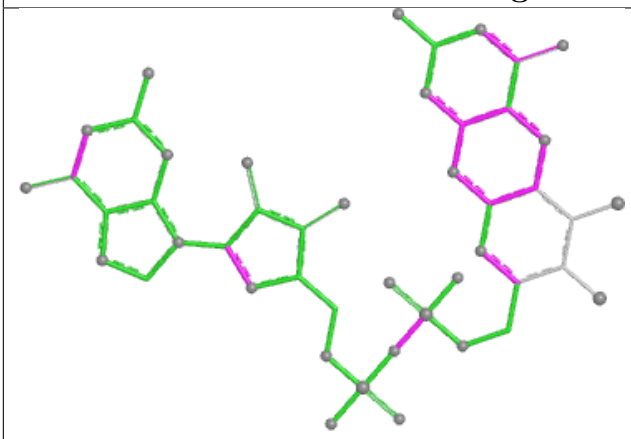


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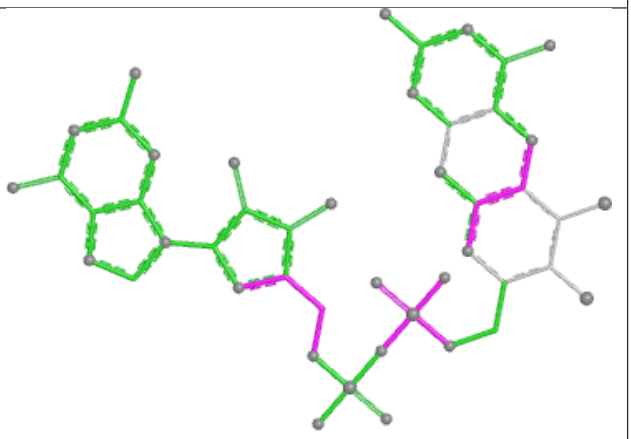


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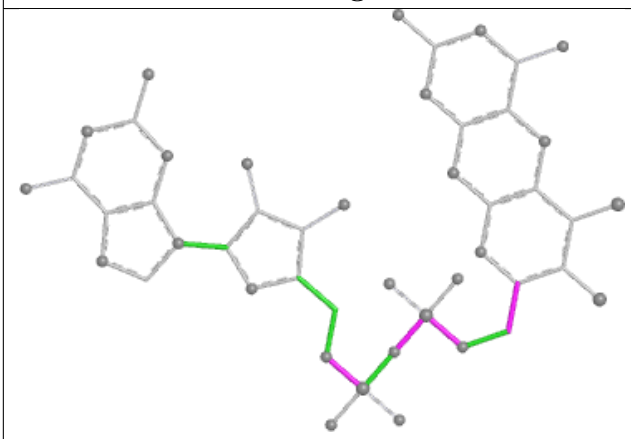
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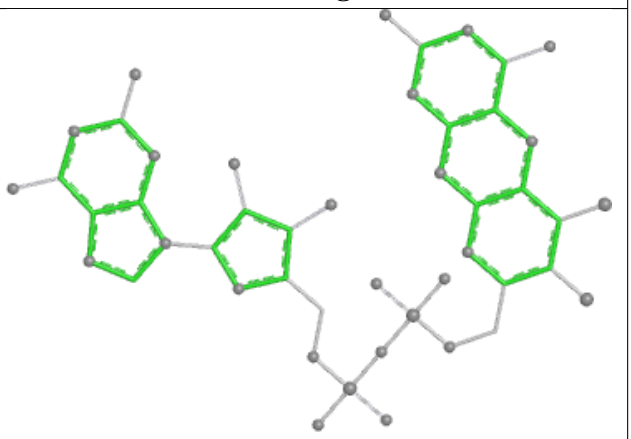
Bond lengths



Bond angles

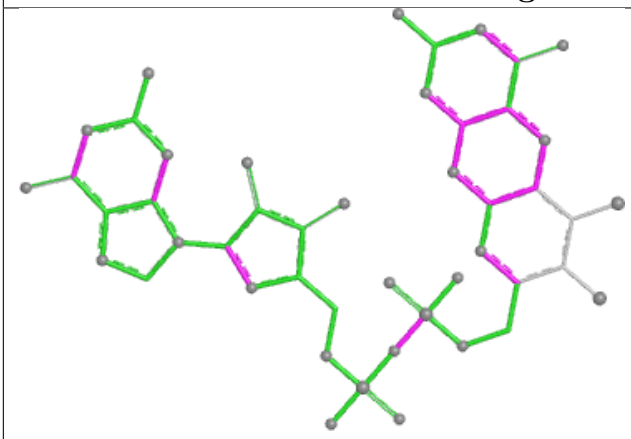


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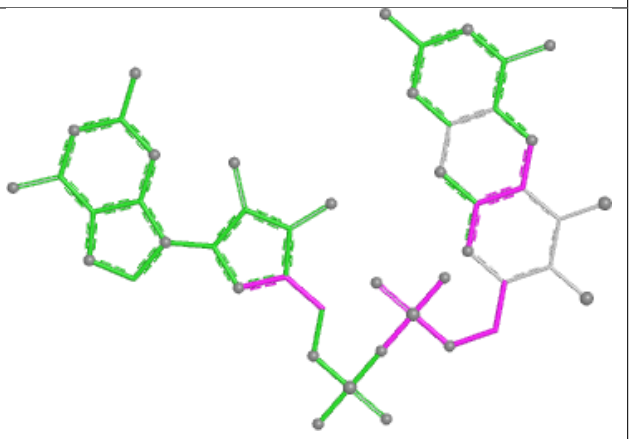


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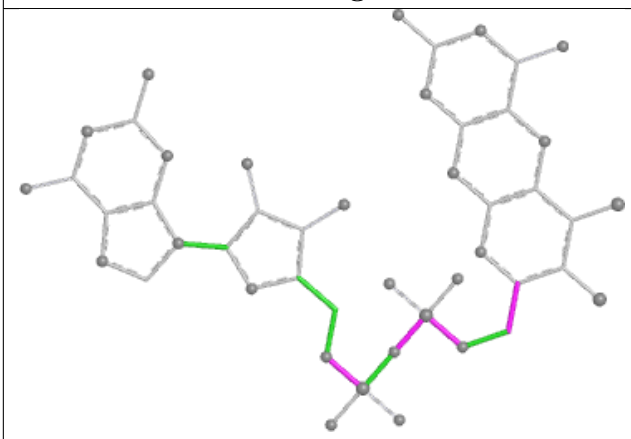
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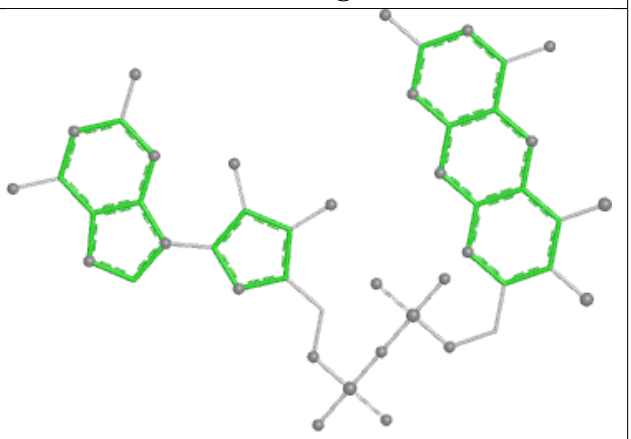
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.