



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:39 am BST

PDB ID : 1HTO
Title : CRYSTALLOGRAPHIC STRUCTURE OF A RELAXED GLUTAMINE
SYNTHETASE FROM MYCOBACTERIUM TUBERCULOSIS
Authors : Gill, H.S.; Eisenberg, D.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2001-01-01
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

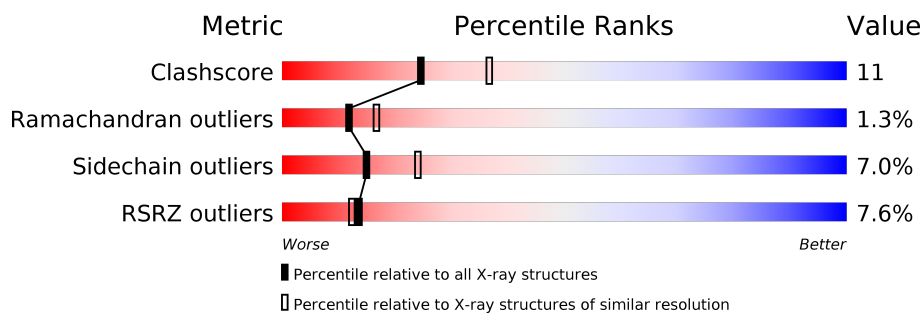
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.






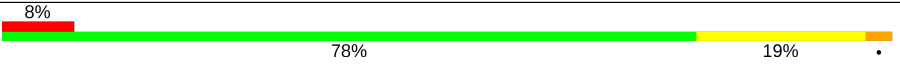
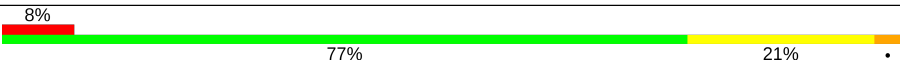

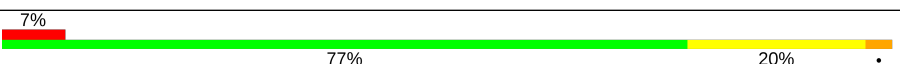
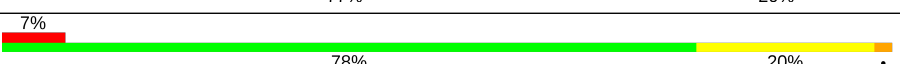
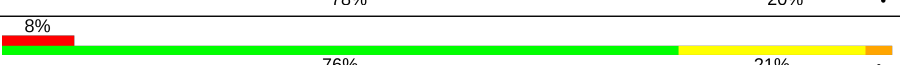
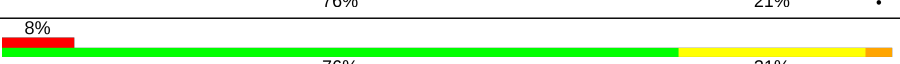
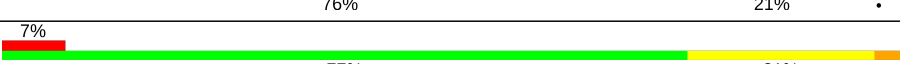
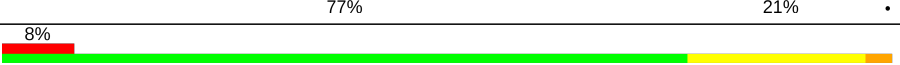

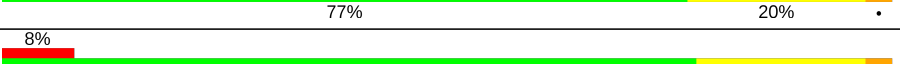



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	477	<div> <div>6%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	B	477	<div> <div>9%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	C	477	<div> <div>9%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	D	477	<div> <div>7%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	E	477	<div> <div>9%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	F	477	<div> <div>7%</div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	G	477	<div> <div>8%</div> <div>76%</div> <div>21%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	477	
1	I	477	
1	J	477	
1	K	477	
1	L	477	
1	M	477	
1	N	477	
1	O	477	
1	P	477	
1	Q	477	
1	R	477	
1	S	477	
1	T	477	
1	U	477	
1	V	477	
1	W	477	
1	X	477	

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
2	MN	O	470	-	-	-	X
3	AMP	A	7475	-	-	X	X
3	AMP	B	7477	-	-	X	X
3	AMP	C	7479	-	-	X	X
3	AMP	D	7481	-	-	X	X
3	AMP	E	7483	-	-	X	X
3	AMP	F	7485	-	-	X	X
3	AMP	G	7487	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AMP	H	7489	-	-	X	X
3	AMP	I	7491	-	-	X	X
3	AMP	J	7493	-	-	X	X
3	AMP	K	7495	-	-	X	X
3	AMP	L	7497	-	-	X	X
3	AMP	M	7499	-	-	X	X
3	AMP	N	7501	-	-	X	X
3	AMP	O	7503	-	-	X	X
3	AMP	P	7505	-	-	X	X
3	AMP	Q	7507	-	-	X	X
3	AMP	R	7509	-	-	X	X
3	AMP	S	7511	-	-	X	X
3	AMP	T	7513	-	-	X	X
3	AMP	U	7515	-	-	X	X
3	AMP	V	7517	-	-	X	X
3	AMP	W	7519	-	-	X	X
3	AMP	X	7521	-	-	X	X
4	CIT	A	7476	-	-	X	-
4	CIT	B	7478	-	-	X	-
4	CIT	D	7482	-	-	X	-
4	CIT	F	7486	-	-	X	X
4	CIT	G	7488	-	-	X	X
4	CIT	H	7490	-	-	X	-
4	CIT	I	7492	-	-	X	-
4	CIT	K	7496	-	-	X	-
4	CIT	L	7498	-	-	X	-
4	CIT	M	7500	-	-	X	-
4	CIT	N	7502	-	-	X	-
4	CIT	P	7506	-	-	X	-
4	CIT	R	7510	-	-	X	X
4	CIT	S	7512	-	-	X	-
4	CIT	T	7514	-	-	X	-
4	CIT	U	7516	-	-	X	-
4	CIT	W	7520	-	-	X	-
4	CIT	X	7522	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 97872 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 GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	E	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	F	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	O	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	P	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

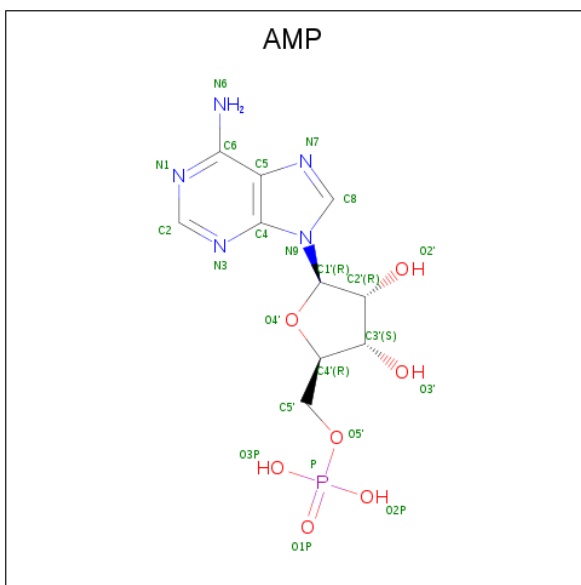
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Mn	0	0
			1	1		
2	K	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	W	1	Total	Mn	0	0
			1	1		
2	N	1	Total	Mn	0	0
			1	1		
2	X	1	Total	Mn	0	0
			1	1		
2	S	1	Total	Mn	0	0
			1	1		
2	J	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	V	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	1	Total 1	Mn 1	0	0
2	M	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0
2	I	1	Total 1	Mn 1	0	0
2	U	1	Total 1	Mn 1	0	0
2	L	1	Total 1	Mn 1	0	0
2	G	1	Total 1	Mn 1	0	0
2	Q	1	Total 1	Mn 1	0	0
2	H	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	T	1	Total 1	Mn 1	0	0
2	O	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



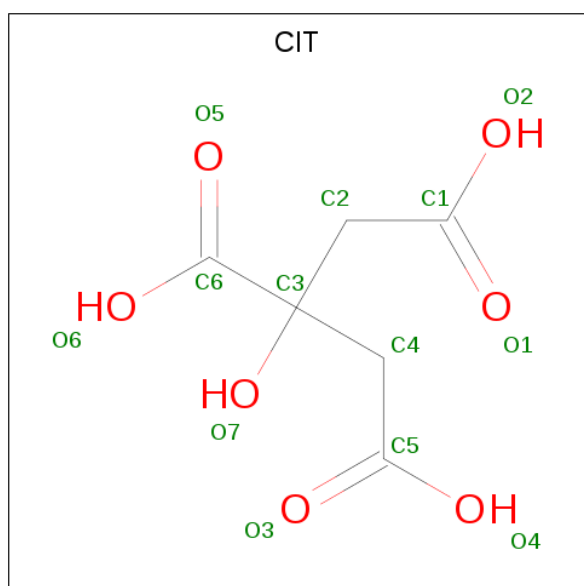
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	I	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	J	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	K	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	L	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	N	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	P	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	R	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	T	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	U	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	V	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	W	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	X	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	E	1	Total	C	O	0	0
			13	6	7		
4	F	1	Total	C	O	0	0
			13	6	7		
4	G	1	Total	C	O	0	0
			13	6	7		
4	H	1	Total	C	O	0	0
			13	6	7		
4	I	1	Total	C	O	0	0
			13	6	7		
4	J	1	Total	C	O	0	0
			13	6	7		
4	K	1	Total	C	O	0	0
			13	6	7		
4	L	1	Total	C	O	0	0
			13	6	7		
4	M	1	Total	C	O	0	0
			13	6	7		
4	N	1	Total	C	O	0	0
			13	6	7		
4	O	1	Total	C	O	0	0
			13	6	7		
4	P	1	Total	C	O	0	0
			13	6	7		
4	Q	1	Total	C	O	0	0
			13	6	7		
4	R	1	Total	C	O	0	0
			13	6	7		
4	S	1	Total	C	O	0	0
			13	6	7		
4	T	1	Total	C	O	0	0
			13	6	7		
4	U	1	Total	C	O	0	0
			13	6	7		
4	V	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	W	1	Total	C	O	0	0
			13	6	7		
4	X	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	261	Total	O		0	0
			261	261			
5	B	262	Total	O		0	0
			262	262			
5	C	264	Total	O		0	0
			264	264			
5	D	262	Total	O		0	0
			262	262			
5	E	261	Total	O		0	0
			261	261			
5	F	267	Total	O		0	0
			267	267			
5	G	262	Total	O		0	0
			262	262			
5	H	263	Total	O		0	0
			263	263			
5	I	263	Total	O		0	0
			263	263			
5	J	262	Total	O		0	0
			262	262			
5	K	267	Total	O		0	0
			267	267			
5	L	262	Total	O		0	0
			262	262			
5	M	263	Total	O		0	0
			263	263			
5	N	262	Total	O		0	0
			262	262			
5	O	265	Total	O		0	0
			265	265			
5	P	265	Total	O		0	0
			265	265			
5	Q	259	Total	O		0	0
			259	259			

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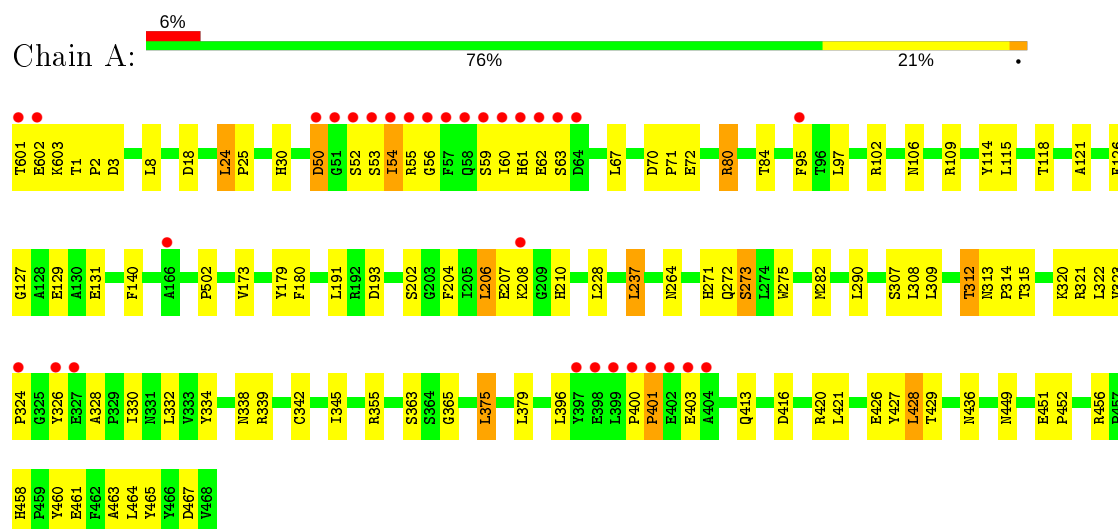
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	269	Total 269	O 269	0	0
5	S	262	Total 262	O 262	0	0
5	T	258	Total 258	O 258	0	0
5	U	265	Total 265	O 265	0	0
5	V	263	Total 263	O 263	0	0
5	W	263	Total 263	O 263	0	0
5	X	262	Total 262	O 262	0	0

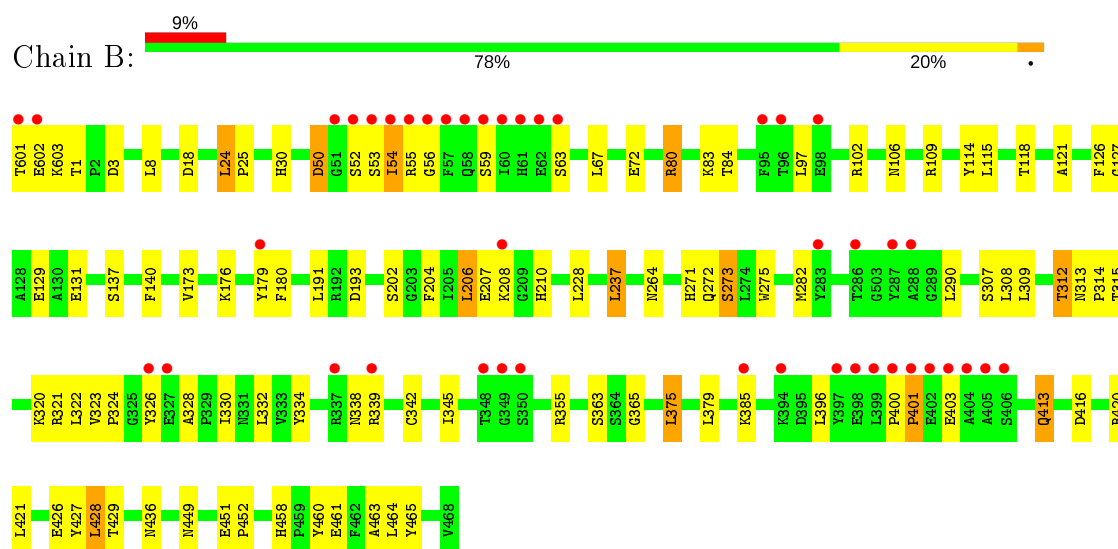
3 Residue-property plots [i](#)

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

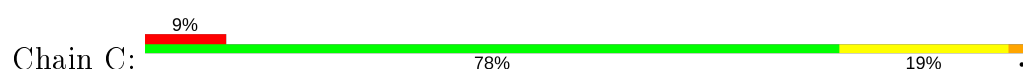
• Molecule 1: GLUTAMINE SYNTHETASE

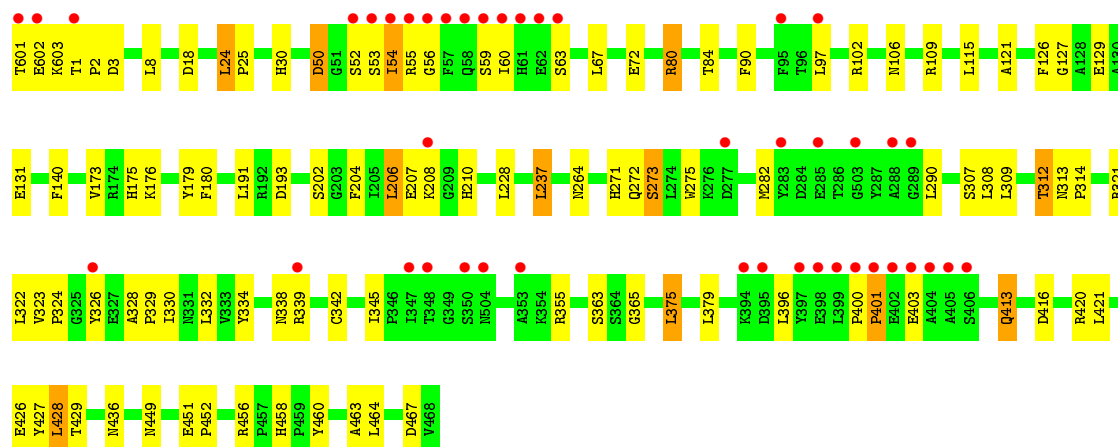


• Molecule 1: GLUTAMINE SYNTHETASE

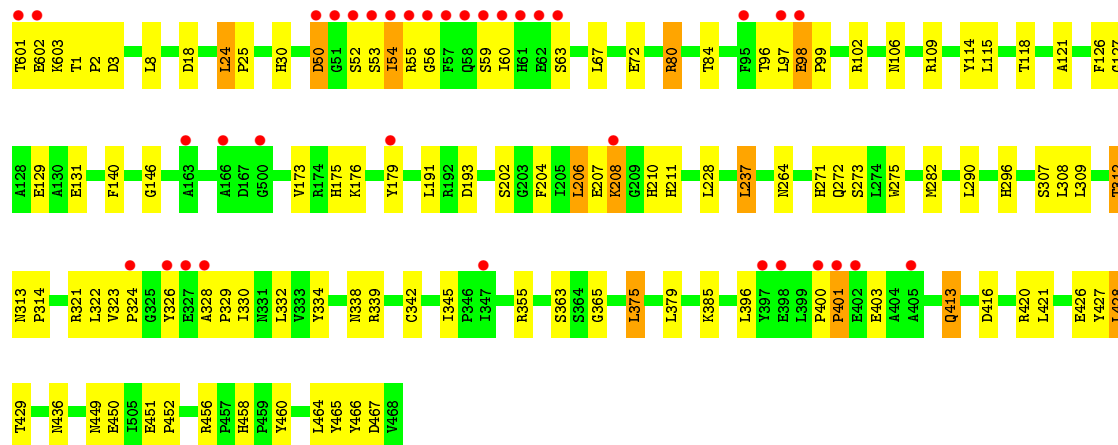
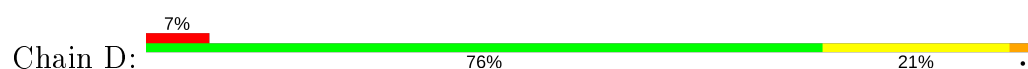


• Molecule 1: GLUTAMINE SYNTHETASE

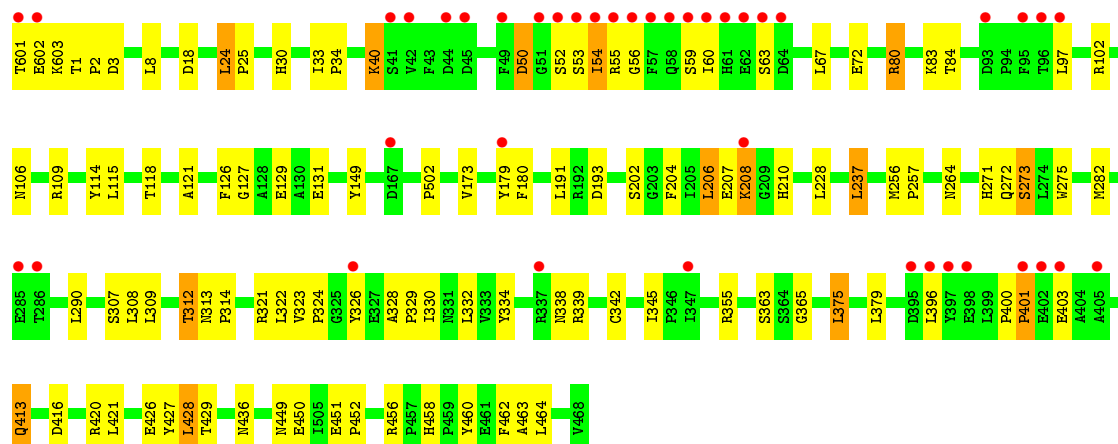
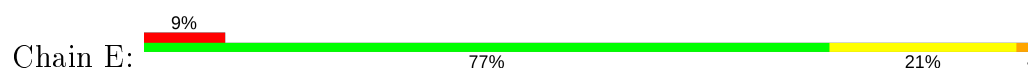




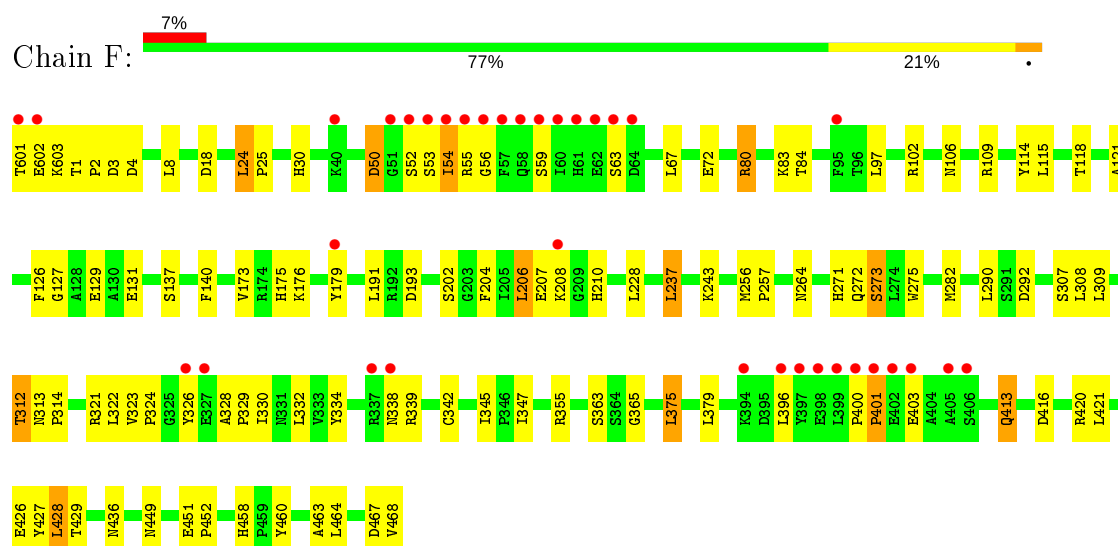
• Molecule 1: GLUTAMINE SYNTHETASE



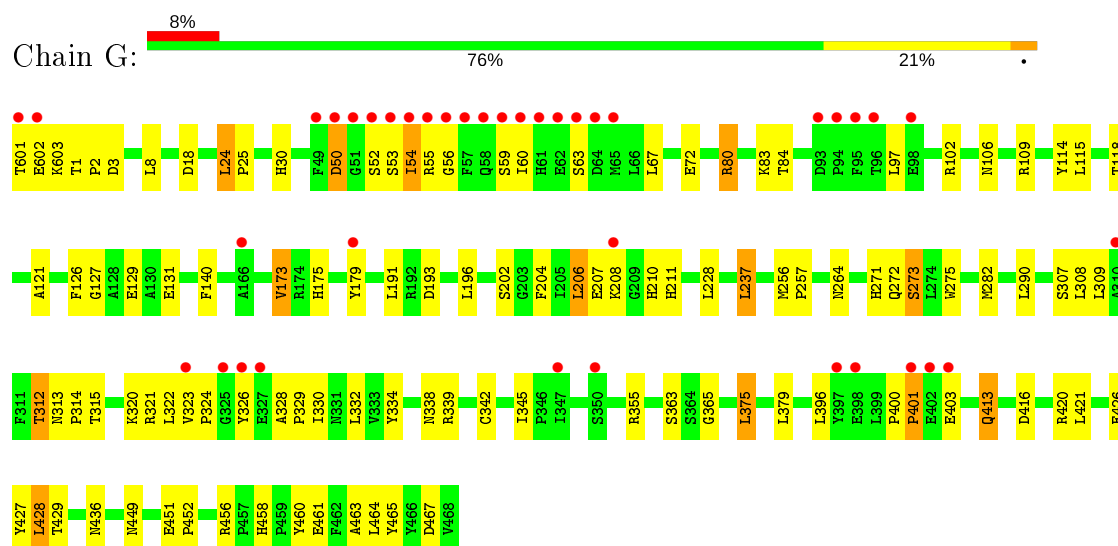
• Molecule 1: GLUTAMINE SYNTHETASE



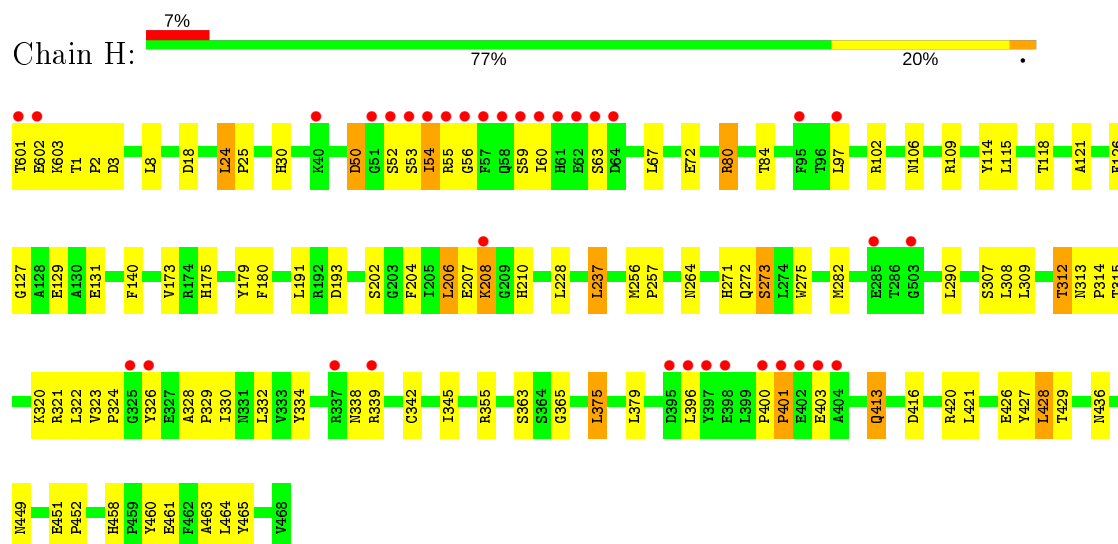
• Molecule 1: GLUTAMINE SYNTHETASE



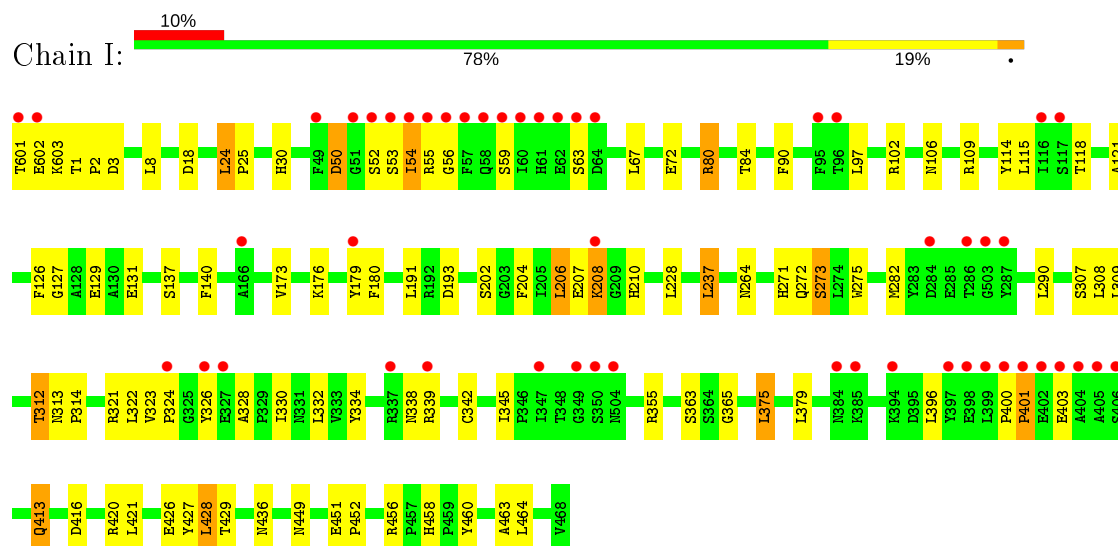
• Molecule 1: GLUTAMINE SYNTHETASE



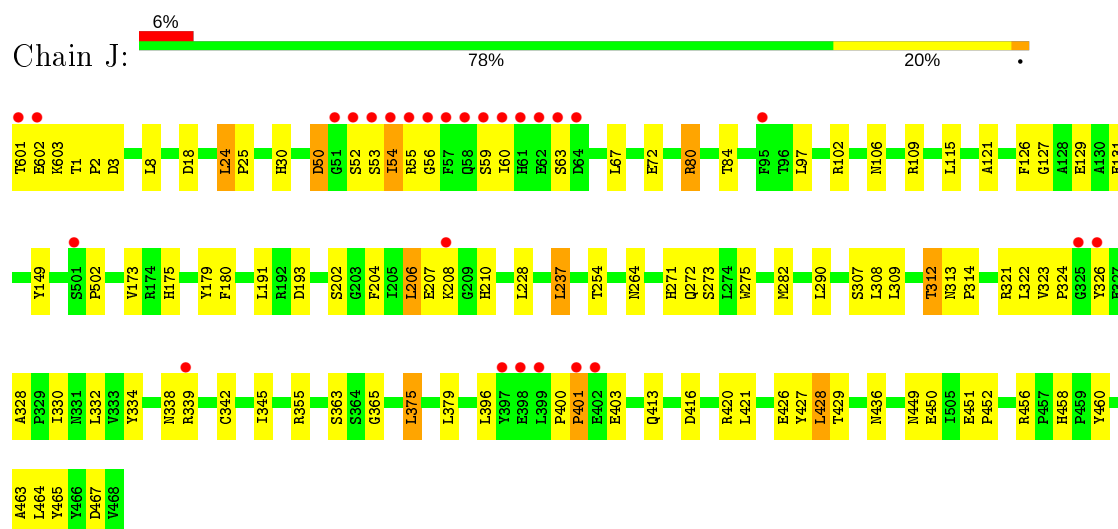
• Molecule 1: GLUTAMINE SYNTHETASE



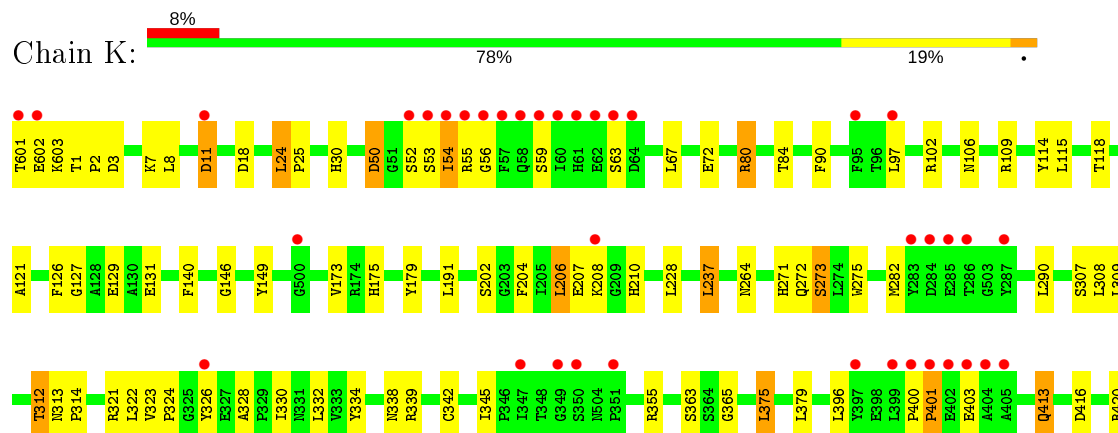
- Molecule 1: GLUTAMINE SYNTHETASE



- Molecule 1: GLUTAMINE SYNTHETASE

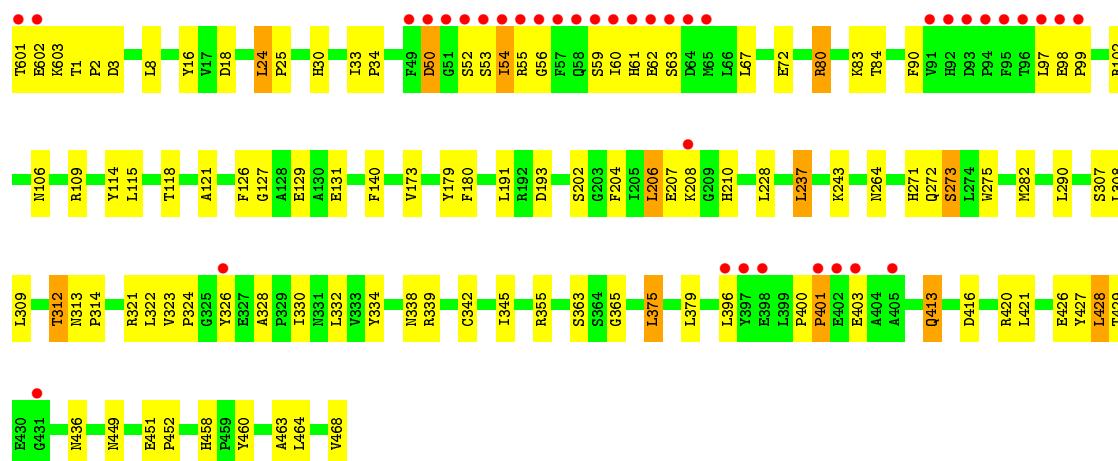
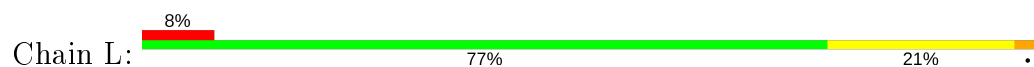


- Molecule 1: GLUTAMINE SYNTHETASE

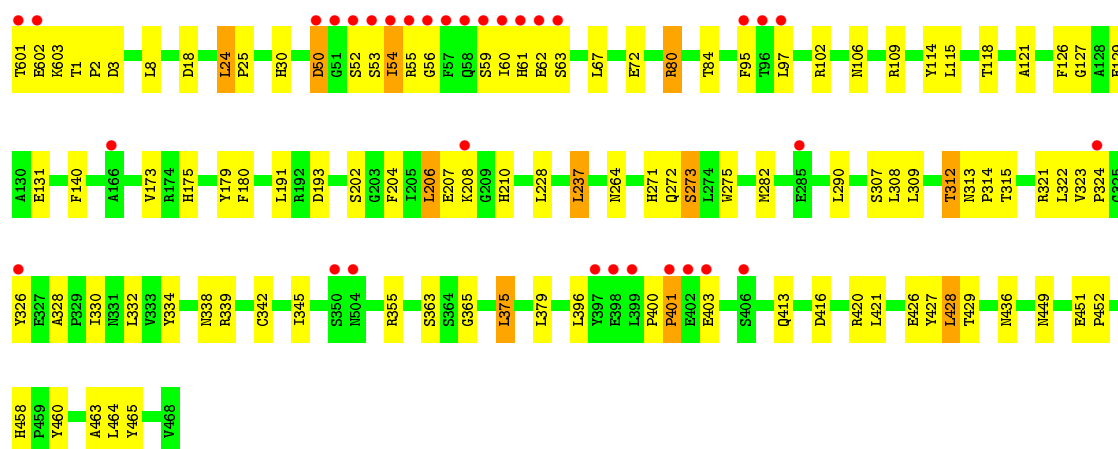
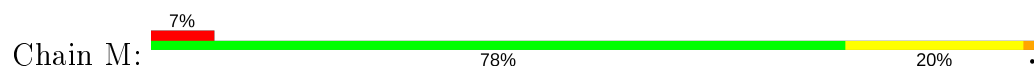




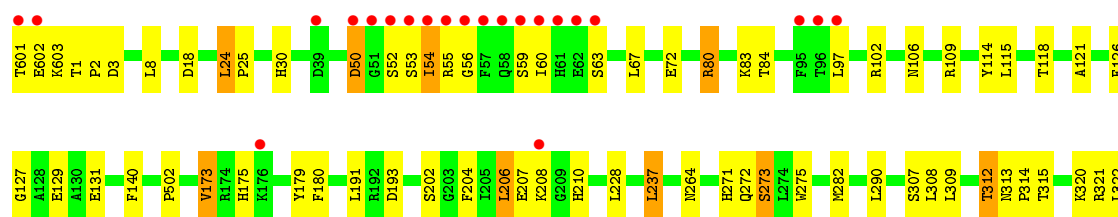
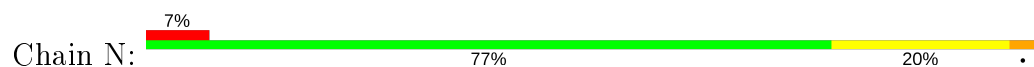
• Molecule 1: GLUTAMINE SYNTHETASE

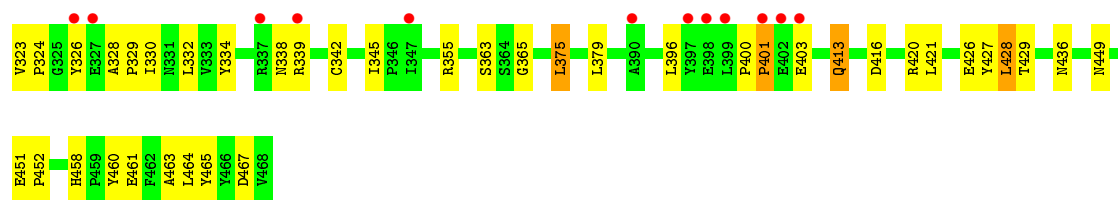


• Molecule 1: GLUTAMINE SYNTHETASE

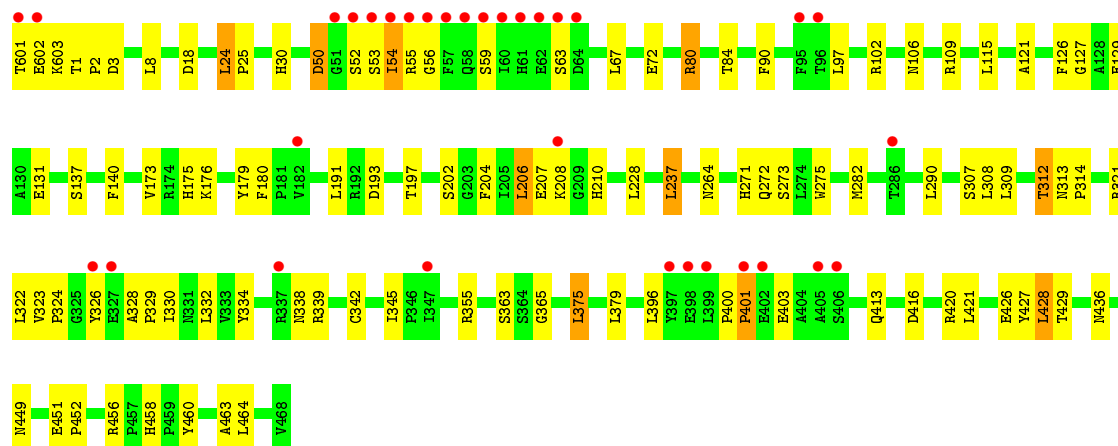
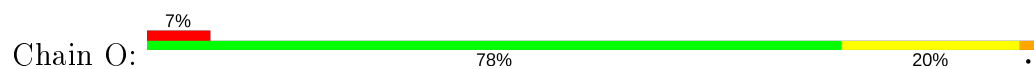


• Molecule 1: GLUTAMINE SYNTHETASE

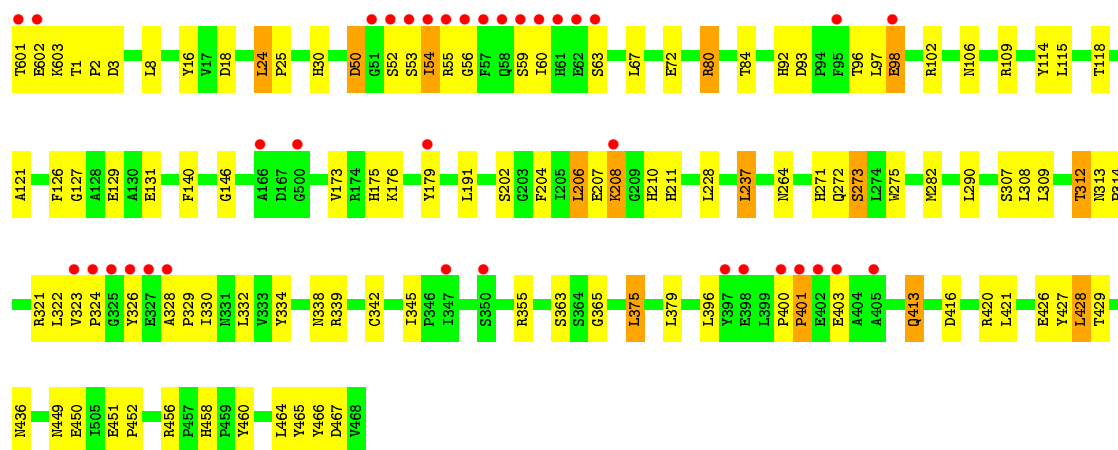
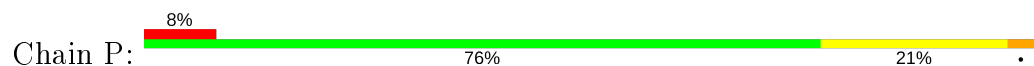




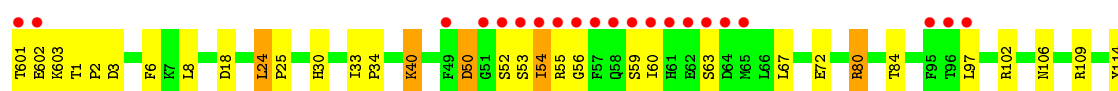
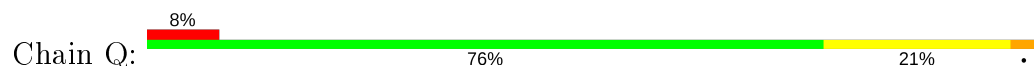
● Molecule 1: GLUTAMINE SYNTHETASE

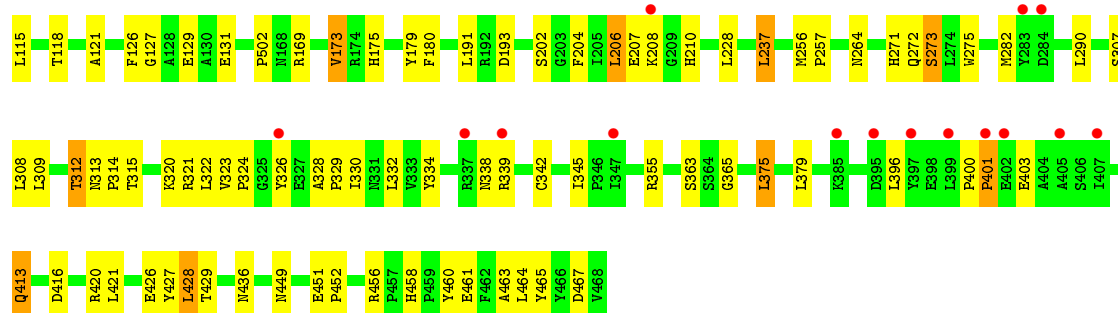


● Molecule 1: GLUTAMINE SYNTHETASE

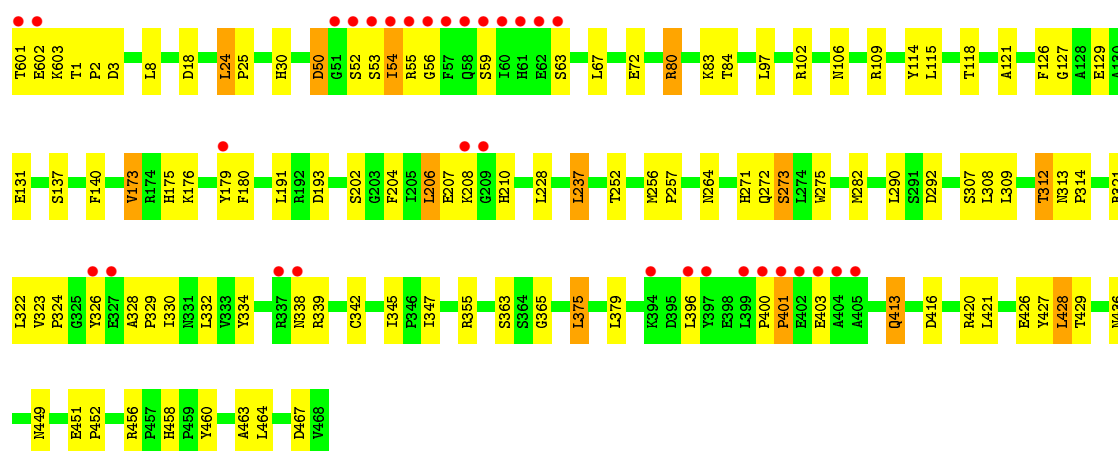
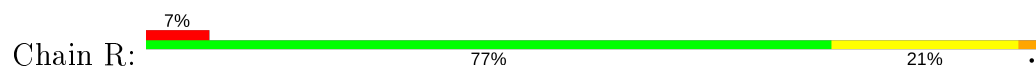


● Molecule 1: GLUTAMINE SYNTHETASE

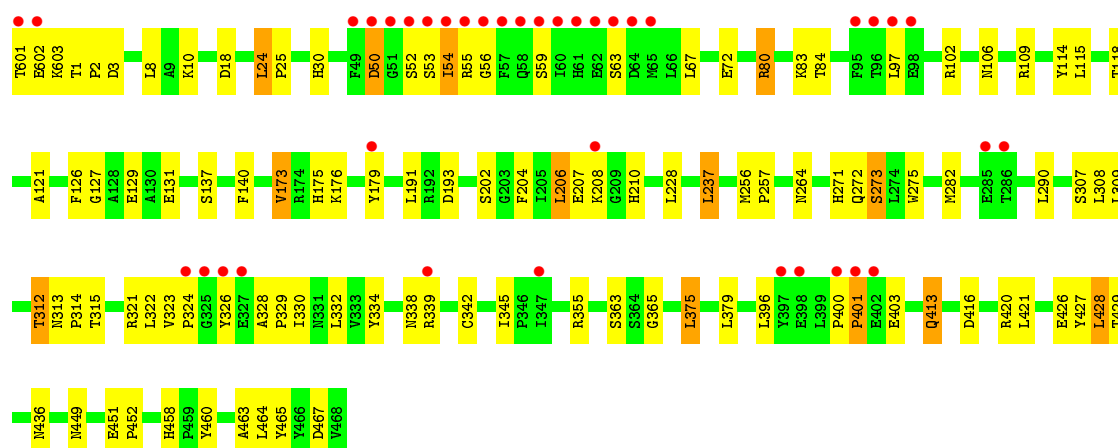
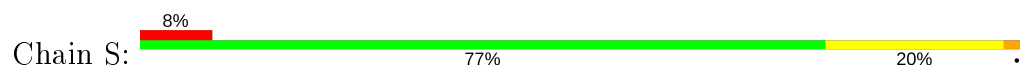




• Molecule 1: GLUTAMINE SYNTHETASE

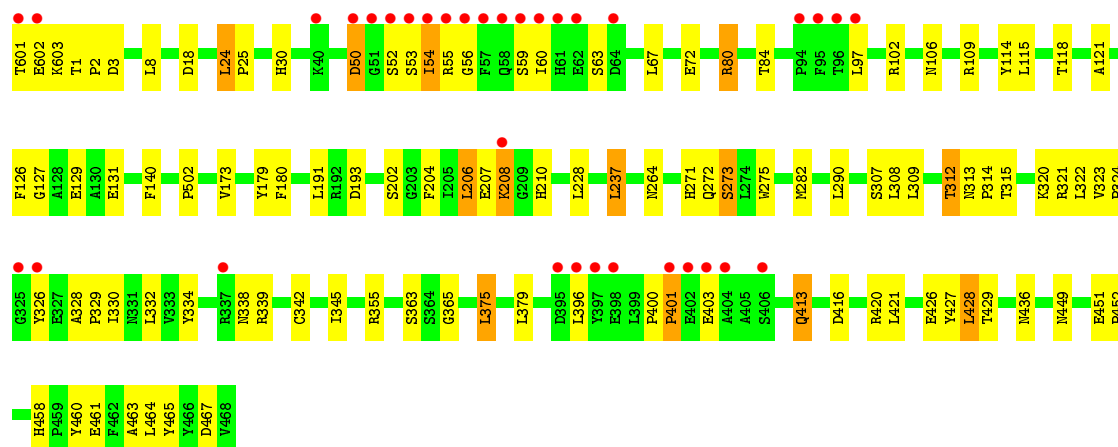


• Molecule 1: GLUTAMINE SYNTHETASE

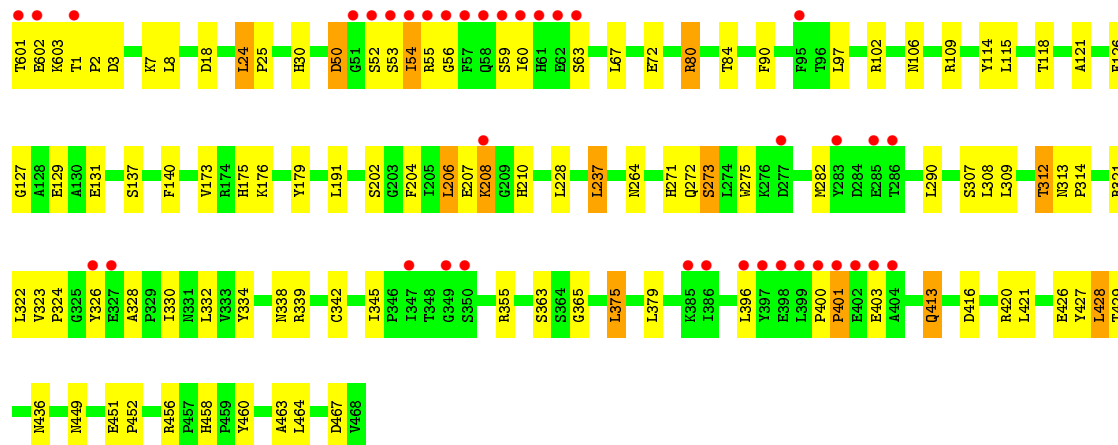
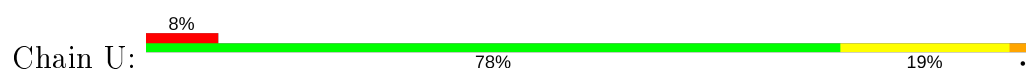


• Molecule 1: GLUTAMINE SYNTHETASE

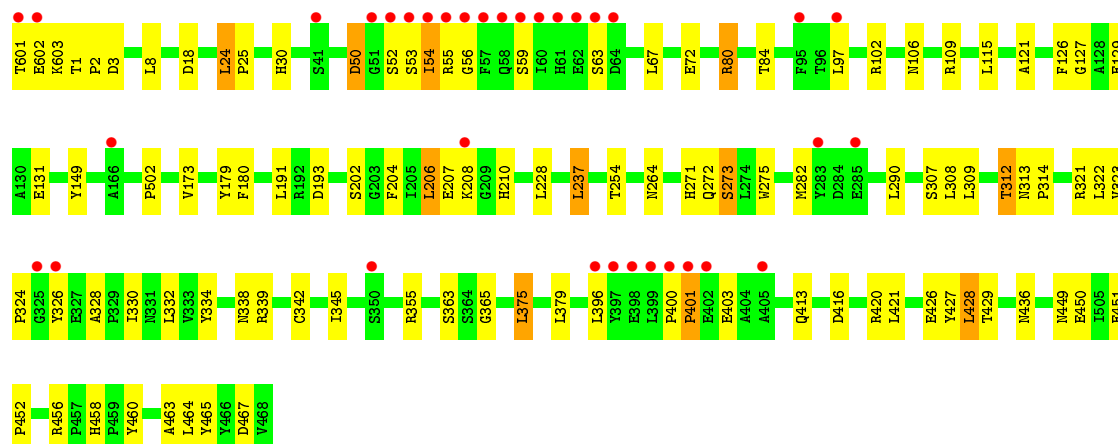
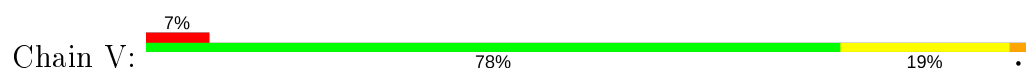




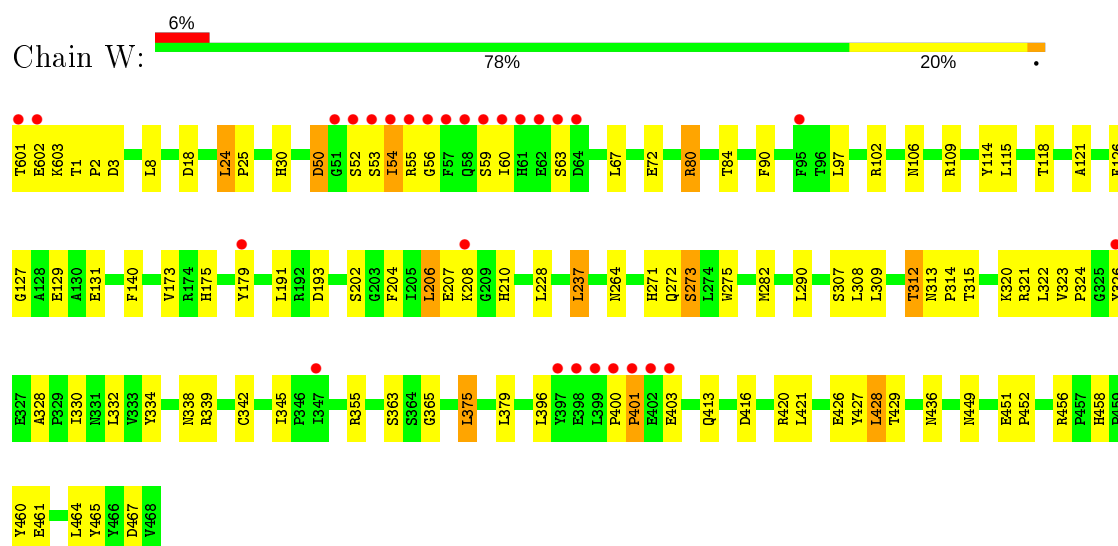
• Molecule 1: GLUTAMINE SYNTHETASE



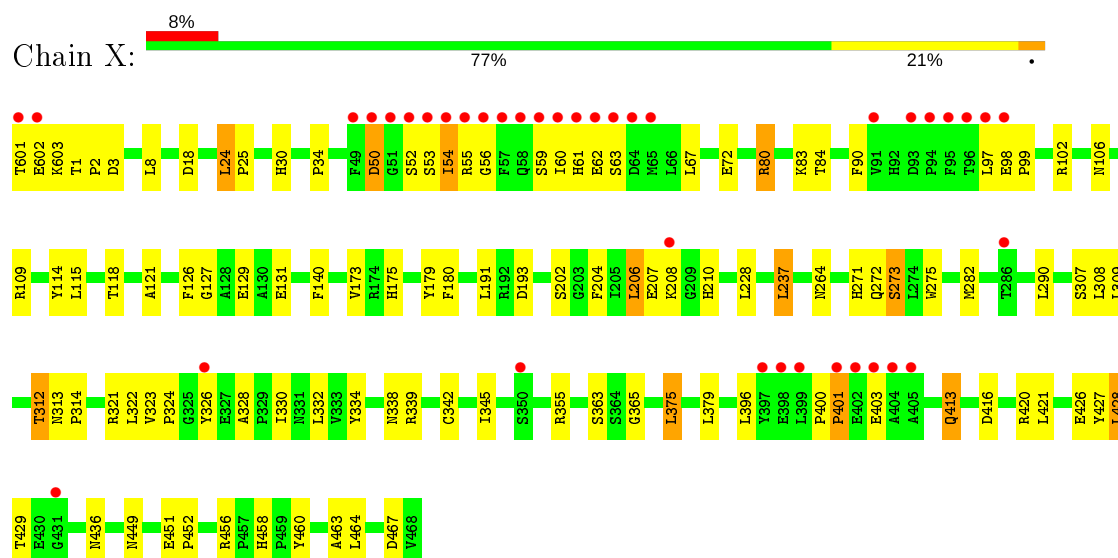
• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.72Å 257.69Å 274.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.40) 99.7 (20.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.38 (at 2.41Å)	Xtrriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.227 , 0.255 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtrriage
Anisotropy	0.287	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	97872	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0949e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, MN, CIT

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	0.35	0/3884	0.68	0/5279
1	B	0.35	0/3884	0.68	0/5279
1	C	0.35	0/3884	0.68	0/5279
1	D	0.35	0/3884	0.69	0/5279
1	E	0.35	0/3884	0.68	0/5279
1	F	0.35	0/3884	0.68	0/5279
1	G	0.35	0/3884	0.68	0/5279
1	H	0.35	0/3884	0.68	0/5279
1	I	0.35	0/3884	0.68	0/5279
1	J	0.35	0/3884	0.68	0/5279
1	K	0.35	0/3884	0.68	0/5279
1	L	0.35	0/3884	0.68	0/5279
1	M	0.35	0/3884	0.68	0/5279
1	N	0.35	0/3884	0.68	0/5279
1	O	0.35	0/3884	0.68	0/5279
1	P	0.35	0/3884	0.69	0/5279
1	Q	0.35	0/3884	0.68	0/5279
1	R	0.35	0/3884	0.68	0/5279
1	S	0.35	0/3884	0.68	0/5279
1	T	0.35	0/3884	0.68	0/5279
1	U	0.35	0/3884	0.68	0/5279
1	V	0.35	0/3884	0.68	0/5279
1	W	0.35	0/3884	0.68	0/5279
1	X	0.35	0/3884	0.68	0/5279
All	All	0.35	0/93216	0.68	0/126696

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3778	0	3604	94	0
1	B	3778	0	3604	93	0
1	C	3778	0	3604	88	0
1	D	3778	0	3604	103	0
1	E	3778	0	3604	99	0
1	F	3778	0	3604	99	0
1	G	3778	0	3604	103	0
1	H	3778	0	3604	96	0
1	I	3778	0	3604	90	0
1	J	3778	0	3604	85	0
1	K	3778	0	3604	100	0
1	L	3778	0	3604	90	0
1	M	3778	0	3604	92	0
1	N	3778	0	3604	99	0
1	O	3778	0	3604	90	0
1	P	3778	0	3604	106	0
1	Q	3778	0	3604	93	0
1	R	3778	0	3604	99	0
1	S	3778	0	3604	94	0
1	T	3778	0	3604	90	0
1	U	3778	0	3604	95	0
1	V	3778	0	3604	88	0
1	W	3778	0	3604	96	0
1	X	3778	0	3604	89	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	A	23	0	10	7	0
3	B	23	0	10	7	0
3	C	23	0	10	7	0
3	D	23	0	10	7	0
3	E	23	0	10	7	0
3	F	23	0	10	7	0
3	G	23	0	10	7	0
3	H	23	0	10	7	0
3	I	23	0	10	7	0
3	J	23	0	10	7	0
3	K	23	0	10	8	0
3	L	23	0	10	7	0
3	M	23	0	10	7	0
3	N	23	0	10	7	0
3	O	23	0	10	7	0
3	P	23	0	10	7	0
3	Q	23	0	10	7	0
3	R	23	0	10	7	0
3	S	23	0	10	7	0
3	T	23	0	10	7	0
3	U	23	0	10	7	0
3	V	23	0	10	7	0
3	W	23	0	10	7	0
3	X	23	0	10	7	0
4	A	13	0	5	6	0
4	B	13	0	5	6	0
4	C	13	0	5	5	0
4	D	13	0	5	6	0
4	E	13	0	5	5	0
4	F	13	0	5	6	0
4	G	13	0	5	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	13	0	5	6	0
4	I	13	0	5	6	0
4	J	13	0	5	5	0
4	K	13	0	5	6	0
4	L	13	0	5	6	0
4	M	13	0	5	6	0
4	N	13	0	5	6	0
4	O	13	0	5	5	0
4	P	13	0	5	6	0
4	Q	13	0	5	5	0
4	R	13	0	5	6	0
4	S	13	0	5	6	0
4	T	13	0	5	6	0
4	U	13	0	5	6	0
4	V	13	0	5	5	0
4	W	13	0	5	6	0
4	X	13	0	5	6	0
5	A	261	0	0	4	0
5	B	262	0	0	5	0
5	C	264	0	0	4	0
5	D	262	0	0	7	0
5	E	261	0	0	4	0
5	F	267	0	0	6	0
5	G	262	0	0	4	0
5	H	263	0	0	4	0
5	I	263	0	0	4	0
5	J	262	0	0	3	0
5	K	267	0	0	5	0
5	L	262	0	0	3	0
5	M	263	0	0	4	0
5	N	262	0	0	4	0
5	O	265	0	0	3	0
5	P	265	0	0	7	0
5	Q	259	0	0	4	0
5	R	269	0	0	6	0
5	S	262	0	0	5	0
5	T	258	0	0	5	0
5	U	265	0	0	5	0
5	V	263	0	0	3	0
5	W	263	0	0	3	0
5	X	262	0	0	5	0
All	All	97872	0	86856	1941	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 11.

All (1941) 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)
3:L:7497:AMP:C1'	3:L:7497:AMP:N9	1.76	1.49
3:X:7521:AMP:N9	3:X:7521:AMP:C1'	1.76	1.49
3:S:7511:AMP:N9	3:S:7511:AMP:C1'	1.76	1.49
3:M:7499:AMP:C1'	3:M:7499:AMP:N9	1.76	1.49
3:H:7489:AMP:C1'	3:H:7489:AMP:N9	1.76	1.49
3:T:7513:AMP:C1'	3:T:7513:AMP:N9	1.76	1.49
3:J:7493:AMP:N9	3:J:7493:AMP:C1'	1.76	1.48
3:V:7517:AMP:C1'	3:V:7517:AMP:N9	1.76	1.48
3:G:7487:AMP:C1'	3:G:7487:AMP:N9	1.76	1.48
3:A:7475:AMP:C1'	3:A:7475:AMP:N9	1.76	1.48
3:Q:7507:AMP:N9	3:Q:7507:AMP:C1'	1.76	1.48
3:E:7483:AMP:C1'	3:E:7483:AMP:N9	1.76	1.48
3:D:7481:AMP:C1'	3:D:7481:AMP:N9	1.76	1.48
3:P:7505:AMP:N9	3:P:7505:AMP:C1'	1.76	1.48
3:N:7501:AMP:N9	3:N:7501:AMP:C1'	1.76	1.47
3:O:7503:AMP:N9	3:O:7503:AMP:C1'	1.76	1.47
3:C:7479:AMP:N9	3:C:7479:AMP:C1'	1.76	1.47
3:B:7477:AMP:N9	3:B:7477:AMP:C1'	1.76	1.46
3:F:7485:AMP:N9	3:F:7485:AMP:C1'	1.76	1.45
3:I:7491:AMP:C1'	3:I:7491:AMP:N9	1.76	1.45
3:K:7495:AMP:C1'	3:K:7495:AMP:N9	1.76	1.45
3:R:7509:AMP:C1'	3:R:7509:AMP:N9	1.76	1.45
3:U:7515:AMP:N9	3:U:7515:AMP:C1'	1.76	1.44
3:W:7519:AMP:N9	3:W:7519:AMP:C1'	1.76	1.43
1:A:179:TYR:HB2	1:B:53:SER:OG	1.48	1.10
1:M:179:TYR:HB2	1:N:53:SER:OG	1.51	1.10
1:R:127:GLY:HA3	3:R:7509:AMP:H1'	1.36	1.07
1:F:127:GLY:HA3	3:F:7485:AMP:H1'	1.36	1.07
1:D:175:HIS:HE1	1:K:467:ASP:OD2	1.38	1.07
1:N:179:TYR:HB2	1:O:53:SER:OG	1.54	1.07
1:U:127:GLY:HA3	3:U:7515:AMP:H1'	1.36	1.06
1:E:179:TYR:HB2	1:F:53:SER:OG	1.55	1.06
1:I:127:GLY:HA3	3:I:7491:AMP:H1'	1.36	1.06
1:G:127:GLY:HA3	3:G:7487:AMP:H1'	1.36	1.06
1:S:127:GLY:HA3	3:S:7511:AMP:H1'	1.36	1.06
1:K:127:GLY:HA3	3:K:7495:AMP:H1'	1.36	1.05
1:W:127:GLY:HA3	3:W:7519:AMP:H1'	1.36	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:53:SER:OG	1:T:179:TYR:HB2	1.55	1.05
1:P:127:GLY:HA3	3:P:7505:AMP:H1'	1.36	1.04
1:W:53:SER:OG	1:X:179:TYR:HB2	1.55	1.04
1:C:127:GLY:HA3	3:C:7479:AMP:H1'	1.36	1.04
1:D:127:GLY:HA3	3:D:7481:AMP:H1'	1.36	1.04
1:O:127:GLY:HA3	3:O:7503:AMP:H1'	1.36	1.04
1:L:127:GLY:HA3	3:L:7497:AMP:H1'	1.36	1.04
1:T:127:GLY:HA3	3:T:7513:AMP:H1'	1.36	1.04
1:H:127:GLY:HA3	3:H:7489:AMP:H1'	1.36	1.03
1:X:127:GLY:HA3	3:X:7521:AMP:H1'	1.36	1.03
1:D:467:ASP:OD2	1:K:175:HIS:HE1	1.41	1.03
1:M:127:GLY:HA3	3:M:7499:AMP:H1'	1.36	1.03
1:J:127:GLY:HA3	3:J:7493:AMP:H1'	1.36	1.02
1:A:127:GLY:HA3	3:A:7475:AMP:H1'	1.36	1.02
1:B:127:GLY:HA3	3:B:7477:AMP:H1'	1.36	1.02
1:H:53:SER:OG	1:I:179:TYR:HB2	1.58	1.02
1:N:127:GLY:HA3	3:N:7501:AMP:H1'	1.36	1.02
1:V:127:GLY:HA3	3:V:7517:AMP:H1'	1.36	1.02
1:Q:127:GLY:HA3	3:Q:7507:AMP:H1'	1.36	1.02
1:E:127:GLY:HA3	3:E:7483:AMP:H1'	1.36	1.02
1:M:53:SER:OG	1:R:179:TYR:HB2	1.60	1.01
1:I:53:SER:OG	1:J:179:TYR:HB2	1.61	1.01
1:G:53:SER:OG	1:H:179:TYR:HB2	1.59	1.01
1:B:179:TYR:HB2	1:C:53:SER:OG	1.60	0.99
1:U:53:SER:OG	1:V:179:TYR:HB2	1.60	0.99
1:J:53:SER:OG	1:K:179:TYR:HB2	1.62	0.99
1:C:179:TYR:HB2	1:D:53:SER:OG	1.63	0.98
1:Q:179:TYR:HB2	1:R:53:SER:OG	1.65	0.97
1:K:53:SER:OG	1:L:179:TYR:HB2	1.66	0.96
1:V:53:SER:OG	1:W:179:TYR:HB2	1.66	0.96
1:O:179:TYR:HB2	1:P:53:SER:OG	1.66	0.95
1:P:467:ASP:OD2	1:W:175:HIS:HE1	1.50	0.95
1:T:53:SER:OG	1:U:179:TYR:HB2	1.66	0.95
1:G:179:TYR:HB2	1:L:53:SER:OG	1.67	0.94
1:A:53:SER:OG	1:F:179:TYR:HB2	1.66	0.94
1:V:207:GLU:H	1:V:210:HIS:HD2	1.16	0.94
1:J:207:GLU:H	1:J:210:HIS:HD2	1.16	0.94
1:O:207:GLU:H	1:O:210:HIS:HD2	1.16	0.93
1:X:207:GLU:H	1:X:210:HIS:HD2	1.16	0.93
1:C:207:GLU:H	1:C:210:HIS:HD2	1.16	0.93
1:H:207:GLU:H	1:H:210:HIS:HD2	1.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:HIS:CE1	1:K:467:ASP:OD2	2.22	0.93
1:T:207:GLU:H	1:T:210:HIS:HD2	1.16	0.92
1:L:207:GLU:H	1:L:210:HIS:HD2	1.16	0.92
1:N:207:GLU:H	1:N:210:HIS:HD2	1.16	0.92
1:W:207:GLU:H	1:W:210:HIS:HD2	1.16	0.92
1:D:175:HIS:CE1	1:K:467:ASP:HB2	2.03	0.92
1:B:207:GLU:H	1:B:210:HIS:HD2	1.16	0.92
1:S:179:TYR:HB2	1:X:53:SER:OG	1.69	0.92
1:K:207:GLU:H	1:K:210:HIS:HD2	1.16	0.91
1:P:179:TYR:HB2	1:Q:53:SER:OG	1.70	0.91
1:E:207:GLU:H	1:E:210:HIS:HD2	1.16	0.91
1:M:207:GLU:H	1:M:210:HIS:HD2	1.16	0.91
1:A:207:GLU:H	1:A:210:HIS:HD2	1.16	0.91
1:J:458:HIS:HD2	1:J:460:TYR:H	1.19	0.90
1:Q:207:GLU:H	1:Q:210:HIS:HD2	1.16	0.90
1:V:458:HIS:HD2	1:V:460:TYR:H	1.19	0.90
1:W:458:HIS:HD2	1:W:460:TYR:H	1.19	0.90
1:C:458:HIS:HD2	1:C:460:TYR:H	1.19	0.90
1:G:207:GLU:H	1:G:210:HIS:HD2	1.16	0.90
1:M:458:HIS:HD2	1:M:460:TYR:H	1.19	0.90
1:A:458:HIS:HD2	1:A:460:TYR:H	1.19	0.90
1:K:458:HIS:HD2	1:K:460:TYR:H	1.19	0.90
1:F:207:GLU:H	1:F:210:HIS:HD2	1.16	0.90
1:D:458:HIS:HD2	1:D:460:TYR:H	1.19	0.89
1:O:458:HIS:HD2	1:O:460:TYR:H	1.19	0.89
1:P:458:HIS:HD2	1:P:460:TYR:H	1.19	0.89
1:R:207:GLU:H	1:R:210:HIS:HD2	1.16	0.89
1:L:458:HIS:HD2	1:L:460:TYR:H	1.19	0.89
1:X:458:HIS:HD2	1:X:460:TYR:H	1.19	0.89
1:B:458:HIS:HD2	1:B:460:TYR:H	1.19	0.89
1:L:54:ILE:O	1:L:54:ILE:HD12	1.73	0.89
1:O:54:ILE:HD12	1:O:54:ILE:O	1.73	0.89
1:X:54:ILE:O	1:X:54:ILE:HD12	1.73	0.89
1:C:54:ILE:O	1:C:54:ILE:HD12	1.73	0.89
1:S:207:GLU:H	1:S:210:HIS:HD2	1.16	0.89
1:T:54:ILE:O	1:T:54:ILE:HD12	1.73	0.89
1:B:54:ILE:O	1:B:54:ILE:HD12	1.73	0.89
1:F:175:HIS:HE1	1:G:467:ASP:OD2	1.53	0.89
1:J:54:ILE:O	1:J:54:ILE:HD12	1.73	0.89
1:V:54:ILE:HD12	1:V:54:ILE:O	1.73	0.89
1:F:54:ILE:HD12	1:F:54:ILE:O	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:ILE:HD12	1:H:54:ILE:O	1.73	0.89
1:N:458:HIS:HD2	1:N:460:TYR:H	1.19	0.89
1:N:54:ILE:HD12	1:N:54:ILE:O	1.73	0.89
1:D:207:GLU:H	1:D:210:HIS:HD2	1.16	0.89
1:K:54:ILE:HD12	1:K:54:ILE:O	1.73	0.88
1:R:54:ILE:HD12	1:R:54:ILE:O	1.73	0.88
1:E:458:HIS:HD2	1:E:460:TYR:H	1.19	0.88
1:E:54:ILE:O	1:E:54:ILE:HD12	1.73	0.88
1:T:458:HIS:HD2	1:T:460:TYR:H	1.19	0.88
1:U:458:HIS:HD2	1:U:460:TYR:H	1.19	0.88
1:W:54:ILE:HD12	1:W:54:ILE:O	1.73	0.88
1:H:458:HIS:HD2	1:H:460:TYR:H	1.19	0.88
1:P:207:GLU:H	1:P:210:HIS:HD2	1.16	0.88
1:Q:54:ILE:HD12	1:Q:54:ILE:O	1.73	0.88
1:S:54:ILE:O	1:S:54:ILE:HD12	1.73	0.88
1:G:54:ILE:HD12	1:G:54:ILE:O	1.73	0.88
1:Q:458:HIS:HD2	1:Q:460:TYR:H	1.19	0.88
1:U:207:GLU:H	1:U:210:HIS:HD2	1.16	0.88
1:I:54:ILE:HD12	1:I:54:ILE:O	1.73	0.88
1:I:458:HIS:HD2	1:I:460:TYR:H	1.19	0.88
1:I:207:GLU:H	1:I:210:HIS:HD2	1.16	0.88
1:U:54:ILE:O	1:U:54:ILE:HD12	1.73	0.88
1:D:54:ILE:HD12	1:D:54:ILE:O	1.73	0.88
1:G:458:HIS:HD2	1:G:460:TYR:H	1.19	0.87
1:P:54:ILE:O	1:P:54:ILE:HD12	1.73	0.87
1:M:54:ILE:O	1:M:54:ILE:HD12	1.73	0.87
1:S:458:HIS:HD2	1:S:460:TYR:H	1.19	0.87
1:A:54:ILE:O	1:A:54:ILE:HD12	1.73	0.87
1:A:321:ARG:HE	4:A:7476:CIT:H42	1.41	0.86
1:M:321:ARG:HE	4:M:7500:CIT:H42	1.41	0.86
1:F:458:HIS:HD2	1:F:460:TYR:H	1.19	0.86
1:N:321:ARG:HE	4:N:7502:CIT:H42	1.41	0.86
1:R:458:HIS:HD2	1:R:460:TYR:H	1.19	0.86
1:S:321:ARG:HE	4:S:7512:CIT:H42	1.41	0.86
1:P:175:HIS:HE1	1:W:467:ASP:OD2	1.58	0.85
1:G:321:ARG:HE	4:G:7488:CIT:H42	1.41	0.85
1:B:321:ARG:HE	4:B:7478:CIT:H42	1.41	0.85
1:R:321:ARG:HE	4:R:7510:CIT:H42	1.41	0.85
1:F:321:ARG:HE	4:F:7486:CIT:H42	1.41	0.85
1:U:321:ARG:HE	4:U:7516:CIT:H42	1.41	0.85
1:G:312:THR:HG22	1:G:313:ASN:HD22	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:HIS:HE1	1:K:467:ASP:CG	1.78	0.85
1:H:321:ARG:HE	4:H:7490:CIT:H42	1.41	0.85
1:I:321:ARG:HE	4:I:7492:CIT:H42	1.41	0.85
1:K:312:THR:HG22	1:K:313:ASN:HD22	1.42	0.85
1:W:312:THR:HG22	1:W:313:ASN:HD22	1.42	0.85
1:L:312:THR:HG22	1:L:313:ASN:HD22	1.42	0.85
1:Q:321:ARG:HE	4:Q:7508:CIT:H42	1.41	0.85
1:S:312:THR:HG22	1:S:313:ASN:HD22	1.42	0.85
1:X:312:THR:HG22	1:X:313:ASN:HD22	1.42	0.85
1:O:321:ARG:HE	4:O:7504:CIT:H42	1.41	0.85
1:P:321:ARG:HE	4:P:7506:CIT:H42	1.41	0.85
1:T:321:ARG:HE	4:T:7514:CIT:H42	1.41	0.85
1:W:321:ARG:HE	4:W:7520:CIT:H42	1.41	0.85
1:X:321:ARG:HE	4:X:7522:CIT:H42	1.41	0.85
1:C:321:ARG:HE	4:C:7480:CIT:H42	1.41	0.84
1:E:321:ARG:HE	4:E:7484:CIT:H42	1.41	0.84
1:O:312:THR:HG22	1:O:313:ASN:HD22	1.42	0.84
1:R:312:THR:HG22	1:R:313:ASN:HD22	1.42	0.84
1:D:321:ARG:HE	4:D:7482:CIT:H42	1.41	0.84
1:C:312:THR:HG22	1:C:313:ASN:HD22	1.42	0.84
1:F:312:THR:HG22	1:F:313:ASN:HD22	1.42	0.84
1:I:312:THR:HG22	1:I:313:ASN:HD22	1.42	0.84
1:K:321:ARG:HE	4:K:7496:CIT:H42	1.41	0.84
1:L:321:ARG:HE	4:L:7498:CIT:H42	1.41	0.84
1:U:312:THR:HG22	1:U:313:ASN:HD22	1.42	0.84
1:B:312:THR:HG22	1:B:313:ASN:HD22	1.42	0.84
1:N:312:THR:HG22	1:N:313:ASN:HD22	1.42	0.84
1:D:312:THR:HG22	1:D:313:ASN:HD22	1.42	0.84
1:P:312:THR:HG22	1:P:313:ASN:HD22	1.42	0.84
1:J:321:ARG:HE	4:J:7494:CIT:H42	1.41	0.83
1:V:321:ARG:HE	4:V:7518:CIT:H42	1.41	0.83
1:D:467:ASP:OD2	1:K:175:HIS:CE1	2.30	0.83
1:T:312:THR:HG22	1:T:313:ASN:HD22	1.42	0.83
1:V:312:THR:HG22	1:V:313:ASN:HD22	1.42	0.83
1:H:312:THR:HG22	1:H:313:ASN:HD22	1.42	0.83
1:J:312:THR:HG22	1:J:313:ASN:HD22	1.42	0.83
1:E:312:THR:HG22	1:E:313:ASN:HD22	1.42	0.83
1:O:180:PHE:HE2	1:P:52:SER:CB	1.91	0.83
1:Q:312:THR:HG22	1:Q:313:ASN:HD22	1.42	0.83
1:A:312:THR:HG22	1:A:313:ASN:HD22	1.42	0.83
1:O:180:PHE:CE2	1:P:52:SER:HB3	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:TYR:HB2	1:E:53:SER:OG	1.78	0.82
1:M:312:THR:HG22	1:M:313:ASN:HD22	1.42	0.82
1:A:179:TYR:CB	1:B:53:SER:OG	2.26	0.81
1:A:179:TYR:HB2	1:B:53:SER:HG	1.45	0.81
1:A:207:GLU:H	1:A:210:HIS:CD2	1.99	0.81
1:C:207:GLU:H	1:C:210:HIS:CD2	1.99	0.81
1:O:207:GLU:H	1:O:210:HIS:CD2	1.99	0.81
1:E:207:GLU:H	1:E:210:HIS:CD2	1.99	0.80
1:M:207:GLU:H	1:M:210:HIS:CD2	1.99	0.80
1:Q:207:GLU:H	1:Q:210:HIS:CD2	1.99	0.80
1:P:207:GLU:H	1:P:210:HIS:CD2	1.99	0.80
1:D:207:GLU:H	1:D:210:HIS:CD2	1.99	0.80
1:E:180:PHE:HE2	1:F:52:SER:CB	1.95	0.80
1:J:207:GLU:H	1:J:210:HIS:CD2	1.99	0.80
1:V:207:GLU:H	1:V:210:HIS:CD2	1.99	0.80
1:H:207:GLU:H	1:H:210:HIS:CD2	1.99	0.79
1:T:207:GLU:H	1:T:210:HIS:CD2	1.99	0.79
1:L:207:GLU:H	1:L:210:HIS:CD2	1.99	0.79
1:X:207:GLU:H	1:X:210:HIS:CD2	1.99	0.79
1:K:207:GLU:H	1:K:210:HIS:CD2	1.99	0.79
1:G:207:GLU:H	1:G:210:HIS:CD2	1.99	0.79
1:I:207:GLU:H	1:I:210:HIS:CD2	1.99	0.79
1:S:207:GLU:H	1:S:210:HIS:CD2	1.99	0.79
1:U:207:GLU:H	1:U:210:HIS:CD2	1.99	0.78
1:W:207:GLU:H	1:W:210:HIS:CD2	1.99	0.78
1:E:179:TYR:CB	1:F:53:SER:OG	2.30	0.78
1:A:60:ILE:HD12	5:F:7676:HOH:O	1.83	0.78
1:B:207:GLU:H	1:B:210:HIS:CD2	1.99	0.78
1:N:207:GLU:H	1:N:210:HIS:CD2	1.99	0.78
1:T:312:THR:CG2	1:T:313:ASN:HD22	1.97	0.78
1:H:312:THR:CG2	1:H:313:ASN:HD22	1.97	0.78
1:M:179:TYR:CB	1:N:53:SER:OG	2.31	0.78
1:U:312:THR:CG2	1:U:313:ASN:HD22	1.97	0.77
1:I:312:THR:CG2	1:I:313:ASN:HD22	1.97	0.77
1:J:312:THR:CG2	1:J:313:ASN:HD22	1.97	0.77
1:O:312:THR:CG2	1:O:313:ASN:HD22	1.97	0.77
1:R:207:GLU:H	1:R:210:HIS:CD2	1.99	0.77
1:V:312:THR:CG2	1:V:313:ASN:HD22	1.97	0.77
1:S:53:SER:OG	1:T:179:TYR:CB	2.30	0.77
1:D:312:THR:CG2	1:D:313:ASN:HD22	1.97	0.77
1:F:207:GLU:H	1:F:210:HIS:CD2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:THR:CG2	1:C:313:ASN:HD22	1.97	0.77
1:P:312:THR:CG2	1:P:313:ASN:HD22	1.97	0.77
1:E:180:PHE:CE2	1:F:52:SER:HB3	2.19	0.77
1:E:312:THR:CG2	1:E:313:ASN:HD22	1.97	0.77
1:N:179:TYR:CB	1:O:53:SER:OG	2.32	0.77
1:R:312:THR:CG2	1:R:313:ASN:HD22	1.97	0.77
1:F:312:THR:CG2	1:F:313:ASN:HD22	1.97	0.77
1:F:4:ASP:OD2	1:S:10:LYS:HE2	1.85	0.77
1:Q:312:THR:CG2	1:Q:313:ASN:HD22	1.97	0.77
1:G:312:THR:CG2	1:G:313:ASN:HD22	1.97	0.76
1:S:312:THR:CG2	1:S:313:ASN:HD22	1.97	0.76
1:M:179:TYR:HB2	1:N:53:SER:HG	1.50	0.76
1:O:180:PHE:CE2	1:P:52:SER:CB	2.68	0.76
1:A:312:THR:CG2	1:A:313:ASN:HD22	1.97	0.76
1:E:180:PHE:CE2	1:F:52:SER:CB	2.68	0.76
1:M:60:ILE:HD12	5:R:4666:HOH:O	1.84	0.76
1:M:312:THR:CG2	1:M:313:ASN:HD22	1.97	0.76
1:X:312:THR:CG2	1:X:313:ASN:HD22	1.97	0.76
1:K:312:THR:CG2	1:K:313:ASN:HD22	1.97	0.76
1:L:312:THR:CG2	1:L:313:ASN:HD22	1.97	0.76
1:N:312:THR:CG2	1:N:313:ASN:HD22	1.97	0.76
1:W:312:THR:CG2	1:W:313:ASN:HD22	1.97	0.76
1:B:312:THR:CG2	1:B:313:ASN:HD22	1.97	0.75
1:D:175:HIS:CE1	1:K:467:ASP:CB	2.70	0.74
1:O:180:PHE:HE2	1:P:52:SER:HB2	1.51	0.74
1:P:175:HIS:CE1	1:W:467:ASP:HB2	2.22	0.74
1:E:180:PHE:HE2	1:F:52:SER:HB2	1.53	0.73
1:D:467:ASP:HB2	1:K:175:HIS:CE1	2.24	0.73
1:D:96:THR:OG1	1:D:98:GLU:HB2	1.88	0.73
1:P:467:ASP:OD2	1:W:175:HIS:CE1	2.40	0.73
1:D:264:ASN:ND2	4:D:7482:CIT:O3	2.22	0.73
1:O:312:THR:CG2	1:O:313:ASN:ND2	2.52	0.73
1:P:264:ASN:ND2	4:P:7506:CIT:O3	2.22	0.73
1:C:312:THR:CG2	1:C:313:ASN:ND2	2.52	0.73
1:E:312:THR:CG2	1:E:313:ASN:ND2	2.52	0.73
1:W:264:ASN:ND2	4:W:7520:CIT:O3	2.22	0.73
1:K:264:ASN:ND2	4:K:7496:CIT:O3	2.22	0.73
1:N:312:THR:CG2	1:N:313:ASN:ND2	2.52	0.73
1:Q:312:THR:CG2	1:Q:313:ASN:ND2	2.52	0.73
1:A:312:THR:CG2	1:A:313:ASN:ND2	2.52	0.72
1:M:312:THR:CG2	1:M:313:ASN:ND2	2.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:312:THR:CG2	1:S:313:ASN:ND2	2.52	0.72
1:B:312:THR:CG2	1:B:313:ASN:ND2	2.52	0.72
1:G:312:THR:CG2	1:G:313:ASN:ND2	2.52	0.72
1:L:312:THR:CG2	1:L:313:ASN:ND2	2.52	0.72
1:R:312:THR:CG2	1:R:313:ASN:ND2	2.52	0.72
1:X:312:THR:CG2	1:X:313:ASN:ND2	2.52	0.72
1:U:264:ASN:ND2	4:U:7516:CIT:O3	2.22	0.72
1:W:312:THR:CG2	1:W:313:ASN:ND2	2.52	0.72
1:F:312:THR:CG2	1:F:313:ASN:ND2	2.52	0.72
1:G:264:ASN:ND2	4:G:7488:CIT:O3	2.22	0.72
1:J:312:THR:CG2	1:J:313:ASN:ND2	2.52	0.72
1:K:312:THR:CG2	1:K:313:ASN:ND2	2.52	0.72
1:V:312:THR:CG2	1:V:313:ASN:ND2	2.52	0.72
1:A:264:ASN:ND2	4:A:7476:CIT:O3	2.22	0.72
1:I:264:ASN:ND2	4:I:7492:CIT:O3	2.22	0.72
1:M:60:ILE:HG22	1:R:339:ARG:HD2	1.70	0.72
1:S:264:ASN:ND2	4:S:7512:CIT:O3	2.22	0.72
1:T:312:THR:CG2	1:T:313:ASN:ND2	2.52	0.72
1:W:53:SER:OG	1:X:179:TYR:CB	2.36	0.72
1:M:264:ASN:ND2	4:M:7500:CIT:O3	2.22	0.72
1:C:264:ASN:ND2	4:C:7480:CIT:O3	2.22	0.72
1:E:264:ASN:ND2	4:E:7484:CIT:O3	2.22	0.72
1:H:312:THR:CG2	1:H:313:ASN:ND2	2.52	0.72
1:I:312:THR:CG2	1:I:313:ASN:ND2	2.52	0.72
1:C:338:ASN:HD21	1:C:396:LEU:H	1.38	0.71
1:J:338:ASN:HD21	1:J:396:LEU:H	1.38	0.71
1:O:264:ASN:ND2	4:O:7504:CIT:O3	2.22	0.71
1:Q:264:ASN:ND2	4:Q:7508:CIT:O3	2.22	0.71
1:V:338:ASN:HD21	1:V:396:LEU:H	1.38	0.71
1:P:312:THR:CG2	1:P:313:ASN:ND2	2.52	0.71
1:R:264:ASN:ND2	4:R:7510:CIT:O3	2.22	0.71
1:T:264:ASN:ND2	4:T:7514:CIT:O3	2.22	0.71
1:U:312:THR:CG2	1:U:313:ASN:ND2	2.52	0.71
1:D:312:THR:CG2	1:D:313:ASN:ND2	2.52	0.71
1:O:338:ASN:HD21	1:O:396:LEU:H	1.38	0.71
1:B:264:ASN:ND2	4:B:7478:CIT:O3	2.22	0.71
1:D:338:ASN:HD22	1:E:60:ILE:HD12	1.56	0.71
1:F:264:ASN:ND2	4:F:7486:CIT:O3	2.22	0.71
1:H:264:ASN:ND2	4:H:7490:CIT:O3	2.22	0.71
1:L:264:ASN:ND2	4:L:7498:CIT:O3	2.22	0.71
1:Q:502:PRO:HB2	1:R:137:SER:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:338:ASN:HD21	1:R:396:LEU:H	1.38	0.71
1:F:338:ASN:HD21	1:F:396:LEU:H	1.38	0.71
1:X:264:ASN:ND2	4:X:7522:CIT:O3	2.22	0.71
1:V:264:ASN:ND2	4:V:7518:CIT:O3	2.22	0.71
1:E:338:ASN:HD21	1:E:396:LEU:H	1.38	0.71
1:Q:338:ASN:HD21	1:Q:396:LEU:H	1.38	0.71
1:S:338:ASN:HD21	1:S:396:LEU:H	1.38	0.71
1:G:338:ASN:HD21	1:G:396:LEU:H	1.38	0.71
1:J:264:ASN:ND2	4:J:7494:CIT:O3	2.22	0.71
1:O:193:ASP:OD2	1:P:80:ARG:HD3	1.90	0.71
1:T:338:ASN:HD21	1:T:396:LEU:H	1.38	0.71
1:N:264:ASN:ND2	4:N:7502:CIT:O3	2.22	0.71
1:N:467:ASP:OD2	1:U:175:HIS:HE1	1.73	0.71
1:G:53:SER:OG	1:H:179:TYR:CB	2.38	0.70
1:S:53:SER:HG	1:T:179:TYR:HB2	1.56	0.70
1:H:338:ASN:HD21	1:H:396:LEU:H	1.38	0.70
1:E:179:TYR:N	1:F:53:SER:OG	2.23	0.70
1:P:458:HIS:HE1	1:V:456:ARG:O	1.73	0.70
1:D:338:ASN:HD21	1:D:396:LEU:H	1.38	0.70
1:F:467:ASP:HB2	1:G:175:HIS:CE1	2.27	0.70
1:I:338:ASN:HD21	1:I:396:LEU:H	1.38	0.70
1:K:80:ARG:HD3	1:L:193:ASP:OD2	1.92	0.70
1:P:338:ASN:HD21	1:P:396:LEU:H	1.38	0.69
1:F:4:ASP:OD2	1:S:10:LYS:CE	2.39	0.69
1:C:175:HIS:HE1	1:J:467:ASP:OD2	1.75	0.69
1:U:338:ASN:HD21	1:U:396:LEU:H	1.38	0.69
1:A:179:TYR:HD2	1:B:53:SER:HB3	1.56	0.69
1:K:338:ASN:HD21	1:K:396:LEU:H	1.38	0.69
1:B:400:PRO:HG2	1:B:403:GLU:HB3	1.75	0.69
1:Q:193:ASP:OD2	1:R:80:ARG:HD3	1.92	0.69
1:W:400:PRO:HG2	1:W:403:GLU:HB3	1.75	0.69
1:A:400:PRO:HG2	1:A:403:GLU:HB3	1.75	0.69
1:F:273:SER:OG	3:F:7485:AMP:N6	2.26	0.69
1:I:273:SER:OG	3:I:7491:AMP:N6	2.26	0.69
1:N:338:ASN:HD21	1:N:396:LEU:H	1.38	0.69
1:N:400:PRO:HG2	1:N:403:GLU:HB3	1.75	0.69
1:O:273:SER:OG	3:O:7503:AMP:N6	2.26	0.69
1:R:273:SER:OG	3:R:7509:AMP:N6	2.26	0.69
1:U:273:SER:OG	3:U:7515:AMP:N6	2.26	0.69
1:V:400:PRO:HG2	1:V:403:GLU:HB3	1.75	0.69
1:W:273:SER:OG	3:W:7519:AMP:N6	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:SER:OG	3:A:7475:AMP:N6	2.26	0.69
1:C:273:SER:OG	3:C:7479:AMP:N6	2.26	0.69
1:J:400:PRO:HG2	1:J:403:GLU:HB3	1.75	0.69
1:K:400:PRO:HG2	1:K:403:GLU:HB3	1.75	0.69
1:K:273:SER:OG	3:K:7495:AMP:N6	2.26	0.69
1:M:273:SER:OG	3:M:7499:AMP:N6	2.26	0.69
1:M:400:PRO:HG2	1:M:403:GLU:HB3	1.75	0.69
1:T:400:PRO:HG2	1:T:403:GLU:HB3	1.75	0.69
1:U:52:SER:HB3	1:V:180:PHE:CE2	2.28	0.69
1:X:400:PRO:HG2	1:X:403:GLU:HB3	1.75	0.69
1:A:338:ASN:HD21	1:A:396:LEU:H	1.38	0.69
1:H:400:PRO:HG2	1:H:403:GLU:HB3	1.75	0.69
1:J:273:SER:OG	3:J:7493:AMP:N6	2.26	0.69
1:M:338:ASN:HD21	1:M:396:LEU:H	1.38	0.69
1:V:273:SER:OG	3:V:7517:AMP:N6	2.26	0.69
1:G:400:PRO:HG2	1:G:403:GLU:HB3	1.75	0.68
1:L:400:PRO:HG2	1:L:403:GLU:HB3	1.75	0.68
1:N:273:SER:OG	3:N:7501:AMP:N6	2.26	0.68
1:W:338:ASN:HD21	1:W:396:LEU:H	1.38	0.68
1:U:52:SER:CB	1:V:180:PHE:HE2	2.05	0.68
1:W:312:THR:HG23	1:W:313:ASN:ND2	2.09	0.68
1:X:338:ASN:HD21	1:X:396:LEU:H	1.38	0.68
1:A:312:THR:HG23	1:A:313:ASN:ND2	2.09	0.68
1:B:273:SER:OG	3:B:7477:AMP:N6	2.26	0.68
1:E:400:PRO:HG2	1:E:403:GLU:HB3	1.75	0.68
1:H:312:THR:HG23	1:H:313:ASN:ND2	2.09	0.68
1:K:312:THR:HG23	1:K:313:ASN:ND2	2.09	0.68
1:M:312:THR:HG23	1:M:313:ASN:ND2	2.09	0.68
1:S:273:SER:OG	3:S:7511:AMP:N6	2.26	0.68
1:T:273:SER:OG	3:T:7513:AMP:N6	2.26	0.68
1:X:312:THR:HG23	1:X:313:ASN:ND2	2.09	0.68
1:B:338:ASN:HD21	1:B:396:LEU:H	1.38	0.68
1:L:312:THR:HG23	1:L:313:ASN:ND2	2.09	0.68
1:Q:400:PRO:HG2	1:Q:403:GLU:HB3	1.75	0.68
1:T:312:THR:HG23	1:T:313:ASN:ND2	2.09	0.68
1:B:312:THR:HG23	1:B:313:ASN:ND2	2.09	0.68
1:C:400:PRO:HG2	1:C:403:GLU:HB3	1.75	0.68
1:H:273:SER:OG	3:H:7489:AMP:N6	2.26	0.68
1:S:400:PRO:HG2	1:S:403:GLU:HB3	1.75	0.68
1:N:312:THR:HG23	1:N:313:ASN:ND2	2.09	0.68
1:O:400:PRO:HG2	1:O:403:GLU:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:312:THR:HG23	1:R:313:ASN:ND2	2.09	0.68
1:D:400:PRO:HG2	1:D:403:GLU:HB3	1.75	0.68
1:D:273:SER:OG	3:D:7481:AMP:N6	2.26	0.68
1:F:312:THR:HG23	1:F:313:ASN:ND2	2.09	0.68
1:G:273:SER:OG	3:G:7487:AMP:N6	2.26	0.68
1:L:338:ASN:HD21	1:L:396:LEU:H	1.38	0.68
1:F:175:HIS:CE1	1:G:467:ASP:OD2	2.43	0.68
1:P:400:PRO:HG2	1:P:403:GLU:HB3	1.75	0.68
1:P:273:SER:OG	3:P:7505:AMP:N6	2.26	0.68
1:G:312:THR:HG23	1:G:313:ASN:ND2	2.09	0.68
1:L:273:SER:OG	3:L:7497:AMP:N6	2.26	0.68
5:P:4140:HOH:O	1:Q:60:ILE:HD12	1.94	0.67
1:R:400:PRO:HG2	1:R:403:GLU:HB3	1.75	0.67
1:O:312:THR:HG23	1:O:313:ASN:ND2	2.09	0.67
1:X:273:SER:OG	3:X:7521:AMP:N6	2.26	0.67
1:F:400:PRO:HG2	1:F:403:GLU:HB3	1.75	0.67
5:M:3330:HOH:O	1:R:176:LYS:HE3	1.93	0.67
1:S:312:THR:HG23	1:S:313:ASN:ND2	2.09	0.67
1:E:273:SER:OG	3:E:7483:AMP:N6	2.26	0.67
1:P:338:ASN:HD22	1:Q:60:ILE:HD12	1.59	0.67
1:Q:273:SER:OG	3:Q:7507:AMP:N6	2.26	0.67
1:V:312:THR:HG23	1:V:313:ASN:ND2	2.09	0.67
1:J:312:THR:HG23	1:J:313:ASN:ND2	2.09	0.67
1:D:312:THR:HG23	1:D:313:ASN:ND2	2.09	0.67
1:D:458:HIS:HE1	1:J:456:ARG:O	1.77	0.67
1:F:175:HIS:CE1	1:G:467:ASP:HB2	2.30	0.67
1:P:312:THR:HG23	1:P:313:ASN:ND2	2.09	0.67
1:C:312:THR:HG23	1:C:313:ASN:ND2	2.09	0.67
1:E:312:THR:HG23	1:E:313:ASN:ND2	2.09	0.67
1:U:400:PRO:HG2	1:U:403:GLU:HB3	1.75	0.67
1:B:179:TYR:CB	1:C:53:SER:OG	2.40	0.67
1:I:400:PRO:HG2	1:I:403:GLU:HB3	1.75	0.67
1:U:53:SER:HG	1:V:179:TYR:HB2	1.59	0.67
1:Q:312:THR:HG23	1:Q:313:ASN:ND2	2.09	0.66
1:S:53:SER:HB3	1:T:179:TYR:HD2	1.58	0.66
1:G:338:ASN:HD22	1:L:60:ILE:HD12	1.61	0.66
1:P:175:HIS:CE1	1:W:467:ASP:OD2	2.45	0.66
1:C:180:PHE:HE2	1:D:52:SER:CB	2.08	0.66
1:I:312:THR:HG23	1:I:313:ASN:ND2	2.09	0.66
1:Q:179:TYR:CB	1:R:53:SER:OG	2.41	0.66
1:I:53:SER:OG	1:J:179:TYR:CB	2.40	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:312:THR:HG23	1:U:313:ASN:ND2	2.09	0.66
1:U:52:SER:CB	1:V:180:PHE:CE2	2.79	0.66
1:R:463:ALA:HA	1:X:140:PHE:CE1	2.30	0.65
1:T:458:HIS:CD2	1:T:460:TYR:H	2.10	0.65
1:H:458:HIS:CD2	1:H:460:TYR:H	2.10	0.65
1:R:175:HIS:CE1	1:S:467:ASP:HB2	2.31	0.65
1:A:60:ILE:HD12	1:F:338:ASN:HD22	1.61	0.65
1:J:458:HIS:CD2	1:J:460:TYR:H	2.10	0.65
1:U:53:SER:OG	1:V:179:TYR:CB	2.39	0.65
1:V:458:HIS:CD2	1:V:460:TYR:H	2.10	0.65
1:D:467:ASP:CG	1:K:175:HIS:HE1	2.00	0.65
1:B:180:PHE:HE2	1:C:52:SER:CB	2.09	0.65
1:C:458:HIS:CD2	1:C:460:TYR:H	2.10	0.65
1:D:206:LEU:HD13	1:D:210:HIS:HB3	1.79	0.65
1:P:206:LEU:HD13	1:P:210:HIS:HB3	1.79	0.65
1:N:179:TYR:HD2	1:O:53:SER:HB3	1.62	0.65
1:J:53:SER:OG	1:K:179:TYR:CB	2.42	0.65
1:C:206:LEU:HD13	1:C:210:HIS:HB3	1.79	0.64
1:E:463:ALA:HA	1:K:140:PHE:CE1	2.32	0.64
1:O:206:LEU:HD13	1:O:210:HIS:HB3	1.79	0.64
1:H:53:SER:OG	1:I:179:TYR:CB	2.42	0.64
1:O:458:HIS:CD2	1:O:460:TYR:H	2.10	0.64
1:C:180:PHE:CE2	1:D:52:SER:HB3	2.31	0.64
1:I:206:LEU:HD13	1:I:210:HIS:HB3	1.79	0.64
1:A:206:LEU:HD13	1:A:210:HIS:HB3	1.79	0.64
1:M:206:LEU:HD13	1:M:210:HIS:HB3	1.79	0.64
1:U:206:LEU:HD13	1:U:210:HIS:HB3	1.79	0.64
1:L:206:LEU:HD13	1:L:210:HIS:HB3	1.79	0.64
1:M:458:HIS:CD2	1:M:460:TYR:H	2.10	0.64
1:X:206:LEU:HD13	1:X:210:HIS:HB3	1.79	0.64
1:A:458:HIS:CD2	1:A:460:TYR:H	2.10	0.64
1:G:458:HIS:CD2	1:G:460:TYR:H	2.10	0.64
1:U:52:SER:HB2	1:V:180:PHE:HE2	1.62	0.64
1:P:467:ASP:HB2	1:W:175:HIS:CE1	2.33	0.64
1:E:179:TYR:HD2	1:F:53:SER:HB3	1.63	0.64
1:G:206:LEU:HB3	1:L:34:PRO:HG3	1.80	0.64
1:J:206:LEU:HD13	1:J:210:HIS:HB3	1.79	0.64
1:K:206:LEU:HD13	1:K:210:HIS:HB3	1.79	0.64
1:O:339:ARG:HD2	1:P:60:ILE:HG22	1.80	0.64
1:W:206:LEU:HD13	1:W:210:HIS:HB3	1.79	0.64
1:F:206:LEU:HD13	1:F:210:HIS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:53:SER:OG	1:L:179:TYR:CB	2.42	0.64
1:P:96:THR:OG1	1:P:98:GLU:HB2	1.98	0.64
1:V:206:LEU:HD13	1:V:210:HIS:HB3	1.79	0.64
1:C:179:TYR:CB	1:D:53:SER:OG	2.44	0.63
1:E:458:HIS:CD2	1:E:460:TYR:H	2.10	0.63
1:G:206:LEU:HD13	1:G:210:HIS:HB3	1.79	0.63
1:H:206:LEU:HD13	1:H:210:HIS:HB3	1.79	0.63
1:Q:458:HIS:CD2	1:Q:460:TYR:H	2.10	0.63
1:R:206:LEU:HD13	1:R:210:HIS:HB3	1.79	0.63
1:S:206:LEU:HD13	1:S:210:HIS:HB3	1.79	0.63
1:B:180:PHE:CE2	1:C:52:SER:HB3	2.32	0.63
1:T:206:LEU:HD13	1:T:210:HIS:HB3	1.79	0.63
1:B:206:LEU:HD13	1:B:210:HIS:HB3	1.79	0.63
1:G:52:SER:CB	1:H:180:PHE:HE2	2.11	0.63
1:N:206:LEU:HD13	1:N:210:HIS:HB3	1.79	0.63
1:C:193:ASP:OD2	1:D:80:ARG:HD3	1.98	0.63
1:P:465:TYR:OH	1:V:450:GLU:HB3	1.98	0.63
1:S:458:HIS:CD2	1:S:460:TYR:H	2.10	0.63
1:C:180:PHE:CE2	1:D:52:SER:CB	2.82	0.63
1:E:206:LEU:HD13	1:E:210:HIS:HB3	1.79	0.62
1:W:416:ASP:O	1:W:420:ARG:HG2	2.00	0.62
1:F:416:ASP:O	1:F:420:ARG:HG2	2.00	0.62
1:K:416:ASP:O	1:K:420:ARG:HG2	2.00	0.62
1:R:416:ASP:O	1:R:420:ARG:HG2	2.00	0.62
1:V:53:SER:OG	1:W:179:TYR:CB	2.44	0.62
1:A:416:ASP:O	1:A:420:ARG:HG2	2.00	0.62
1:B:463:ALA:HA	1:H:140:PHE:CE1	2.34	0.62
1:M:416:ASP:O	1:M:420:ARG:HG2	2.00	0.62
1:R:467:ASP:HB2	1:S:175:HIS:CE1	2.35	0.62
1:N:416:ASP:O	1:N:420:ARG:HG2	2.00	0.62
1:P:339:ARG:HH21	1:P:339:ARG:HG3	1.65	0.62
1:Q:206:LEU:HD13	1:Q:210:HIS:HB3	1.79	0.62
1:A:339:ARG:HH21	1:A:339:ARG:HG3	1.65	0.62
1:B:339:ARG:HG3	1:B:339:ARG:HH21	1.65	0.62
1:B:416:ASP:O	1:B:420:ARG:HG2	2.00	0.62
1:D:339:ARG:HH21	1:D:339:ARG:HG3	1.65	0.62
1:F:458:HIS:CD2	1:F:460:TYR:H	2.10	0.62
1:G:52:SER:HB2	1:H:180:PHE:HE2	1.65	0.62
1:J:339:ARG:HG3	1:J:339:ARG:HH21	1.65	0.62
1:M:339:ARG:HG3	1:M:339:ARG:HH21	1.65	0.62
1:P:93:ASP:HB3	1:P:98:GLU:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:458:HIS:CD2	1:R:460:TYR:H	2.10	0.62
1:Q:180:PHE:HE2	1:R:52:SER:CB	2.13	0.62
1:W:339:ARG:HH21	1:W:339:ARG:HG3	1.65	0.62
1:C:339:ARG:HH21	1:C:339:ARG:HG3	1.65	0.62
1:B:180:PHE:CE2	1:C:52:SER:CB	2.83	0.62
1:D:416:ASP:O	1:D:420:ARG:HG2	2.00	0.62
1:N:339:ARG:HH21	1:N:339:ARG:HG3	1.65	0.62
1:P:416:ASP:O	1:P:420:ARG:HG2	2.00	0.62
1:I:339:ARG:HH21	1:I:339:ARG:HG3	1.65	0.62
1:K:339:ARG:HH21	1:K:339:ARG:HG3	1.65	0.62
1:L:416:ASP:O	1:L:420:ARG:HG2	2.00	0.62
1:F:140:PHE:CE1	1:L:463:ALA:HA	2.35	0.62
1:V:339:ARG:HH21	1:V:339:ARG:HG3	1.65	0.62
1:O:339:ARG:HH21	1:O:339:ARG:HG3	1.65	0.62
1:O:416:ASP:O	1:O:420:ARG:HG2	2.00	0.62
1:U:339:ARG:HG3	1:U:339:ARG:HH21	1.65	0.62
1:U:458:HIS:CD2	1:U:460:TYR:H	2.10	0.62
1:X:416:ASP:O	1:X:420:ARG:HG2	2.00	0.62
1:C:416:ASP:O	1:C:420:ARG:HG2	2.00	0.62
1:D:175:HIS:HE1	1:K:467:ASP:CB	2.10	0.62
1:C:180:PHE:HE2	1:D:52:SER:HB2	1.64	0.62
1:E:193:ASP:OD2	1:F:80:ARG:HD3	1.99	0.62
1:G:339:ARG:HH21	1:G:339:ARG:HG3	1.65	0.62
1:H:416:ASP:O	1:H:420:ARG:HG2	2.00	0.62
1:S:339:ARG:HH21	1:S:339:ARG:HG3	1.65	0.62
1:B:180:PHE:HE2	1:C:52:SER:HB2	1.65	0.61
1:G:52:SER:HB3	1:H:180:PHE:CE2	2.34	0.61
1:X:339:ARG:HH21	1:X:339:ARG:HG3	1.65	0.61
1:J:416:ASP:O	1:J:420:ARG:HG2	2.00	0.61
1:M:179:TYR:HD2	1:N:53:SER:HB3	1.64	0.61
1:T:416:ASP:O	1:T:420:ARG:HG2	2.00	0.61
1:E:456:ARG:O	1:K:458:HIS:HE1	1.83	0.61
1:G:416:ASP:O	1:G:420:ARG:HG2	2.00	0.61
1:L:339:ARG:HH21	1:L:339:ARG:HG3	1.65	0.61
1:V:416:ASP:O	1:V:420:ARG:HG2	2.00	0.61
1:R:140:PHE:CE1	1:X:463:ALA:HA	2.35	0.61
1:F:339:ARG:HH21	1:F:339:ARG:HG3	1.65	0.61
1:H:339:ARG:HG3	1:H:339:ARG:HH21	1.65	0.61
1:I:416:ASP:O	1:I:420:ARG:HG2	2.00	0.61
1:I:458:HIS:CD2	1:I:460:TYR:H	2.10	0.61
1:R:339:ARG:HH21	1:R:339:ARG:HG3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:ARG:HD3	1:H:193:ASP:OD2	2.01	0.61
1:S:416:ASP:O	1:S:420:ARG:HG2	2.00	0.61
1:S:53:SER:OG	1:T:179:TYR:N	2.33	0.61
1:X:458:HIS:CD2	1:X:460:TYR:H	2.10	0.61
1:L:458:HIS:CD2	1:L:460:TYR:H	2.10	0.61
1:T:339:ARG:HH21	1:T:339:ARG:HG3	1.65	0.61
1:U:416:ASP:O	1:U:420:ARG:HG2	2.00	0.61
1:G:52:SER:CB	1:H:180:PHE:CE2	2.84	0.61
1:B:55:ARG:HD3	5:B:7664:HOH:O	2.01	0.61
1:E:339:ARG:HH21	1:E:339:ARG:HG3	1.65	0.61
1:D:456:ARG:O	1:J:458:HIS:HE1	1.83	0.61
1:J:55:ARG:HD3	5:J:2568:HOH:O	2.01	0.60
1:O:55:ARG:HD3	5:O:3883:HOH:O	2.01	0.60
1:O:179:TYR:CB	1:P:53:SER:OG	2.45	0.60
1:Q:339:ARG:HG3	1:Q:339:ARG:HH21	1.65	0.60
1:N:467:ASP:HB2	1:U:175:HIS:CE1	2.36	0.60
1:V:55:ARG:HD3	5:V:5724:HOH:O	2.01	0.60
1:N:55:ARG:HD3	5:N:3620:HOH:O	2.01	0.60
1:O:463:ALA:HA	1:U:140:PHE:CE1	2.36	0.60
1:X:55:ARG:HD3	5:X:6250:HOH:O	2.01	0.60
1:A:204:PHE:CE1	1:A:237:LEU:HD13	2.36	0.60
1:A:55:ARG:HD3	5:A:7655:HOH:O	2.01	0.60
1:C:55:ARG:HD3	5:C:7670:HOH:O	2.01	0.60
1:E:416:ASP:O	1:E:420:ARG:HG2	2.00	0.60
1:L:55:ARG:HD3	5:L:3094:HOH:O	2.01	0.60
1:M:204:PHE:CE1	1:M:237:LEU:HD13	2.36	0.60
1:M:55:ARG:HD3	5:M:3357:HOH:O	2.01	0.60
1:Q:416:ASP:O	1:Q:420:ARG:HG2	2.00	0.60
1:N:204:PHE:CE1	1:N:237:LEU:HD13	2.36	0.60
1:P:55:ARG:HD3	5:P:4146:HOH:O	2.01	0.60
1:S:55:ARG:HD3	5:S:4935:HOH:O	2.01	0.60
1:N:458:HIS:CD2	1:N:460:TYR:H	2.10	0.60
1:Q:204:PHE:CE1	1:Q:237:LEU:HD13	2.36	0.60
1:W:55:ARG:HD3	5:W:5987:HOH:O	2.01	0.60
1:B:204:PHE:CE1	1:B:237:LEU:HD13	2.36	0.60
1:C:204:PHE:CE1	1:C:237:LEU:HD13	2.36	0.60
1:D:55:ARG:HD3	5:D:990:HOH:O	2.01	0.60
1:E:204:PHE:CE1	1:E:237:LEU:HD13	2.36	0.60
1:J:204:PHE:CE1	1:J:237:LEU:HD13	2.36	0.60
1:I:204:PHE:CE1	1:I:237:LEU:HD13	2.36	0.60
1:Q:180:PHE:CE2	1:R:52:SER:HB3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:204:PHE:CE1	1:U:237:LEU:HD13	2.36	0.60
1:V:204:PHE:CE1	1:V:237:LEU:HD13	2.36	0.60
1:E:55:ARG:HD3	5:E:1253:HOH:O	2.01	0.60
1:F:204:PHE:CE1	1:F:237:LEU:HD13	2.36	0.60
1:G:55:ARG:HD3	5:G:7677:HOH:O	2.01	0.60
1:K:458:HIS:CD2	1:K:460:TYR:H	2.10	0.60
1:O:204:PHE:CE1	1:O:237:LEU:HD13	2.36	0.60
1:P:456:ARG:O	1:V:458:HIS:HE1	1.85	0.60
3:X:7521:AMP:H1'	3:X:7521:AMP:N9	2.08	0.60
1:A:179:TYR:CD2	1:B:53:SER:HB3	2.35	0.60
1:K:55:ARG:HD3	5:K:2831:HOH:O	2.01	0.60
1:Q:55:ARG:HD3	5:Q:4409:HOH:O	2.01	0.60
1:R:204:PHE:CE1	1:R:237:LEU:HD13	2.36	0.60
1:R:55:ARG:HD3	5:R:4672:HOH:O	2.01	0.60
1:S:204:PHE:CE1	1:S:237:LEU:HD13	2.36	0.60
1:W:458:HIS:CD2	1:W:460:TYR:H	2.10	0.60
3:L:7497:AMP:H1'	3:L:7497:AMP:N9	2.08	0.60
1:G:204:PHE:CE1	1:G:237:LEU:HD13	2.36	0.59
1:N:315:THR:HB	1:T:465:TYR:CZ	2.37	0.59
1:T:55:ARG:HD3	5:T:5198:HOH:O	2.01	0.59
1:E:149:TYR:CE1	1:K:146:GLY:HA2	2.38	0.59
1:F:55:ARG:HD3	5:F:7682:HOH:O	2.01	0.59
1:H:55:ARG:HD3	5:H:7685:HOH:O	2.01	0.59
1:R:175:HIS:HE1	1:S:467:ASP:OD2	1.85	0.59
1:W:53:SER:HG	1:X:179:TYR:HB2	1.65	0.59
1:K:204:PHE:CE1	1:K:237:LEU:HD13	2.36	0.59
1:L:204:PHE:CE1	1:L:237:LEU:HD13	2.36	0.59
1:T:204:PHE:CE1	1:T:237:LEU:HD13	2.36	0.59
1:W:204:PHE:CE1	1:W:237:LEU:HD13	2.36	0.59
1:B:458:HIS:CD2	1:B:460:TYR:H	2.10	0.59
1:D:204:PHE:CE1	1:D:237:LEU:HD13	2.36	0.59
1:D:458:HIS:CD2	1:D:460:TYR:H	2.10	0.59
1:P:204:PHE:CE1	1:P:237:LEU:HD13	2.36	0.59
1:P:458:HIS:CD2	1:P:460:TYR:H	2.10	0.59
1:P:175:HIS:HE1	1:W:467:ASP:CG	2.05	0.59
1:E:450:GLU:HB3	1:K:465:TYR:OH	2.02	0.59
1:H:204:PHE:CE1	1:H:237:LEU:HD13	2.36	0.59
1:N:193:ASP:OD2	1:O:80:ARG:HD3	2.02	0.59
1:X:204:PHE:CE1	1:X:237:LEU:HD13	2.36	0.59
1:S:80:ARG:HD3	1:T:193:ASP:OD2	2.02	0.59
5:G:7671:HOH:O	1:L:60:ILE:HD12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:193:ASP:OD2	1:X:80:ARG:HD3	2.01	0.59
1:U:55:ARG:HD3	5:U:5461:HOH:O	2.01	0.59
1:Q:179:TYR:N	1:R:53:SER:OG	2.35	0.59
1:S:338:ASN:HD22	1:X:60:ILE:HD12	1.68	0.59
1:E:601:THR:N	1:E:72:GLU:HG3	2.18	0.59
1:Q:601:THR:N	1:Q:72:GLU:HG3	2.18	0.59
1:D:601:THR:N	1:D:72:GLU:HG3	2.18	0.59
1:J:601:THR:N	1:J:72:GLU:HG3	2.18	0.59
1:V:601:THR:N	1:V:72:GLU:HG3	2.18	0.59
1:E:40:LYS:HG2	1:U:7:LYS:HE2	1.84	0.58
1:I:55:ARG:HD3	5:I:7687:HOH:O	2.01	0.58
1:P:601:THR:N	1:P:72:GLU:HG3	2.18	0.58
1:B:601:THR:N	1:B:72:GLU:HG3	2.18	0.58
1:O:601:THR:N	1:O:72:GLU:HG3	2.18	0.58
1:C:601:THR:N	1:C:72:GLU:HG3	2.18	0.58
5:A:7631:HOH:O	1:F:176:LYS:HE3	2.02	0.58
1:U:80:ARG:HD3	1:V:193:ASP:OD2	2.04	0.58
1:K:601:THR:N	1:K:72:GLU:HG3	2.18	0.58
1:N:601:THR:N	1:N:72:GLU:HG3	2.18	0.58
1:S:601:THR:N	1:S:72:GLU:HG3	2.18	0.58
1:A:601:THR:N	1:A:72:GLU:HG3	2.18	0.58
1:I:601:THR:N	1:I:72:GLU:HG3	2.18	0.58
1:L:601:THR:N	1:L:72:GLU:HG3	2.18	0.58
1:M:601:THR:N	1:M:72:GLU:HG3	2.18	0.58
1:U:601:THR:N	1:U:72:GLU:HG3	2.18	0.58
1:X:601:THR:N	1:X:72:GLU:HG3	2.18	0.58
1:G:601:THR:N	1:G:72:GLU:HG3	2.18	0.58
1:W:601:THR:N	1:W:72:GLU:HG3	2.18	0.58
1:C:55:ARG:HD2	1:C:449:ASN:HD21	1.69	0.58
1:F:601:THR:N	1:F:72:GLU:HG3	2.18	0.58
1:J:55:ARG:HD2	1:J:449:ASN:HD21	1.69	0.58
1:O:55:ARG:HD2	1:O:449:ASN:HD21	1.69	0.58
1:S:52:SER:CB	1:T:180:PHE:HE2	2.17	0.58
1:V:55:ARG:HD2	1:V:449:ASN:HD21	1.69	0.58
1:E:55:ARG:HD2	1:E:449:ASN:HD21	1.69	0.58
1:H:55:ARG:HD2	1:H:449:ASN:HD21	1.69	0.58
1:R:55:ARG:HD2	1:R:449:ASN:HD21	1.69	0.58
1:R:601:THR:N	1:R:72:GLU:HG3	2.18	0.58
1:T:55:ARG:HD2	1:T:449:ASN:HD21	1.69	0.58
1:F:55:ARG:HD2	1:F:449:ASN:HD21	1.69	0.58
1:Q:55:ARG:HD2	1:Q:449:ASN:HD21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:52:SER:CB	1:T:180:PHE:CE2	2.87	0.58
1:U:55:ARG:HD2	1:U:449:ASN:HD21	1.69	0.57
1:I:55:ARG:HD2	1:I:449:ASN:HD21	1.69	0.57
3:J:7493:AMP:N9	3:J:7493:AMP:H1'	2.08	0.57
1:P:55:ARG:HD2	1:P:449:ASN:HD21	1.69	0.57
1:T:601:THR:N	1:T:72:GLU:HG3	2.18	0.57
3:U:7515:AMP:N9	3:U:7515:AMP:H1'	2.08	0.57
3:V:7517:AMP:H1'	3:V:7517:AMP:N9	2.08	0.57
1:A:55:ARG:HD2	1:A:449:ASN:HD21	1.69	0.57
1:H:601:THR:N	1:H:72:GLU:HG3	2.18	0.57
1:M:180:PHE:HE2	1:N:52:SER:HB2	1.68	0.57
1:D:55:ARG:HD2	1:D:449:ASN:HD21	1.69	0.57
1:M:55:ARG:HD2	1:M:449:ASN:HD21	1.69	0.57
1:M:60:ILE:CD1	5:R:4666:HOH:O	2.46	0.57
1:E:40:LYS:HG2	1:U:7:LYS:HZ1	1.68	0.57
1:E:40:LYS:HG2	1:U:7:LYS:CE	2.35	0.57
1:T:60:ILE:HD12	5:U:5455:HOH:O	2.04	0.57
1:Q:180:PHE:CE2	1:R:52:SER:CB	2.88	0.57
1:B:290:LEU:HD11	1:B:345:ILE:HG12	1.87	0.57
1:N:290:LEU:HD11	1:N:345:ILE:HG12	1.87	0.57
3:I:7491:AMP:H1'	3:I:7491:AMP:N9	2.08	0.57
1:Q:290:LEU:HD11	1:Q:345:ILE:HG12	1.87	0.57
1:E:290:LEU:HD11	1:E:345:ILE:HG12	1.87	0.57
1:K:52:SER:CB	1:L:180:PHE:HE2	2.17	0.57
1:S:55:ARG:HD2	1:S:449:ASN:HD21	1.69	0.57
1:W:290:LEU:HD11	1:W:345:ILE:HG12	1.87	0.57
1:E:40:LYS:HD2	1:E:40:LYS:H	1.70	0.57
1:K:290:LEU:HD11	1:K:345:ILE:HG12	1.87	0.57
1:A:290:LEU:HD11	1:A:345:ILE:HG12	1.87	0.56
1:M:290:LEU:HD11	1:M:345:ILE:HG12	1.87	0.56
1:K:55:ARG:HD2	1:K:449:ASN:HD21	1.69	0.56
1:Q:179:TYR:HB2	1:R:53:SER:HG	1.69	0.56
1:V:1:THR:HG22	1:V:3:ASP:H	1.70	0.56
1:A:180:PHE:HE2	1:B:52:SER:HB2	1.70	0.56
1:G:55:ARG:HD2	1:G:449:ASN:HD21	1.69	0.56
1:O:197:THR:HG1	1:P:16:TYR:HH	1.51	0.56
1:W:55:ARG:HD2	1:W:449:ASN:HD21	1.69	0.56
1:A:180:PHE:CE2	1:B:52:SER:CB	2.88	0.56
1:F:290:LEU:HD11	1:F:345:ILE:HG12	1.87	0.56
1:L:55:ARG:HD2	1:L:449:ASN:HD21	1.69	0.56
1:R:290:LEU:HD11	1:R:345:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:ASP:OD2	1:S:10:LYS:NZ	2.38	0.56
1:D:467:ASP:CB	1:K:175:HIS:CE1	2.88	0.56
1:S:52:SER:HB2	1:T:180:PHE:HE2	1.70	0.56
1:S:53:SER:HB3	1:T:179:TYR:CD2	2.41	0.56
1:A:1:THR:HG22	1:A:3:ASP:H	1.71	0.56
1:C:140:PHE:CE1	1:I:463:ALA:HA	2.41	0.56
1:N:465:TYR:CZ	1:T:315:THR:HB	2.41	0.56
1:G:1:THR:HG22	1:G:3:ASP:H	1.71	0.56
1:H:290:LEU:HD11	1:H:345:ILE:HG12	1.87	0.56
1:J:1:THR:HG22	1:J:3:ASP:H	1.71	0.56
1:O:290:LEU:HD11	1:O:345:ILE:HG12	1.87	0.56
1:T:290:LEU:HD11	1:T:345:ILE:HG12	1.87	0.56
1:X:55:ARG:HD2	1:X:449:ASN:HD21	1.69	0.56
1:C:290:LEU:HD11	1:C:345:ILE:HG12	1.87	0.56
1:C:1:THR:HG22	1:C:3:ASP:H	1.71	0.56
1:E:1:THR:HG22	1:E:3:ASP:H	1.71	0.56
1:G:290:LEU:HD11	1:G:345:ILE:HG12	1.87	0.56
1:C:463:ALA:HA	1:I:140:PHE:CE1	2.41	0.56
1:O:1:THR:HG22	1:O:3:ASP:H	1.71	0.56
1:M:1:THR:HG22	1:M:3:ASP:H	1.71	0.56
1:N:502:PRO:HB2	1:O:137:SER:HB3	1.88	0.56
3:O:7503:AMP:N9	3:O:7503:AMP:H1'	2.08	0.56
1:P:53:SER:HB2	5:P:3802:HOH:O	2.06	0.56
1:R:1:THR:HG22	1:R:3:ASP:H	1.71	0.56
1:S:1:THR:HG22	1:S:3:ASP:H	1.71	0.56
1:F:1:THR:HG22	1:F:3:ASP:H	1.71	0.56
1:Q:1:THR:HG22	1:Q:3:ASP:H	1.71	0.56
1:S:290:LEU:HD11	1:S:345:ILE:HG12	1.87	0.56
1:W:1:THR:HG22	1:W:3:ASP:H	1.71	0.56
3:C:7479:AMP:H1'	3:C:7479:AMP:N9	2.08	0.56
1:J:290:LEU:HD11	1:J:345:ILE:HG12	1.87	0.56
1:L:1:THR:HG22	1:L:3:ASP:H	1.71	0.56
1:V:290:LEU:HD11	1:V:345:ILE:HG12	1.87	0.56
1:X:1:THR:HG22	1:X:3:ASP:H	1.71	0.56
1:B:55:ARG:HD2	1:B:449:ASN:HD21	1.69	0.55
1:N:1:THR:HG22	1:N:3:ASP:H	1.71	0.55
1:M:180:PHE:CE2	1:N:52:SER:CB	2.89	0.55
1:W:53:SER:HB3	1:X:179:TYR:HD2	1.71	0.55
1:A:179:TYR:N	1:B:53:SER:OG	2.39	0.55
1:D:131:GLU:OE1	4:D:7482:CIT:O1	2.25	0.55
1:G:131:GLU:OE1	4:G:7488:CIT:O1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:ARG:HD3	1:I:193:ASP:OD2	2.06	0.55
1:K:1:THR:HG22	1:K:3:ASP:H	1.71	0.55
1:M:180:PHE:HE2	1:N:52:SER:CB	2.19	0.55
1:T:131:GLU:OE1	4:T:7514:CIT:O1	2.25	0.55
1:B:1:THR:HG22	1:B:3:ASP:H	1.71	0.55
1:F:131:GLU:OE1	4:F:7486:CIT:O1	2.25	0.55
1:H:131:GLU:OE1	4:H:7490:CIT:O1	2.25	0.55
1:R:131:GLU:OE1	4:R:7510:CIT:O1	2.25	0.55
1:S:131:GLU:OE1	4:S:7512:CIT:O1	2.25	0.55
1:T:1:THR:HG22	1:T:3:ASP:H	1.71	0.55
1:U:1:THR:HG22	1:U:3:ASP:H	1.71	0.55
1:D:1:THR:HG22	1:D:3:ASP:H	1.71	0.55
1:G:211:HIS:HD2	1:L:33:ILE:HG22	1.72	0.55
1:N:55:ARG:HD2	1:N:449:ASN:HD21	1.69	0.55
1:P:131:GLU:OE1	4:P:7506:CIT:O1	2.25	0.55
1:T:60:ILE:HD12	1:U:338:ASN:HD22	1.71	0.55
1:E:131:GLU:OE1	4:E:7484:CIT:O1	2.25	0.55
1:G:53:SER:HG	1:H:179:TYR:HB2	1.67	0.55
1:K:52:SER:HB3	1:L:180:PHE:CE2	2.42	0.55
1:Q:179:TYR:HD2	1:R:53:SER:HB3	1.71	0.55
1:X:290:LEU:HD11	1:X:345:ILE:HG12	1.87	0.55
1:D:290:LEU:HD11	1:D:345:ILE:HG12	1.87	0.55
1:I:1:THR:HG22	1:I:3:ASP:H	1.71	0.55
1:Q:131:GLU:OE1	4:Q:7508:CIT:O1	2.25	0.55
1:S:52:SER:HB3	1:T:180:PHE:CE2	2.42	0.55
1:X:131:GLU:OE1	4:X:7522:CIT:O1	2.25	0.55
1:A:180:PHE:HE2	1:B:52:SER:CB	2.19	0.55
1:H:1:THR:HG22	1:H:3:ASP:H	1.72	0.55
1:J:131:GLU:OE1	4:J:7494:CIT:O1	2.25	0.55
1:K:52:SER:HB2	1:L:180:PHE:HE2	1.72	0.55
1:L:131:GLU:OE1	4:L:7498:CIT:O1	2.25	0.55
1:K:52:SER:CB	1:L:180:PHE:CE2	2.90	0.55
1:L:290:LEU:HD11	1:L:345:ILE:HG12	1.87	0.55
1:P:290:LEU:HD11	1:P:345:ILE:HG12	1.87	0.55
1:P:1:THR:HG22	1:P:3:ASP:H	1.71	0.55
1:S:56:GLY:O	1:S:102:ARG:NE	2.40	0.55
1:V:131:GLU:OE1	4:V:7518:CIT:O1	2.25	0.55
1:I:80:ARG:HD3	1:J:193:ASP:OD2	2.06	0.55
3:N:7501:AMP:H1'	3:N:7501:AMP:N9	2.08	0.55
1:U:290:LEU:HD11	1:U:345:ILE:HG12	1.87	0.55
1:O:140:PHE:CE1	1:U:463:ALA:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:204:PHE:HE1	1:W:237:LEU:HD13	1.72	0.55
3:B:7477:AMP:H1'	3:B:7477:AMP:N9	2.08	0.55
1:G:56:GLY:O	1:G:102:ARG:NE	2.40	0.55
1:I:290:LEU:HD11	1:I:345:ILE:HG12	1.87	0.55
1:Q:180:PHE:HE2	1:R:52:SER:HB2	1.72	0.55
1:T:204:PHE:HE1	1:T:237:LEU:HD13	1.72	0.55
1:U:131:GLU:OE1	4:U:7516:CIT:O1	2.25	0.55
1:U:451:GLU:HB3	1:U:452:PRO:HD3	1.89	0.55
1:B:193:ASP:OD2	1:C:80:ARG:HD3	2.07	0.54
1:E:204:PHE:HE1	1:E:237:LEU:HD13	1.72	0.54
1:G:204:PHE:HE1	1:G:237:LEU:HD13	1.72	0.54
1:G:451:GLU:HB3	1:G:452:PRO:HD3	1.89	0.54
1:H:204:PHE:HE1	1:H:237:LEU:HD13	1.72	0.54
1:I:131:GLU:OE1	4:I:7492:CIT:O1	2.25	0.54
1:I:451:GLU:HB3	1:I:452:PRO:HD3	1.89	0.54
1:K:204:PHE:HE1	1:K:237:LEU:HD13	1.73	0.54
1:O:175:HIS:HE1	1:V:467:ASP:OD2	1.91	0.54
1:A:451:GLU:HB3	1:A:452:PRO:HD3	1.89	0.54
1:B:204:PHE:HE1	1:B:237:LEU:HD13	1.72	0.54
1:D:451:GLU:HB3	1:D:452:PRO:HD3	1.89	0.54
1:D:465:TYR:OH	1:J:450:GLU:HB3	2.07	0.54
1:K:53:SER:OG	1:L:179:TYR:N	2.40	0.54
1:O:131:GLU:OE1	4:O:7504:CIT:O1	2.25	0.54
1:S:204:PHE:HE1	1:S:237:LEU:HD13	1.72	0.54
1:C:131:GLU:OE1	4:C:7480:CIT:O1	2.25	0.54
1:I:53:SER:HB3	1:J:179:TYR:HD2	1.72	0.54
1:P:451:GLU:HB3	1:P:452:PRO:HD3	1.89	0.54
1:R:451:GLU:HB3	1:R:452:PRO:HD3	1.89	0.54
1:S:451:GLU:HB3	1:S:452:PRO:HD3	1.89	0.54
1:U:53:SER:OG	1:V:179:TYR:N	2.40	0.54
1:P:467:ASP:CG	1:W:175:HIS:HE1	2.10	0.54
1:D:204:PHE:HE1	1:D:237:LEU:HD13	1.72	0.54
1:E:179:TYR:H	1:F:53:SER:CB	2.19	0.54
1:F:451:GLU:HB3	1:F:452:PRO:HD3	1.89	0.54
1:J:204:PHE:HE1	1:J:237:LEU:HD13	1.72	0.54
1:K:131:GLU:OE1	4:K:7496:CIT:O1	2.25	0.54
1:M:451:GLU:HB3	1:M:452:PRO:HD3	1.89	0.54
1:N:179:TYR:N	1:O:53:SER:OG	2.40	0.54
1:Q:204:PHE:HE1	1:Q:237:LEU:HD13	1.73	0.54
1:V:204:PHE:HE1	1:V:237:LEU:HD13	1.72	0.54
1:G:193:ASP:OD2	1:L:80:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:451:GLU:HB3	1:L:452:PRO:HD3	1.89	0.54
1:N:204:PHE:HE1	1:N:237:LEU:HD13	1.72	0.54
1:P:204:PHE:HE1	1:P:237:LEU:HD13	1.72	0.54
1:A:204:PHE:HE1	1:A:237:LEU:HD13	1.72	0.54
1:G:53:SER:HB3	1:H:179:TYR:HD2	1.72	0.54
1:M:204:PHE:HE1	1:M:237:LEU:HD13	1.72	0.54
1:N:131:GLU:OE1	4:N:7502:CIT:O1	2.25	0.54
1:N:451:GLU:HB3	1:N:452:PRO:HD3	1.89	0.54
1:B:451:GLU:HB3	1:B:452:PRO:HD3	1.89	0.54
1:B:131:GLU:OE1	4:B:7478:CIT:O1	2.25	0.54
1:C:204:PHE:HE1	1:C:237:LEU:HD13	1.72	0.54
1:E:451:GLU:HB3	1:E:452:PRO:HD3	1.89	0.54
1:K:7:LYS:HG2	1:K:11:ASP:OD2	2.07	0.54
1:N:180:PHE:HE2	1:O:52:SER:CB	2.21	0.54
1:E:40:LYS:HG2	1:U:7:LYS:NZ	2.23	0.54
1:W:131:GLU:OE1	4:W:7520:CIT:O1	2.25	0.54
1:A:467:ASP:OD2	1:H:175:HIS:HE1	1.91	0.54
1:N:179:TYR:CD2	1:O:53:SER:HB3	2.42	0.54
1:Q:451:GLU:HB3	1:Q:452:PRO:HD3	1.89	0.54
1:X:204:PHE:HE1	1:X:237:LEU:HD13	1.72	0.54
1:L:204:PHE:HE1	1:L:237:LEU:HD13	1.72	0.54
1:P:98:GLU:HB3	5:P:4174:HOH:O	2.08	0.54
1:Q:173:VAL:HG21	5:X:6107:HOH:O	2.08	0.54
1:J:53:SER:HB3	1:K:179:TYR:HD2	1.73	0.54
1:O:204:PHE:HE1	1:O:237:LEU:HD13	1.73	0.54
1:T:451:GLU:HB3	1:T:452:PRO:HD3	1.89	0.54
1:V:53:SER:HB3	1:W:179:TYR:HD2	1.73	0.54
1:X:451:GLU:HB3	1:X:452:PRO:HD3	1.90	0.54
1:F:467:ASP:OD2	1:G:175:HIS:HE1	1.91	0.53
1:H:451:GLU:HB3	1:H:452:PRO:HD3	1.89	0.53
1:A:56:GLY:O	1:A:102:ARG:NE	2.40	0.53
1:H:60:ILE:HG22	1:I:339:ARG:HD2	1.90	0.53
1:M:140:PHE:CE1	1:S:463:ALA:HA	2.43	0.53
1:U:204:PHE:HE1	1:U:237:LEU:HD13	1.72	0.53
1:I:204:PHE:HE1	1:I:237:LEU:HD13	1.72	0.53
1:I:56:GLY:O	1:I:102:ARG:NE	2.40	0.53
1:M:131:GLU:OE1	4:M:7500:CIT:O1	2.25	0.53
1:W:451:GLU:HB3	1:W:452:PRO:HD3	1.89	0.53
1:A:131:GLU:OE1	4:A:7476:CIT:O1	2.25	0.53
1:B:315:THR:HB	1:H:465:TYR:CZ	2.43	0.53
1:U:56:GLY:O	1:U:102:ARG:NE	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:603:LYS:HD2	5:J:2579:HOH:O	2.09	0.53
1:F:463:ALA:HA	1:L:140:PHE:CE1	2.42	0.53
1:M:56:GLY:O	1:M:102:ARG:NE	2.40	0.53
1:N:180:PHE:CE2	1:O:52:SER:CB	2.91	0.53
5:T:5171:HOH:O	1:U:176:LYS:HE3	2.08	0.53
1:V:603:LYS:HD2	5:V:5735:HOH:O	2.09	0.53
1:C:451:GLU:HB3	1:C:452:PRO:HD3	1.89	0.53
1:F:204:PHE:HE1	1:F:237:LEU:HD13	1.72	0.53
1:L:603:LYS:HD2	5:L:3105:HOH:O	2.09	0.53
3:M:7499:AMP:N9	3:M:7499:AMP:H1'	2.08	0.53
1:B:56:GLY:O	1:B:102:ARG:NE	2.40	0.53
1:R:204:PHE:HE1	1:R:237:LEU:HD13	1.72	0.53
1:X:603:LYS:HD2	5:X:6261:HOH:O	2.09	0.53
1:A:180:PHE:CE2	1:B:52:SER:HB3	2.43	0.53
1:A:60:ILE:HG22	1:F:339:ARG:HD2	1.89	0.53
1:J:451:GLU:HB3	1:J:452:PRO:HD3	1.89	0.53
1:K:451:GLU:HB3	1:K:452:PRO:HD3	1.89	0.53
1:M:95:PHE:CE2	1:R:347:ILE:HG21	2.44	0.53
1:O:451:GLU:HB3	1:O:452:PRO:HD3	1.89	0.53
1:M:463:ALA:HA	1:S:140:PHE:CE1	2.44	0.53
1:U:53:SER:HB3	1:V:179:TYR:HD2	1.74	0.53
1:V:451:GLU:HB3	1:V:452:PRO:HD3	1.89	0.53
1:X:18:ASP:OD2	1:X:30:HIS:HD2	1.92	0.53
1:A:18:ASP:OD2	1:A:30:HIS:HD2	1.92	0.53
1:M:18:ASP:OD2	1:M:30:HIS:HD2	1.92	0.53
1:O:603:LYS:HD2	5:O:3894:HOH:O	2.09	0.53
1:U:18:ASP:OD2	1:U:30:HIS:HD2	1.92	0.53
1:H:18:ASP:OD2	1:H:30:HIS:HD2	1.92	0.53
1:I:18:ASP:OD2	1:I:30:HIS:HD2	1.92	0.53
1:K:53:SER:HB3	1:L:179:TYR:HD2	1.74	0.53
1:N:180:PHE:HE2	1:O:52:SER:HB2	1.73	0.53
1:M:60:ILE:HD12	1:R:338:ASN:HD22	1.73	0.53
1:C:603:LYS:HD2	5:C:7680:HOH:O	2.09	0.52
1:F:467:ASP:HB2	1:G:175:HIS:HE1	1.73	0.52
1:L:18:ASP:OD2	1:L:30:HIS:HD2	1.92	0.52
1:M:180:PHE:CE2	1:N:52:SER:HB3	2.43	0.52
1:T:18:ASP:OD2	1:T:30:HIS:HD2	1.92	0.52
1:F:18:ASP:OD2	1:F:30:HIS:HD2	1.92	0.52
1:J:53:SER:HB3	1:K:179:TYR:CD2	2.45	0.52
1:M:179:TYR:CD2	1:N:53:SER:HB3	2.42	0.52
1:N:56:GLY:O	1:N:102:ARG:NE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:95:PHE:CZ	1:R:347:ILE:HD13	2.44	0.52
3:A:7475:AMP:H1'	3:A:7475:AMP:N9	2.08	0.52
1:F:175:HIS:HE1	1:G:467:ASP:CG	2.10	0.52
1:G:18:ASP:OD2	1:G:30:HIS:HD2	1.92	0.52
1:N:603:LYS:HD2	5:N:3631:HOH:O	2.09	0.52
1:R:18:ASP:OD2	1:R:30:HIS:HD2	1.92	0.52
1:B:207:GLU:N	1:B:210:HIS:HD2	1.98	0.52
1:B:603:LYS:HD2	5:B:7674:HOH:O	2.09	0.52
1:I:603:LYS:HD2	5:I:7697:HOH:O	2.09	0.52
1:M:603:LYS:HD2	5:M:3368:HOH:O	2.09	0.52
1:S:18:ASP:OD2	1:S:30:HIS:HD2	1.92	0.52
1:U:603:LYS:HD2	5:U:5472:HOH:O	2.09	0.52
1:Q:465:TYR:CZ	1:W:315:THR:HB	2.44	0.52
1:H:207:GLU:N	1:H:210:HIS:HD2	1.98	0.52
1:R:603:LYS:HD2	5:R:4683:HOH:O	2.09	0.52
1:W:56:GLY:O	1:W:102:ARG:NE	2.40	0.52
1:A:603:LYS:HD2	5:A:7666:HOH:O	2.09	0.52
1:B:179:TYR:HD2	1:C:53:SER:HB3	1.75	0.52
1:D:18:ASP:OD2	1:D:30:HIS:HD2	1.92	0.52
1:F:603:LYS:HD2	5:F:7692:HOH:O	2.09	0.52
1:H:52:SER:HB2	1:I:180:PHE:HE2	1.75	0.52
1:H:56:GLY:O	1:H:102:ARG:NE	2.40	0.52
1:V:18:ASP:OD2	1:V:30:HIS:HD2	1.92	0.52
1:A:60:ILE:CD1	5:F:7676:HOH:O	2.48	0.52
5:D:984:HOH:O	1:E:60:ILE:HD12	2.09	0.52
1:J:18:ASP:OD2	1:J:30:HIS:HD2	1.92	0.52
1:K:56:GLY:O	1:K:102:ARG:NE	2.40	0.52
1:P:18:ASP:OD2	1:P:30:HIS:HD2	1.92	0.52
1:O:180:PHE:CZ	1:P:52:SER:HB3	2.44	0.52
1:T:56:GLY:O	1:T:102:ARG:NE	2.40	0.52
1:C:18:ASP:OD2	1:C:30:HIS:HD2	1.92	0.52
1:E:307:SER:HB2	1:E:421:LEU:HA	1.92	0.52
1:L:56:GLY:O	1:L:102:ARG:NE	2.40	0.52
1:O:18:ASP:OD2	1:O:30:HIS:HD2	1.92	0.52
1:Q:307:SER:HB2	1:Q:421:LEU:HA	1.92	0.52
1:I:307:SER:HB2	1:I:421:LEU:HA	1.92	0.52
1:U:307:SER:HB2	1:U:421:LEU:HA	1.92	0.52
1:W:18:ASP:OD2	1:W:30:HIS:HD2	1.92	0.52
1:X:56:GLY:O	1:X:102:ARG:NE	2.40	0.52
1:B:18:ASP:OD2	1:B:30:HIS:HD2	1.92	0.51
1:D:307:SER:HB2	1:D:421:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:603:LYS:HD2	5:G:7688:HOH:O	2.09	0.51
1:P:307:SER:HB2	1:P:421:LEU:HA	1.92	0.51
1:Q:18:ASP:OD2	1:Q:30:HIS:HD2	1.92	0.51
1:W:80:ARG:HD2	1:W:84:THR:OG1	2.10	0.51
1:X:80:ARG:HD2	1:X:84:THR:OG1	2.10	0.51
1:A:207:GLU:N	1:A:210:HIS:HD2	1.98	0.51
1:E:18:ASP:OD2	1:E:30:HIS:HD2	1.92	0.51
1:E:40:LYS:H	1:E:40:LYS:CD	2.23	0.51
1:E:603:LYS:HD2	5:E:1264:HOH:O	2.09	0.51
1:J:307:SER:HB2	1:J:421:LEU:HA	1.92	0.51
1:J:80:ARG:HD2	1:J:84:THR:OG1	2.11	0.51
1:K:7:LYS:HD3	5:K:2861:HOH:O	2.09	0.51
1:K:80:ARG:HD2	1:K:84:THR:OG1	2.11	0.51
1:L:80:ARG:HD2	1:L:84:THR:OG1	2.11	0.51
1:Q:603:LYS:HD2	5:Q:4420:HOH:O	2.09	0.51
1:V:307:SER:HB2	1:V:421:LEU:HA	1.92	0.51
1:W:603:LYS:HD2	5:W:5998:HOH:O	2.09	0.51
5:F:7548:HOH:O	1:G:173:VAL:HG21	2.11	0.51
1:K:18:ASP:OD2	1:K:30:HIS:HD2	1.92	0.51
1:K:603:LYS:HD2	5:K:2842:HOH:O	2.09	0.51
3:K:7495:AMP:HI'	3:K:7495:AMP:N9	2.08	0.51
1:M:207:GLU:N	1:M:210:HIS:HD2	1.98	0.51
1:N:207:GLU:N	1:N:210:HIS:HD2	1.98	0.51
1:N:80:ARG:HD2	1:N:84:THR:OG1	2.10	0.51
1:S:603:LYS:HD2	5:S:4946:HOH:O	2.09	0.51
1:T:207:GLU:N	1:T:210:HIS:HD2	1.98	0.51
1:V:80:ARG:HD2	1:V:84:THR:OG1	2.11	0.51
1:A:95:PHE:CZ	1:F:347:ILE:HD13	2.46	0.51
1:C:307:SER:HB2	1:C:421:LEU:HA	1.92	0.51
1:O:307:SER:HB2	1:O:421:LEU:HA	1.92	0.51
1:T:307:SER:HB2	1:T:421:LEU:HA	1.92	0.51
1:B:80:ARG:HD2	1:B:84:THR:OG1	2.11	0.51
1:C:56:GLY:O	1:C:102:ARG:NE	2.40	0.51
1:H:307:SER:HB2	1:H:421:LEU:HA	1.92	0.51
1:N:180:PHE:CE2	1:O:52:SER:HB3	2.45	0.51
1:F:80:ARG:HD2	1:F:84:THR:OG1	2.11	0.51
1:N:18:ASP:OD2	1:N:30:HIS:HD2	1.92	0.51
1:O:179:TYR:N	1:P:53:SER:OG	2.41	0.51
1:R:307:SER:HB2	1:R:421:LEU:HA	1.92	0.51
1:R:80:ARG:HD2	1:R:84:THR:OG1	2.10	0.51
5:R:4529:HOH:O	1:S:173:VAL:HG21	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:ARG:HD2	1:C:84:THR:OG1	2.10	0.51
1:D:603:LYS:HD2	5:D:1001:HOH:O	2.09	0.51
1:F:307:SER:HB2	1:F:421:LEU:HA	1.92	0.51
1:M:80:ARG:HD2	1:M:84:THR:OG1	2.10	0.51
1:P:603:LYS:HD2	5:P:4157:HOH:O	2.09	0.51
1:V:56:GLY:O	1:V:102:ARG:NE	2.40	0.51
1:C:339:ARG:HD2	1:D:60:ILE:HG22	1.91	0.51
1:E:56:GLY:O	1:E:102:ARG:NE	2.40	0.51
1:H:603:LYS:HD2	5:H:7696:HOH:O	2.09	0.51
1:J:56:GLY:O	1:J:102:ARG:NE	2.40	0.51
1:K:307:SER:HB2	1:K:421:LEU:HA	1.92	0.51
1:O:80:ARG:HD2	1:O:84:THR:OG1	2.10	0.51
1:T:603:LYS:HD2	5:T:5209:HOH:O	2.09	0.51
1:A:80:ARG:HD2	1:A:84:THR:OG1	2.11	0.51
1:P:466:TYR:CZ	1:V:254:THR:HB	2.45	0.51
1:Q:56:GLY:O	1:Q:102:ARG:NE	2.40	0.51
1:S:307:SER:HB2	1:S:421:LEU:HA	1.92	0.51
1:S:80:ARG:HD2	1:S:84:THR:OG1	2.10	0.51
1:P:146:GLY:HA2	1:V:149:TYR:CE1	2.46	0.51
1:W:307:SER:HB2	1:W:421:LEU:HA	1.92	0.51
1:W:52:SER:HB2	1:X:180:PHE:HE2	1.76	0.51
1:B:179:TYR:N	1:C:53:SER:OG	2.44	0.50
1:G:126:PHE:CE2	1:G:272:GLN:HG2	2.46	0.50
1:G:307:SER:HB2	1:G:421:LEU:HA	1.92	0.50
1:N:413:GLN:HG2	5:T:5239:HOH:O	2.10	0.50
1:V:207:GLU:N	1:V:210:HIS:HD2	1.98	0.50
1:A:307:SER:HB2	1:A:421:LEU:HA	1.92	0.50
1:C:126:PHE:CE2	1:C:272:GLN:HG2	2.46	0.50
1:F:126:PHE:CE2	1:F:272:GLN:HG2	2.46	0.50
1:H:80:ARG:HD2	1:H:84:THR:OG1	2.10	0.50
1:L:207:GLU:N	1:L:210:HIS:HD2	1.98	0.50
1:M:60:ILE:HG21	1:R:339:ARG:HB2	1.92	0.50
1:Q:80:ARG:HD2	1:Q:84:THR:OG1	2.10	0.50
1:R:126:PHE:CE2	1:R:272:GLN:HG2	2.46	0.50
1:S:126:PHE:CE2	1:S:272:GLN:HG2	2.46	0.50
1:T:126:PHE:CE2	1:T:272:GLN:HG2	2.46	0.50
1:X:126:PHE:CE2	1:X:272:GLN:HG2	2.46	0.50
1:X:207:GLU:N	1:X:210:HIS:HD2	1.98	0.50
1:E:80:ARG:HD2	1:E:84:THR:OG1	2.11	0.50
1:G:80:ARG:HD2	1:G:84:THR:OG1	2.10	0.50
1:O:126:PHE:CE2	1:O:272:GLN:HG2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7505:AMP:N9	3:P:7505:AMP:H1'	2.08	0.50
1:N:320:LYS:HE3	1:T:461:GLU:OE1	2.11	0.50
1:T:80:ARG:HD2	1:T:84:THR:OG1	2.11	0.50
1:X:307:SER:HB2	1:X:421:LEU:HA	1.92	0.50
3:D:7481:AMP:H1'	3:D:7481:AMP:N9	2.08	0.50
1:I:126:PHE:CE2	1:I:272:GLN:HG2	2.46	0.50
1:I:80:ARG:HD2	1:I:84:THR:OG1	2.10	0.50
1:J:207:GLU:N	1:J:210:HIS:HD2	1.98	0.50
1:J:126:PHE:CE2	1:J:272:GLN:HG2	2.46	0.50
1:M:307:SER:HB2	1:M:421:LEU:HA	1.92	0.50
1:Q:126:PHE:CE2	1:Q:272:GLN:HG2	2.46	0.50
1:V:126:PHE:CE2	1:V:272:GLN:HG2	2.46	0.50
1:B:307:SER:HB2	1:B:421:LEU:HA	1.92	0.50
1:D:126:PHE:CE2	1:D:272:GLN:HG2	2.46	0.50
1:D:56:GLY:O	1:D:102:ARG:NE	2.40	0.50
1:D:80:ARG:HD2	1:D:84:THR:OG1	2.11	0.50
1:E:126:PHE:CE2	1:E:272:GLN:HG2	2.46	0.50
1:H:126:PHE:CE2	1:H:272:GLN:HG2	2.46	0.50
1:L:307:SER:HB2	1:L:421:LEU:HA	1.92	0.50
1:N:307:SER:HB2	1:N:421:LEU:HA	1.92	0.50
1:P:126:PHE:CE2	1:P:272:GLN:HG2	2.46	0.50
1:P:80:ARG:HD2	1:P:84:THR:OG1	2.10	0.50
1:U:126:PHE:CE2	1:U:272:GLN:HG2	2.46	0.50
1:G:53:SER:OG	1:H:179:TYR:N	2.43	0.50
1:J:60:ILE:HD12	1:K:338:ASN:HD22	1.75	0.50
1:L:126:PHE:CE2	1:L:272:GLN:HG2	2.47	0.50
1:M:95:PHE:HZ	1:R:347:ILE:HD13	1.76	0.50
5:N:3661:HOH:O	1:T:413:GLN:HG2	2.11	0.50
1:U:80:ARG:HD2	1:U:84:THR:OG1	2.11	0.50
1:W:53:SER:HB3	1:X:179:TYR:CD2	2.47	0.50
3:W:7519:AMP:N9	3:W:7519:AMP:H1'	2.08	0.50
1:K:126:PHE:CE2	1:K:272:GLN:HG2	2.46	0.50
1:P:56:GLY:O	1:P:102:ARG:NE	2.40	0.50
1:W:126:PHE:CE2	1:W:272:GLN:HG2	2.46	0.50
1:N:461:GLU:OE1	1:T:320:LYS:HE3	2.12	0.50
1:O:456:ARG:O	1:U:458:HIS:HE1	1.95	0.50
1:E:40:LYS:HE3	1:U:7:LYS:HE2	1.93	0.50
1:C:207:GLU:N	1:C:210:HIS:HD2	1.98	0.49
1:H:52:SER:HB3	1:I:180:PHE:CE2	2.47	0.49
1:N:126:PHE:CE2	1:N:272:GLN:HG2	2.46	0.49
1:O:207:GLU:N	1:O:210:HIS:HD2	1.98	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:450:GLU:HB3	1:V:465:TYR:OH	2.12	0.49
1:A:458:HIS:HE1	1:G:456:ARG:O	1.95	0.49
1:P:211:HIS:HD2	1:Q:33:ILE:HG22	1.76	0.49
1:R:56:GLY:O	1:R:102:ARG:NE	2.40	0.49
1:W:129:GLU:OE1	3:W:7519:AMP:H5'1	2.13	0.49
1:Q:463:ALA:HA	1:W:140:PHE:CE1	2.47	0.49
1:A:193:ASP:OD2	1:B:80:ARG:HD3	2.12	0.49
1:B:126:PHE:CE2	1:B:272:GLN:HG2	2.46	0.49
1:E:502:PRO:HB2	1:F:137:SER:HB3	1.94	0.49
1:A:456:ARG:O	1:G:458:HIS:HE1	1.95	0.49
1:I:207:GLU:N	1:I:210:HIS:HD2	1.98	0.49
1:K:129:GLU:OE1	3:K:7495:AMP:H5'1	2.13	0.49
1:B:320:LYS:HE3	1:H:461:GLU:OE1	2.13	0.49
1:B:465:TYR:CZ	1:H:315:THR:HB	2.47	0.49
1:D:296:HIS:NE2	1:D:385:LYS:HG2	2.27	0.49
1:N:315:THR:HB	1:T:465:TYR:CE1	2.46	0.49
1:B:321:ARG:NE	4:B:7478:CIT:H42	2.21	0.49
1:F:56:GLY:O	1:F:102:ARG:NE	2.40	0.49
1:O:56:GLY:O	1:O:102:ARG:NE	2.40	0.49
1:P:321:ARG:NE	4:P:7506:CIT:H42	2.21	0.49
1:V:129:GLU:OE1	3:V:7517:AMP:H5'1	2.13	0.49
5:S:4929:HOH:O	1:X:60:ILE:HD12	2.13	0.49
1:G:129:GLU:OE1	3:G:7487:AMP:H5'1	2.13	0.49
1:J:129:GLU:OE1	3:J:7493:AMP:H5'1	2.13	0.49
1:S:176:LYS:HE3	5:X:6223:HOH:O	2.13	0.49
1:A:126:PHE:CE2	1:A:272:GLN:HG2	2.46	0.49
1:C:175:HIS:CE1	1:J:467:ASP:HB2	2.48	0.49
1:G:179:TYR:CB	1:L:53:SER:OG	2.51	0.49
1:L:129:GLU:OE1	3:L:7497:AMP:H5'1	2.13	0.49
1:L:98:GLU:OE1	1:L:99:PRO:HD2	2.13	0.49
1:M:126:PHE:CE2	1:M:272:GLN:HG2	2.46	0.49
1:M:80:ARG:HD3	1:R:193:ASP:OD2	2.12	0.49
1:D:321:ARG:NE	4:D:7482:CIT:H42	2.21	0.49
3:G:7487:AMP:H1'	3:G:7487:AMP:N9	2.08	0.49
1:H:52:SER:CB	1:I:180:PHE:CE2	2.96	0.49
1:N:129:GLU:OE1	3:N:7501:AMP:H5'1	2.13	0.49
1:Q:6:PHE:CE1	1:Q:40:LYS:HG3	2.48	0.49
1:X:129:GLU:OE1	3:X:7521:AMP:H5'1	2.13	0.49
3:E:7483:AMP:H1'	3:E:7483:AMP:N9	2.08	0.49
1:H:52:SER:CB	1:I:180:PHE:HE2	2.25	0.49
1:I:129:GLU:OE1	3:I:7491:AMP:H5'1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:140:PHE:CE1	1:V:463:ALA:HA	2.47	0.49
1:S:129:GLU:OE1	3:S:7511:AMP:H5'1	2.13	0.49
1:U:129:GLU:OE1	3:U:7515:AMP:H5'1	2.13	0.49
1:B:129:GLU:OE1	3:B:7477:AMP:H5'1	2.13	0.49
1:C:129:GLU:OE1	3:C:7479:AMP:H5'1	2.13	0.49
1:F:339:ARG:NH2	1:F:339:ARG:HG3	2.28	0.49
1:H:129:GLU:OE1	3:H:7489:AMP:H5'1	2.13	0.49
1:M:339:ARG:HG3	1:M:339:ARG:NH2	2.28	0.49
1:T:129:GLU:OE1	3:T:7513:AMP:H5'1	2.13	0.49
1:U:207:GLU:N	1:U:210:HIS:HD2	1.98	0.49
1:M:338:ASN:HB3	5:M:3351:HOH:O	2.13	0.48
1:N:321:ARG:NE	4:N:7502:CIT:H42	2.21	0.48
1:O:129:GLU:OE1	3:O:7503:AMP:H5'1	2.13	0.48
1:O:338:ASN:HB3	5:O:3877:HOH:O	2.14	0.48
1:R:339:ARG:NH2	1:R:339:ARG:HG3	2.28	0.48
1:R:467:ASP:HB2	1:S:175:HIS:HE1	1.76	0.48
1:A:338:ASN:HB3	5:A:7649:HOH:O	2.14	0.48
1:A:339:ARG:HG3	1:A:339:ARG:NH2	2.28	0.48
1:A:129:GLU:OE1	3:A:7475:AMP:H5'1	2.13	0.48
1:C:338:ASN:HB3	5:C:7664:HOH:O	2.14	0.48
1:H:339:ARG:NH2	1:H:339:ARG:HG3	2.28	0.48
5:H:7661:HOH:O	1:I:176:LYS:HE3	2.11	0.48
1:K:339:ARG:NH2	1:K:339:ARG:HG3	2.28	0.48
1:M:129:GLU:OE1	3:M:7499:AMP:H5'1	2.13	0.48
1:Q:338:ASN:HB3	5:Q:4403:HOH:O	2.13	0.48
1:T:338:ASN:HB3	5:T:5192:HOH:O	2.13	0.48
1:T:339:ARG:NH2	1:T:339:ARG:HG3	2.28	0.48
1:X:98:GLU:OE1	1:X:99:PRO:HD2	2.13	0.48
1:B:458:HIS:HD2	1:B:460:TYR:N	2.01	0.48
1:H:338:ASN:HB3	5:H:7679:HOH:O	2.13	0.48
1:Q:129:GLU:OE1	3:Q:7507:AMP:H5'1	2.13	0.48
1:W:339:ARG:NH2	1:W:339:ARG:HG3	2.28	0.48
1:A:502:PRO:HB2	1:B:137:SER:HB3	1.94	0.48
1:D:211:HIS:HD2	1:E:33:ILE:HG22	1.77	0.48
1:E:338:ASN:HB3	5:E:1247:HOH:O	2.14	0.48
1:E:129:GLU:OE1	3:E:7483:AMP:H5'1	2.13	0.48
1:F:129:GLU:OE1	3:F:7485:AMP:H5'1	2.13	0.48
1:X:339:ARG:HG3	1:X:339:ARG:NH2	2.28	0.48
1:I:52:SER:CB	1:J:180:PHE:HE2	2.26	0.48
1:L:339:ARG:NH2	1:L:339:ARG:HG3	2.28	0.48
1:R:129:GLU:OE1	3:R:7509:AMP:H5'1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:129:GLU:OE1	3:P:7505:AMP:H5'1	2.13	0.48
3:Q:7507:AMP:N9	3:Q:7507:AMP:H1'	2.08	0.48
3:S:7511:AMP:H1'	3:S:7511:AMP:N9	2.08	0.48
1:W:80:ARG:HD3	1:X:193:ASP:OD2	2.13	0.48
1:X:321:ARG:NE	4:X:7522:CIT:H42	2.21	0.48
1:B:339:ARG:HD2	1:C:60:ILE:HG22	1.95	0.48
1:D:129:GLU:OE1	3:D:7481:AMP:H5'1	2.13	0.48
1:M:52:SER:HB2	1:R:180:PHE:HE2	1.78	0.48
1:S:273:SER:HB2	1:S:282:MET:HG3	1.96	0.48
1:P:175:HIS:CE1	1:W:467:ASP:CB	2.93	0.48
1:R:456:ARG:O	1:X:458:HIS:HE1	1.95	0.48
1:A:320:LYS:HE3	1:G:461:GLU:OE1	2.14	0.48
1:B:273:SER:HB2	1:B:282:MET:HG3	1.96	0.48
1:C:339:ARG:NH2	1:C:339:ARG:HG3	2.28	0.48
1:G:273:SER:HB2	1:G:282:MET:HG3	1.96	0.48
1:L:338:ASN:HB3	5:L:3088:HOH:O	2.13	0.48
1:S:338:ASN:HB3	5:S:4929:HOH:O	2.14	0.48
1:R:175:HIS:HE1	1:S:467:ASP:HB2	1.79	0.48
1:X:338:ASN:HB3	5:X:6244:HOH:O	2.14	0.48
1:L:321:ARG:NE	4:L:7498:CIT:H42	2.21	0.48
1:M:179:TYR:N	1:N:53:SER:OG	2.46	0.48
1:Q:273:SER:HB2	1:Q:282:MET:HG3	1.96	0.48
1:E:273:SER:HB2	1:E:282:MET:HG3	1.96	0.48
1:F:338:ASN:HB3	5:F:7676:HOH:O	2.14	0.48
1:J:273:SER:HB2	1:J:282:MET:HG3	1.96	0.48
1:N:467:ASP:OD2	1:U:175:HIS:CE1	2.62	0.48
1:O:339:ARG:NH2	1:O:339:ARG:HG3	2.28	0.48
1:P:207:GLU:N	1:P:210:HIS:HD2	1.98	0.48
1:T:60:ILE:HG22	1:U:339:ARG:HD2	1.95	0.48
1:G:338:ASN:HB3	5:G:7671:HOH:O	2.14	0.47
1:B:140:PHE:CE1	1:H:463:ALA:HA	2.49	0.47
1:K:375:LEU:HD22	1:K:379:LEU:HG	1.96	0.47
1:L:273:SER:HB2	1:L:282:MET:HG3	1.96	0.47
1:M:465:TYR:CZ	1:S:315:THR:HB	2.49	0.47
1:N:273:SER:HB2	1:N:282:MET:HG3	1.96	0.47
1:Q:339:ARG:HG3	1:Q:339:ARG:NH2	2.28	0.47
1:R:273:SER:HB2	1:R:282:MET:HG3	1.96	0.47
1:R:338:ASN:HB3	5:R:4666:HOH:O	2.14	0.47
1:V:273:SER:HB2	1:V:282:MET:HG3	1.96	0.47
1:V:338:ASN:HB3	5:V:5718:HOH:O	2.13	0.47
1:X:273:SER:HB2	1:X:282:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:THR:HB	1:G:465:TYR:CE1	2.49	0.47
1:E:339:ARG:NH2	1:E:339:ARG:HG3	2.28	0.47
1:F:273:SER:HB2	1:F:282:MET:HG3	1.96	0.47
1:G:264:ASN:HD21	4:G:7488:CIT:H22	1.80	0.47
1:J:338:ASN:HB3	5:J:2562:HOH:O	2.14	0.47
1:P:175:HIS:HE1	1:W:467:ASP:CB	2.27	0.47
1:P:339:ARG:HG3	1:P:339:ARG:NH2	2.28	0.47
1:W:338:ASN:HB3	5:W:5981:HOH:O	2.14	0.47
1:S:179:TYR:CB	1:X:53:SER:OG	2.54	0.47
1:D:207:GLU:N	1:D:210:HIS:HD2	1.98	0.47
1:D:375:LEU:HD22	1:D:379:LEU:HG	1.96	0.47
1:F:264:ASN:HD21	4:F:7486:CIT:H22	1.80	0.47
1:G:339:ARG:NH2	1:G:339:ARG:HG3	2.28	0.47
1:G:375:LEU:HD22	1:G:379:LEU:HG	1.96	0.47
1:H:53:SER:HB3	1:I:179:TYR:HD2	1.79	0.47
1:K:338:ASN:HB3	5:K:2825:HOH:O	2.14	0.47
1:M:309:LEU:HA	1:M:312:THR:HG22	1.96	0.47
1:R:264:ASN:HD21	4:R:7510:CIT:H22	1.80	0.47
1:S:264:ASN:HD21	4:S:7512:CIT:H22	1.80	0.47
1:W:375:LEU:HD22	1:W:379:LEU:HG	1.96	0.47
1:D:339:ARG:HG3	1:D:339:ARG:NH2	2.28	0.47
1:L:309:LEU:HA	1:L:312:THR:HG22	1.97	0.47
1:N:338:ASN:HB3	5:N:3614:HOH:O	2.13	0.47
1:N:339:ARG:NH2	1:N:339:ARG:HG3	2.28	0.47
1:R:321:ARG:NE	4:R:7510:CIT:H42	2.21	0.47
1:S:375:LEU:HD22	1:S:379:LEU:HG	1.96	0.47
1:T:375:LEU:HD22	1:T:379:LEU:HG	1.96	0.47
1:U:309:LEU:HA	1:U:312:THR:HG22	1.97	0.47
1:V:309:LEU:HA	1:V:312:THR:HG22	1.97	0.47
1:Q:456:ARG:O	1:W:458:HIS:HE1	1.97	0.47
1:X:309:LEU:HA	1:X:312:THR:HG22	1.97	0.47
1:A:309:LEU:HA	1:A:312:THR:HG22	1.97	0.47
1:A:264:ASN:HD21	4:A:7476:CIT:H22	1.80	0.47
1:E:179:TYR:CA	1:F:53:SER:OG	2.62	0.47
1:H:309:LEU:HA	1:H:312:THR:HG22	1.97	0.47
1:J:309:LEU:HA	1:J:312:THR:HG22	1.97	0.47
1:O:273:SER:HB2	1:O:282:MET:HG3	1.96	0.47
1:P:375:LEU:HD22	1:P:379:LEU:HG	1.96	0.47
1:R:375:LEU:HD22	1:R:379:LEU:HG	1.96	0.47
3:T:7513:AMP:H1'	3:T:7513:AMP:N9	2.08	0.47
1:W:52:SER:CB	1:X:180:PHE:CE2	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ARG:HG3	1:B:339:ARG:NH2	2.28	0.47
1:C:273:SER:HB2	1:C:282:MET:HG3	1.96	0.47
1:F:375:LEU:HD22	1:F:379:LEU:HG	1.96	0.47
1:H:375:LEU:HD22	1:H:379:LEU:HG	1.96	0.47
1:I:52:SER:HB3	1:J:180:PHE:CE2	2.49	0.47
1:M:264:ASN:HD21	4:M:7500:CIT:H22	1.80	0.47
1:T:309:LEU:HA	1:T:312:THR:HG22	1.97	0.47
1:Q:467:ASP:OD2	1:X:175:HIS:HE1	1.97	0.47
1:C:309:LEU:HA	1:C:312:THR:HG22	1.97	0.47
1:F:321:ARG:NE	4:F:7486:CIT:H42	2.21	0.47
1:I:309:LEU:HA	1:I:312:THR:HG22	1.97	0.47
1:L:264:ASN:HD21	4:L:7498:CIT:H22	1.80	0.47
1:M:273:SER:HB2	1:M:282:MET:HG3	1.96	0.47
1:O:309:LEU:HA	1:O:312:THR:HG22	1.97	0.47
1:P:309:LEU:HA	1:P:312:THR:HG22	1.97	0.47
1:P:98:GLU:OE1	1:P:98:GLU:HA	2.15	0.47
1:X:264:ASN:HD21	4:X:7522:CIT:H22	1.80	0.47
1:A:273:SER:HB2	1:A:282:MET:HG3	1.96	0.47
1:B:338:ASN:HB3	5:B:7658:HOH:O	2.14	0.47
1:D:309:LEU:HA	1:D:312:THR:HG22	1.97	0.47
1:D:450:GLU:HB3	1:J:465:TYR:OH	2.15	0.47
1:J:339:ARG:HG3	1:J:339:ARG:NH2	2.28	0.47
1:S:339:ARG:NH2	1:S:339:ARG:HG3	2.28	0.47
1:T:50:ASP:OD1	1:T:52:SER:OG	2.28	0.47
1:V:53:SER:HB3	1:W:179:TYR:CD2	2.50	0.47
1:C:179:TYR:N	1:D:53:SER:OG	2.46	0.47
1:D:338:ASN:HB3	5:D:984:HOH:O	2.14	0.47
1:E:375:LEU:HD22	1:E:379:LEU:HG	1.96	0.47
3:H:7489:AMP:H1'	3:H:7489:AMP:N9	2.08	0.47
1:I:52:SER:CB	1:J:180:PHE:CE2	2.98	0.47
1:J:375:LEU:HD22	1:J:379:LEU:HG	1.96	0.47
1:M:193:ASP:OD2	1:N:80:ARG:HD3	2.14	0.47
1:N:375:LEU:HD22	1:N:379:LEU:HG	1.96	0.47
1:Q:375:LEU:HD22	1:Q:379:LEU:HG	1.96	0.47
1:U:273:SER:HB2	1:U:282:MET:HG3	1.96	0.47
1:U:338:ASN:HB3	5:U:5455:HOH:O	2.13	0.47
1:W:264:ASN:HD21	4:W:7520:CIT:H22	1.79	0.47
1:E:309:LEU:HA	1:E:312:THR:HG22	1.97	0.47
1:I:273:SER:HB2	1:I:282:MET:HG3	1.96	0.47
1:I:375:LEU:HD22	1:I:379:LEU:HG	1.96	0.47
1:K:273:SER:HB2	1:K:282:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:427:TYR:CE1	1:K:428:LEU:HD13	2.50	0.47
1:K:264:ASN:HD21	4:K:7496:CIT:H22	1.80	0.47
1:P:338:ASN:HB3	5:P:4140:HOH:O	2.14	0.47
1:T:264:ASN:HD21	4:T:7514:CIT:H22	1.80	0.47
1:V:339:ARG:NH2	1:V:339:ARG:HG3	2.28	0.47
1:I:338:ASN:HB3	5:I:7681:HOH:O	2.14	0.47
1:O:264:ASN:HD21	4:O:7504:CIT:H22	1.80	0.47
1:Q:309:LEU:HA	1:Q:312:THR:HG22	1.97	0.47
1:U:375:LEU:HD22	1:U:379:LEU:HG	1.96	0.47
1:V:375:LEU:HD22	1:V:379:LEU:HG	1.96	0.47
1:C:264:ASN:HD21	4:C:7480:CIT:H22	1.80	0.46
1:I:332:LEU:HD23	1:I:342:CYS:SG	2.56	0.46
1:I:52:SER:HB2	1:J:180:PHE:HE2	1.79	0.46
1:L:332:LEU:HD23	1:L:342:CYS:SG	2.56	0.46
1:S:137:SER:HB3	1:T:502:PRO:HB2	1.97	0.46
1:V:264:ASN:HD21	4:V:7518:CIT:H22	1.80	0.46
1:V:80:ARG:HD3	1:W:193:ASP:OD2	2.14	0.46
1:W:427:TYR:CE1	1:W:428:LEU:HD13	2.50	0.46
1:X:375:LEU:HD22	1:X:379:LEU:HG	1.96	0.46
1:D:427:TYR:CE1	1:D:428:LEU:HD13	2.50	0.46
1:E:264:ASN:HD21	4:E:7484:CIT:H22	1.80	0.46
3:F:7485:AMP:N9	3:F:7485:AMP:H1'	2.08	0.46
1:H:264:ASN:HD21	4:H:7490:CIT:H22	1.80	0.46
1:J:264:ASN:HD21	4:J:7494:CIT:H22	1.80	0.46
1:M:332:LEU:HD23	1:M:342:CYS:SG	2.56	0.46
1:P:427:TYR:CE1	1:P:428:LEU:HD13	2.50	0.46
1:U:332:LEU:HD23	1:U:342:CYS:SG	2.56	0.46
1:V:332:LEU:HD23	1:V:342:CYS:SG	2.56	0.46
1:W:273:SER:HB2	1:W:282:MET:HG3	1.96	0.46
1:X:332:LEU:HD23	1:X:342:CYS:SG	2.56	0.46
1:B:309:LEU:HA	1:B:312:THR:HG22	1.97	0.46
1:B:375:LEU:HD22	1:B:379:LEU:HG	1.96	0.46
1:B:413:GLN:HG2	5:B:7738:HOH:O	2.15	0.46
1:B:427:TYR:CE1	1:B:428:LEU:HD13	2.50	0.46
1:F:332:LEU:HD23	1:F:342:CYS:SG	2.56	0.46
1:G:427:TYR:CE1	1:G:428:LEU:HD13	2.50	0.46
1:H:321:ARG:NE	4:H:7490:CIT:H42	2.21	0.46
1:L:375:LEU:HD22	1:L:379:LEU:HG	1.96	0.46
1:N:427:TYR:CE1	1:N:428:LEU:HD13	2.50	0.46
1:S:321:ARG:NE	4:S:7512:CIT:H42	2.21	0.46
1:W:52:SER:CB	1:X:180:PHE:HE2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LEU:HD23	1:A:342:CYS:SG	2.56	0.46
1:C:375:LEU:HD22	1:C:379:LEU:HG	1.96	0.46
1:C:50:ASP:O	1:C:52:SER:N	2.49	0.46
1:D:176:LYS:HE3	5:E:1226:HOH:O	2.15	0.46
1:I:264:ASN:HD21	4:I:7492:CIT:H22	1.80	0.46
1:J:332:LEU:HD23	1:J:342:CYS:SG	2.56	0.46
1:L:427:TYR:CE1	1:L:428:LEU:HD13	2.50	0.46
1:N:264:ASN:HD21	4:N:7502:CIT:H22	1.80	0.46
1:O:176:LYS:HE3	5:P:4119:HOH:O	2.15	0.46
1:P:206:LEU:HB3	1:Q:34:PRO:HG3	1.97	0.46
1:P:273:SER:HB2	1:P:282:MET:HG3	1.96	0.46
1:Q:264:ASN:HD21	4:Q:7508:CIT:H22	1.80	0.46
3:R:7509:AMP:H1'	3:R:7509:AMP:N9	2.08	0.46
1:T:321:ARG:NE	4:T:7514:CIT:H42	2.21	0.46
1:U:207:GLU:HB3	1:U:208:LYS:H	1.44	0.46
1:U:60:ILE:HG22	1:V:339:ARG:HD2	1.96	0.46
1:A:315:THR:HB	1:G:465:TYR:CZ	2.51	0.46
1:B:332:LEU:HD23	1:B:342:CYS:SG	2.56	0.46
1:E:427:TYR:CE1	1:E:428:LEU:HD13	2.50	0.46
1:G:309:LEU:HA	1:G:312:THR:HG22	1.97	0.46
1:L:50:ASP:O	1:L:52:SER:N	2.49	0.46
1:O:375:LEU:HD22	1:O:379:LEU:HG	1.96	0.46
1:Q:427:TYR:CE1	1:Q:428:LEU:HD13	2.50	0.46
1:R:332:LEU:HD23	1:R:342:CYS:SG	2.56	0.46
1:R:427:TYR:CE1	1:R:428:LEU:HD13	2.50	0.46
1:S:427:TYR:CE1	1:S:428:LEU:HD13	2.50	0.46
1:S:50:ASP:O	1:S:52:SER:N	2.49	0.46
1:T:273:SER:HB2	1:T:282:MET:HG3	1.96	0.46
1:U:264:ASN:HD21	4:U:7516:CIT:H22	1.79	0.46
1:A:375:LEU:HD22	1:A:379:LEU:HG	1.96	0.46
1:A:50:ASP:O	1:A:52:SER:N	2.49	0.46
1:C:332:LEU:HD23	1:C:342:CYS:SG	2.56	0.46
1:C:427:TYR:CE1	1:C:428:LEU:HD13	2.50	0.46
1:D:273:SER:HB2	1:D:282:MET:HG3	1.96	0.46
1:D:466:TYR:CZ	1:J:254:THR:HB	2.51	0.46
1:F:427:TYR:CE1	1:F:428:LEU:HD13	2.50	0.46
1:G:50:ASP:O	1:G:52:SER:N	2.49	0.46
1:I:339:ARG:NH2	1:I:339:ARG:HG3	2.28	0.46
1:M:50:ASP:O	1:M:52:SER:N	2.49	0.46
1:O:332:LEU:HD23	1:O:342:CYS:SG	2.56	0.46
1:O:427:TYR:CE1	1:O:428:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:50:ASP:O	1:O:52:SER:N	2.49	0.46
1:P:332:LEU:HD23	1:P:342:CYS:SG	2.56	0.46
1:O:339:ARG:HD2	1:P:60:ILE:CG2	2.43	0.46
1:V:264:ASN:ND2	4:V:7518:CIT:C5	2.79	0.46
1:V:50:ASP:O	1:V:52:SER:N	2.49	0.46
1:B:264:ASN:HD21	4:B:7478:CIT:H22	1.80	0.46
1:D:332:LEU:HD23	1:D:342:CYS:SG	2.56	0.46
1:H:273:SER:HB2	1:H:282:MET:HG3	1.96	0.46
1:J:264:ASN:ND2	4:J:7494:CIT:C5	2.79	0.46
1:J:50:ASP:O	1:J:52:SER:N	2.49	0.46
1:L:106:ASN:ND2	1:L:109:ARG:HH11	2.14	0.46
1:N:309:LEU:HA	1:N:312:THR:HG22	1.97	0.46
1:O:458:HIS:HE1	1:U:456:ARG:O	1.98	0.46
1:U:339:ARG:NH2	1:U:339:ARG:HG3	2.28	0.46
1:X:427:TYR:CE1	1:X:428:LEU:HD13	2.50	0.46
1:X:50:ASP:O	1:X:52:SER:N	2.49	0.46
1:G:321:ARG:NE	4:G:7488:CIT:H42	2.21	0.46
1:H:50:ASP:O	1:H:52:SER:N	2.49	0.46
1:I:427:TYR:CE1	1:I:428:LEU:HD13	2.50	0.46
1:K:332:LEU:HD23	1:K:342:CYS:SG	2.56	0.46
1:K:264:ASN:ND2	4:K:7496:CIT:C5	2.79	0.46
1:N:332:LEU:HD23	1:N:342:CYS:SG	2.56	0.46
1:O:179:TYR:H	1:P:53:SER:CB	2.28	0.46
1:P:50:ASP:O	1:P:52:SER:N	2.49	0.46
1:Q:332:LEU:HD23	1:Q:342:CYS:SG	2.56	0.46
1:T:50:ASP:O	1:T:52:SER:N	2.49	0.46
1:U:427:TYR:CE1	1:U:428:LEU:HD13	2.50	0.46
1:A:264:ASN:ND2	4:A:7476:CIT:C5	2.79	0.46
1:N:465:TYR:CE1	1:T:315:THR:HB	2.51	0.46
1:S:309:LEU:HA	1:S:312:THR:HG22	1.97	0.46
1:W:309:LEU:HA	1:W:312:THR:HG22	1.97	0.46
1:W:332:LEU:HD23	1:W:342:CYS:SG	2.56	0.46
1:W:264:ASN:ND2	4:W:7520:CIT:C5	2.79	0.46
1:X:106:ASN:ND2	1:X:109:ARG:HH11	2.14	0.46
1:A:106:ASN:ND2	1:A:109:ARG:HH11	2.14	0.46
1:D:50:ASP:O	1:D:52:SER:N	2.49	0.46
1:E:332:LEU:HD23	1:E:342:CYS:SG	2.56	0.46
1:F:309:LEU:HA	1:F:312:THR:HG22	1.97	0.46
1:M:375:LEU:HD22	1:M:379:LEU:HG	1.96	0.46
1:M:264:ASN:ND2	4:M:7500:CIT:C5	2.79	0.46
1:R:50:ASP:O	1:R:52:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:332:LEU:HD23	1:S:342:CYS:SG	2.56	0.46
1:A:461:GLU:OE1	1:G:320:LYS:HE3	2.17	0.45
1:F:50:ASP:O	1:F:52:SER:N	2.49	0.45
1:H:427:TYR:CE1	1:H:428:LEU:HD13	2.50	0.45
1:M:106:ASN:ND2	1:M:109:ARG:HH11	2.14	0.45
1:T:427:TYR:CE1	1:T:428:LEU:HD13	2.50	0.45
1:D:264:ASN:HD21	4:D:7482:CIT:H22	1.80	0.45
1:G:332:LEU:HD23	1:G:342:CYS:SG	2.56	0.45
1:G:264:ASN:ND2	4:G:7488:CIT:C5	2.79	0.45
1:K:309:LEU:HA	1:K:312:THR:HG22	1.97	0.45
1:M:339:ARG:HD2	1:N:60:ILE:HG22	1.98	0.45
1:P:264:ASN:HD21	4:P:7506:CIT:H22	1.80	0.45
1:Q:264:ASN:ND2	4:Q:7508:CIT:C5	2.79	0.45
1:Q:50:ASP:O	1:Q:52:SER:N	2.49	0.45
1:D:264:ASN:ND2	4:D:7482:CIT:C5	2.79	0.45
1:E:50:ASP:O	1:E:52:SER:N	2.49	0.45
1:H:332:LEU:HD23	1:H:342:CYS:SG	2.56	0.45
1:I:106:ASN:ND2	1:I:109:ARG:HH11	2.14	0.45
1:I:264:ASN:ND2	4:I:7492:CIT:C5	2.79	0.45
1:P:264:ASN:ND2	4:P:7506:CIT:C5	2.79	0.45
1:R:309:LEU:HA	1:R:312:THR:HG22	1.97	0.45
1:T:332:LEU:HD23	1:T:342:CYS:SG	2.56	0.45
1:A:427:TYR:CE1	1:A:428:LEU:HD13	2.50	0.45
1:B:50:ASP:O	1:B:52:SER:N	2.49	0.45
1:C:106:ASN:ND2	1:C:109:ARG:HH11	2.14	0.45
1:C:264:ASN:ND2	4:C:7480:CIT:C5	2.79	0.45
1:D:206:LEU:HB3	1:E:34:PRO:HG3	1.98	0.45
1:F:264:ASN:ND2	4:F:7486:CIT:C5	2.79	0.45
1:C:458:HIS:HE1	1:I:456:ARG:O	1.99	0.45
1:I:53:SER:HB3	1:J:179:TYR:CD2	2.51	0.45
1:J:106:ASN:ND2	1:J:109:ARG:HH11	2.14	0.45
1:K:106:ASN:ND2	1:K:109:ARG:HH11	2.14	0.45
1:M:427:TYR:CE1	1:M:428:LEU:HD13	2.50	0.45
1:M:53:SER:OG	1:R:179:TYR:CB	2.48	0.45
1:O:264:ASN:ND2	4:O:7504:CIT:C5	2.79	0.45
1:R:264:ASN:ND2	4:R:7510:CIT:C5	2.79	0.45
1:T:106:ASN:ND2	1:T:109:ARG:HH11	2.14	0.45
1:U:458:HIS:HD2	1:U:460:TYR:N	2.01	0.45
1:V:106:ASN:ND2	1:V:109:ARG:HH11	2.14	0.45
1:W:106:ASN:ND2	1:W:109:ARG:HH11	2.14	0.45
1:B:106:ASN:ND2	1:B:109:ARG:HH11	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:450:GLU:HA	1:K:464:LEU:HD21	1.98	0.45
1:F:243:LYS:NZ	1:L:468:VAL:O	2.45	0.45
1:O:106:ASN:ND2	1:O:109:ARG:HH11	2.14	0.45
1:U:106:ASN:ND2	1:U:109:ARG:HH11	2.14	0.45
1:V:427:TYR:CE1	1:V:428:LEU:HD13	2.50	0.45
1:R:458:HIS:HE1	1:X:456:ARG:O	2.00	0.45
1:H:106:ASN:ND2	1:H:109:ARG:HH11	2.14	0.45
1:C:456:ARG:O	1:I:458:HIS:HE1	1.99	0.45
1:J:427:TYR:CE1	1:J:428:LEU:HD13	2.50	0.45
1:D:467:ASP:CB	1:K:175:HIS:HE1	2.27	0.45
1:K:207:GLU:N	1:K:210:HIS:HD2	1.98	0.45
1:S:264:ASN:ND2	4:S:7512:CIT:C5	2.79	0.45
1:U:264:ASN:ND2	4:U:7516:CIT:C5	2.79	0.45
1:H:53:SER:HG	1:I:179:TYR:HB2	1.73	0.45
1:N:106:ASN:ND2	1:N:109:ARG:HH11	2.14	0.45
1:N:50:ASP:O	1:N:52:SER:N	2.49	0.45
1:W:207:GLU:N	1:W:210:HIS:HD2	1.98	0.45
1:C:179:TYR:HD2	1:D:53:SER:HB3	1.81	0.45
1:D:106:ASN:ND2	1:D:109:ARG:HH11	2.14	0.45
1:E:207:GLU:N	1:E:210:HIS:HD2	1.98	0.45
1:H:429:THR:HG21	1:H:436:ASN:OD1	2.17	0.45
1:K:321:ARG:NE	4:K:7496:CIT:H42	2.21	0.45
1:Q:207:GLU:N	1:Q:210:HIS:HD2	1.98	0.45
1:T:429:THR:HG21	1:T:436:ASN:OD1	2.17	0.45
1:A:429:THR:HG21	1:A:436:ASN:OD1	2.17	0.45
1:H:264:ASN:ND2	4:H:7490:CIT:C5	2.79	0.45
1:J:429:THR:HG21	1:J:436:ASN:OD1	2.17	0.45
1:M:429:THR:HG21	1:M:436:ASN:OD1	2.17	0.45
1:P:106:ASN:ND2	1:P:109:ARG:HH11	2.14	0.45
1:V:429:THR:HG21	1:V:436:ASN:OD1	2.17	0.45
1:C:458:HIS:HD2	1:C:460:TYR:N	2.01	0.45
1:D:207:GLU:HB3	1:D:208:LYS:H	1.44	0.45
1:I:50:ASP:O	1:I:52:SER:N	2.49	0.45
1:G:206:LEU:CB	1:L:34:PRO:HG3	2.45	0.45
1:Q:465:TYR:CE1	1:W:315:THR:HB	2.51	0.45
1:S:429:THR:HG21	1:S:436:ASN:OD1	2.17	0.45
1:W:50:ASP:O	1:W:52:SER:N	2.49	0.45
1:W:52:SER:HB3	1:X:180:PHE:CE2	2.52	0.45
1:B:264:ASN:ND2	4:B:7478:CIT:C5	2.79	0.44
1:E:264:ASN:ND2	4:E:7484:CIT:C5	2.79	0.44
1:G:429:THR:HG21	1:G:436:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:429:THR:HG21	1:R:436:ASN:OD1	2.17	0.44
1:N:140:PHE:CE1	1:T:463:ALA:HA	2.52	0.44
1:X:429:THR:HG21	1:X:436:ASN:OD1	2.17	0.44
1:E:429:THR:HG21	1:E:436:ASN:OD1	2.17	0.44
1:F:429:THR:HG21	1:F:436:ASN:OD1	2.17	0.44
1:I:53:SER:OG	1:J:179:TYR:N	2.49	0.44
1:J:458:HIS:HD2	1:J:460:TYR:N	2.01	0.44
1:K:50:ASP:O	1:K:52:SER:N	2.49	0.44
1:L:429:THR:HG21	1:L:436:ASN:OD1	2.17	0.44
1:P:176:LYS:HE3	5:Q:4382:HOH:O	2.16	0.44
1:Q:106:ASN:ND2	1:Q:109:ARG:HH11	2.14	0.44
1:T:264:ASN:ND2	4:T:7514:CIT:C5	2.79	0.44
1:U:50:ASP:O	1:U:52:SER:N	2.49	0.44
1:V:458:HIS:HD2	1:V:460:TYR:N	2.01	0.44
1:A:80:ARG:HD3	1:F:193:ASP:OD2	2.18	0.44
1:E:106:ASN:ND2	1:E:109:ARG:HH11	2.14	0.44
1:F:106:ASN:ND2	1:F:109:ARG:HH11	2.14	0.44
1:I:458:HIS:HD2	1:I:460:TYR:N	2.01	0.44
1:D:175:HIS:CE1	1:K:467:ASP:CG	2.69	0.44
1:M:315:THR:HB	1:S:465:TYR:CZ	2.52	0.44
1:Q:429:THR:HG21	1:Q:436:ASN:OD1	2.17	0.44
1:P:207:GLU:HB3	1:P:208:LYS:H	1.44	0.44
1:U:50:ASP:OD1	1:U:52:SER:OG	2.28	0.44
1:W:321:ARG:NE	4:W:7520:CIT:H42	2.21	0.44
1:X:264:ASN:ND2	4:X:7522:CIT:C5	2.79	0.44
1:F:175:HIS:CE1	1:G:467:ASP:CB	2.98	0.44
1:N:264:ASN:ND2	4:N:7502:CIT:C5	2.79	0.44
1:R:106:ASN:ND2	1:R:109:ARG:HH11	2.14	0.44
1:J:60:ILE:HD12	5:K:2825:HOH:O	2.18	0.44
1:K:429:THR:HG21	1:K:436:ASN:OD1	2.17	0.44
1:L:264:ASN:ND2	4:L:7498:CIT:C5	2.79	0.44
1:R:328:ALA:HA	1:R:329:PRO:HD3	1.87	0.44
1:S:106:ASN:ND2	1:S:109:ARG:HH11	2.14	0.44
1:W:60:ILE:HG22	1:X:339:ARG:HD2	1.99	0.44
1:D:429:THR:HG21	1:D:436:ASN:OD1	2.17	0.44
1:F:328:ALA:HA	1:F:329:PRO:HD3	1.87	0.44
1:G:106:ASN:ND2	1:G:109:ARG:HH11	2.14	0.44
1:O:458:HIS:HD2	1:O:460:TYR:N	2.01	0.44
1:P:429:THR:HG21	1:P:436:ASN:OD1	2.17	0.44
1:U:429:THR:HG21	1:U:436:ASN:OD1	2.17	0.44
1:D:146:GLY:HA2	1:J:149:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:429:THR:HG21	1:O:436:ASN:OD1	2.17	0.44
1:T:53:SER:OG	1:U:179:TYR:CB	2.51	0.44
1:Q:315:THR:HB	1:W:465:TYR:CZ	2.52	0.44
1:Q:467:ASP:HB2	1:X:175:HIS:CE1	2.53	0.44
1:K:50:ASP:OD1	1:K:52:SER:OG	2.28	0.44
1:R:173:VAL:HG21	5:S:4792:HOH:O	2.17	0.44
1:W:429:THR:HG21	1:W:436:ASN:OD1	2.17	0.44
1:W:50:ASP:OD1	1:W:52:SER:OG	2.28	0.44
1:C:429:THR:HG21	1:C:436:ASN:OD1	2.17	0.43
1:I:429:THR:HG21	1:I:436:ASN:OD1	2.17	0.43
1:Q:320:LYS:HE3	1:W:461:GLU:OE1	2.18	0.43
1:N:463:ALA:HA	1:T:140:PHE:CE1	2.53	0.43
1:N:328:ALA:HA	1:N:329:PRO:HD3	1.87	0.43
1:S:328:ALA:HA	1:S:329:PRO:HD3	1.87	0.43
1:X:345:ILE:N	1:X:345:ILE:HD12	2.34	0.43
1:X:458:HIS:HD2	1:X:460:TYR:N	2.01	0.43
1:A:345:ILE:HD12	1:A:345:ILE:N	2.34	0.43
1:B:429:THR:HG21	1:B:436:ASN:OD1	2.17	0.43
1:D:98:GLU:OE1	1:D:99:PRO:HD2	2.19	0.43
1:L:345:ILE:N	1:L:345:ILE:HD12	2.34	0.43
1:L:458:HIS:HD2	1:L:460:TYR:N	2.01	0.43
1:C:345:ILE:HD12	1:C:345:ILE:N	2.34	0.43
1:D:98:GLU:HB3	5:D:1018:HOH:O	2.18	0.43
1:E:180:PHE:CZ	1:F:52:SER:HB3	2.52	0.43
1:M:345:ILE:N	1:M:345:ILE:HD12	2.34	0.43
1:N:429:THR:HG21	1:N:436:ASN:OD1	2.17	0.43
1:Q:169:ARG:HB3	1:R:252:THR:HB	2.01	0.43
1:S:256:MET:HA	1:S:257:PRO:HD3	1.90	0.43
1:V:345:ILE:HD12	1:V:345:ILE:N	2.34	0.43
1:D:467:ASP:HB2	5:D:2709:HOH:O	2.18	0.43
1:F:345:ILE:HD12	1:F:345:ILE:N	2.34	0.43
1:G:53:SER:HB3	1:H:179:TYR:CD2	2.53	0.43
1:H:121:ALA:HB1	1:H:275:TRP:O	2.19	0.43
1:K:345:ILE:HD12	1:K:345:ILE:N	2.34	0.43
1:M:121:ALA:HB1	1:M:275:TRP:O	2.19	0.43
1:M:52:SER:HB3	1:R:180:PHE:CE2	2.53	0.43
1:O:345:ILE:HD12	1:O:345:ILE:N	2.34	0.43
1:Q:458:HIS:HD2	1:Q:460:TYR:N	2.01	0.43
1:Q:461:GLU:OE1	1:W:320:LYS:HE3	2.18	0.43
1:R:345:ILE:HD12	1:R:345:ILE:N	2.34	0.43
1:U:328:ALA:O	1:U:330:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ALA:O	1:B:330:ILE:HG12	2.19	0.43
1:E:458:HIS:HD2	1:E:460:TYR:N	2.01	0.43
1:I:328:ALA:O	1:I:330:ILE:HG12	2.19	0.43
1:I:345:ILE:HD12	1:I:345:ILE:N	2.34	0.43
1:J:345:ILE:HD12	1:J:345:ILE:N	2.34	0.43
1:L:54:ILE:HD13	1:L:54:ILE:HA	1.86	0.43
1:O:121:ALA:HB1	1:O:275:TRP:O	2.19	0.43
1:M:52:SER:CB	1:R:180:PHE:HE2	2.32	0.43
1:T:121:ALA:HB1	1:T:275:TRP:O	2.19	0.43
1:U:323:VAL:HG22	1:U:324:PRO:HD2	2.01	0.43
1:P:467:ASP:CB	1:W:175:HIS:CE1	2.99	0.43
1:W:345:ILE:N	1:W:345:ILE:HD12	2.34	0.43
1:A:121:ALA:HB1	1:A:275:TRP:O	2.19	0.43
1:A:321:ARG:NE	4:A:7476:CIT:H42	2.21	0.43
1:C:121:ALA:HB1	1:C:275:TRP:O	2.19	0.43
1:E:179:TYR:CD2	1:F:53:SER:HB3	2.48	0.43
1:G:345:ILE:HD12	1:G:345:ILE:N	2.34	0.43
1:A:467:ASP:HB2	1:H:175:HIS:CE1	2.54	0.43
1:H:345:ILE:N	1:H:345:ILE:HD12	2.34	0.43
1:M:321:ARG:NE	4:M:7500:CIT:H42	2.21	0.43
1:R:256:MET:HA	1:R:257:PRO:HD3	1.90	0.43
1:T:323:VAL:HG22	1:T:324:PRO:HD2	2.01	0.43
1:U:345:ILE:N	1:U:345:ILE:HD12	2.34	0.43
1:X:323:VAL:HG22	1:X:324:PRO:HD2	2.01	0.43
1:H:323:VAL:HG22	1:H:324:PRO:HD2	2.01	0.43
1:I:323:VAL:HG22	1:I:324:PRO:HD2	2.01	0.43
1:K:323:VAL:HG22	1:K:324:PRO:HD2	2.01	0.43
1:L:323:VAL:HG22	1:L:324:PRO:HD2	2.01	0.43
1:N:328:ALA:O	1:N:330:ILE:HG12	2.19	0.43
1:S:323:VAL:HG22	1:S:324:PRO:HD2	2.01	0.43
1:A:463:ALA:HA	1:G:140:PHE:CE1	2.54	0.43
1:A:465:TYR:CE1	1:G:315:THR:HB	2.54	0.43
1:B:323:VAL:HG22	1:B:324:PRO:HD2	2.01	0.43
1:C:323:VAL:HG22	1:C:324:PRO:HD2	2.01	0.43
1:D:328:ALA:O	1:D:330:ILE:HG12	2.19	0.43
1:E:271:HIS:CD2	3:E:7483:AMP:H4'	2.54	0.43
1:F:271:HIS:CD2	3:F:7485:AMP:H4'	2.54	0.43
1:G:121:ALA:HB1	1:G:275:TRP:O	2.19	0.43
1:G:323:VAL:HG22	1:G:324:PRO:HD2	2.01	0.43
1:H:458:HIS:HD2	1:H:460:TYR:N	2.01	0.43
1:N:323:VAL:HG22	1:N:324:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:345:ILE:HD12	1:N:345:ILE:N	2.34	0.43
1:P:328:ALA:O	1:P:330:ILE:HG12	2.19	0.43
1:S:345:ILE:N	1:S:345:ILE:HD12	2.34	0.43
1:T:271:HIS:CD2	3:T:7513:AMP:H4'	2.54	0.43
1:T:345:ILE:N	1:T:345:ILE:HD12	2.34	0.43
1:W:323:VAL:HG22	1:W:324:PRO:HD2	2.01	0.43
1:F:323:VAL:HG22	1:F:324:PRO:HD2	2.01	0.43
1:G:328:ALA:O	1:G:330:ILE:HG12	2.19	0.43
1:H:271:HIS:CD2	3:H:7489:AMP:H4'	2.54	0.43
1:J:328:ALA:O	1:J:330:ILE:HG12	2.19	0.43
1:E:463:ALA:HA	1:K:140:PHE:CZ	2.54	0.43
1:M:52:SER:CB	1:R:180:PHE:CE2	3.02	0.43
1:M:271:HIS:CD2	3:M:7499:AMP:H4'	2.54	0.43
1:N:121:ALA:HB1	1:N:275:TRP:O	2.19	0.43
1:O:323:VAL:HG22	1:O:324:PRO:HD2	2.01	0.43
1:Q:345:ILE:N	1:Q:345:ILE:HD12	2.34	0.43
1:R:271:HIS:CD2	3:R:7509:AMP:H4'	2.54	0.43
1:T:458:HIS:HD2	1:T:460:TYR:N	2.01	0.43
1:A:271:HIS:CD2	3:A:7475:AMP:H4'	2.54	0.42
1:A:95:PHE:HZ	1:F:347:ILE:HD13	1.84	0.42
1:B:121:ALA:HB1	1:B:275:TRP:O	2.19	0.42
1:C:328:ALA:O	1:C:330:ILE:HG12	2.19	0.42
1:D:271:HIS:CD2	3:D:7481:AMP:H4'	2.54	0.42
1:E:323:VAL:HG22	1:E:324:PRO:HD2	2.01	0.42
1:E:345:ILE:N	1:E:345:ILE:HD12	2.34	0.42
1:F:256:MET:HA	1:F:257:PRO:HD3	1.90	0.42
1:I:137:SER:HB3	1:J:502:PRO:HB2	2.01	0.42
1:O:328:ALA:O	1:O:330:ILE:HG12	2.19	0.42
1:P:271:HIS:CD2	3:P:7505:AMP:H4'	2.54	0.42
1:Q:121:ALA:HB1	1:Q:275:TRP:O	2.19	0.42
1:Q:271:HIS:CD2	3:Q:7507:AMP:H4'	2.54	0.42
1:Q:323:VAL:HG22	1:Q:324:PRO:HD2	2.01	0.42
1:R:323:VAL:HG22	1:R:324:PRO:HD2	2.01	0.42
1:S:121:ALA:HB1	1:S:275:TRP:O	2.19	0.42
1:S:328:ALA:O	1:S:330:ILE:HG12	2.19	0.42
1:V:328:ALA:O	1:V:330:ILE:HG12	2.19	0.42
1:B:345:ILE:HD12	1:B:345:ILE:N	2.34	0.42
1:E:121:ALA:HB1	1:E:275:TRP:O	2.19	0.42
1:F:121:ALA:HB1	1:F:275:TRP:O	2.19	0.42
1:G:256:MET:HA	1:G:257:PRO:HD3	1.90	0.42
1:J:323:VAL:HG22	1:J:324:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:173:VAL:HG21	5:U:5318:HOH:O	2.18	0.42
1:T:328:ALA:HA	1:T:329:PRO:HD3	1.87	0.42
1:W:121:ALA:HB1	1:W:275:TRP:O	2.19	0.42
1:L:271:HIS:CD2	3:L:7497:AMP:H4'	2.54	0.42
1:M:175:HIS:HE1	1:T:467:ASP:OD2	2.02	0.42
1:R:121:ALA:HB1	1:R:275:TRP:O	2.19	0.42
1:T:53:SER:HG	1:U:179:TYR:HB2	1.76	0.42
1:X:271:HIS:CD2	3:X:7521:AMP:H4'	2.54	0.42
1:K:121:ALA:HB1	1:K:275:TRP:O	2.19	0.42
1:S:271:HIS:CD2	3:S:7511:AMP:H4'	2.54	0.42
1:V:323:VAL:HG22	1:V:324:PRO:HD2	2.01	0.42
1:D:121:ALA:HB1	1:D:275:TRP:O	2.19	0.42
1:G:179:TYR:CD2	1:L:53:SER:HB3	2.54	0.42
1:G:271:HIS:CD2	3:G:7487:AMP:H4'	2.54	0.42
1:H:24:LEU:HB3	1:H:25:PRO:CD	2.50	0.42
1:H:328:ALA:HA	1:H:329:PRO:HD3	1.87	0.42
1:M:24:LEU:HB3	1:M:25:PRO:CD	2.50	0.42
1:O:175:HIS:CE1	1:V:467:ASP:HB2	2.54	0.42
1:P:121:ALA:HB1	1:P:275:TRP:O	2.19	0.42
1:Q:24:LEU:HB3	1:Q:25:PRO:CD	2.50	0.42
1:S:206:LEU:HB3	1:X:34:PRO:HG3	2.01	0.42
1:A:24:LEU:HB3	1:A:25:PRO:CD	2.50	0.42
1:B:461:GLU:OE1	1:H:320:LYS:HE3	2.19	0.42
1:D:24:LEU:HB3	1:D:25:PRO:CD	2.50	0.42
1:E:24:LEU:HB3	1:E:25:PRO:CD	2.50	0.42
1:E:314:PRO:HG3	1:E:365:GLY:HA3	2.02	0.42
1:G:60:ILE:HG22	1:H:339:ARG:HD2	2.01	0.42
5:B:7704:HOH:O	1:H:413:GLN:HG2	2.19	0.42
1:I:207:GLU:HB3	1:I:208:LYS:H	1.44	0.42
1:D:140:PHE:CE1	1:J:463:ALA:HA	2.54	0.42
1:K:24:LEU:HB3	1:K:25:PRO:CD	2.50	0.42
1:L:121:ALA:HB1	1:L:275:TRP:O	2.19	0.42
1:O:271:HIS:CD2	3:O:7503:AMP:H4'	2.54	0.42
1:P:24:LEU:HB3	1:P:25:PRO:CD	2.50	0.42
1:Q:314:PRO:HG3	1:Q:365:GLY:HA3	2.02	0.42
1:Q:328:ALA:O	1:Q:330:ILE:HG12	2.19	0.42
1:R:467:ASP:OD2	1:S:175:HIS:HE1	2.02	0.42
1:N:175:HIS:CE1	1:U:467:ASP:HB2	2.55	0.42
1:W:24:LEU:HB3	1:W:25:PRO:CD	2.50	0.42
1:X:121:ALA:HB1	1:X:275:TRP:O	2.19	0.42
1:E:328:ALA:O	1:E:330:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:468:VAL:O	1:L:243:LYS:NZ	2.49	0.42
1:L:314:PRO:HG3	1:L:365:GLY:HA3	2.02	0.42
1:T:24:LEU:HB3	1:T:25:PRO:CD	2.50	0.42
1:U:121:ALA:HB1	1:U:275:TRP:O	2.19	0.42
1:X:314:PRO:HG3	1:X:365:GLY:HA3	2.02	0.42
1:C:314:PRO:HG3	1:C:365:GLY:HA3	2.02	0.42
1:F:467:ASP:CB	1:G:175:HIS:HE1	2.33	0.42
1:G:328:ALA:HA	1:G:329:PRO:HD3	1.87	0.42
1:I:121:ALA:HB1	1:I:275:TRP:O	2.19	0.42
1:J:121:ALA:HB1	1:J:275:TRP:O	2.19	0.42
1:J:24:LEU:HB3	1:J:25:PRO:CD	2.50	0.42
1:E:462:PHE:CZ	1:K:149:TYR:CE1	3.07	0.42
1:O:314:PRO:HG3	1:O:365:GLY:HA3	2.02	0.42
1:S:207:GLU:N	1:S:210:HIS:HD2	1.98	0.42
1:S:24:LEU:HB3	1:S:25:PRO:CD	2.50	0.42
1:T:314:PRO:HG3	1:T:365:GLY:HA3	2.02	0.42
1:V:24:LEU:HB3	1:V:25:PRO:CD	2.50	0.42
1:A:314:PRO:HG3	1:A:365:GLY:HA3	2.02	0.42
1:A:328:ALA:O	1:A:330:ILE:HG12	2.19	0.42
1:C:271:HIS:CD2	3:C:7479:AMP:H4'	2.54	0.42
1:D:345:ILE:N	1:D:345:ILE:HD12	2.34	0.42
1:F:328:ALA:O	1:F:330:ILE:HG12	2.19	0.42
1:I:321:ARG:NE	4:I:7492:CIT:H42	2.21	0.42
1:K:400:PRO:HG2	1:K:403:GLU:CB	2.49	0.42
1:M:314:PRO:HG3	1:M:365:GLY:HA3	2.02	0.42
1:N:271:HIS:CD2	3:N:7501:AMP:H4'	2.54	0.42
1:R:328:ALA:O	1:R:330:ILE:HG12	2.19	0.42
1:V:314:PRO:HG3	1:V:365:GLY:HA3	2.02	0.42
1:A:465:TYR:CZ	1:G:315:THR:HB	2.55	0.42
1:A:60:ILE:HG21	1:F:339:ARG:HB2	2.02	0.42
1:F:83:LYS:HD3	1:F:83:LYS:HA	1.94	0.42
1:G:24:LEU:HB3	1:G:25:PRO:CD	2.50	0.42
1:H:314:PRO:HG3	1:H:365:GLY:HA3	2.02	0.42
1:H:328:ALA:O	1:H:330:ILE:HG12	2.19	0.42
1:J:314:PRO:HG3	1:J:365:GLY:HA3	2.02	0.42
1:K:328:ALA:O	1:K:330:ILE:HG12	2.19	0.42
1:L:338:ASN:ND2	1:L:396:LEU:H	2.13	0.42
1:M:400:PRO:HG2	1:M:403:GLU:CB	2.49	0.42
1:P:345:ILE:HD12	1:P:345:ILE:N	2.34	0.42
1:S:314:PRO:HG3	1:S:365:GLY:HA3	2.02	0.42
1:U:271:HIS:CD2	3:U:7515:AMP:H4'	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:121:ALA:HB1	1:V:275:TRP:O	2.19	0.42
1:W:271:HIS:CD2	3:W:7519:AMP:H4'	2.54	0.42
1:A:400:PRO:HG2	1:A:403:GLU:CB	2.49	0.41
1:B:271:HIS:CD2	3:B:7477:AMP:H4'	2.54	0.41
1:D:193:ASP:OD2	1:E:80:ARG:HD3	2.20	0.41
1:L:24:LEU:HB3	1:L:25:PRO:CD	2.50	0.41
1:M:328:ALA:O	1:M:330:ILE:HG12	2.19	0.41
1:R:207:GLU:N	1:R:210:HIS:HD2	1.98	0.41
1:W:400:PRO:HG2	1:W:403:GLU:CB	2.49	0.41
1:Q:175:HIS:CE1	1:X:467:ASP:HB2	2.55	0.41
1:C:24:LEU:HB3	1:C:25:PRO:CD	2.50	0.41
1:F:24:LEU:HB3	1:F:25:PRO:CD	2.50	0.41
1:G:314:PRO:HG3	1:G:365:GLY:HA3	2.02	0.41
1:I:314:PRO:HG3	1:I:365:GLY:HA3	2.02	0.41
1:I:271:HIS:CD2	3:I:7491:AMP:H4'	2.54	0.41
1:K:271:HIS:CD2	3:K:7495:AMP:H4'	2.54	0.41
1:E:323:VAL:HG21	1:K:455:ILE:HG22	2.02	0.41
1:O:24:LEU:HB3	1:O:25:PRO:CD	2.50	0.41
1:P:328:ALA:HA	1:P:329:PRO:HD3	1.87	0.41
1:R:314:PRO:HG3	1:R:365:GLY:HA3	2.02	0.41
1:M:95:PHE:HE2	1:R:347:ILE:HG21	1.85	0.41
1:S:83:LYS:HA	1:S:83:LYS:HD3	1.94	0.41
1:T:328:ALA:O	1:T:330:ILE:HG12	2.19	0.41
1:U:314:PRO:HG3	1:U:365:GLY:HA3	2.02	0.41
1:W:328:ALA:O	1:W:330:ILE:HG12	2.19	0.41
1:X:24:LEU:HB3	1:X:25:PRO:CD	2.50	0.41
1:A:323:VAL:HG22	1:A:324:PRO:HD2	2.01	0.41
1:D:323:VAL:HG22	1:D:324:PRO:HD2	2.01	0.41
1:F:207:GLU:N	1:F:210:HIS:HD2	1.98	0.41
1:F:314:PRO:HG3	1:F:365:GLY:HA3	2.02	0.41
1:G:83:LYS:HD3	1:G:83:LYS:HA	1.94	0.41
1:H:129:GLU:OE1	3:H:7489:AMP:P	2.79	0.41
1:I:24:LEU:HB3	1:I:25:PRO:CD	2.50	0.41
1:P:314:PRO:HG3	1:P:365:GLY:HA3	2.02	0.41
1:R:83:LYS:HA	1:R:83:LYS:HD3	1.94	0.41
1:T:207:GLU:HB3	1:T:208:LYS:H	1.44	0.41
1:V:338:ASN:ND2	1:V:396:LEU:H	2.14	0.41
1:A:179:TYR:CD2	1:B:53:SER:CB	3.01	0.41
1:B:54:ILE:HA	1:B:54:ILE:HD13	1.86	0.41
1:D:328:ALA:HA	1:D:329:PRO:HD3	1.87	0.41
1:D:338:ASN:ND2	1:E:60:ILE:HD12	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:LEU:CD2	1:L:16:TYR:CE2	3.04	0.41
1:N:24:LEU:HB3	1:N:25:PRO:CD	2.50	0.41
1:P:323:VAL:HG22	1:P:324:PRO:HD2	2.01	0.41
1:T:129:GLU:OE1	3:T:7513:AMP:P	2.79	0.41
1:U:24:LEU:HB3	1:U:25:PRO:CD	2.50	0.41
1:U:321:ARG:NE	4:U:7516:CIT:H42	2.21	0.41
1:U:53:SER:CB	1:V:179:TYR:H	2.33	0.41
1:X:328:ALA:O	1:X:330:ILE:HG12	2.19	0.41
1:B:129:GLU:OE1	3:B:7477:AMP:P	2.79	0.41
1:B:24:LEU:HB3	1:B:25:PRO:CD	2.50	0.41
1:C:338:ASN:ND2	1:C:396:LEU:H	2.13	0.41
1:D:314:PRO:HG3	1:D:365:GLY:HA3	2.02	0.41
1:E:400:PRO:HG2	1:E:403:GLU:CB	2.49	0.41
1:G:114:TYR:O	1:G:118:THR:HG23	2.21	0.41
1:I:114:TYR:O	1:I:118:THR:HG23	2.21	0.41
1:J:338:ASN:ND2	1:J:396:LEU:H	2.14	0.41
1:K:7:LYS:HE3	1:K:11:ASP:OD2	2.20	0.41
1:M:323:VAL:HG22	1:M:324:PRO:HD2	2.01	0.41
1:O:328:ALA:HA	1:O:329:PRO:HD3	1.87	0.41
1:P:179:TYR:CB	1:Q:53:SER:OG	2.56	0.41
1:R:24:LEU:HB3	1:R:25:PRO:CD	2.50	0.41
1:S:114:TYR:O	1:S:118:THR:HG23	2.21	0.41
1:U:114:TYR:O	1:U:118:THR:HG23	2.21	0.41
1:P:466:TYR:CE1	1:V:254:THR:HB	2.55	0.41
1:H:53:SER:HB3	1:I:179:TYR:CD2	2.55	0.41
1:J:271:HIS:CD2	3:J:7493:AMP:H4'	2.54	0.41
1:L:129:GLU:OE1	3:L:7497:AMP:P	2.79	0.41
1:N:114:TYR:O	1:N:118:THR:HG23	2.21	0.41
1:N:129:GLU:OE1	3:N:7501:AMP:P	2.79	0.41
1:P:129:GLU:OE1	3:P:7505:AMP:P	2.79	0.41
1:Q:400:PRO:HG2	1:Q:403:GLU:CB	2.49	0.41
1:V:53:SER:OG	1:W:179:TYR:N	2.54	0.41
1:B:114:TYR:O	1:B:118:THR:HG23	2.21	0.41
1:D:129:GLU:OE1	3:D:7481:AMP:P	2.79	0.41
1:E:129:GLU:OE1	3:E:7483:AMP:P	2.79	0.41
1:Q:129:GLU:OE1	3:Q:7507:AMP:P	2.79	0.41
1:V:271:HIS:CD2	3:V:7517:AMP:H4'	2.54	0.41
1:X:129:GLU:OE1	3:X:7521:AMP:P	2.79	0.41
1:E:328:ALA:HA	1:E:329:PRO:HD3	1.87	0.41
1:J:129:GLU:OE1	3:J:7493:AMP:P	2.79	0.41
1:L:114:TYR:O	1:L:118:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:328:ALA:O	1:L:330:ILE:HG12	2.19	0.41
1:N:83:LYS:HA	1:N:83:LYS:HD3	1.94	0.41
1:O:338:ASN:ND2	1:O:396:LEU:H	2.14	0.41
1:T:114:TYR:O	1:T:118:THR:HG23	2.21	0.41
1:B:83:LYS:HD3	1:B:83:LYS:HA	1.94	0.41
1:F:413:GLN:O	1:F:416:ASP:HB2	2.21	0.41
1:A:140:PHE:CE1	1:G:463:ALA:HA	2.56	0.41
1:H:114:TYR:O	1:H:118:THR:HG23	2.21	0.41
1:H:60:ILE:HD12	5:I:7681:HOH:O	2.19	0.41
1:K:314:PRO:HG3	1:K:365:GLY:HA3	2.02	0.41
1:L:83:LYS:HD3	1:L:83:LYS:HA	1.94	0.41
1:R:413:GLN:O	1:R:416:ASP:HB2	2.21	0.41
1:V:129:GLU:OE1	3:V:7517:AMP:P	2.79	0.41
1:W:114:TYR:O	1:W:118:THR:HG23	2.21	0.41
1:X:114:TYR:O	1:X:118:THR:HG23	2.21	0.41
1:A:70:ASP:HA	1:A:71:PRO:HD2	1.94	0.41
1:C:129:GLU:OE1	3:C:7479:AMP:P	2.79	0.41
1:G:413:GLN:O	1:G:416:ASP:HB2	2.21	0.41
1:G:129:GLU:OE1	3:G:7487:AMP:P	2.79	0.41
1:P:338:ASN:ND2	1:P:396:LEU:H	2.13	0.41
1:Q:328:ALA:HA	1:Q:329:PRO:HD3	1.87	0.41
1:W:314:PRO:HG3	1:W:365:GLY:HA3	2.02	0.41
1:X:83:LYS:HD3	1:X:83:LYS:HA	1.94	0.41
1:B:176:LYS:HE3	5:C:7646:HOH:O	2.20	0.41
1:B:400:PRO:HG2	1:B:403:GLU:CB	2.49	0.41
1:K:114:TYR:O	1:K:118:THR:HG23	2.21	0.41
1:K:129:GLU:OE1	3:K:7495:AMP:P	2.79	0.41
1:N:54:ILE:HA	1:N:54:ILE:HD13	1.86	0.41
1:R:129:GLU:OE1	3:R:7509:AMP:P	2.79	0.41
1:S:129:GLU:OE1	3:S:7511:AMP:P	2.79	0.41
1:V:54:ILE:HA	1:V:54:ILE:HD13	1.86	0.41
1:W:129:GLU:OE1	3:W:7519:AMP:P	2.79	0.41
1:Q:458:HIS:HE1	1:W:456:ARG:O	2.04	0.41
1:D:338:ASN:ND2	1:D:396:LEU:H	2.13	0.40
1:E:114:TYR:O	1:E:118:THR:HG23	2.21	0.40
1:F:129:GLU:OE1	3:F:7485:AMP:P	2.79	0.40
1:H:207:GLU:HB3	1:H:208:LYS:H	1.44	0.40
1:K:53:SER:HB3	1:L:179:TYR:CD2	2.56	0.40
1:N:314:PRO:HG3	1:N:365:GLY:HA3	2.02	0.40
1:N:400:PRO:HG2	1:N:403:GLU:CB	2.49	0.40
1:O:129:GLU:OE1	3:O:7503:AMP:P	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:114:TYR:O	1:Q:118:THR:HG23	2.21	0.40
1:S:339:ARG:HD2	1:X:60:ILE:HG22	2.04	0.40
1:S:413:GLN:O	1:S:416:ASP:HB2	2.21	0.40
1:U:129:GLU:OE1	3:U:7515:AMP:P	2.79	0.40
1:U:52:SER:HB3	1:V:180:PHE:CZ	2.56	0.40
1:B:314:PRO:HG3	1:B:365:GLY:HA3	2.02	0.40
1:C:176:LYS:HE3	5:D:963:HOH:O	2.20	0.40
1:D:114:TYR:O	1:D:118:THR:HG23	2.21	0.40
1:D:413:GLN:O	1:D:416:ASP:HB2	2.21	0.40
1:E:256:MET:HA	1:E:257:PRO:HD3	1.90	0.40
1:F:114:TYR:O	1:F:118:THR:HG23	2.21	0.40
1:G:207:GLU:N	1:G:210:HIS:HD2	1.98	0.40
1:H:60:ILE:HD12	1:I:338:ASN:HD22	1.87	0.40
1:I:413:GLN:O	1:I:416:ASP:HB2	2.21	0.40
1:I:129:GLU:OE1	3:I:7491:AMP:P	2.79	0.40
1:J:54:ILE:HD13	1:J:54:ILE:HA	1.86	0.40
1:N:413:GLN:O	1:N:416:ASP:HB2	2.21	0.40
1:P:114:TYR:O	1:P:118:THR:HG23	2.21	0.40
1:P:413:GLN:O	1:P:416:ASP:HB2	2.21	0.40
1:R:114:TYR:O	1:R:118:THR:HG23	2.21	0.40
1:B:413:GLN:O	1:B:416:ASP:HB2	2.21	0.40
1:H:256:MET:HA	1:H:257:PRO:HD3	1.90	0.40
1:I:90:PHE:HB3	1:I:106:ASN:HD21	1.87	0.40
1:I:54:ILE:HA	1:I:54:ILE:HD13	1.86	0.40
3:K:7495:AMP:C8	3:K:7495:AMP:C1'	2.92	0.40
1:L:413:GLN:O	1:L:416:ASP:HB2	2.21	0.40
1:M:114:TYR:O	1:M:118:THR:HG23	2.21	0.40
1:Q:175:HIS:HE1	1:X:467:ASP:HB2	1.86	0.40
1:U:90:PHE:HB3	1:U:106:ASN:HD21	1.87	0.40
1:U:137:SER:HB3	1:V:502:PRO:HB2	2.04	0.40
1:U:413:GLN:O	1:U:416:ASP:HB2	2.21	0.40
1:X:61:HIS:HD2	1:X:62:GLU:HB2	1.87	0.40
1:A:114:TYR:O	1:A:118:THR:HG23	2.21	0.40
1:A:61:HIS:HD2	1:A:62:GLU:HB2	1.87	0.40
1:C:328:ALA:HA	1:C:329:PRO:HD3	1.87	0.40
1:E:207:GLU:HB3	1:E:208:LYS:H	1.44	0.40
1:H:413:GLN:O	1:H:416:ASP:HB2	2.21	0.40
1:G:179:TYR:HD2	1:L:53:SER:HB3	1.86	0.40
1:M:61:HIS:HD2	1:M:62:GLU:HB2	1.87	0.40
1:M:129:GLU:OE1	3:M:7499:AMP:P	2.79	0.40
1:O:90:PHE:HB3	1:O:106:ASN:HD21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:54:ILE:HA	1:P:54:ILE:HD13	1.86	0.40
1:Q:256:MET:HA	1:Q:257:PRO:HD3	1.90	0.40
1:T:413:GLN:O	1:T:416:ASP:HB2	2.21	0.40
1:W:90:PHE:HB3	1:W:106:ASN:HD21	1.87	0.40
1:X:413:GLN:O	1:X:416:ASP:HB2	2.21	0.40
1:X:90:PHE:HB3	1:X:106:ASN:HD21	1.87	0.40
1:A:129:GLU:OE1	3:A:7475:AMP:P	2.79	0.40
1:C:413:GLN:O	1:C:416:ASP:HB2	2.21	0.40
1:C:467:ASP:HB2	1:J:175:HIS:CE1	2.57	0.40
1:C:90:PHE:HB3	1:C:106:ASN:HD21	1.87	0.40
1:E:413:GLN:O	1:E:416:ASP:HB2	2.21	0.40
1:E:83:LYS:HA	1:E:83:LYS:HD3	1.94	0.40
1:K:90:PHE:HB3	1:K:106:ASN:HD21	1.87	0.40
1:K:413:GLN:O	1:K:416:ASP:HB2	2.21	0.40
1:L:61:HIS:HD2	1:L:62:GLU:HB2	1.87	0.40
1:L:90:PHE:HB3	1:L:106:ASN:HD21	1.87	0.40
1:P:92:HIS:HA	1:P:98:GLU:O	2.21	0.40
1:Q:413:GLN:O	1:Q:416:ASP:HB2	2.21	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	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	B	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	C	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	12	17
1	D	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	E	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	12	17
1	F	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	12	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	H	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	I	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	12	17
1	J	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	K	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	L	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	12	17
1	M	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	N	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	O	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	P	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	12	17
1	Q	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	R	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	S	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	T	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	U	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	12	17
1	V	475/477 (100%)	446 (94%)	23 (5%)	6 (1%)	12	17
1	W	475/477 (100%)	447 (94%)	22 (5%)	6 (1%)	12	17
1	X	475/477 (100%)	445 (94%)	24 (5%)	6 (1%)	12	17
All	All	11400/11448 (100%)	10718 (94%)	538 (5%)	144 (1%)	12	17

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	208	LYS
1	B	63	SER
1	B	208	LYS
1	C	63	SER
1	C	208	LYS
1	D	63	SER
1	D	208	LYS
1	E	63	SER
1	E	208	LYS
1	F	63	SER
1	F	208	LYS
1	G	63	SER

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Mol	Chain	Res	Type
1	G	208	LYS
1	H	63	SER
1	H	208	LYS
1	I	63	SER
1	I	208	LYS
1	J	63	SER
1	J	208	LYS
1	K	63	SER
1	K	208	LYS
1	L	63	SER
1	L	208	LYS
1	M	63	SER
1	M	208	LYS
1	N	63	SER
1	N	208	LYS
1	O	63	SER
1	O	208	LYS
1	P	63	SER
1	P	208	LYS
1	Q	63	SER
1	Q	208	LYS
1	R	63	SER
1	R	208	LYS
1	S	63	SER
1	S	208	LYS
1	T	63	SER
1	T	208	LYS
1	U	63	SER
1	U	208	LYS
1	V	63	SER
1	V	208	LYS
1	W	63	SER
1	W	208	LYS
1	X	63	SER
1	X	208	LYS
1	A	326	TYR
1	B	326	TYR
1	C	326	TYR
1	D	326	TYR
1	E	326	TYR
1	F	326	TYR
1	G	326	TYR

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Mol	Chain	Res	Type
1	H	326	TYR
1	I	326	TYR
1	J	326	TYR
1	K	326	TYR
1	L	326	TYR
1	M	326	TYR
1	N	326	TYR
1	O	326	TYR
1	P	326	TYR
1	Q	326	TYR
1	R	326	TYR
1	S	326	TYR
1	T	326	TYR
1	U	326	TYR
1	V	326	TYR
1	W	326	TYR
1	X	326	TYR
1	A	59	SER
1	B	59	SER
1	C	59	SER
1	D	59	SER
1	E	59	SER
1	F	59	SER
1	G	59	SER
1	H	59	SER
1	I	59	SER
1	J	59	SER
1	K	59	SER
1	L	59	SER
1	M	59	SER
1	N	59	SER
1	O	59	SER
1	P	59	SER
1	Q	59	SER
1	R	59	SER
1	S	59	SER
1	T	59	SER
1	U	59	SER
1	V	59	SER
1	W	59	SER
1	X	59	SER
1	A	401	PRO

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Mol	Chain	Res	Type
1	B	401	PRO
1	C	401	PRO
1	D	401	PRO
1	E	401	PRO
1	F	401	PRO
1	G	401	PRO
1	H	401	PRO
1	I	401	PRO
1	J	401	PRO
1	K	401	PRO
1	L	401	PRO
1	M	401	PRO
1	N	401	PRO
1	O	401	PRO
1	P	401	PRO
1	Q	401	PRO
1	R	401	PRO
1	S	401	PRO
1	T	401	PRO
1	U	401	PRO
1	V	401	PRO
1	W	401	PRO
1	X	401	PRO
1	A	228	LEU
1	B	228	LEU
1	C	228	LEU
1	D	228	LEU
1	E	228	LEU
1	F	228	LEU
1	G	228	LEU
1	H	228	LEU
1	I	228	LEU
1	J	228	LEU
1	K	228	LEU
1	L	228	LEU
1	M	228	LEU
1	N	228	LEU
1	O	228	LEU
1	P	228	LEU
1	Q	228	LEU
1	R	228	LEU
1	S	228	LEU

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Mol	Chain	Res	Type
1	T	228	LEU
1	U	228	LEU
1	V	228	LEU
1	W	228	LEU
1	X	228	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	B	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	C	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	D	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	E	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	F	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	G	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	H	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	I	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	J	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	K	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	L	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	M	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	N	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	O	404/404 (100%)	377 (93%)	27 (7%)	16	26
1	P	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	Q	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	R	404/404 (100%)	375 (93%)	29 (7%)	14	23
1	S	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	T	404/404 (100%)	376 (93%)	28 (7%)	15	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	V	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	W	404/404 (100%)	376 (93%)	28 (7%)	15	25
1	X	404/404 (100%)	376 (93%)	28 (7%)	15	25
All	All	9696/9696 (100%)	9020 (93%)	676 (7%)	15	24

All (676) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	602	GLU
1	A	2	PRO
1	A	8	LEU
1	A	24	LEU
1	A	50	ASP
1	A	54	ILE
1	A	67	LEU
1	A	80	ARG
1	A	97	LEU
1	A	115	LEU
1	A	173	VAL
1	A	191	LEU
1	A	202	SER
1	A	206	LEU
1	A	237	LEU
1	A	273	SER
1	A	308	LEU
1	A	312	THR
1	A	322	LEU
1	A	334	TYR
1	A	355	ARG
1	A	363	SER
1	A	375	LEU
1	A	401	PRO
1	A	413	GLN
1	A	426	GLU
1	A	428	LEU
1	A	464	LEU
1	B	602	GLU
1	B	8	LEU
1	B	24	LEU
1	B	50	ASP

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Mol	Chain	Res	Type
1	B	54	ILE
1	B	67	LEU
1	B	80	ARG
1	B	97	LEU
1	B	115	LEU
1	B	173	VAL
1	B	191	LEU
1	B	202	SER
1	B	206	LEU
1	B	237	LEU
1	B	273	SER
1	B	308	LEU
1	B	312	THR
1	B	322	LEU
1	B	334	TYR
1	B	355	ARG
1	B	363	SER
1	B	375	LEU
1	B	385	LYS
1	B	401	PRO
1	B	413	GLN
1	B	426	GLU
1	B	428	LEU
1	B	464	LEU
1	C	602	GLU
1	C	2	PRO
1	C	8	LEU
1	C	24	LEU
1	C	50	ASP
1	C	54	ILE
1	C	67	LEU
1	C	80	ARG
1	C	97	LEU
1	C	115	LEU
1	C	173	VAL
1	C	191	LEU
1	C	202	SER
1	C	206	LEU
1	C	237	LEU
1	C	273	SER
1	C	308	LEU
1	C	312	THR

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Mol	Chain	Res	Type
1	C	322	LEU
1	C	334	TYR
1	C	355	ARG
1	C	363	SER
1	C	375	LEU
1	C	401	PRO
1	C	413	GLN
1	C	426	GLU
1	C	428	LEU
1	C	464	LEU
1	D	602	GLU
1	D	2	PRO
1	D	8	LEU
1	D	24	LEU
1	D	50	ASP
1	D	54	ILE
1	D	67	LEU
1	D	80	ARG
1	D	97	LEU
1	D	98	GLU
1	D	115	LEU
1	D	173	VAL
1	D	191	LEU
1	D	202	SER
1	D	206	LEU
1	D	237	LEU
1	D	308	LEU
1	D	312	THR
1	D	322	LEU
1	D	334	TYR
1	D	355	ARG
1	D	363	SER
1	D	375	LEU
1	D	401	PRO
1	D	413	GLN
1	D	426	GLU
1	D	428	LEU
1	D	464	LEU
1	E	602	GLU
1	E	2	PRO
1	E	8	LEU
1	E	24	LEU

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Mol	Chain	Res	Type
1	E	40	LYS
1	E	50	ASP
1	E	54	ILE
1	E	67	LEU
1	E	80	ARG
1	E	97	LEU
1	E	115	LEU
1	E	173	VAL
1	E	191	LEU
1	E	202	SER
1	E	206	LEU
1	E	237	LEU
1	E	273	SER
1	E	308	LEU
1	E	312	THR
1	E	322	LEU
1	E	334	TYR
1	E	355	ARG
1	E	363	SER
1	E	375	LEU
1	E	401	PRO
1	E	413	GLN
1	E	426	GLU
1	E	428	LEU
1	E	464	LEU
1	F	602	GLU
1	F	2	PRO
1	F	8	LEU
1	F	24	LEU
1	F	50	ASP
1	F	54	ILE
1	F	67	LEU
1	F	80	ARG
1	F	97	LEU
1	F	115	LEU
1	F	173	VAL
1	F	191	LEU
1	F	202	SER
1	F	206	LEU
1	F	237	LEU
1	F	273	SER
1	F	292	ASP

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Mol	Chain	Res	Type
1	F	308	LEU
1	F	312	THR
1	F	322	LEU
1	F	334	TYR
1	F	355	ARG
1	F	363	SER
1	F	375	LEU
1	F	401	PRO
1	F	413	GLN
1	F	426	GLU
1	F	428	LEU
1	F	464	LEU
1	G	602	GLU
1	G	2	PRO
1	G	8	LEU
1	G	24	LEU
1	G	50	ASP
1	G	54	ILE
1	G	67	LEU
1	G	80	ARG
1	G	97	LEU
1	G	115	LEU
1	G	173	VAL
1	G	191	LEU
1	G	202	SER
1	G	206	LEU
1	G	237	LEU
1	G	273	SER
1	G	308	LEU
1	G	312	THR
1	G	322	LEU
1	G	334	TYR
1	G	355	ARG
1	G	363	SER
1	G	375	LEU
1	G	401	PRO
1	G	413	GLN
1	G	426	GLU
1	G	428	LEU
1	G	464	LEU
1	H	602	GLU
1	H	2	PRO

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Mol	Chain	Res	Type
1	H	8	LEU
1	H	24	LEU
1	H	50	ASP
1	H	54	ILE
1	H	67	LEU
1	H	80	ARG
1	H	97	LEU
1	H	115	LEU
1	H	173	VAL
1	H	191	LEU
1	H	202	SER
1	H	206	LEU
1	H	237	LEU
1	H	273	SER
1	H	308	LEU
1	H	312	THR
1	H	322	LEU
1	H	334	TYR
1	H	355	ARG
1	H	363	SER
1	H	375	LEU
1	H	401	PRO
1	H	413	GLN
1	H	426	GLU
1	H	428	LEU
1	H	464	LEU
1	I	602	GLU
1	I	2	PRO
1	I	8	LEU
1	I	24	LEU
1	I	50	ASP
1	I	54	ILE
1	I	67	LEU
1	I	80	ARG
1	I	97	LEU
1	I	115	LEU
1	I	173	VAL
1	I	191	LEU
1	I	202	SER
1	I	206	LEU
1	I	237	LEU
1	I	273	SER

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Mol	Chain	Res	Type
1	I	308	LEU
1	I	312	THR
1	I	322	LEU
1	I	334	TYR
1	I	355	ARG
1	I	363	SER
1	I	375	LEU
1	I	401	PRO
1	I	413	GLN
1	I	426	GLU
1	I	428	LEU
1	I	464	LEU
1	J	602	GLU
1	J	2	PRO
1	J	8	LEU
1	J	24	LEU
1	J	50	ASP
1	J	54	ILE
1	J	67	LEU
1	J	80	ARG
1	J	97	LEU
1	J	115	LEU
1	J	173	VAL
1	J	191	LEU
1	J	202	SER
1	J	206	LEU
1	J	237	LEU
1	J	308	LEU
1	J	312	THR
1	J	322	LEU
1	J	334	TYR
1	J	355	ARG
1	J	363	SER
1	J	375	LEU
1	J	401	PRO
1	J	413	GLN
1	J	426	GLU
1	J	428	LEU
1	J	464	LEU
1	K	602	GLU
1	K	2	PRO
1	K	8	LEU

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Mol	Chain	Res	Type
1	K	11	ASP
1	K	24	LEU
1	K	50	ASP
1	K	54	ILE
1	K	67	LEU
1	K	80	ARG
1	K	97	LEU
1	K	115	LEU
1	K	173	VAL
1	K	191	LEU
1	K	202	SER
1	K	206	LEU
1	K	237	LEU
1	K	273	SER
1	K	308	LEU
1	K	312	THR
1	K	322	LEU
1	K	334	TYR
1	K	355	ARG
1	K	363	SER
1	K	375	LEU
1	K	401	PRO
1	K	413	GLN
1	K	426	GLU
1	K	428	LEU
1	K	464	LEU
1	L	602	GLU
1	L	2	PRO
1	L	8	LEU
1	L	24	LEU
1	L	50	ASP
1	L	54	ILE
1	L	67	LEU
1	L	80	ARG
1	L	97	LEU
1	L	115	LEU
1	L	173	VAL
1	L	191	LEU
1	L	202	SER
1	L	206	LEU
1	L	237	LEU
1	L	273	SER

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Mol	Chain	Res	Type
1	L	308	LEU
1	L	312	THR
1	L	322	LEU
1	L	334	TYR
1	L	355	ARG
1	L	363	SER
1	L	375	LEU
1	L	401	PRO
1	L	413	GLN
1	L	426	GLU
1	L	428	LEU
1	L	464	LEU
1	M	602	GLU
1	M	2	PRO
1	M	8	LEU
1	M	24	LEU
1	M	50	ASP
1	M	54	ILE
1	M	67	LEU
1	M	80	ARG
1	M	97	LEU
1	M	115	LEU
1	M	173	VAL
1	M	191	LEU
1	M	202	SER
1	M	206	LEU
1	M	237	LEU
1	M	273	SER
1	M	308	LEU
1	M	312	THR
1	M	322	LEU
1	M	334	TYR
1	M	355	ARG
1	M	363	SER
1	M	375	LEU
1	M	401	PRO
1	M	413	GLN
1	M	426	GLU
1	M	428	LEU
1	M	464	LEU
1	N	602	GLU
1	N	2	PRO

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Mol	Chain	Res	Type
1	N	8	LEU
1	N	24	LEU
1	N	50	ASP
1	N	54	ILE
1	N	67	LEU
1	N	80	ARG
1	N	97	LEU
1	N	115	LEU
1	N	173	VAL
1	N	191	LEU
1	N	202	SER
1	N	206	LEU
1	N	237	LEU
1	N	273	SER
1	N	308	LEU
1	N	312	THR
1	N	322	LEU
1	N	334	TYR
1	N	355	ARG
1	N	363	SER
1	N	375	LEU
1	N	401	PRO
1	N	413	GLN
1	N	426	GLU
1	N	428	LEU
1	N	464	LEU
1	O	602	GLU
1	O	2	PRO
1	O	8	LEU
1	O	24	LEU
1	O	50	ASP
1	O	54	ILE
1	O	67	LEU
1	O	80	ARG
1	O	97	LEU
1	O	115	LEU
1	O	173	VAL
1	O	191	LEU
1	O	202	SER
1	O	206	LEU
1	O	237	LEU
1	O	308	LEU

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Mol	Chain	Res	Type
1	O	312	THR
1	O	322	LEU
1	O	334	TYR
1	O	355	ARG
1	O	363	SER
1	O	375	LEU
1	O	401	PRO
1	O	413	GLN
1	O	426	GLU
1	O	428	LEU
1	O	464	LEU
1	P	602	GLU
1	P	2	PRO
1	P	8	LEU
1	P	24	LEU
1	P	50	ASP
1	P	54	ILE
1	P	67	LEU
1	P	80	ARG
1	P	97	LEU
1	P	98	GLU
1	P	115	LEU
1	P	173	VAL
1	P	191	LEU
1	P	202	SER
1	P	206	LEU
1	P	237	LEU
1	P	273	SER
1	P	308	LEU
1	P	312	THR
1	P	322	LEU
1	P	334	TYR
1	P	355	ARG
1	P	363	SER
1	P	375	LEU
1	P	401	PRO
1	P	413	GLN
1	P	426	GLU
1	P	428	LEU
1	P	464	LEU
1	Q	602	GLU
1	Q	2	PRO

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Mol	Chain	Res	Type
1	Q	8	LEU
1	Q	24	LEU
1	Q	40	LYS
1	Q	50	ASP
1	Q	54	ILE
1	Q	67	LEU
1	Q	80	ARG
1	Q	97	LEU
1	Q	115	LEU
1	Q	173	VAL
1	Q	191	LEU
1	Q	202	SER
1	Q	206	LEU
1	Q	237	LEU
1	Q	273	SER
1	Q	308	LEU
1	Q	312	THR
1	Q	322	LEU
1	Q	334	TYR
1	Q	355	ARG
1	Q	363	SER
1	Q	375	LEU
1	Q	401	PRO
1	Q	413	GLN
1	Q	426	GLU
1	Q	428	LEU
1	Q	464	LEU
1	R	602	GLU
1	R	2	PRO
1	R	8	LEU
1	R	24	LEU
1	R	50	ASP
1	R	54	ILE
1	R	67	LEU
1	R	80	ARG
1	R	97	LEU
1	R	115	LEU
1	R	173	VAL
1	R	191	LEU
1	R	202	SER
1	R	206	LEU
1	R	237	LEU

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Mol	Chain	Res	Type
1	R	273	SER
1	R	292	ASP
1	R	308	LEU
1	R	312	THR
1	R	322	LEU
1	R	334	TYR
1	R	355	ARG
1	R	363	SER
1	R	375	LEU
1	R	401	PRO
1	R	413	GLN
1	R	426	GLU
1	R	428	LEU
1	R	464	LEU
1	S	602	GLU
1	S	2	PRO
1	S	8	LEU
1	S	24	LEU
1	S	50	ASP
1	S	54	ILE
1	S	67	LEU
1	S	80	ARG
1	S	97	LEU
1	S	115	LEU
1	S	173	VAL
1	S	191	LEU
1	S	202	SER
1	S	206	LEU
1	S	237	LEU
1	S	273	SER
1	S	308	LEU
1	S	312	THR
1	S	322	LEU
1	S	334	TYR
1	S	355	ARG
1	S	363	SER
1	S	375	LEU
1	S	401	PRO
1	S	413	GLN
1	S	426	GLU
1	S	428	LEU
1	S	464	LEU

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Mol	Chain	Res	Type
1	T	602	GLU
1	T	2	PRO
1	T	8	LEU
1	T	24	LEU
1	T	50	ASP
1	T	54	ILE
1	T	67	LEU
1	T	80	ARG
1	T	97	LEU
1	T	115	LEU
1	T	173	VAL
1	T	191	LEU
1	T	202	SER
1	T	206	LEU
1	T	237	LEU
1	T	273	SER
1	T	308	LEU
1	T	312	THR
1	T	322	LEU
1	T	334	TYR
1	T	355	ARG
1	T	363	SER
1	T	375	LEU
1	T	401	PRO
1	T	413	GLN
1	T	426	GLU
1	T	428	LEU
1	T	464	LEU
1	U	602	GLU
1	U	2	PRO
1	U	8	LEU
1	U	24	LEU
1	U	50	ASP
1	U	54	ILE
1	U	67	LEU
1	U	80	ARG
1	U	97	LEU
1	U	115	LEU
1	U	173	VAL
1	U	191	LEU
1	U	202	SER
1	U	206	LEU

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Mol	Chain	Res	Type
1	U	237	LEU
1	U	273	SER
1	U	308	LEU
1	U	312	THR
1	U	322	LEU
1	U	334	TYR
1	U	355	ARG
1	U	363	SER
1	U	375	LEU
1	U	401	PRO
1	U	413	GLN
1	U	426	GLU
1	U	428	LEU
1	U	464	LEU
1	V	602	GLU
1	V	2	PRO
1	V	8	LEU
1	V	24	LEU
1	V	50	ASP
1	V	54	ILE
1	V	67	LEU
1	V	80	ARG
1	V	97	LEU
1	V	115	LEU
1	V	173	VAL
1	V	191	LEU
1	V	202	SER
1	V	206	LEU
1	V	237	LEU
1	V	273	SER
1	V	308	LEU
1	V	312	THR
1	V	322	LEU
1	V	334	TYR
1	V	355	ARG
1	V	363	SER
1	V	375	LEU
1	V	401	PRO
1	V	413	GLN
1	V	426	GLU
1	V	428	LEU
1	V	464	LEU

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Mol	Chain	Res	Type
1	W	602	GLU
1	W	2	PRO
1	W	8	LEU
1	W	24	LEU
1	W	50	ASP
1	W	54	ILE
1	W	67	LEU
1	W	80	ARG
1	W	97	LEU
1	W	115	LEU
1	W	173	VAL
1	W	191	LEU
1	W	202	SER
1	W	206	LEU
1	W	237	LEU
1	W	273	SER
1	W	308	LEU
1	W	312	THR
1	W	322	LEU
1	W	334	TYR
1	W	355	ARG
1	W	363	SER
1	W	375	LEU
1	W	401	PRO
1	W	413	GLN
1	W	426	GLU
1	W	428	LEU
1	W	464	LEU
1	X	602	GLU
1	X	2	PRO
1	X	8	LEU
1	X	24	LEU
1	X	50	ASP
1	X	54	ILE
1	X	67	LEU
1	X	80	ARG
1	X	97	LEU
1	X	115	LEU
1	X	173	VAL
1	X	191	LEU
1	X	202	SER
1	X	206	LEU

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Mol	Chain	Res	Type
1	X	237	LEU
1	X	273	SER
1	X	308	LEU
1	X	312	THR
1	X	322	LEU
1	X	334	TYR
1	X	355	ARG
1	X	363	SER
1	X	375	LEU
1	X	401	PRO
1	X	413	GLN
1	X	426	GLU
1	X	428	LEU
1	X	464	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (416) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	61	HIS
1	A	86	ASN
1	A	106	ASN
1	A	113	ASN
1	A	175	HIS
1	A	187	GLN
1	A	210	HIS
1	A	218	GLN
1	A	230	HIS
1	A	244	ASN
1	A	248	GLN
1	A	272	GLN
1	A	296	HIS
1	A	313	ASN
1	A	338	ASN
1	A	458	HIS
1	B	30	HIS
1	B	61	HIS
1	B	86	ASN
1	B	106	ASN
1	B	113	ASN
1	B	175	HIS
1	B	187	GLN

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Mol	Chain	Res	Type
1	B	210	HIS
1	B	218	GLN
1	B	230	HIS
1	B	244	ASN
1	B	248	GLN
1	B	272	GLN
1	B	296	HIS
1	B	313	ASN
1	B	338	ASN
1	B	458	HIS
1	C	30	HIS
1	C	61	HIS
1	C	86	ASN
1	C	106	ASN
1	C	113	ASN
1	C	175	HIS
1	C	187	GLN
1	C	210	HIS
1	C	218	GLN
1	C	230	HIS
1	C	244	ASN
1	C	248	GLN
1	C	272	GLN
1	C	296	HIS
1	C	313	ASN
1	C	338	ASN
1	C	458	HIS
1	D	30	HIS
1	D	61	HIS
1	D	86	ASN
1	D	106	ASN
1	D	113	ASN
1	D	175	HIS
1	D	187	GLN
1	D	210	HIS
1	D	211	HIS
1	D	218	GLN
1	D	230	HIS
1	D	244	ASN
1	D	248	GLN
1	D	272	GLN
1	D	313	ASN

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Mol	Chain	Res	Type
1	D	338	ASN
1	D	458	HIS
1	E	30	HIS
1	E	61	HIS
1	E	86	ASN
1	E	106	ASN
1	E	113	ASN
1	E	187	GLN
1	E	210	HIS
1	E	218	GLN
1	E	230	HIS
1	E	244	ASN
1	E	248	GLN
1	E	272	GLN
1	E	296	HIS
1	E	313	ASN
1	E	338	ASN
1	E	458	HIS
1	F	30	HIS
1	F	61	HIS
1	F	86	ASN
1	F	106	ASN
1	F	113	ASN
1	F	175	HIS
1	F	187	GLN
1	F	210	HIS
1	F	218	GLN
1	F	230	HIS
1	F	244	ASN
1	F	248	GLN
1	F	272	GLN
1	F	296	HIS
1	F	313	ASN
1	F	338	ASN
1	F	458	HIS
1	G	30	HIS
1	G	61	HIS
1	G	86	ASN
1	G	106	ASN
1	G	113	ASN
1	G	175	HIS
1	G	187	GLN

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Mol	Chain	Res	Type
1	G	210	HIS
1	G	211	HIS
1	G	218	GLN
1	G	230	HIS
1	G	244	ASN
1	G	248	GLN
1	G	264	ASN
1	G	272	GLN
1	G	296	HIS
1	G	313	ASN
1	G	338	ASN
1	G	458	HIS
1	H	30	HIS
1	H	61	HIS
1	H	86	ASN
1	H	106	ASN
1	H	113	ASN
1	H	175	HIS
1	H	187	GLN
1	H	210	HIS
1	H	218	GLN
1	H	230	HIS
1	H	244	ASN
1	H	248	GLN
1	H	272	GLN
1	H	296	HIS
1	H	313	ASN
1	H	338	ASN
1	H	458	HIS
1	I	30	HIS
1	I	61	HIS
1	I	86	ASN
1	I	106	ASN
1	I	113	ASN
1	I	175	HIS
1	I	187	GLN
1	I	210	HIS
1	I	218	GLN
1	I	230	HIS
1	I	244	ASN
1	I	248	GLN
1	I	272	GLN

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Mol	Chain	Res	Type
1	I	296	HIS
1	I	313	ASN
1	I	338	ASN
1	I	458	HIS
1	J	61	HIS
1	J	86	ASN
1	J	106	ASN
1	J	113	ASN
1	J	175	HIS
1	J	187	GLN
1	J	210	HIS
1	J	218	GLN
1	J	230	HIS
1	J	244	ASN
1	J	248	GLN
1	J	264	ASN
1	J	272	GLN
1	J	296	HIS
1	J	313	ASN
1	J	338	ASN
1	J	458	HIS
1	K	30	HIS
1	K	61	HIS
1	K	86	ASN
1	K	106	ASN
1	K	113	ASN
1	K	175	HIS
1	K	187	GLN
1	K	210	HIS
1	K	211	HIS
1	K	218	GLN
1	K	230	HIS
1	K	244	ASN
1	K	248	GLN
1	K	272	GLN
1	K	296	HIS
1	K	313	ASN
1	K	338	ASN
1	K	458	HIS
1	L	61	HIS
1	L	86	ASN
1	L	106	ASN

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Mol	Chain	Res	Type
1	L	113	ASN
1	L	175	HIS
1	L	187	GLN
1	L	210	HIS
1	L	218	GLN
1	L	230	HIS
1	L	244	ASN
1	L	248	GLN
1	L	272	GLN
1	L	296	HIS
1	L	313	ASN
1	L	338	ASN
1	L	458	HIS
1	M	30	HIS
1	M	61	HIS
1	M	86	ASN
1	M	106	ASN
1	M	113	ASN
1	M	175	HIS
1	M	187	GLN
1	M	210	HIS
1	M	218	GLN
1	M	230	HIS
1	M	244	ASN
1	M	248	GLN
1	M	272	GLN
1	M	296	HIS
1	M	313	ASN
1	M	338	ASN
1	M	458	HIS
1	N	30	HIS
1	N	61	HIS
1	N	86	ASN
1	N	106	ASN
1	N	113	ASN
1	N	175	HIS
1	N	187	GLN
1	N	210	HIS
1	N	218	GLN
1	N	230	HIS
1	N	244	ASN
1	N	248	GLN

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Mol	Chain	Res	Type
1	N	272	GLN
1	N	296	HIS
1	N	313	ASN
1	N	338	ASN
1	N	458	HIS
1	O	30	HIS
1	O	61	HIS
1	O	86	ASN
1	O	106	ASN
1	O	113	ASN
1	O	175	HIS
1	O	187	GLN
1	O	210	HIS
1	O	211	HIS
1	O	218	GLN
1	O	230	HIS
1	O	244	ASN
1	O	248	GLN
1	O	272	GLN
1	O	296	HIS
1	O	313	ASN
1	O	338	ASN
1	O	458	HIS
1	P	30	HIS
1	P	61	HIS
1	P	86	ASN
1	P	106	ASN
1	P	113	ASN
1	P	175	HIS
1	P	187	GLN
1	P	210	HIS
1	P	211	HIS
1	P	218	GLN
1	P	230	HIS
1	P	244	ASN
1	P	248	GLN
1	P	264	ASN
1	P	272	GLN
1	P	313	ASN
1	P	338	ASN
1	P	458	HIS
1	Q	30	HIS

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Mol	Chain	Res	Type
1	Q	61	HIS
1	Q	86	ASN
1	Q	106	ASN
1	Q	113	ASN
1	Q	175	HIS
1	Q	187	GLN
1	Q	210	HIS
1	Q	218	GLN
1	Q	230	HIS
1	Q	244	ASN
1	Q	248	GLN
1	Q	264	ASN
1	Q	272	GLN
1	Q	296	HIS
1	Q	313	ASN
1	Q	338	ASN
1	Q	458	HIS
1	R	30	HIS
1	R	61	HIS
1	R	86	ASN
1	R	106	ASN
1	R	113	ASN
1	R	175	HIS
1	R	187	GLN
1	R	210	HIS
1	R	218	GLN
1	R	230	HIS
1	R	244	ASN
1	R	248	GLN
1	R	272	GLN
1	R	296	HIS
1	R	313	ASN
1	R	338	ASN
1	R	458	HIS
1	S	30	HIS
1	S	61	HIS
1	S	86	ASN
1	S	106	ASN
1	S	113	ASN
1	S	175	HIS
1	S	187	GLN
1	S	210	HIS

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Mol	Chain	Res	Type
1	S	211	HIS
1	S	218	GLN
1	S	230	HIS
1	S	244	ASN
1	S	248	GLN
1	S	272	GLN
1	S	296	HIS
1	S	313	ASN
1	S	338	ASN
1	S	458	HIS
1	T	30	HIS
1	T	61	HIS
1	T	86	ASN
1	T	106	ASN
1	T	113	ASN
1	T	175	HIS
1	T	187	GLN
1	T	210	HIS
1	T	218	GLN
1	T	230	HIS
1	T	244	ASN
1	T	248	GLN
1	T	272	GLN
1	T	296	HIS
1	T	313	ASN
1	T	338	ASN
1	T	458	HIS
1	U	30	HIS
1	U	61	HIS
1	U	86	ASN
1	U	106	ASN
1	U	113	ASN
1	U	175	HIS
1	U	187	GLN
1	U	210	HIS
1	U	218	GLN
1	U	230	HIS
1	U	244	ASN
1	U	248	GLN
1	U	272	GLN
1	U	296	HIS
1	U	313	ASN

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Mol	Chain	Res	Type
1	U	338	ASN
1	U	458	HIS
1	V	30	HIS
1	V	61	HIS
1	V	86	ASN
1	V	106	ASN
1	V	113	ASN
1	V	175	HIS
1	V	187	GLN
1	V	210	HIS
1	V	218	GLN
1	V	230	HIS
1	V	244	ASN
1	V	248	GLN
1	V	264	ASN
1	V	272	GLN
1	V	296	HIS
1	V	313	ASN
1	V	338	ASN
1	V	458	HIS
1	W	30	HIS
1	W	61	HIS
1	W	86	ASN
1	W	106	ASN
1	W	113	ASN
1	W	175	HIS
1	W	187	GLN
1	W	210	HIS
1	W	218	GLN
1	W	230	HIS
1	W	244	ASN
1	W	248	GLN
1	W	264	ASN
1	W	272	GLN
1	W	296	HIS
1	W	313	ASN
1	W	338	ASN
1	W	458	HIS
1	X	30	HIS
1	X	61	HIS
1	X	86	ASN
1	X	106	ASN

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Mol	Chain	Res	Type
1	X	113	ASN
1	X	175	HIS
1	X	187	GLN
1	X	210	HIS
1	X	218	GLN
1	X	230	HIS
1	X	244	ASN
1	X	248	GLN
1	X	264	ASN
1	X	272	GLN
1	X	296	HIS
1	X	313	ASN
1	X	338	ASN
1	X	458	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 24 are monoatomic - leaving 48 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CIT	Q	7508	-	3,12,12	2.99	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	I	7491	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	M	7499	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	A	7476	-	3,12,12	2.98	2 (66%)	3,17,17	1.67	1 (33%)
4	CIT	H	7490	-	3,12,12	2.98	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	E	7483	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	M	7500	-	3,12,12	2.97	2 (66%)	3,17,17	1.68	1 (33%)
3	AMP	Q	7507	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	L	7498	-	3,12,12	3.01	2 (66%)	3,17,17	1.67	1 (33%)
4	CIT	D	7482	-	3,12,12	2.99	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	H	7489	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	S	7511	-	22,25,25	3.45	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	R	7509	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
4	CIT	G	7488	-	3,12,12	2.97	2 (66%)	3,17,17	1.67	1 (33%)
4	CIT	I	7492	-	3,12,12	2.99	2 (66%)	3,17,17	1.67	1 (33%)
4	CIT	X	7522	-	3,12,12	2.96	2 (66%)	3,17,17	1.67	1 (33%)
4	CIT	J	7494	-	3,12,12	2.98	2 (66%)	3,17,17	1.66	1 (33%)
4	CIT	C	7480	-	3,12,12	3.01	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	N	7501	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	E	7484	-	3,12,12	2.99	2 (66%)	3,17,17	1.68	1 (33%)
4	CIT	P	7506	-	3,12,12	2.98	2 (66%)	3,17,17	1.67	1 (33%)
4	CIT	W	7520	-	3,12,12	2.99	2 (66%)	3,17,17	1.68	1 (33%)
3	AMP	L	7497	-	22,25,25	3.46	13 (59%)	25,38,38	4.15	10 (40%)
3	AMP	A	7475	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	N	7502	-	3,12,12	2.99	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	B	7477	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	R	7510	-	3,12,12	2.98	2 (66%)	3,17,17	1.66	1 (33%)
3	AMP	P	7505	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	O	7504	-	3,12,12	2.97	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	O	7503	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	B	7478	-	3,12,12	2.99	2 (66%)	3,17,17	1.68	1 (33%)
3	AMP	X	7521	-	22,25,25	3.47	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	U	7515	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	G	7487	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	C	7479	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	V	7517	-	22,25,25	3.45	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	S	7512	-	3,12,12	3.00	2 (66%)	3,17,17	1.67	1 (33%)
4	CIT	U	7516	-	3,12,12	2.98	2 (66%)	3,17,17	1.66	1 (33%)
4	CIT	V	7518	-	3,12,12	3.02	2 (66%)	3,17,17	1.66	1 (33%)
4	CIT	K	7496	-	3,12,12	2.96	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	W	7519	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	J	7493	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	F	7485	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	T	7514	-	3,12,12	2.97	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	D	7481	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
4	CIT	F	7486	-	3,12,12	2.99	2 (66%)	3,17,17	1.67	1 (33%)
3	AMP	T	7513	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)
3	AMP	K	7495	-	22,25,25	3.46	13 (59%)	25,38,38	4.16	10 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	Q	7508	-	-	4/6/16/16	-
3	AMP	I	7491	-	-	3/6/26/26	0/3/3/3
3	AMP	M	7499	-	-	3/6/26/26	0/3/3/3
4	CIT	A	7476	-	-	4/6/16/16	-
4	CIT	H	7490	-	-	4/6/16/16	-
3	AMP	E	7483	-	-	3/6/26/26	0/3/3/3
4	CIT	M	7500	-	-	4/6/16/16	-
3	AMP	Q	7507	-	-	3/6/26/26	0/3/3/3
4	CIT	L	7498	-	-	4/6/16/16	-
4	CIT	D	7482	-	-	4/6/16/16	-
3	AMP	H	7489	-	-	3/6/26/26	0/3/3/3
3	AMP	S	7511	-	-	3/6/26/26	0/3/3/3
3	AMP	R	7509	-	-	3/6/26/26	0/3/3/3
4	CIT	G	7488	-	-	4/6/16/16	-
4	CIT	I	7492	-	-	4/6/16/16	-
4	CIT	X	7522	-	-	4/6/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	J	7494	-	-	4/6/16/16	-
4	CIT	C	7480	-	-	4/6/16/16	-
3	AMP	N	7501	-	-	3/6/26/26	0/3/3/3
4	CIT	E	7484	-	-	4/6/16/16	-
4	CIT	P	7506	-	-	4/6/16/16	-
4	CIT	W	7520	-	-	4/6/16/16	-
3	AMP	L	7497	-	-	3/6/26/26	0/3/3/3
3	AMP	A	7475	-	-	3/6/26/26	0/3/3/3
4	CIT	N	7502	-	-	4/6/16/16	-
3	AMP	B	7477	-	-	3/6/26/26	0/3/3/3
4	CIT	R	7510	-	-	4/6/16/16	-
3	AMP	P	7505	-	-	3/6/26/26	0/3/3/3
4	CIT	O	7504	-	-	4/6/16/16	-
3	AMP	O	7503	-	-	3/6/26/26	0/3/3/3
4	CIT	B	7478	-	-	4/6/16/16	-
3	AMP	X	7521	-	-	3/6/26/26	0/3/3/3
3	AMP	U	7515	-	-	3/6/26/26	0/3/3/3
3	AMP	G	7487	-	-	3/6/26/26	0/3/3/3
3	AMP	C	7479	-	-	3/6/26/26	0/3/3/3
3	AMP	V	7517	-	-	3/6/26/26	0/3/3/3
4	CIT	S	7512	-	-	4/6/16/16	-
4	CIT	U	7516	-	-	4/6/16/16	-
4	CIT	V	7518	-	-	4/6/16/16	-
4	CIT	K	7496	-	-	4/6/16/16	-
3	AMP	W	7519	-	-	3/6/26/26	0/3/3/3
3	AMP	J	7493	-	-	3/6/26/26	0/3/3/3
3	AMP	F	7485	-	-	3/6/26/26	0/3/3/3
4	CIT	T	7514	-	-	4/6/16/16	-
3	AMP	D	7481	-	-	3/6/26/26	0/3/3/3
4	CIT	F	7486	-	-	4/6/16/16	-
3	AMP	T	7513	-	-	3/6/26/26	0/3/3/3
3	AMP	K	7495	-	-	3/6/26/26	0/3/3/3

All (360) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	7521	AMP	O4'-C1'	8.64	1.53	1.41
3	N	7501	AMP	O4'-C1'	8.63	1.53	1.41
3	B	7477	AMP	O4'-C1'	8.62	1.53	1.41
3	K	7495	AMP	O4'-C1'	8.62	1.53	1.41
3	W	7519	AMP	O4'-C1'	8.62	1.53	1.41
3	C	7479	AMP	O4'-C1'	8.61	1.53	1.41
3	G	7487	AMP	O4'-C1'	8.60	1.53	1.41
3	P	7505	AMP	O4'-C1'	8.60	1.53	1.41
3	E	7483	AMP	O4'-C1'	8.60	1.53	1.41
3	M	7499	AMP	O4'-C1'	8.59	1.53	1.41
3	J	7493	AMP	O4'-C1'	8.59	1.53	1.41
3	T	7513	AMP	O4'-C1'	8.59	1.53	1.41
3	A	7475	AMP	O4'-C1'	8.58	1.53	1.41
3	F	7485	AMP	O4'-C1'	8.58	1.53	1.41
3	D	7481	AMP	O4'-C1'	8.58	1.53	1.41
3	S	7511	AMP	O4'-C1'	8.58	1.53	1.41
3	O	7503	AMP	O4'-C1'	8.58	1.53	1.41
3	R	7509	AMP	O4'-C1'	8.57	1.53	1.41
3	L	7497	AMP	O4'-C1'	8.57	1.53	1.41
3	U	7515	AMP	O4'-C1'	8.56	1.53	1.41
3	H	7489	AMP	O4'-C1'	8.56	1.53	1.41
3	Q	7507	AMP	O4'-C1'	8.55	1.53	1.41
3	I	7491	AMP	O4'-C1'	8.53	1.53	1.41
3	V	7517	AMP	O4'-C1'	8.52	1.53	1.41
3	L	7497	AMP	C4-N3	6.53	1.44	1.35
3	H	7489	AMP	C4-N3	6.53	1.44	1.35
3	B	7477	AMP	C4-N3	6.52	1.44	1.35
3	U	7515	AMP	C4-N3	6.52	1.44	1.35
3	J	7493	AMP	C4-N3	6.50	1.44	1.35
3	D	7481	AMP	C4-N3	6.50	1.44	1.35
3	W	7519	AMP	C4-N3	6.50	1.44	1.35
3	I	7491	AMP	C4-N3	6.49	1.44	1.35
3	F	7485	AMP	C4-N3	6.49	1.44	1.35
3	M	7499	AMP	C4-N3	6.48	1.44	1.35
3	N	7501	AMP	C4-N3	6.48	1.44	1.35
3	A	7475	AMP	C4-N3	6.48	1.44	1.35
3	V	7517	AMP	C4-N3	6.47	1.44	1.35
3	G	7487	AMP	C4-N3	6.47	1.44	1.35
3	P	7505	AMP	C4-N3	6.47	1.44	1.35
3	T	7513	AMP	C4-N3	6.47	1.44	1.35
3	R	7509	AMP	C4-N3	6.47	1.44	1.35
3	X	7521	AMP	C4-N3	6.47	1.44	1.35
3	O	7503	AMP	C4-N3	6.47	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	7483	AMP	C4-N3	6.47	1.44	1.35
3	S	7511	AMP	C4-N3	6.46	1.44	1.35
3	Q	7507	AMP	C4-N3	6.46	1.44	1.35
3	C	7479	AMP	C4-N3	6.45	1.44	1.35
3	K	7495	AMP	C4-N3	6.42	1.44	1.35
3	F	7485	AMP	C2-N3	5.65	1.41	1.32
3	R	7509	AMP	C2-N3	5.65	1.41	1.32
3	C	7479	AMP	C2-N3	5.65	1.41	1.32
3	U	7515	AMP	C2-N3	5.63	1.41	1.32
3	D	7481	AMP	C2-N3	5.63	1.41	1.32
3	X	7521	AMP	C2-N3	5.63	1.41	1.32
3	T	7513	AMP	C2-N3	5.63	1.41	1.32
3	K	7495	AMP	C2-N3	5.63	1.41	1.32
3	I	7491	AMP	C2-N3	5.62	1.41	1.32
3	W	7519	AMP	C2-N3	5.62	1.41	1.32
3	J	7493	AMP	C2-N3	5.62	1.41	1.32
3	L	7497	AMP	C2-N3	5.62	1.41	1.32
3	O	7503	AMP	C2-N3	5.62	1.41	1.32
3	A	7475	AMP	C2-N3	5.61	1.41	1.32
3	B	7477	AMP	C2-N3	5.61	1.41	1.32
3	G	7487	AMP	C2-N3	5.61	1.41	1.32
3	Q	7507	AMP	C2-N3	5.61	1.41	1.32
3	H	7489	AMP	C2-N3	5.61	1.41	1.32
3	N	7501	AMP	C2-N3	5.60	1.41	1.32
3	E	7483	AMP	C2-N3	5.60	1.41	1.32
3	P	7505	AMP	C2-N3	5.60	1.41	1.32
3	V	7517	AMP	C2-N3	5.60	1.41	1.32
3	M	7499	AMP	C2-N3	5.58	1.41	1.32
3	S	7511	AMP	C2-N3	5.57	1.41	1.32
3	N	7501	AMP	P-O3P	4.86	1.73	1.54
3	W	7519	AMP	P-O3P	4.85	1.73	1.54
3	B	7477	AMP	P-O3P	4.85	1.73	1.54
3	X	7521	AMP	P-O3P	4.85	1.73	1.54
3	J	7493	AMP	P-O3P	4.84	1.73	1.54
3	M	7499	AMP	P-O3P	4.84	1.73	1.54
3	Q	7507	AMP	P-O3P	4.84	1.73	1.54
3	R	7509	AMP	P-O3P	4.84	1.73	1.54
3	C	7479	AMP	P-O3P	4.84	1.73	1.54
3	L	7497	AMP	P-O3P	4.84	1.73	1.54
3	F	7485	AMP	P-O3P	4.84	1.73	1.54
3	A	7475	AMP	P-O3P	4.84	1.73	1.54
3	E	7483	AMP	P-O3P	4.84	1.73	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	7503	AMP	P-O3P	4.83	1.73	1.54
3	P	7505	AMP	P-O3P	4.83	1.73	1.54
3	K	7495	AMP	P-O3P	4.83	1.73	1.54
3	I	7491	AMP	P-O3P	4.83	1.73	1.54
3	V	7517	AMP	P-O3P	4.83	1.73	1.54
3	D	7481	AMP	P-O3P	4.83	1.73	1.54
3	G	7487	AMP	P-O3P	4.83	1.73	1.54
3	U	7515	AMP	P-O3P	4.83	1.73	1.54
3	T	7513	AMP	P-O3P	4.82	1.73	1.54
3	H	7489	AMP	P-O3P	4.81	1.73	1.54
3	S	7511	AMP	P-O3P	4.81	1.73	1.54
3	Q	7507	AMP	O4'-C4'	4.31	1.54	1.45
3	S	7511	AMP	O4'-C4'	4.30	1.54	1.45
3	M	7499	AMP	O4'-C4'	4.30	1.54	1.45
3	H	7489	AMP	O4'-C4'	4.30	1.54	1.45
3	V	7517	AMP	O4'-C4'	4.30	1.54	1.45
3	F	7485	AMP	O4'-C4'	4.30	1.54	1.45
3	X	7521	AMP	O4'-C4'	4.30	1.54	1.45
3	I	7491	AMP	O4'-C4'	4.30	1.54	1.45
3	J	7493	AMP	O4'-C4'	4.29	1.54	1.45
3	B	7477	AMP	O4'-C4'	4.29	1.54	1.45
3	A	7475	AMP	O4'-C4'	4.28	1.54	1.45
3	O	7503	AMP	O4'-C4'	4.28	1.54	1.45
3	L	7497	AMP	O4'-C4'	4.28	1.54	1.45
3	G	7487	AMP	O4'-C4'	4.28	1.54	1.45
3	K	7495	AMP	O4'-C4'	4.28	1.54	1.45
3	D	7481	AMP	O4'-C4'	4.28	1.54	1.45
3	U	7515	AMP	O4'-C4'	4.28	1.54	1.45
3	E	7483	AMP	O4'-C4'	4.27	1.54	1.45
3	R	7509	AMP	O4'-C4'	4.26	1.54	1.45
3	W	7519	AMP	O4'-C4'	4.26	1.54	1.45
3	N	7501	AMP	O4'-C4'	4.26	1.54	1.45
3	T	7513	AMP	O4'-C4'	4.26	1.54	1.45
3	P	7505	AMP	O4'-C4'	4.26	1.54	1.45
3	C	7479	AMP	O4'-C4'	4.25	1.54	1.45
4	L	7498	CIT	C2-C3	4.25	1.60	1.54
4	C	7480	CIT	C2-C3	4.22	1.60	1.54
4	V	7518	CIT	C2-C3	4.21	1.60	1.54
4	I	7492	CIT	C2-C3	4.19	1.60	1.54
4	N	7502	CIT	C2-C3	4.19	1.60	1.54
4	F	7486	CIT	C2-C3	4.18	1.60	1.54
4	D	7482	CIT	C2-C3	4.18	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	W	7520	CIT	C2-C3	4.17	1.60	1.54
4	E	7484	CIT	C2-C3	4.17	1.60	1.54
4	S	7512	CIT	C2-C3	4.17	1.60	1.54
4	A	7476	CIT	C2-C3	4.16	1.60	1.54
4	Q	7508	CIT	C2-C3	4.16	1.60	1.54
4	B	7478	CIT	C2-C3	4.16	1.60	1.54
4	G	7488	CIT	C2-C3	4.16	1.60	1.54
4	O	7504	CIT	C2-C3	4.15	1.60	1.54
4	J	7494	CIT	C2-C3	4.15	1.60	1.54
4	P	7506	CIT	C2-C3	4.14	1.60	1.54
4	U	7516	CIT	C2-C3	4.14	1.60	1.54
4	K	7496	CIT	C2-C3	4.13	1.60	1.54
4	H	7490	CIT	C2-C3	4.13	1.60	1.54
4	R	7510	CIT	C2-C3	4.13	1.60	1.54
4	X	7522	CIT	C2-C3	4.12	1.60	1.54
4	M	7500	CIT	C2-C3	4.11	1.60	1.54
4	T	7514	CIT	C2-C3	4.10	1.60	1.54
3	R	7509	AMP	C3'-C4'	-4.10	1.42	1.53
3	M	7499	AMP	C3'-C4'	-4.09	1.42	1.53
3	H	7489	AMP	C3'-C4'	-4.08	1.42	1.53
3	K	7495	AMP	C3'-C4'	-4.08	1.42	1.53
3	U	7515	AMP	C3'-C4'	-4.08	1.42	1.53
3	W	7519	AMP	C3'-C4'	-4.08	1.42	1.53
3	N	7501	AMP	C3'-C4'	-4.06	1.42	1.53
3	I	7491	AMP	C3'-C4'	-4.06	1.42	1.53
3	O	7503	AMP	C3'-C4'	-4.06	1.42	1.53
3	P	7505	AMP	C3'-C4'	-4.06	1.42	1.53
3	E	7483	AMP	C3'-C4'	-4.06	1.42	1.53
3	D	7481	AMP	C3'-C4'	-4.06	1.42	1.53
3	A	7475	AMP	C3'-C4'	-4.06	1.42	1.53
3	S	7511	AMP	C3'-C4'	-4.05	1.42	1.53
3	F	7485	AMP	C3'-C4'	-4.05	1.42	1.53
3	Q	7507	AMP	C3'-C4'	-4.05	1.42	1.53
3	T	7513	AMP	C3'-C4'	-4.05	1.42	1.53
3	C	7479	AMP	C3'-C4'	-4.05	1.42	1.53
3	L	7497	AMP	C3'-C4'	-4.05	1.42	1.53
3	X	7521	AMP	C3'-C4'	-4.05	1.42	1.53
3	V	7517	AMP	C3'-C4'	-4.05	1.42	1.53
3	J	7493	AMP	C3'-C4'	-4.04	1.42	1.53
3	G	7487	AMP	C3'-C4'	-4.04	1.42	1.53
3	B	7477	AMP	C3'-C4'	-4.04	1.42	1.53
3	E	7483	AMP	C2'-C1'	3.20	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7487	AMP	C2'-C1'	3.19	1.58	1.53
3	T	7513	AMP	C2'-C1'	3.18	1.58	1.53
3	P	7505	AMP	C2'-C1'	3.18	1.58	1.53
3	X	7521	AMP	C2'-C1'	3.18	1.58	1.53
3	D	7481	AMP	C2'-C1'	3.17	1.58	1.53
3	F	7485	AMP	C2'-C1'	3.17	1.58	1.53
3	N	7501	AMP	C2'-C1'	3.17	1.58	1.53
3	L	7497	AMP	C2'-C1'	3.16	1.58	1.53
3	J	7493	AMP	C2'-C1'	3.16	1.58	1.53
3	O	7503	AMP	C2'-C1'	3.15	1.58	1.53
3	A	7475	AMP	C2'-C1'	3.15	1.58	1.53
3	S	7511	AMP	C6-N6	-3.14	1.22	1.34
3	L	7497	AMP	C6-N6	-3.14	1.22	1.34
3	D	7481	AMP	C6-N6	-3.14	1.22	1.34
3	K	7495	AMP	C6-N6	-3.14	1.22	1.34
3	K	7495	AMP	C2'-C1'	3.14	1.58	1.53
3	U	7515	AMP	C6-N6	-3.13	1.22	1.34
3	Q	7507	AMP	C6-N6	-3.13	1.22	1.34
3	V	7517	AMP	C2'-C1'	3.13	1.58	1.53
3	R	7509	AMP	C6-N6	-3.13	1.22	1.34
3	R	7509	AMP	C2'-C1'	3.13	1.58	1.53
3	C	7479	AMP	C2'-C1'	3.13	1.58	1.53
3	M	7499	AMP	C2'-C1'	3.13	1.58	1.53
3	B	7477	AMP	C2'-C1'	3.13	1.58	1.53
3	J	7493	AMP	C6-N6	-3.13	1.22	1.34
3	I	7491	AMP	C6-N6	-3.13	1.22	1.34
3	Q	7507	AMP	C2'-C1'	3.13	1.58	1.53
3	U	7515	AMP	C2'-C1'	3.13	1.58	1.53
3	W	7519	AMP	C6-N6	-3.12	1.22	1.34
3	I	7491	AMP	C2'-C1'	3.12	1.58	1.53
3	E	7483	AMP	C6-N6	-3.12	1.22	1.34
3	X	7521	AMP	C6-N6	-3.12	1.22	1.34
3	C	7479	AMP	C6-N6	-3.12	1.22	1.34
3	A	7475	AMP	C6-N6	-3.12	1.22	1.34
3	T	7513	AMP	C6-N6	-3.12	1.22	1.34
3	W	7519	AMP	C2'-C1'	3.12	1.58	1.53
3	B	7477	AMP	P-O1P	3.12	1.60	1.50
3	H	7489	AMP	C2'-C1'	3.12	1.58	1.53
3	G	7487	AMP	C6-N6	-3.11	1.22	1.34
3	S	7511	AMP	C2'-C1'	3.11	1.58	1.53
3	N	7501	AMP	C6-N6	-3.11	1.22	1.34
3	M	7499	AMP	C6-N6	-3.11	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	7485	AMP	C6-N6	-3.11	1.22	1.34
3	P	7505	AMP	C6-N6	-3.11	1.22	1.34
3	H	7489	AMP	C6-N6	-3.11	1.22	1.34
3	B	7477	AMP	C6-N6	-3.11	1.22	1.34
3	V	7517	AMP	C6-N6	-3.11	1.22	1.34
3	I	7491	AMP	P-O1P	3.11	1.60	1.50
3	E	7483	AMP	P-O1P	3.10	1.60	1.50
3	O	7503	AMP	C6-N6	-3.10	1.22	1.34
3	O	7503	AMP	P-O1P	3.10	1.60	1.50
3	U	7515	AMP	P-O1P	3.10	1.60	1.50
3	Q	7507	AMP	P-O1P	3.09	1.60	1.50
3	G	7487	AMP	P-O1P	3.09	1.60	1.50
3	L	7497	AMP	P-O1P	3.09	1.60	1.50
3	D	7481	AMP	P-O1P	3.09	1.60	1.50
3	H	7489	AMP	P-O1P	3.09	1.60	1.50
3	T	7513	AMP	P-O1P	3.09	1.60	1.50
3	J	7493	AMP	P-O1P	3.09	1.60	1.50
3	A	7475	AMP	P-O1P	3.09	1.60	1.50
3	P	7505	AMP	P-O1P	3.09	1.60	1.50
3	K	7495	AMP	P-O1P	3.09	1.60	1.50
3	X	7521	AMP	P-O1P	3.09	1.60	1.50
3	M	7499	AMP	P-O1P	3.09	1.60	1.50
3	W	7519	AMP	P-O1P	3.08	1.60	1.50
3	R	7509	AMP	P-O1P	3.08	1.60	1.50
3	N	7501	AMP	P-O1P	3.08	1.60	1.50
3	S	7511	AMP	P-O1P	3.08	1.60	1.50
3	V	7517	AMP	P-O1P	3.07	1.60	1.50
3	F	7485	AMP	P-O1P	3.07	1.60	1.50
3	C	7479	AMP	P-O1P	3.07	1.60	1.50
4	T	7514	CIT	C4-C3	2.64	1.58	1.54
4	Q	7508	CIT	C4-C3	2.63	1.58	1.54
4	V	7518	CIT	C4-C3	2.63	1.58	1.54
4	R	7510	CIT	C4-C3	2.62	1.58	1.54
4	B	7478	CIT	C4-C3	2.62	1.58	1.54
4	W	7520	CIT	C4-C3	2.62	1.58	1.54
4	H	7490	CIT	C4-C3	2.62	1.58	1.54
4	E	7484	CIT	C4-C3	2.61	1.58	1.54
4	P	7506	CIT	C4-C3	2.61	1.58	1.54
4	J	7494	CIT	C4-C3	2.61	1.58	1.54
4	D	7482	CIT	C4-C3	2.60	1.58	1.54
4	M	7500	CIT	C4-C3	2.60	1.58	1.54
4	S	7512	CIT	C4-C3	2.60	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	7480	CIT	C4-C3	2.60	1.58	1.54
4	F	7486	CIT	C4-C3	2.59	1.58	1.54
4	A	7476	CIT	C4-C3	2.59	1.58	1.54
4	N	7502	CIT	C4-C3	2.59	1.58	1.54
4	G	7488	CIT	C4-C3	2.58	1.58	1.54
4	U	7516	CIT	C4-C3	2.58	1.58	1.54
4	X	7522	CIT	C4-C3	2.57	1.58	1.54
4	K	7496	CIT	C4-C3	2.57	1.58	1.54
4	O	7504	CIT	C4-C3	2.57	1.58	1.54
3	T	7513	AMP	P-O5'	2.56	1.68	1.60
3	O	7503	AMP	P-O5'	2.55	1.68	1.60
4	L	7498	CIT	C4-C3	2.55	1.58	1.54
3	Q	7507	AMP	P-O5'	2.55	1.68	1.60
3	S	7511	AMP	C5-C4	2.55	1.47	1.40
3	S	7511	AMP	P-O5'	2.55	1.68	1.60
3	U	7515	AMP	P-O5'	2.55	1.68	1.60
3	X	7521	AMP	C5-C4	2.55	1.47	1.40
3	B	7477	AMP	C5-C4	2.55	1.47	1.40
4	I	7492	CIT	C4-C3	2.55	1.58	1.54
3	L	7497	AMP	P-O5'	2.54	1.68	1.60
3	W	7519	AMP	P-O5'	2.54	1.68	1.60
3	T	7513	AMP	C5-C4	2.54	1.47	1.40
3	F	7485	AMP	P-O5'	2.54	1.68	1.60
3	D	7481	AMP	P-O5'	2.54	1.68	1.60
3	I	7491	AMP	P-O5'	2.54	1.68	1.60
3	A	7475	AMP	P-O5'	2.54	1.68	1.60
3	P	7505	AMP	C5-C4	2.54	1.47	1.40
3	R	7509	AMP	P-O5'	2.54	1.68	1.60
3	R	7509	AMP	C5-C4	2.54	1.47	1.40
3	U	7515	AMP	C5-C4	2.54	1.47	1.40
3	X	7521	AMP	P-O5'	2.53	1.68	1.60
3	K	7495	AMP	P-O5'	2.53	1.68	1.60
3	M	7499	AMP	P-O5'	2.53	1.68	1.60
3	N	7501	AMP	P-O5'	2.53	1.68	1.60
3	D	7481	AMP	C5-C4	2.53	1.47	1.40
3	J	7493	AMP	P-O5'	2.53	1.68	1.60
3	B	7477	AMP	P-O5'	2.53	1.68	1.60
3	C	7479	AMP	C5-C4	2.53	1.47	1.40
3	C	7479	AMP	P-O5'	2.53	1.68	1.60
3	H	7489	AMP	P-O5'	2.53	1.68	1.60
3	M	7499	AMP	C5-C4	2.53	1.47	1.40
3	F	7485	AMP	C5-C4	2.52	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	7517	AMP	P-O5'	2.52	1.68	1.60
3	K	7495	AMP	C5-C4	2.52	1.47	1.40
3	I	7491	AMP	C5-C4	2.52	1.47	1.40
3	G	7487	AMP	P-O5'	2.52	1.68	1.60
3	P	7505	AMP	P-O5'	2.52	1.68	1.60
3	A	7475	AMP	C5-C4	2.52	1.47	1.40
3	E	7483	AMP	P-O5'	2.52	1.68	1.60
3	W	7519	AMP	C5-C4	2.52	1.47	1.40
3	G	7487	AMP	C5-C4	2.52	1.47	1.40
3	Q	7507	AMP	C5-C4	2.52	1.47	1.40
3	N	7501	AMP	C5-C4	2.51	1.47	1.40
3	H	7489	AMP	C5-C4	2.51	1.47	1.40
3	O	7503	AMP	C5-C4	2.51	1.47	1.40
3	V	7517	AMP	C5-C4	2.51	1.47	1.40
3	J	7493	AMP	C5-C4	2.50	1.47	1.40
3	E	7483	AMP	C5-C4	2.49	1.47	1.40
3	L	7497	AMP	C5-C4	2.48	1.47	1.40
3	G	7487	AMP	P-O2P	2.39	1.64	1.54
3	V	7517	AMP	P-O2P	2.39	1.64	1.54
3	S	7511	AMP	P-O2P	2.39	1.64	1.54
3	O	7503	AMP	P-O2P	2.38	1.64	1.54
3	T	7513	AMP	P-O2P	2.38	1.64	1.54
3	C	7479	AMP	P-O2P	2.38	1.64	1.54
3	J	7493	AMP	P-O2P	2.38	1.64	1.54
3	B	7477	AMP	P-O2P	2.38	1.64	1.54
3	D	7481	AMP	P-O2P	2.38	1.64	1.54
3	A	7475	AMP	P-O2P	2.38	1.64	1.54
3	Q	7507	AMP	P-O2P	2.38	1.64	1.54
3	R	7509	AMP	P-O2P	2.38	1.64	1.54
3	P	7505	AMP	P-O2P	2.37	1.64	1.54
3	F	7485	AMP	P-O2P	2.37	1.64	1.54
3	H	7489	AMP	P-O2P	2.37	1.64	1.54
3	W	7519	AMP	P-O2P	2.37	1.64	1.54
3	K	7495	AMP	P-O2P	2.37	1.64	1.54
3	I	7491	AMP	P-O2P	2.37	1.64	1.54
3	N	7501	AMP	P-O2P	2.37	1.64	1.54
3	U	7515	AMP	P-O2P	2.37	1.64	1.54
3	X	7521	AMP	P-O2P	2.37	1.64	1.54
3	E	7483	AMP	P-O2P	2.36	1.63	1.54
3	M	7499	AMP	P-O2P	2.36	1.63	1.54
3	L	7497	AMP	P-O2P	2.36	1.63	1.54
3	K	7495	AMP	C2'-C3'	2.33	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	7515	AMP	C2'-C3'	2.32	1.59	1.53
3	N	7501	AMP	C2'-C3'	2.32	1.59	1.53
3	B	7477	AMP	C2'-C3'	2.32	1.59	1.53
3	F	7485	AMP	C2'-C3'	2.32	1.59	1.53
3	O	7503	AMP	C2'-C3'	2.32	1.59	1.53
3	H	7489	AMP	C2'-C3'	2.32	1.59	1.53
3	V	7517	AMP	C2'-C3'	2.31	1.59	1.53
3	I	7491	AMP	C2'-C3'	2.31	1.59	1.53
3	X	7521	AMP	C2'-C3'	2.31	1.59	1.53
3	R	7509	AMP	C2'-C3'	2.30	1.59	1.53
3	Q	7507	AMP	C2'-C3'	2.30	1.59	1.53
3	A	7475	AMP	C2'-C3'	2.30	1.59	1.53
3	W	7519	AMP	C2'-C3'	2.30	1.59	1.53
3	P	7505	AMP	C2'-C3'	2.30	1.59	1.53
3	D	7481	AMP	C2'-C3'	2.30	1.59	1.53
3	C	7479	AMP	C2'-C3'	2.30	1.59	1.53
3	G	7487	AMP	C2'-C3'	2.30	1.59	1.53
3	T	7513	AMP	C2'-C3'	2.30	1.59	1.53
3	J	7493	AMP	C2'-C3'	2.29	1.59	1.53
3	E	7483	AMP	C2'-C3'	2.29	1.59	1.53
3	M	7499	AMP	C2'-C3'	2.29	1.59	1.53
3	S	7511	AMP	C2'-C3'	2.28	1.59	1.53
3	L	7497	AMP	C2'-C3'	2.28	1.59	1.53

All (264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	7505	AMP	O4'-C1'-C2'	-13.64	87.00	106.93
3	J	7493	AMP	O4'-C1'-C2'	-13.63	87.00	106.93
3	E	7483	AMP	O4'-C1'-C2'	-13.63	87.00	106.93
3	N	7501	AMP	O4'-C1'-C2'	-13.63	87.01	106.93
3	G	7487	AMP	O4'-C1'-C2'	-13.63	87.01	106.93
3	O	7503	AMP	O4'-C1'-C2'	-13.62	87.02	106.93
3	M	7499	AMP	O4'-C1'-C2'	-13.62	87.02	106.93
3	C	7479	AMP	O4'-C1'-C2'	-13.62	87.03	106.93
3	F	7485	AMP	O4'-C1'-C2'	-13.61	87.03	106.93
3	W	7519	AMP	O4'-C1'-C2'	-13.61	87.04	106.93
3	K	7495	AMP	O4'-C1'-C2'	-13.61	87.04	106.93
3	H	7489	AMP	O4'-C1'-C2'	-13.61	87.04	106.93
3	X	7521	AMP	O4'-C1'-C2'	-13.61	87.04	106.93
3	A	7475	AMP	O4'-C1'-C2'	-13.61	87.04	106.93
3	D	7481	AMP	O4'-C1'-C2'	-13.61	87.04	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	7515	AMP	O4'-C1'-C2'	-13.60	87.05	106.93
3	T	7513	AMP	O4'-C1'-C2'	-13.60	87.05	106.93
3	L	7497	AMP	O4'-C1'-C2'	-13.60	87.05	106.93
3	Q	7507	AMP	O4'-C1'-C2'	-13.60	87.06	106.93
3	I	7491	AMP	O4'-C1'-C2'	-13.60	87.06	106.93
3	B	7477	AMP	O4'-C1'-C2'	-13.59	87.06	106.93
3	V	7517	AMP	O4'-C1'-C2'	-13.59	87.06	106.93
3	R	7509	AMP	O4'-C1'-C2'	-13.59	87.06	106.93
3	S	7511	AMP	O4'-C1'-C2'	-13.59	87.06	106.93
3	X	7521	AMP	O5'-C5'-C4'	8.40	137.89	108.99
3	P	7505	AMP	O5'-C5'-C4'	8.39	137.88	108.99
3	I	7491	AMP	O5'-C5'-C4'	8.39	137.87	108.99
3	C	7479	AMP	O5'-C5'-C4'	8.39	137.87	108.99
3	T	7513	AMP	O5'-C5'-C4'	8.39	137.86	108.99
3	V	7517	AMP	O5'-C5'-C4'	8.39	137.86	108.99
3	M	7499	AMP	O5'-C5'-C4'	8.39	137.86	108.99
3	U	7515	AMP	O5'-C5'-C4'	8.39	137.86	108.99
3	S	7511	AMP	O5'-C5'-C4'	8.39	137.85	108.99
3	W	7519	AMP	O5'-C5'-C4'	8.39	137.85	108.99
3	Q	7507	AMP	O5'-C5'-C4'	8.38	137.85	108.99
3	K	7495	AMP	O5'-C5'-C4'	8.38	137.85	108.99
3	E	7483	AMP	O5'-C5'-C4'	8.38	137.85	108.99
3	G	7487	AMP	O5'-C5'-C4'	8.38	137.85	108.99
3	A	7475	AMP	O5'-C5'-C4'	8.38	137.84	108.99
3	O	7503	AMP	O5'-C5'-C4'	8.38	137.84	108.99
3	N	7501	AMP	O5'-C5'-C4'	8.38	137.84	108.99
3	H	7489	AMP	O5'-C5'-C4'	8.38	137.83	108.99
3	R	7509	AMP	O5'-C5'-C4'	8.38	137.83	108.99
3	J	7493	AMP	O5'-C5'-C4'	8.38	137.83	108.99
3	D	7481	AMP	O5'-C5'-C4'	8.38	137.82	108.99
3	B	7477	AMP	O5'-C5'-C4'	8.38	137.82	108.99
3	L	7497	AMP	O5'-C5'-C4'	8.37	137.80	108.99
3	F	7485	AMP	O5'-C5'-C4'	8.37	137.79	108.99
3	V	7517	AMP	P-O5'-C5'	7.49	138.93	118.30
3	X	7521	AMP	P-O5'-C5'	7.49	138.92	118.30
3	I	7491	AMP	P-O5'-C5'	7.49	138.91	118.30
3	S	7511	AMP	P-O5'-C5'	7.49	138.91	118.30
3	G	7487	AMP	P-O5'-C5'	7.48	138.91	118.30
3	E	7483	AMP	P-O5'-C5'	7.48	138.90	118.30
3	P	7505	AMP	P-O5'-C5'	7.48	138.90	118.30
3	N	7501	AMP	P-O5'-C5'	7.48	138.89	118.30
3	M	7499	AMP	P-O5'-C5'	7.48	138.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	7479	AMP	P-O5'-C5'	7.48	138.89	118.30
3	K	7495	AMP	P-O5'-C5'	7.47	138.88	118.30
3	A	7475	AMP	P-O5'-C5'	7.47	138.88	118.30
3	J	7493	AMP	P-O5'-C5'	7.47	138.87	118.30
3	F	7485	AMP	P-O5'-C5'	7.47	138.87	118.30
3	Q	7507	AMP	P-O5'-C5'	7.47	138.87	118.30
3	D	7481	AMP	P-O5'-C5'	7.47	138.87	118.30
3	U	7515	AMP	P-O5'-C5'	7.47	138.87	118.30
3	W	7519	AMP	P-O5'-C5'	7.47	138.86	118.30
3	T	7513	AMP	P-O5'-C5'	7.47	138.86	118.30
3	O	7503	AMP	P-O5'-C5'	7.46	138.85	118.30
3	H	7489	AMP	P-O5'-C5'	7.46	138.85	118.30
3	R	7509	AMP	P-O5'-C5'	7.46	138.85	118.30
3	B	7477	AMP	P-O5'-C5'	7.46	138.84	118.30
3	L	7497	AMP	P-O5'-C5'	7.45	138.82	118.30
3	I	7491	AMP	O4'-C4'-C5'	4.68	124.79	109.37
3	E	7483	AMP	O4'-C4'-C5'	4.68	124.78	109.37
3	T	7513	AMP	O4'-C4'-C5'	4.68	124.77	109.37
3	V	7517	AMP	O4'-C4'-C5'	4.68	124.76	109.37
3	P	7505	AMP	O4'-C4'-C5'	4.68	124.76	109.37
3	U	7515	AMP	O4'-C4'-C5'	4.67	124.75	109.37
3	F	7485	AMP	O4'-C4'-C5'	4.67	124.75	109.37
3	S	7511	AMP	O4'-C4'-C5'	4.67	124.75	109.37
3	A	7475	AMP	O4'-C4'-C5'	4.67	124.75	109.37
3	J	7493	AMP	O4'-C4'-C5'	4.67	124.74	109.37
3	W	7519	AMP	O4'-C4'-C5'	4.67	124.73	109.37
3	D	7481	AMP	O4'-C4'-C5'	4.67	124.73	109.37
3	H	7489	AMP	O4'-C4'-C5'	4.67	124.73	109.37
3	L	7497	AMP	O4'-C4'-C5'	4.67	124.73	109.37
3	O	7503	AMP	O4'-C4'-C5'	4.67	124.73	109.37
3	N	7501	AMP	O4'-C4'-C5'	4.67	124.72	109.37
3	M	7499	AMP	O4'-C4'-C5'	4.66	124.72	109.37
3	B	7477	AMP	O4'-C4'-C5'	4.66	124.72	109.37
3	X	7521	AMP	O4'-C4'-C5'	4.66	124.72	109.37
3	C	7479	AMP	O4'-C4'-C5'	4.66	124.72	109.37
3	R	7509	AMP	O4'-C4'-C5'	4.66	124.72	109.37
3	Q	7507	AMP	O4'-C4'-C5'	4.66	124.71	109.37
3	K	7495	AMP	O4'-C4'-C5'	4.66	124.71	109.37
3	G	7487	AMP	O4'-C4'-C5'	4.66	124.70	109.37
3	P	7505	AMP	C1'-N9-C4	4.41	134.40	126.64
3	L	7497	AMP	C1'-N9-C4	4.41	134.39	126.64
3	D	7481	AMP	C1'-N9-C4	4.40	134.37	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	7515	AMP	C1'-N9-C4	4.40	134.37	126.64
3	N	7501	AMP	C1'-N9-C4	4.39	134.35	126.64
3	V	7517	AMP	C1'-N9-C4	4.39	134.35	126.64
3	O	7503	AMP	C1'-N9-C4	4.39	134.35	126.64
3	W	7519	AMP	C1'-N9-C4	4.39	134.35	126.64
3	Q	7507	AMP	C1'-N9-C4	4.39	134.35	126.64
3	B	7477	AMP	C1'-N9-C4	4.39	134.35	126.64
3	E	7483	AMP	C1'-N9-C4	4.39	134.35	126.64
3	J	7493	AMP	C1'-N9-C4	4.38	134.34	126.64
3	F	7485	AMP	C1'-N9-C4	4.38	134.34	126.64
3	A	7475	AMP	C1'-N9-C4	4.38	134.34	126.64
3	G	7487	AMP	C1'-N9-C4	4.38	134.33	126.64
3	T	7513	AMP	C1'-N9-C4	4.38	134.33	126.64
3	H	7489	AMP	C1'-N9-C4	4.37	134.32	126.64
3	S	7511	AMP	C1'-N9-C4	4.37	134.32	126.64
3	K	7495	AMP	C1'-N9-C4	4.37	134.32	126.64
3	M	7499	AMP	C1'-N9-C4	4.37	134.31	126.64
3	I	7491	AMP	C1'-N9-C4	4.37	134.31	126.64
3	R	7509	AMP	C1'-N9-C4	4.36	134.30	126.64
3	C	7479	AMP	C1'-N9-C4	4.35	134.29	126.64
3	X	7521	AMP	C1'-N9-C4	4.35	134.29	126.64
3	V	7517	AMP	O2'-C2'-C1'	4.29	126.70	110.85
3	R	7509	AMP	O2'-C2'-C1'	4.28	126.67	110.85
3	B	7477	AMP	O2'-C2'-C1'	4.28	126.67	110.85
3	U	7515	AMP	O2'-C2'-C1'	4.28	126.67	110.85
3	L	7497	AMP	O2'-C2'-C1'	4.28	126.66	110.85
3	I	7491	AMP	O2'-C2'-C1'	4.28	126.65	110.85
3	D	7481	AMP	O2'-C2'-C1'	4.28	126.65	110.85
3	Q	7507	AMP	O2'-C2'-C1'	4.28	126.64	110.85
3	T	7513	AMP	O2'-C2'-C1'	4.28	126.64	110.85
3	P	7505	AMP	O2'-C2'-C1'	4.28	126.64	110.85
3	A	7475	AMP	O2'-C2'-C1'	4.27	126.64	110.85
3	K	7495	AMP	O2'-C2'-C1'	4.27	126.63	110.85
3	G	7487	AMP	O2'-C2'-C1'	4.27	126.63	110.85
3	W	7519	AMP	O2'-C2'-C1'	4.27	126.63	110.85
3	X	7521	AMP	O2'-C2'-C1'	4.27	126.63	110.85
3	E	7483	AMP	O2'-C2'-C1'	4.27	126.62	110.85
3	N	7501	AMP	O2'-C2'-C1'	4.27	126.62	110.85
3	C	7479	AMP	O2'-C2'-C1'	4.27	126.61	110.85
3	S	7511	AMP	O2'-C2'-C1'	4.27	126.61	110.85
3	F	7485	AMP	O2'-C2'-C1'	4.27	126.61	110.85
3	H	7489	AMP	O2'-C2'-C1'	4.27	126.61	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	7493	AMP	O2'-C2'-C1'	4.27	126.60	110.85
3	M	7499	AMP	O2'-C2'-C1'	4.26	126.59	110.85
3	O	7503	AMP	O2'-C2'-C1'	4.26	126.59	110.85
3	N	7501	AMP	C4-C5-N7	4.23	113.81	109.40
3	H	7489	AMP	C4-C5-N7	4.21	113.79	109.40
3	X	7521	AMP	C4-C5-N7	4.21	113.78	109.40
3	E	7483	AMP	C4-C5-N7	4.20	113.78	109.40
3	J	7493	AMP	C4-C5-N7	4.20	113.78	109.40
3	K	7495	AMP	C4-C5-N7	4.19	113.76	109.40
3	M	7499	AMP	C4-C5-N7	4.18	113.76	109.40
3	A	7475	AMP	C4-C5-N7	4.18	113.76	109.40
3	D	7481	AMP	C4-C5-N7	4.18	113.75	109.40
3	R	7509	AMP	C4-C5-N7	4.18	113.75	109.40
3	O	7503	AMP	C4-C5-N7	4.17	113.75	109.40
3	V	7517	AMP	C4-C5-N7	4.17	113.75	109.40
3	T	7513	AMP	C4-C5-N7	4.17	113.75	109.40
3	G	7487	AMP	C4-C5-N7	4.17	113.75	109.40
3	C	7479	AMP	C4-C5-N7	4.17	113.75	109.40
3	W	7519	AMP	C4-C5-N7	4.17	113.75	109.40
3	L	7497	AMP	C4-C5-N7	4.17	113.74	109.40
3	Q	7507	AMP	C4-C5-N7	4.16	113.74	109.40
3	P	7505	AMP	C4-C5-N7	4.16	113.74	109.40
3	U	7515	AMP	C4-C5-N7	4.16	113.74	109.40
3	I	7491	AMP	C4-C5-N7	4.16	113.73	109.40
3	F	7485	AMP	C4-C5-N7	4.15	113.73	109.40
3	B	7477	AMP	C4-C5-N7	4.15	113.73	109.40
3	S	7511	AMP	C4-C5-N7	4.14	113.72	109.40
3	E	7483	AMP	O3'-C3'-C2'	4.03	124.87	111.82
3	C	7479	AMP	O3'-C3'-C2'	4.03	124.86	111.82
3	O	7503	AMP	O3'-C3'-C2'	4.02	124.84	111.82
3	T	7513	AMP	O3'-C3'-C2'	4.02	124.84	111.82
3	V	7517	AMP	O3'-C3'-C2'	4.02	124.84	111.82
3	M	7499	AMP	O3'-C3'-C2'	4.02	124.84	111.82
3	K	7495	AMP	O3'-C3'-C2'	4.02	124.83	111.82
3	S	7511	AMP	O3'-C3'-C2'	4.02	124.83	111.82
3	G	7487	AMP	O3'-C3'-C2'	4.02	124.83	111.82
3	R	7509	AMP	O3'-C3'-C2'	4.02	124.82	111.82
3	B	7477	AMP	O3'-C3'-C2'	4.02	124.82	111.82
3	X	7521	AMP	O3'-C3'-C2'	4.02	124.82	111.82
3	J	7493	AMP	O3'-C3'-C2'	4.02	124.82	111.82
3	F	7485	AMP	O3'-C3'-C2'	4.02	124.82	111.82
3	H	7489	AMP	O3'-C3'-C2'	4.02	124.81	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7475	AMP	O3'-C3'-C2'	4.02	124.81	111.82
3	W	7519	AMP	O3'-C3'-C2'	4.02	124.81	111.82
3	L	7497	AMP	O3'-C3'-C2'	4.02	124.81	111.82
3	P	7505	AMP	O3'-C3'-C2'	4.02	124.81	111.82
3	I	7491	AMP	O3'-C3'-C2'	4.01	124.81	111.82
3	Q	7507	AMP	O3'-C3'-C2'	4.01	124.80	111.82
3	D	7481	AMP	O3'-C3'-C2'	4.01	124.79	111.82
3	U	7515	AMP	O3'-C3'-C2'	4.00	124.78	111.82
3	N	7501	AMP	O3'-C3'-C2'	4.00	124.77	111.82
3	B	7477	AMP	C5'-C4'-C3'	-3.38	102.52	115.18
3	N	7501	AMP	C5'-C4'-C3'	-3.38	102.52	115.18
3	D	7481	AMP	C5'-C4'-C3'	-3.38	102.52	115.18
3	G	7487	AMP	C5'-C4'-C3'	-3.38	102.52	115.18
3	K	7495	AMP	C5'-C4'-C3'	-3.38	102.53	115.18
3	J	7493	AMP	C5'-C4'-C3'	-3.38	102.53	115.18
3	F	7485	AMP	C5'-C4'-C3'	-3.38	102.53	115.18
3	Q	7507	AMP	C5'-C4'-C3'	-3.37	102.54	115.18
3	O	7503	AMP	C5'-C4'-C3'	-3.37	102.54	115.18
3	L	7497	AMP	C5'-C4'-C3'	-3.37	102.55	115.18
3	A	7475	AMP	C5'-C4'-C3'	-3.37	102.55	115.18
3	H	7489	AMP	C5'-C4'-C3'	-3.37	102.55	115.18
3	S	7511	AMP	C5'-C4'-C3'	-3.37	102.55	115.18
3	I	7491	AMP	C5'-C4'-C3'	-3.37	102.56	115.18
3	E	7483	AMP	C5'-C4'-C3'	-3.37	102.57	115.18
3	U	7515	AMP	C5'-C4'-C3'	-3.37	102.57	115.18
3	V	7517	AMP	C5'-C4'-C3'	-3.36	102.57	115.18
3	X	7521	AMP	C5'-C4'-C3'	-3.36	102.57	115.18
3	W	7519	AMP	C5'-C4'-C3'	-3.36	102.57	115.18
3	M	7499	AMP	C5'-C4'-C3'	-3.36	102.58	115.18
3	P	7505	AMP	C5'-C4'-C3'	-3.36	102.58	115.18
3	T	7513	AMP	C5'-C4'-C3'	-3.36	102.58	115.18
3	C	7479	AMP	C5'-C4'-C3'	-3.36	102.58	115.18
3	R	7509	AMP	C5'-C4'-C3'	-3.36	102.59	115.18
4	W	7520	CIT	C3-C4-C5	2.61	119.17	114.98
4	M	7500	CIT	C3-C4-C5	2.61	119.17	114.98
4	O	7504	CIT	C3-C4-C5	2.61	119.17	114.98
4	K	7496	CIT	C3-C4-C5	2.61	119.17	114.98
4	E	7484	CIT	C3-C4-C5	2.61	119.16	114.98
4	B	7478	CIT	C3-C4-C5	2.61	119.16	114.98
4	X	7522	CIT	C3-C4-C5	2.61	119.16	114.98
4	G	7488	CIT	C3-C4-C5	2.61	119.16	114.98
4	D	7482	CIT	C3-C4-C5	2.60	119.15	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	7476	CIT	C3-C4-C5	2.60	119.14	114.98
4	F	7486	CIT	C3-C4-C5	2.59	119.14	114.98
4	I	7492	CIT	C3-C4-C5	2.59	119.14	114.98
4	P	7506	CIT	C3-C4-C5	2.59	119.14	114.98
4	T	7514	CIT	C3-C4-C5	2.59	119.13	114.98
4	N	7502	CIT	C3-C4-C5	2.59	119.13	114.98
4	V	7518	CIT	C3-C4-C5	2.59	119.13	114.98
4	L	7498	CIT	C3-C4-C5	2.59	119.13	114.98
4	S	7512	CIT	C3-C4-C5	2.59	119.13	114.98
4	R	7510	CIT	C3-C4-C5	2.59	119.12	114.98
4	Q	7508	CIT	C3-C4-C5	2.58	119.12	114.98
4	J	7494	CIT	C3-C4-C5	2.58	119.12	114.98
4	U	7516	CIT	C3-C4-C5	2.58	119.11	114.98
4	C	7480	CIT	C3-C4-C5	2.58	119.11	114.98
4	H	7490	CIT	C3-C4-C5	2.57	119.11	114.98
3	D	7481	AMP	O3P-P-O5'	2.23	112.68	106.73
3	V	7517	AMP	O3P-P-O5'	2.23	112.66	106.73
3	P	7505	AMP	O3P-P-O5'	2.23	112.66	106.73
3	H	7489	AMP	O3P-P-O5'	2.23	112.66	106.73
3	C	7479	AMP	O3P-P-O5'	2.22	112.65	106.73
3	S	7511	AMP	O3P-P-O5'	2.22	112.65	106.73
3	G	7487	AMP	O3P-P-O5'	2.22	112.64	106.73
3	F	7485	AMP	O3P-P-O5'	2.22	112.64	106.73
3	E	7483	AMP	O3P-P-O5'	2.22	112.64	106.73
3	I	7491	AMP	O3P-P-O5'	2.22	112.64	106.73
3	A	7475	AMP	O3P-P-O5'	2.22	112.63	106.73
3	R	7509	AMP	O3P-P-O5'	2.22	112.63	106.73
3	J	7493	AMP	O3P-P-O5'	2.22	112.63	106.73
3	B	7477	AMP	O3P-P-O5'	2.21	112.63	106.73
3	K	7495	AMP	O3P-P-O5'	2.21	112.62	106.73
3	O	7503	AMP	O3P-P-O5'	2.21	112.62	106.73
3	Q	7507	AMP	O3P-P-O5'	2.21	112.62	106.73
3	N	7501	AMP	O3P-P-O5'	2.21	112.61	106.73
3	T	7513	AMP	O3P-P-O5'	2.21	112.60	106.73
3	L	7497	AMP	O3P-P-O5'	2.21	112.60	106.73
3	U	7515	AMP	O3P-P-O5'	2.21	112.60	106.73
3	W	7519	AMP	O3P-P-O5'	2.20	112.60	106.73
3	X	7521	AMP	O3P-P-O5'	2.20	112.59	106.73
3	M	7499	AMP	O3P-P-O5'	2.19	112.57	106.73

There are no chirality outliers.

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	7491	AMP	C5'-O5'-P-O2P
3	I	7491	AMP	C5'-O5'-P-O3P
3	M	7499	AMP	C5'-O5'-P-O2P
3	M	7499	AMP	C5'-O5'-P-O3P
3	E	7483	AMP	C5'-O5'-P-O2P
3	E	7483	AMP	C5'-O5'-P-O3P
3	G	7487	AMP	C5'-O5'-P-O2P
3	G	7487	AMP	C5'-O5'-P-O3P
3	Q	7507	AMP	C5'-O5'-P-O2P
3	Q	7507	AMP	C5'-O5'-P-O3P
3	H	7489	AMP	C5'-O5'-P-O2P
3	H	7489	AMP	C5'-O5'-P-O3P
3	S	7511	AMP	C5'-O5'-P-O2P
3	S	7511	AMP	C5'-O5'-P-O3P
3	X	7521	AMP	C5'-O5'-P-O2P
3	X	7521	AMP	C5'-O5'-P-O3P
3	R	7509	AMP	C5'-O5'-P-O2P
3	R	7509	AMP	C5'-O5'-P-O3P
3	N	7501	AMP	C5'-O5'-P-O2P
3	N	7501	AMP	C5'-O5'-P-O3P
3	L	7497	AMP	C5'-O5'-P-O2P
3	L	7497	AMP	C5'-O5'-P-O3P
3	A	7475	AMP	C5'-O5'-P-O2P
3	A	7475	AMP	C5'-O5'-P-O3P
3	B	7477	AMP	C5'-O5'-P-O2P
3	B	7477	AMP	C5'-O5'-P-O3P
3	P	7505	AMP	C5'-O5'-P-O2P
3	P	7505	AMP	C5'-O5'-P-O3P
3	O	7503	AMP	C5'-O5'-P-O2P
3	O	7503	AMP	C5'-O5'-P-O3P
3	U	7515	AMP	C5'-O5'-P-O2P
3	U	7515	AMP	C5'-O5'-P-O3P
3	C	7479	AMP	C5'-O5'-P-O2P
3	C	7479	AMP	C5'-O5'-P-O3P
3	V	7517	AMP	C5'-O5'-P-O2P
3	V	7517	AMP	C5'-O5'-P-O3P
3	T	7513	AMP	C5'-O5'-P-O2P
3	T	7513	AMP	C5'-O5'-P-O3P
3	W	7519	AMP	C5'-O5'-P-O2P
3	W	7519	AMP	C5'-O5'-P-O3P
3	J	7493	AMP	C5'-O5'-P-O2P
3	J	7493	AMP	C5'-O5'-P-O3P
3	F	7485	AMP	C5'-O5'-P-O2P

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Mol	Chain	Res	Type	Atoms
3	F	7485	AMP	C5'-O5'-P-O3P
3	D	7481	AMP	C5'-O5'-P-O2P
3	D	7481	AMP	C5'-O5'-P-O3P
3	K	7495	AMP	C5'-O5'-P-O2P
3	K	7495	AMP	C5'-O5'-P-O3P
3	I	7491	AMP	C5'-O5'-P-O1P
3	M	7499	AMP	C5'-O5'-P-O1P
3	E	7483	AMP	C5'-O5'-P-O1P
3	G	7487	AMP	C5'-O5'-P-O1P
3	Q	7507	AMP	C5'-O5'-P-O1P
3	H	7489	AMP	C5'-O5'-P-O1P
3	S	7511	AMP	C5'-O5'-P-O1P
3	X	7521	AMP	C5'-O5'-P-O1P
3	R	7509	AMP	C5'-O5'-P-O1P
3	N	7501	AMP	C5'-O5'-P-O1P
3	L	7497	AMP	C5'-O5'-P-O1P
3	A	7475	AMP	C5'-O5'-P-O1P
3	B	7477	AMP	C5'-O5'-P-O1P
3	P	7505	AMP	C5'-O5'-P-O1P
3	O	7503	AMP	C5'-O5'-P-O1P
3	U	7515	AMP	C5'-O5'-P-O1P
3	C	7479	AMP	C5'-O5'-P-O1P
3	V	7517	AMP	C5'-O5'-P-O1P
3	T	7513	AMP	C5'-O5'-P-O1P
3	W	7519	AMP	C5'-O5'-P-O1P
3	J	7493	AMP	C5'-O5'-P-O1P
3	F	7485	AMP	C5'-O5'-P-O1P
3	D	7481	AMP	C5'-O5'-P-O1P
3	K	7495	AMP	C5'-O5'-P-O1P
4	X	7522	CIT	C1-C2-C3-C6
4	A	7476	CIT	C1-C2-C3-C6
4	M	7500	CIT	C1-C2-C3-C6
4	H	7490	CIT	C1-C2-C3-C6
4	O	7504	CIT	C1-C2-C3-C6
4	L	7498	CIT	C1-C2-C3-C6
4	Q	7508	CIT	C1-C2-C3-C6
4	D	7482	CIT	C1-C2-C3-C6
4	G	7488	CIT	C1-C2-C3-C6
4	I	7492	CIT	C1-C2-C3-C6
4	J	7494	CIT	C1-C2-C3-C6
4	C	7480	CIT	C1-C2-C3-C6
4	E	7484	CIT	C1-C2-C3-C6

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Mol	Chain	Res	Type	Atoms
4	P	7506	CIT	C1-C2-C3-C6
4	W	7520	CIT	C1-C2-C3-C6
4	N	7502	CIT	C1-C2-C3-C6
4	R	7510	CIT	C1-C2-C3-C6
4	S	7512	CIT	C1-C2-C3-C6
4	B	7478	CIT	C1-C2-C3-C6
4	F	7486	CIT	C1-C2-C3-C6
4	U	7516	CIT	C1-C2-C3-C6
4	V	7518	CIT	C1-C2-C3-C6
4	K	7496	CIT	C1-C2-C3-C6
4	T	7514	CIT	C1-C2-C3-C6
4	X	7522	CIT	C1-C2-C3-O7
4	X	7522	CIT	O7-C3-C4-C5
4	A	7476	CIT	C1-C2-C3-O7
4	A	7476	CIT	O7-C3-C4-C5
4	M	7500	CIT	C1-C2-C3-O7
4	M	7500	CIT	O7-C3-C4-C5
4	H	7490	CIT	C1-C2-C3-O7
4	H	7490	CIT	O7-C3-C4-C5
4	O	7504	CIT	C1-C2-C3-O7
4	O	7504	CIT	O7-C3-C4-C5
4	L	7498	CIT	C1-C2-C3-O7
4	L	7498	CIT	O7-C3-C4-C5
4	Q	7508	CIT	C1-C2-C3-O7
4	Q	7508	CIT	O7-C3-C4-C5
4	D	7482	CIT	C1-C2-C3-O7
4	D	7482	CIT	O7-C3-C4-C5
4	G	7488	CIT	C1-C2-C3-O7
4	G	7488	CIT	O7-C3-C4-C5
4	I	7492	CIT	C1-C2-C3-O7
4	I	7492	CIT	O7-C3-C4-C5
4	J	7494	CIT	C1-C2-C3-O7
4	J	7494	CIT	O7-C3-C4-C5
4	C	7480	CIT	C1-C2-C3-O7
4	C	7480	CIT	O7-C3-C4-C5
4	E	7484	CIT	C1-C2-C3-O7
4	E	7484	CIT	O7-C3-C4-C5
4	P	7506	CIT	C1-C2-C3-O7
4	P	7506	CIT	O7-C3-C4-C5
4	W	7520	CIT	C1-C2-C3-O7
4	W	7520	CIT	O7-C3-C4-C5
4	N	7502	CIT	C1-C2-C3-O7

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Mol	Chain	Res	Type	Atoms
4	N	7502	CIT	O7-C3-C4-C5
4	R	7510	CIT	C1-C2-C3-O7
4	R	7510	CIT	O7-C3-C4-C5
4	S	7512	CIT	C1-C2-C3-O7
4	S	7512	CIT	O7-C3-C4-C5
4	B	7478	CIT	C1-C2-C3-O7
4	B	7478	CIT	O7-C3-C4-C5
4	F	7486	CIT	C1-C2-C3-O7
4	F	7486	CIT	O7-C3-C4-C5
4	U	7516	CIT	C1-C2-C3-O7
4	U	7516	CIT	O7-C3-C4-C5
4	V	7518	CIT	C1-C2-C3-O7
4	V	7518	CIT	O7-C3-C4-C5
4	K	7496	CIT	C1-C2-C3-O7
4	K	7496	CIT	O7-C3-C4-C5
4	T	7514	CIT	C1-C2-C3-O7
4	T	7514	CIT	O7-C3-C4-C5
4	X	7522	CIT	C1-C2-C3-C4
4	A	7476	CIT	C1-C2-C3-C4
4	M	7500	CIT	C1-C2-C3-C4
4	H	7490	CIT	C1-C2-C3-C4
4	O	7504	CIT	C1-C2-C3-C4
4	L	7498	CIT	C1-C2-C3-C4
4	Q	7508	CIT	C1-C2-C3-C4
4	D	7482	CIT	C1-C2-C3-C4
4	G	7488	CIT	C1-C2-C3-C4
4	I	7492	CIT	C1-C2-C3-C4
4	J	7494	CIT	C1-C2-C3-C4
4	C	7480	CIT	C1-C2-C3-C4
4	E	7484	CIT	C1-C2-C3-C4
4	P	7506	CIT	C1-C2-C3-C4
4	W	7520	CIT	C1-C2-C3-C4
4	N	7502	CIT	C1-C2-C3-C4
4	R	7510	CIT	C1-C2-C3-C4
4	S	7512	CIT	C1-C2-C3-C4
4	B	7478	CIT	C1-C2-C3-C4
4	F	7486	CIT	C1-C2-C3-C4
4	U	7516	CIT	C1-C2-C3-C4
4	V	7518	CIT	C1-C2-C3-C4
4	K	7496	CIT	C1-C2-C3-C4
4	T	7514	CIT	C1-C2-C3-C4

There are no ring outliers.

48 monomers are involved in 307 short contacts:

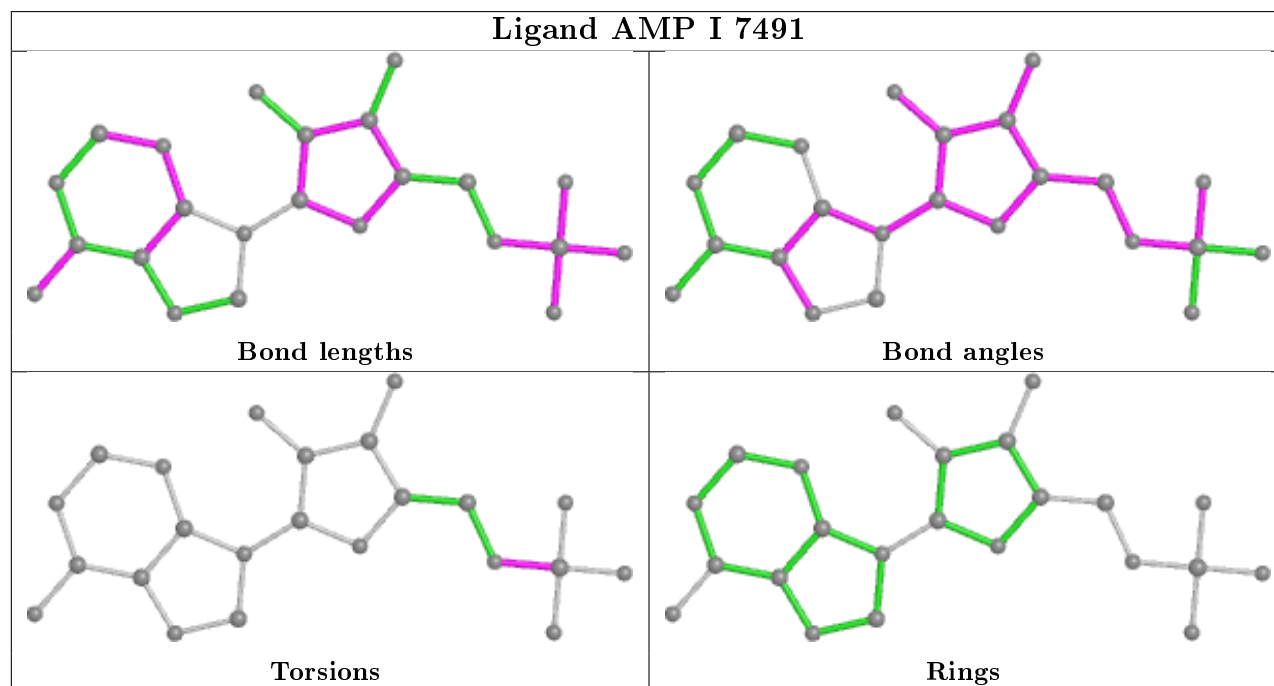
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	7508	CIT	5	0
3	I	7491	AMP	7	0
3	M	7499	AMP	7	0
4	A	7476	CIT	6	0
4	H	7490	CIT	6	0
3	E	7483	AMP	7	0
4	M	7500	CIT	6	0
3	Q	7507	AMP	7	0
4	L	7498	CIT	6	0
4	D	7482	CIT	6	0
3	H	7489	AMP	7	0
3	S	7511	AMP	7	0
3	R	7509	AMP	7	0
4	G	7488	CIT	6	0
4	I	7492	CIT	6	0
4	X	7522	CIT	6	0
4	J	7494	CIT	5	0
4	C	7480	CIT	5	0
3	N	7501	AMP	7	0
4	E	7484	CIT	5	0
4	P	7506	CIT	6	0
4	W	7520	CIT	6	0
3	L	7497	AMP	7	0
3	A	7475	AMP	7	0
4	N	7502	CIT	6	0
3	B	7477	AMP	7	0
4	R	7510	CIT	6	0
3	P	7505	AMP	7	0
4	O	7504	CIT	5	0
3	O	7503	AMP	7	0
4	B	7478	CIT	6	0
3	X	7521	AMP	7	0
3	U	7515	AMP	7	0
3	G	7487	AMP	7	0
3	C	7479	AMP	7	0
3	V	7517	AMP	7	0
4	S	7512	CIT	6	0
4	U	7516	CIT	6	0
4	V	7518	CIT	5	0
4	K	7496	CIT	6	0
3	W	7519	AMP	7	0
3	J	7493	AMP	7	0

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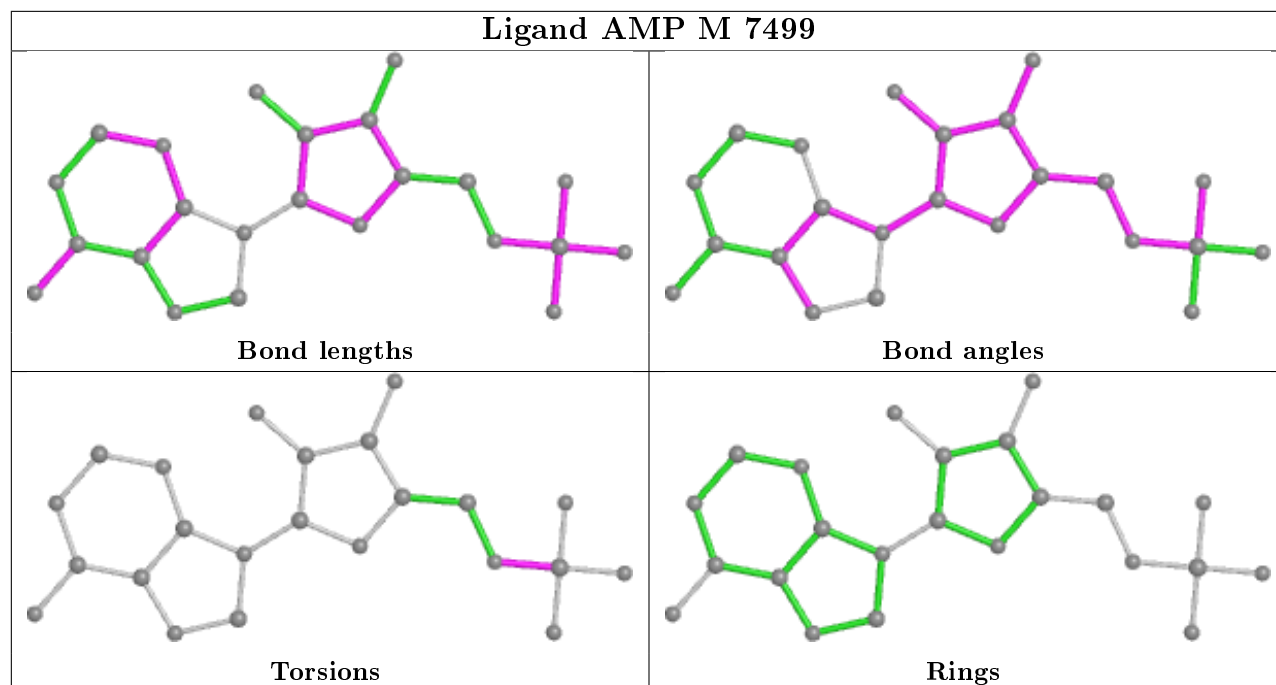
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	7485	AMP	7	0
4	T	7514	CIT	6	0
3	D	7481	AMP	7	0
4	F	7486	CIT	6	0
3	T	7513	AMP	7	0
3	K	7495	AMP	8	0

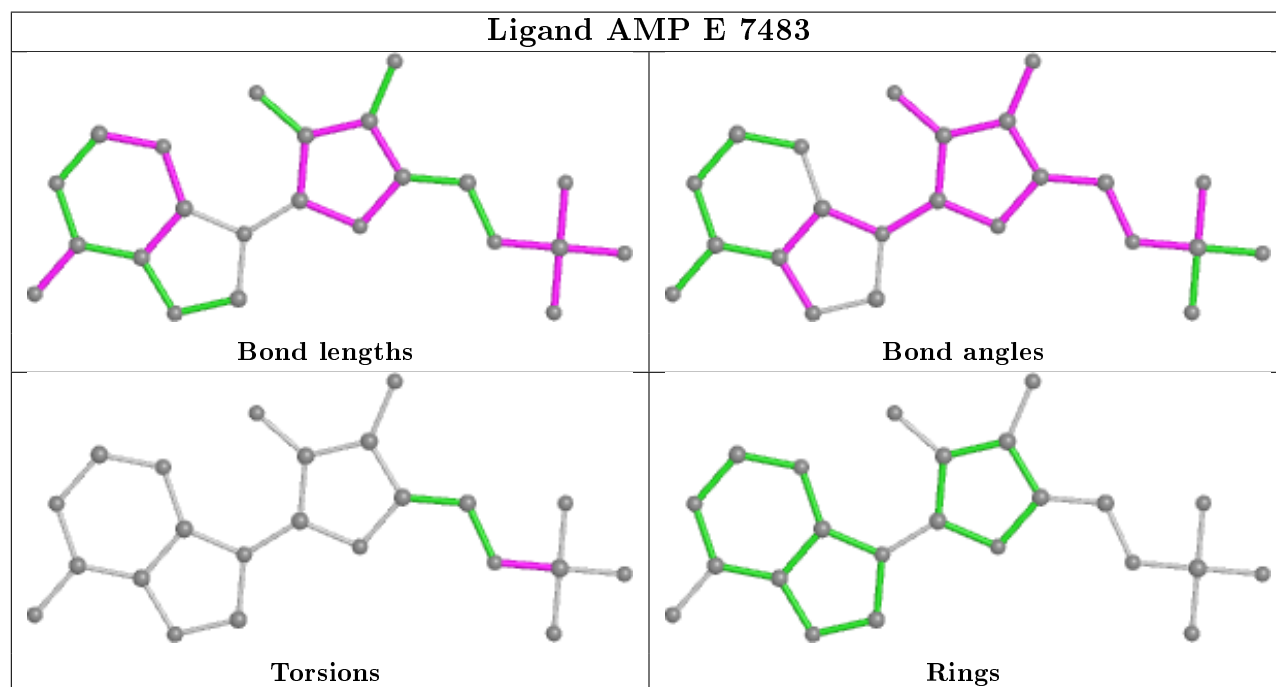
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



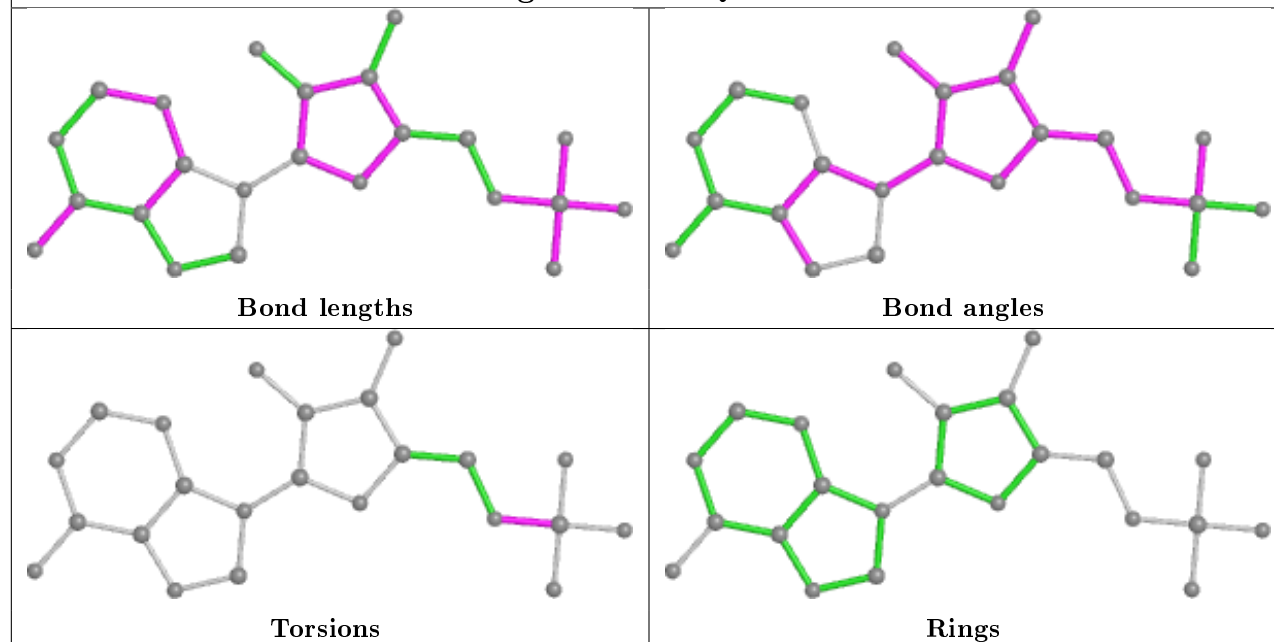
Ligand AMP M 7499



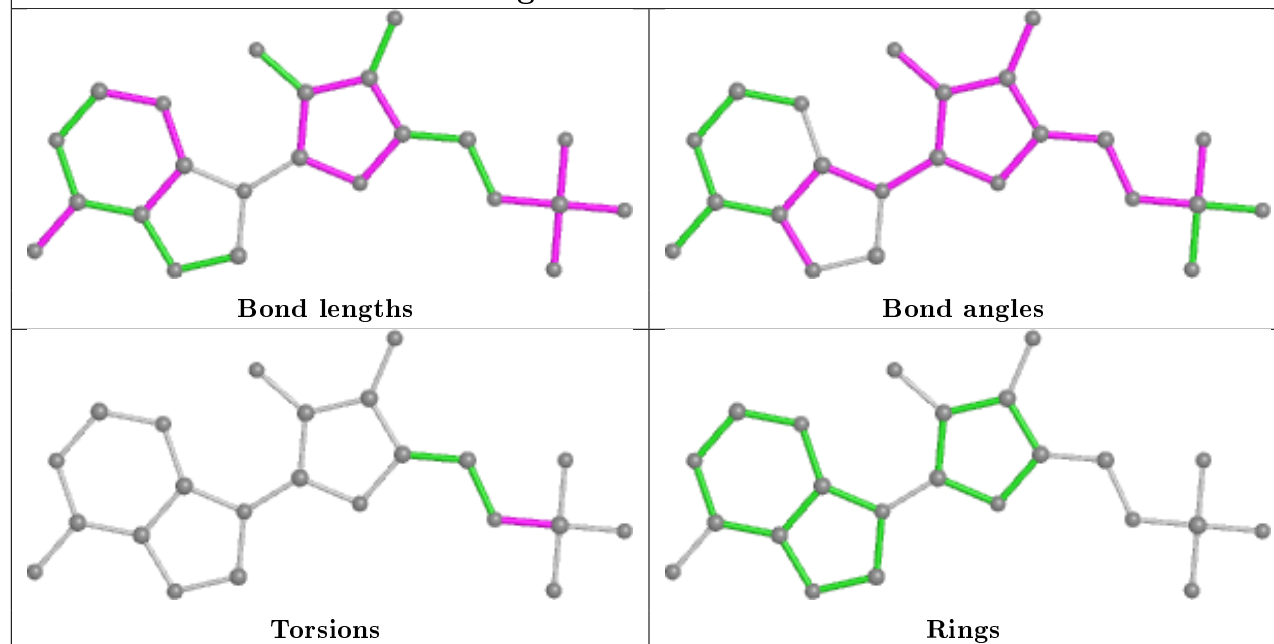
Ligand AMP E 7483



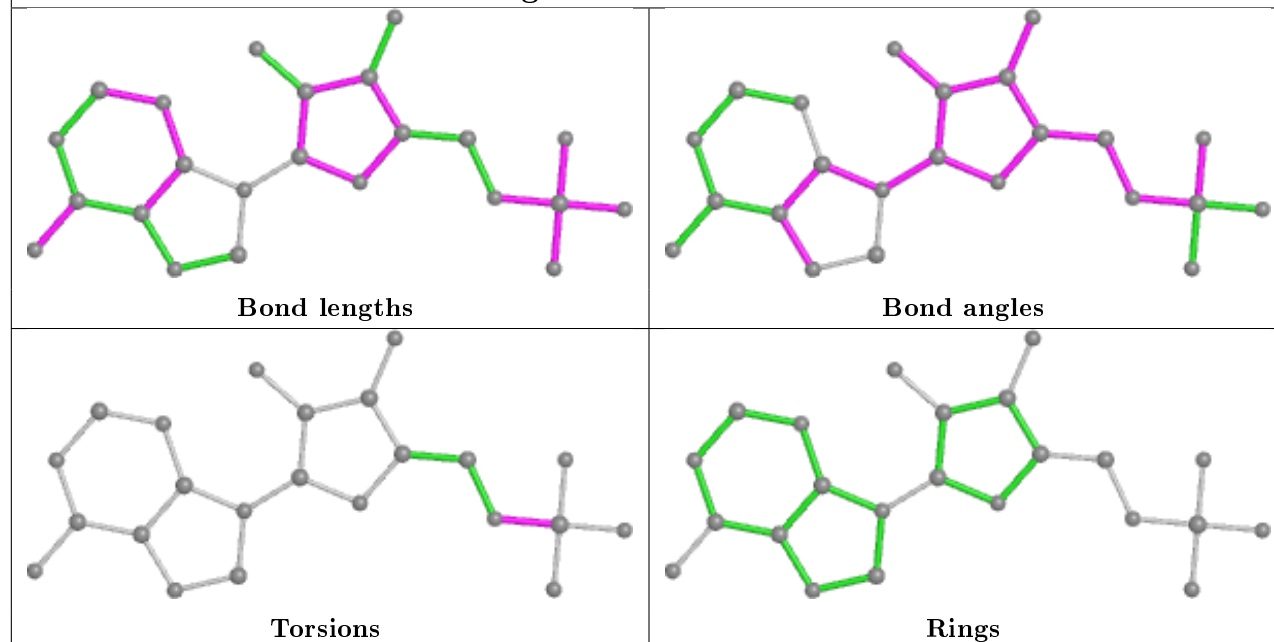
Ligand AMP Q 7507



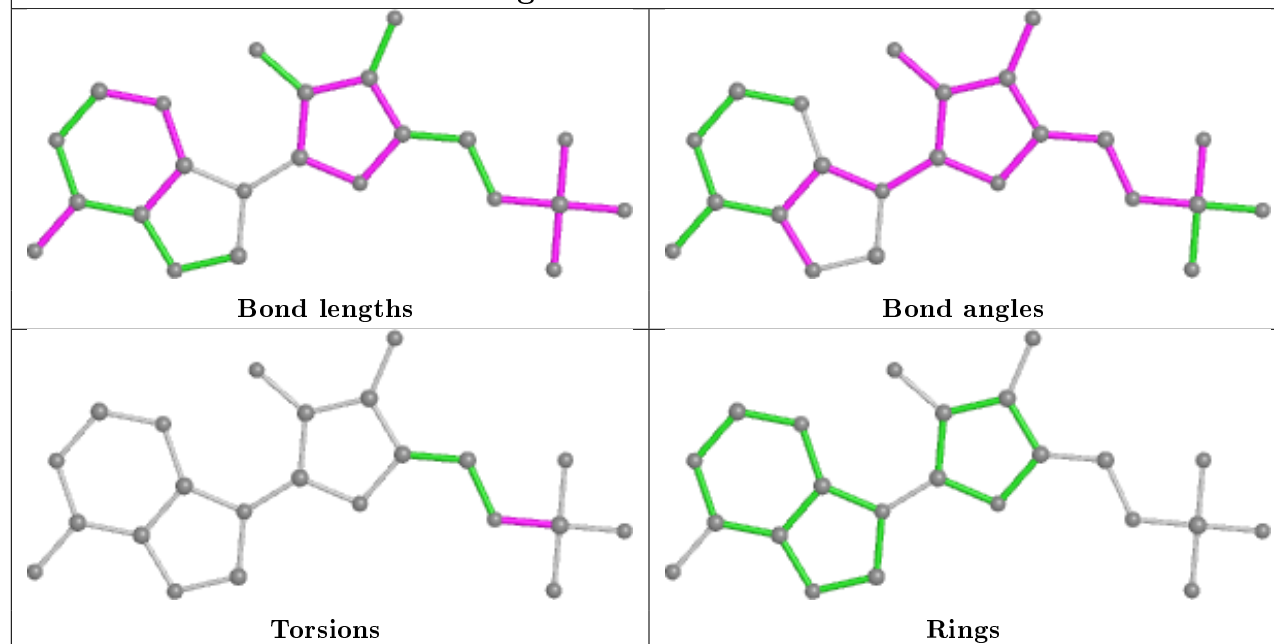
Ligand AMP H 7489



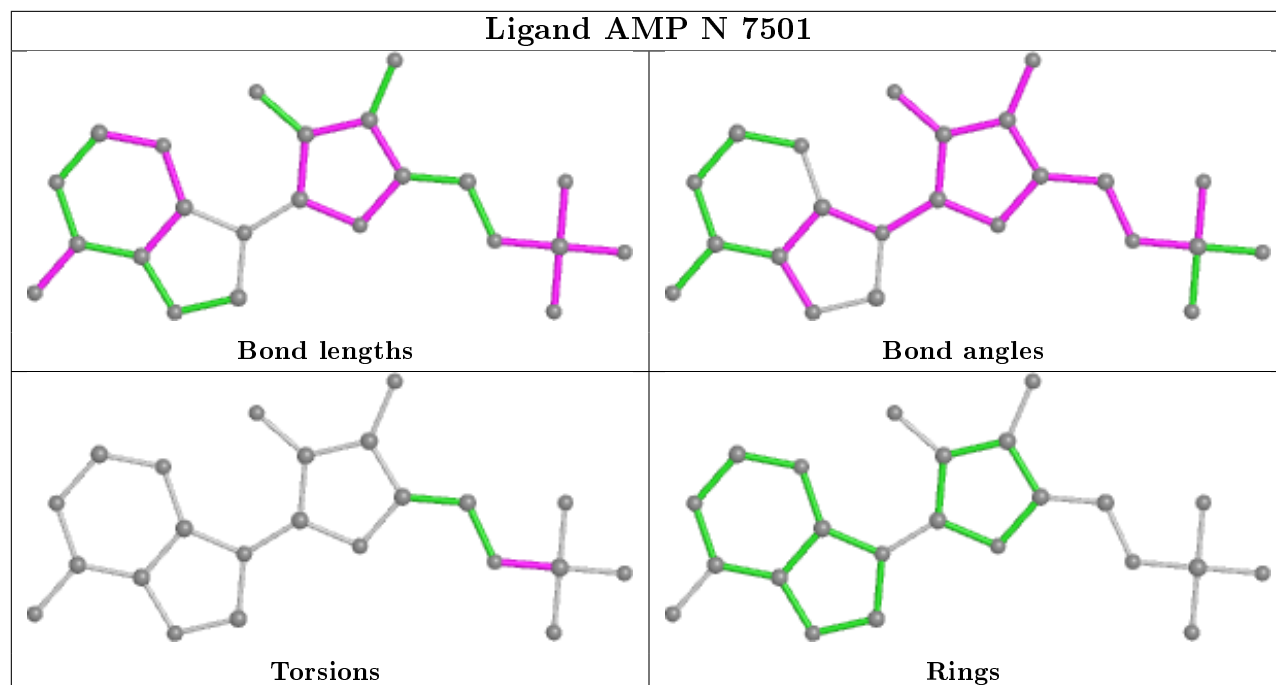
Ligand AMP S 7511



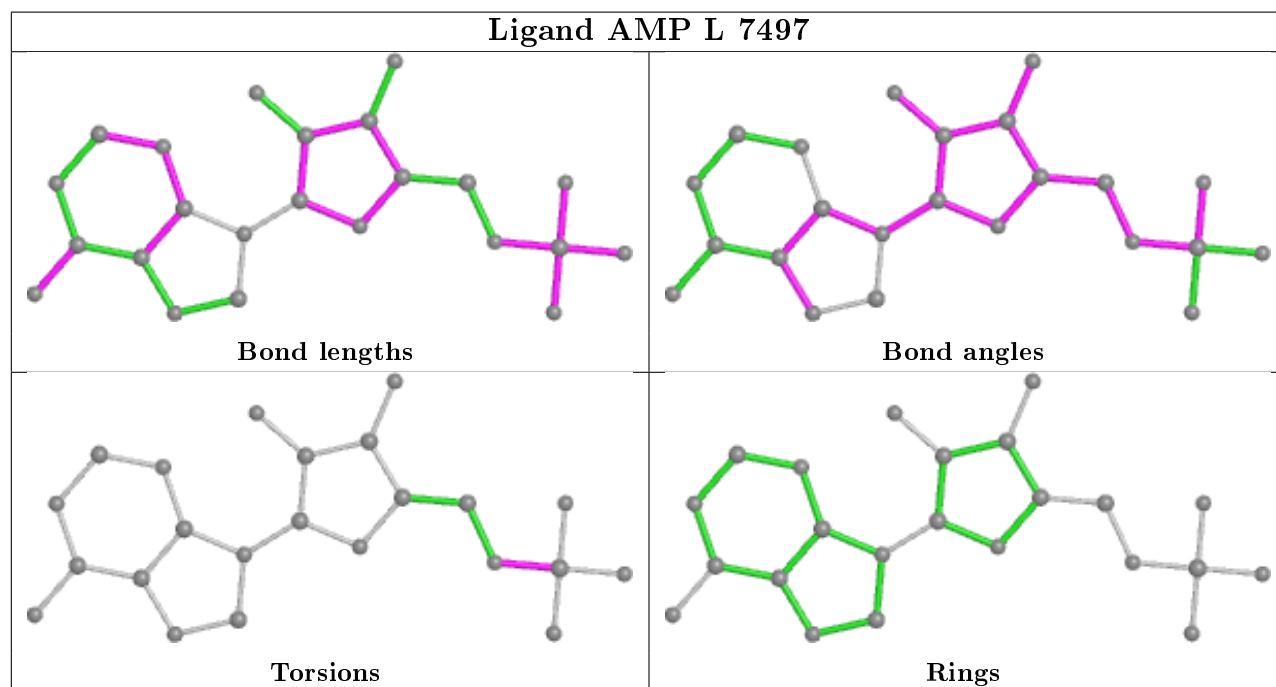
Ligand AMP R 7509



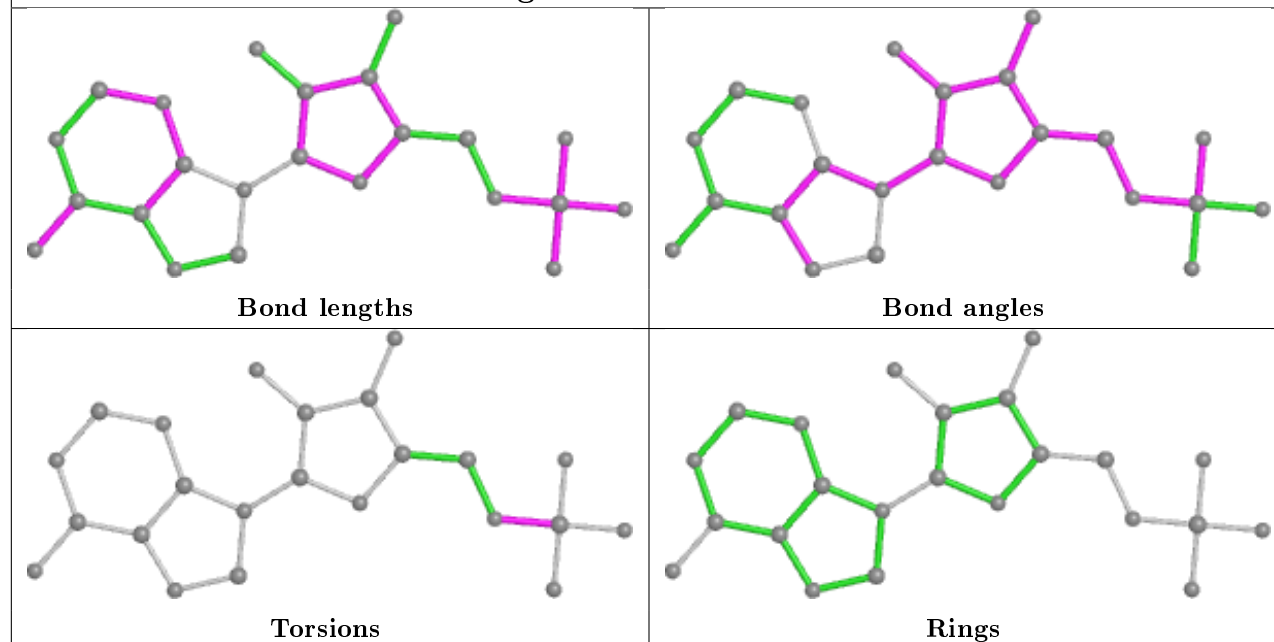
Ligand AMP N 7501



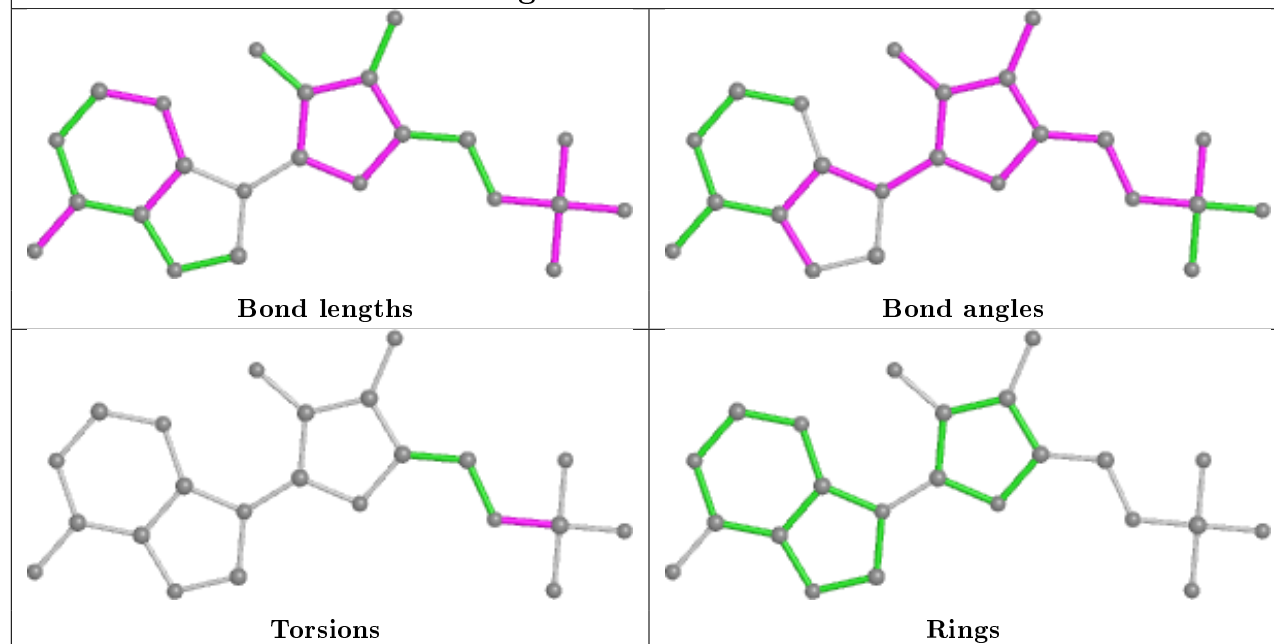
Ligand AMP L 7497



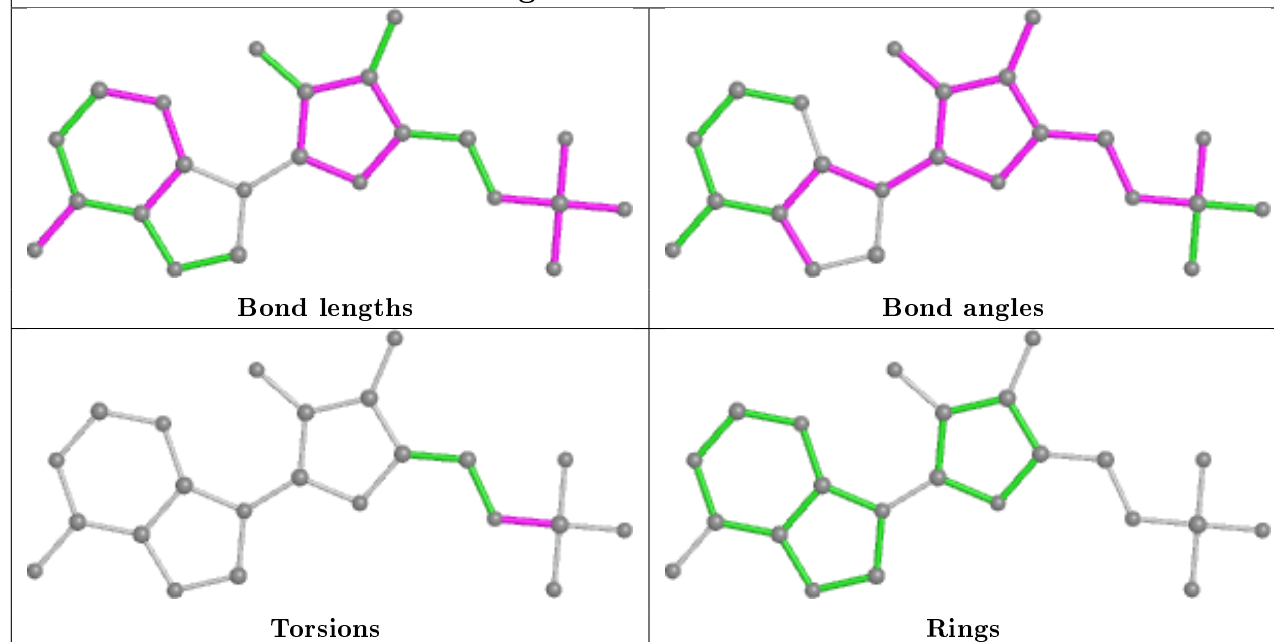
Ligand AMP A 7475



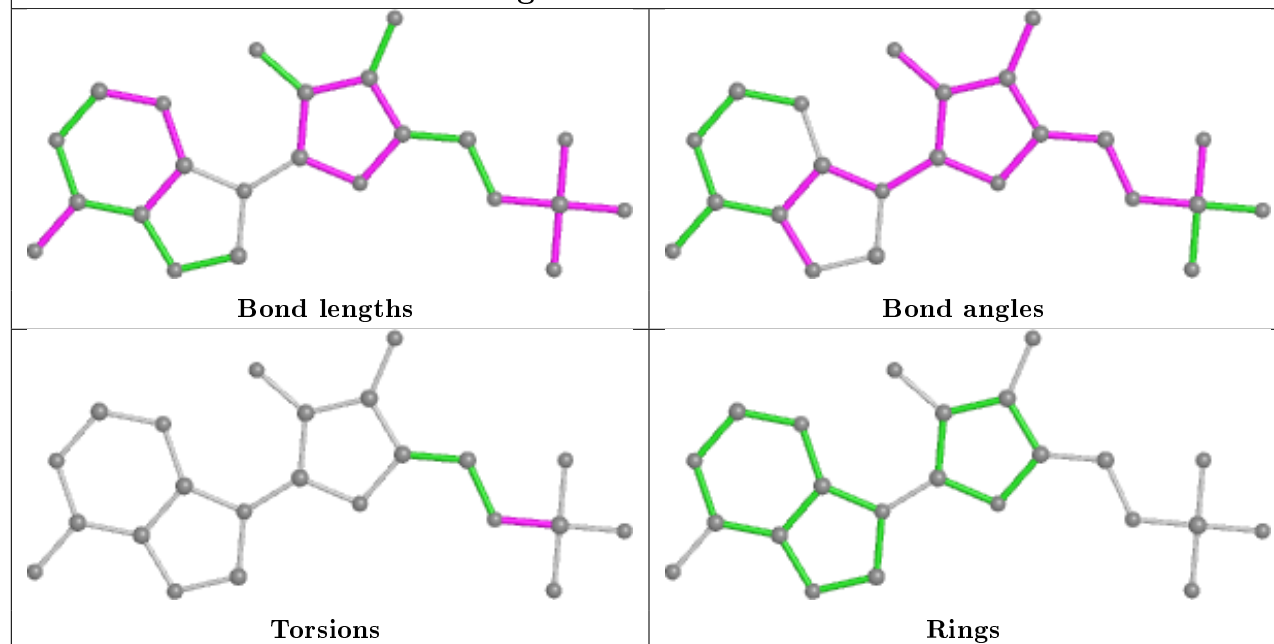
Ligand AMP B 7477



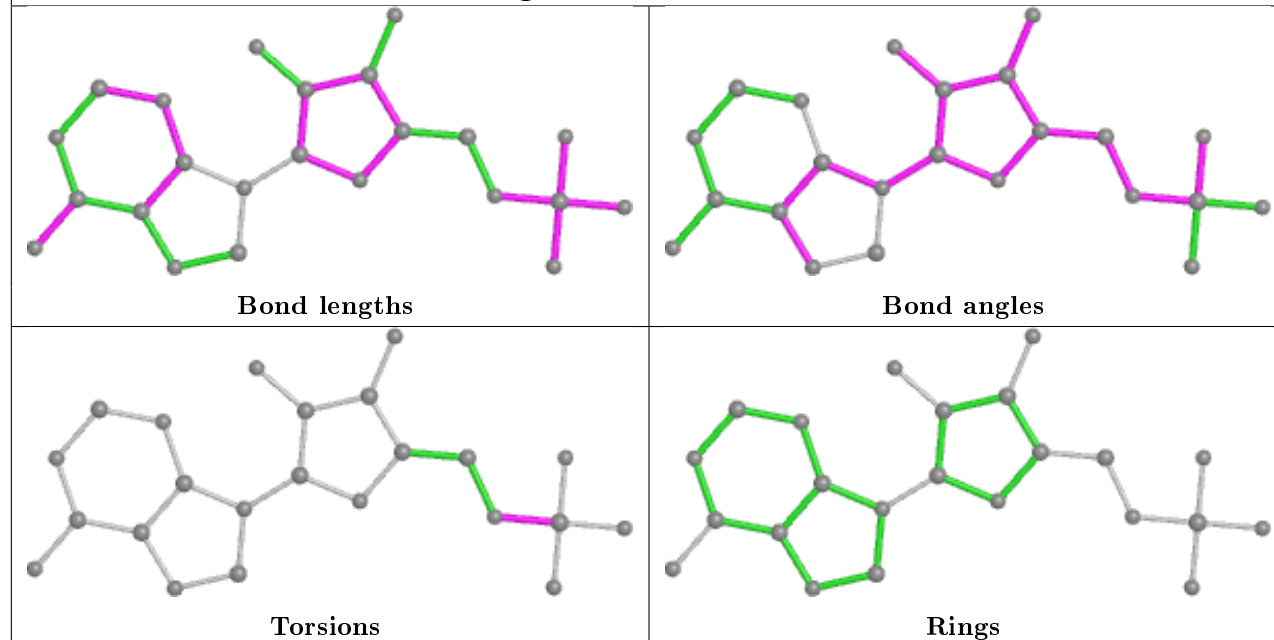
Ligand AMP P 7505



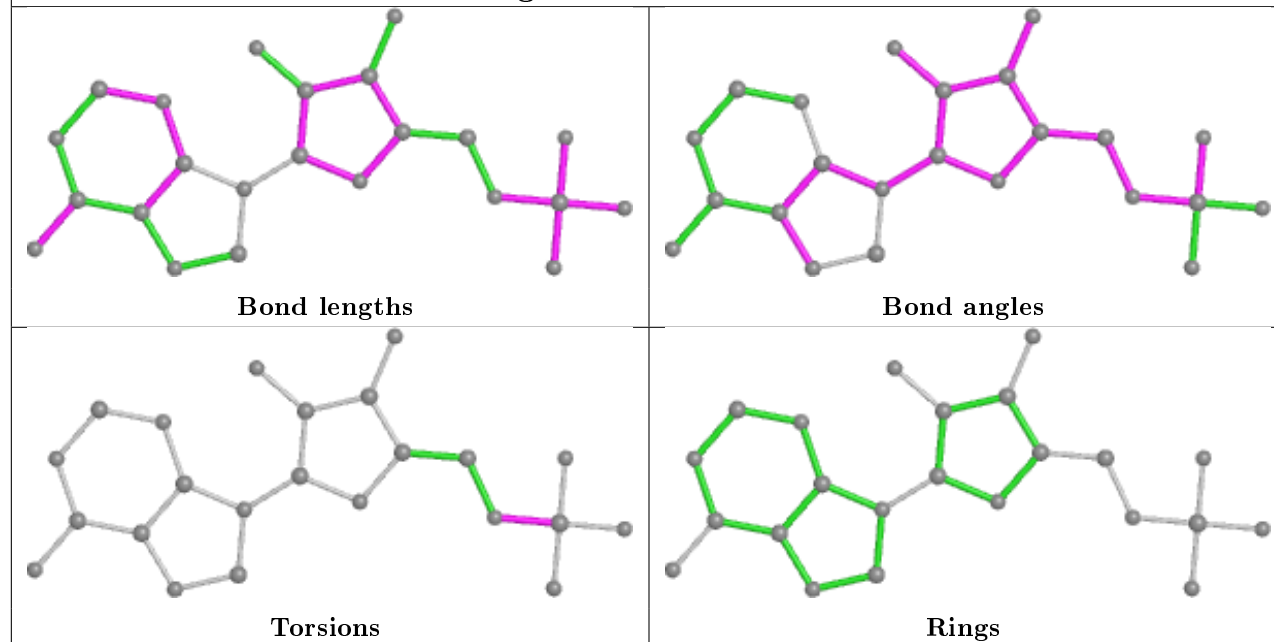
Ligand AMP O 7503



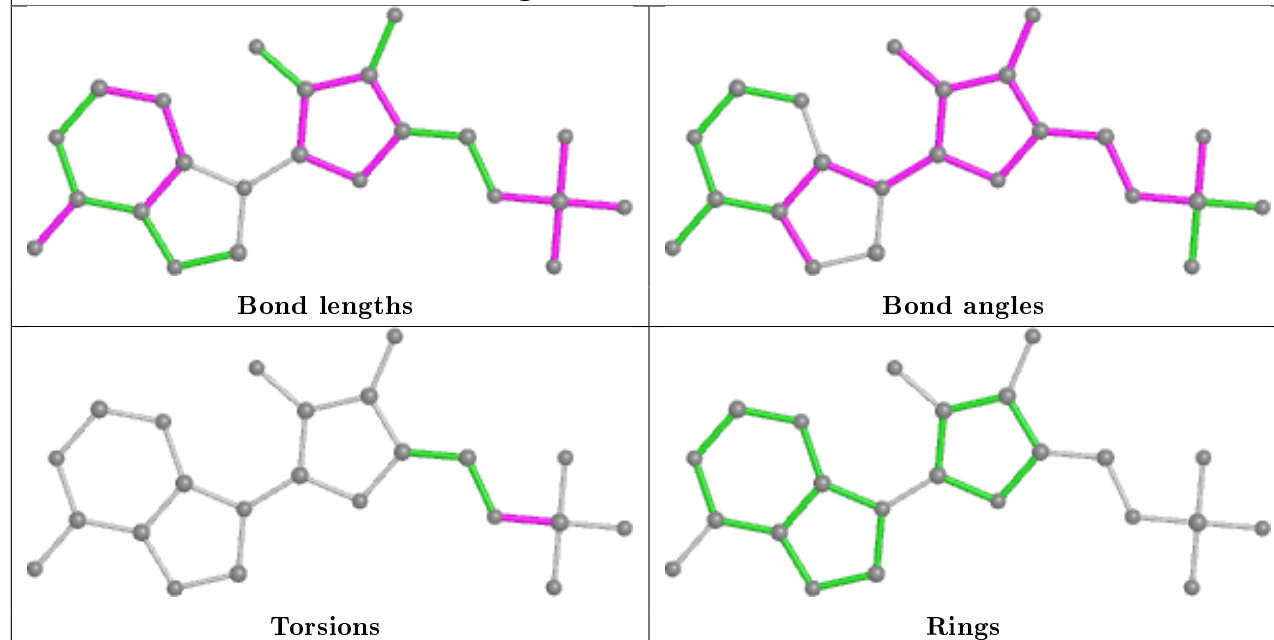
Ligand AMP X 7521



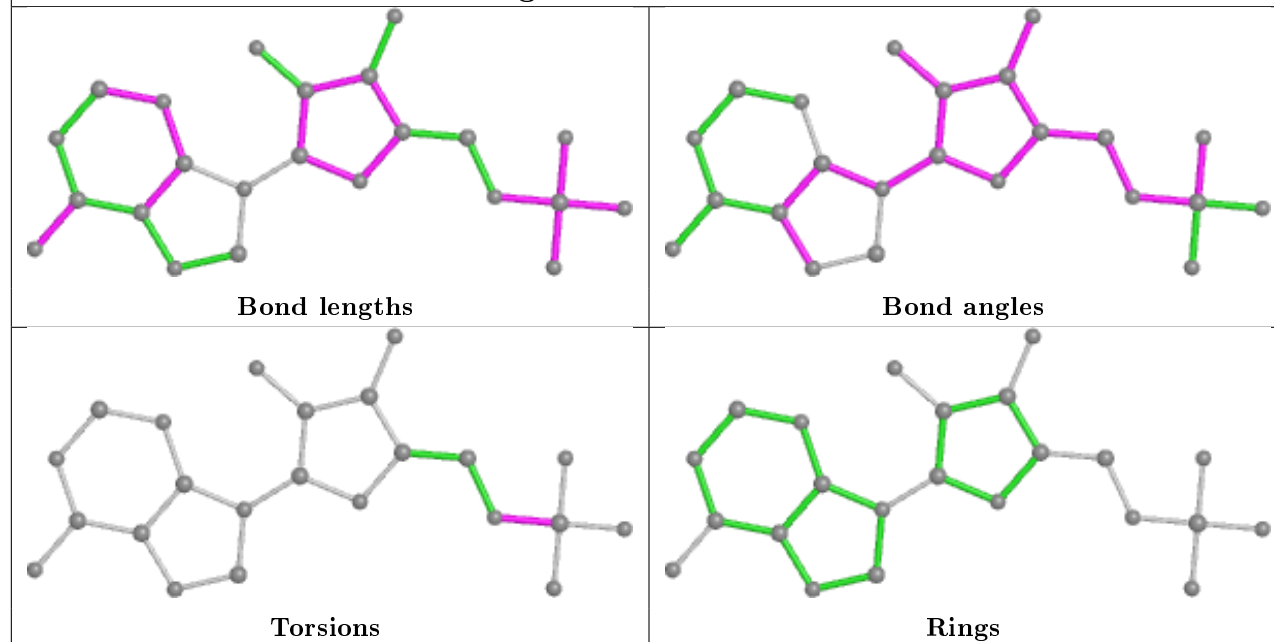
Ligand AMP U 7515



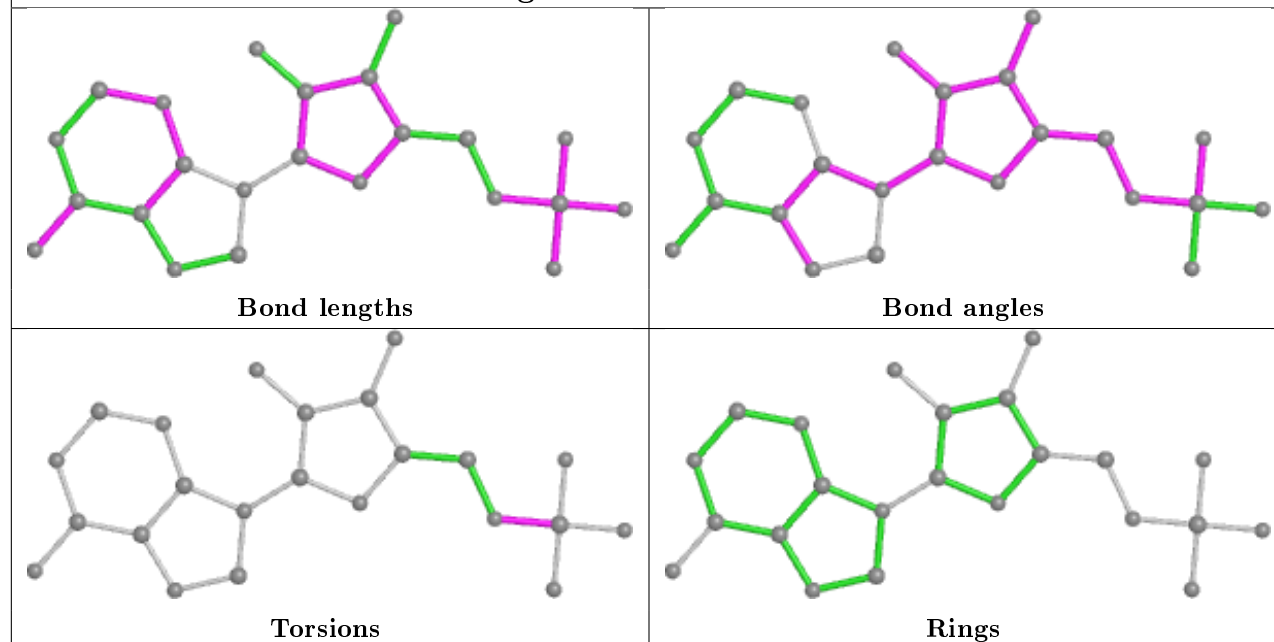
Ligand AMP G 7487



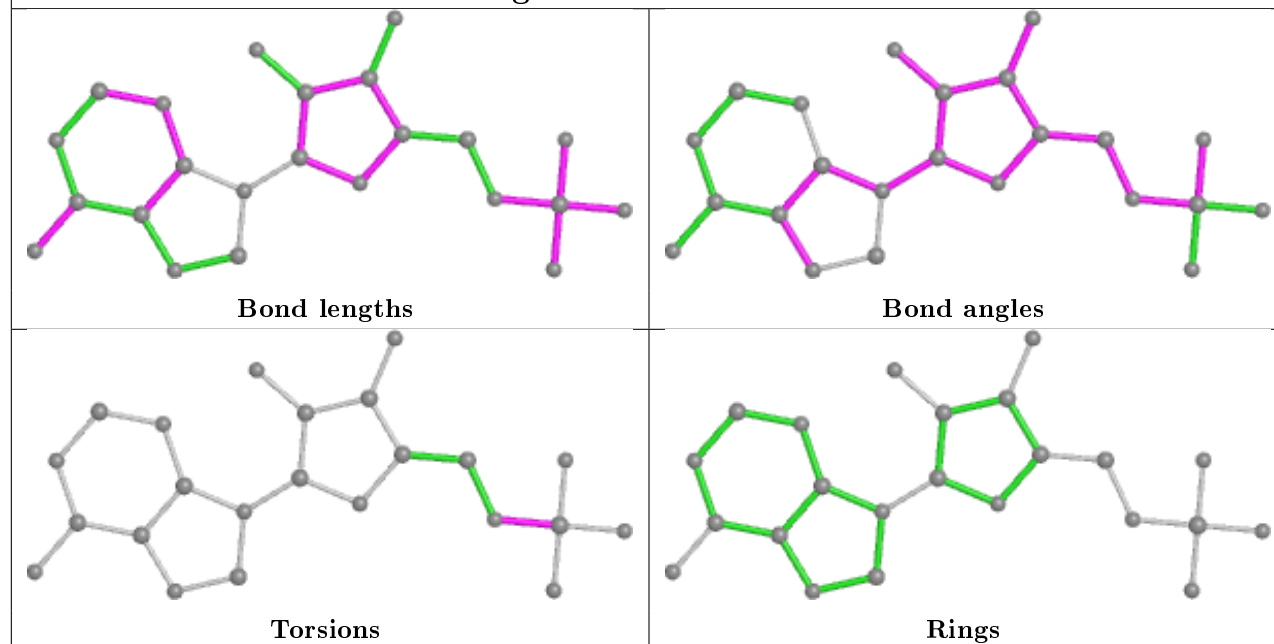
Ligand AMP C 7479



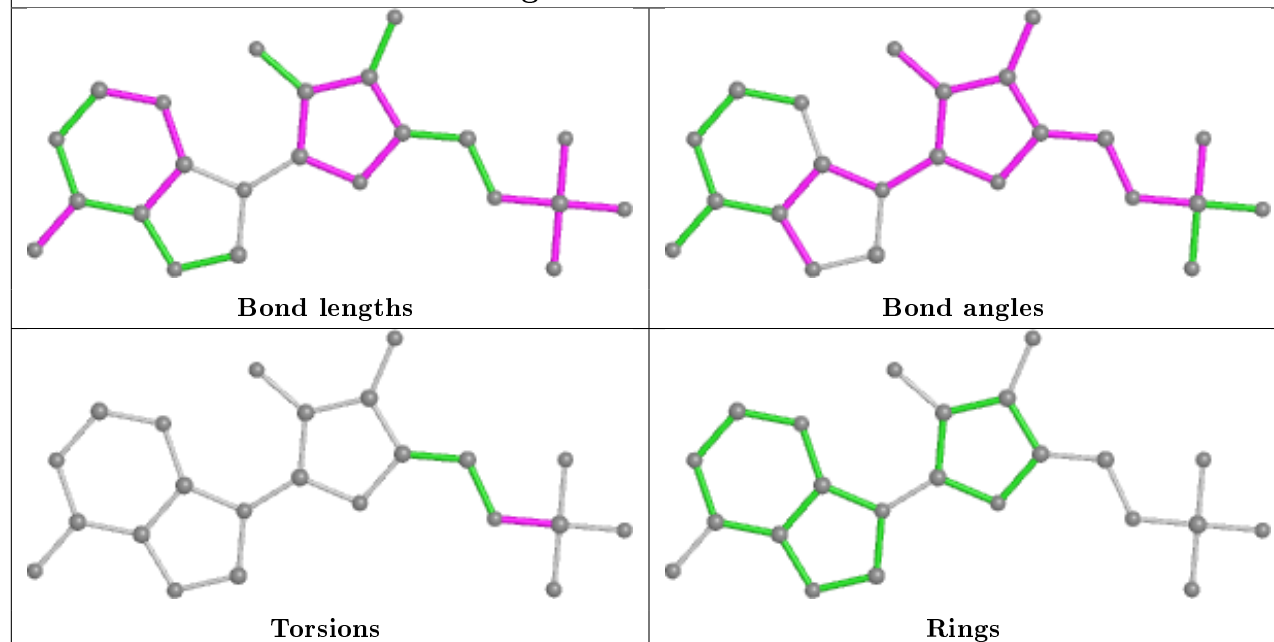
Ligand AMP V 7517



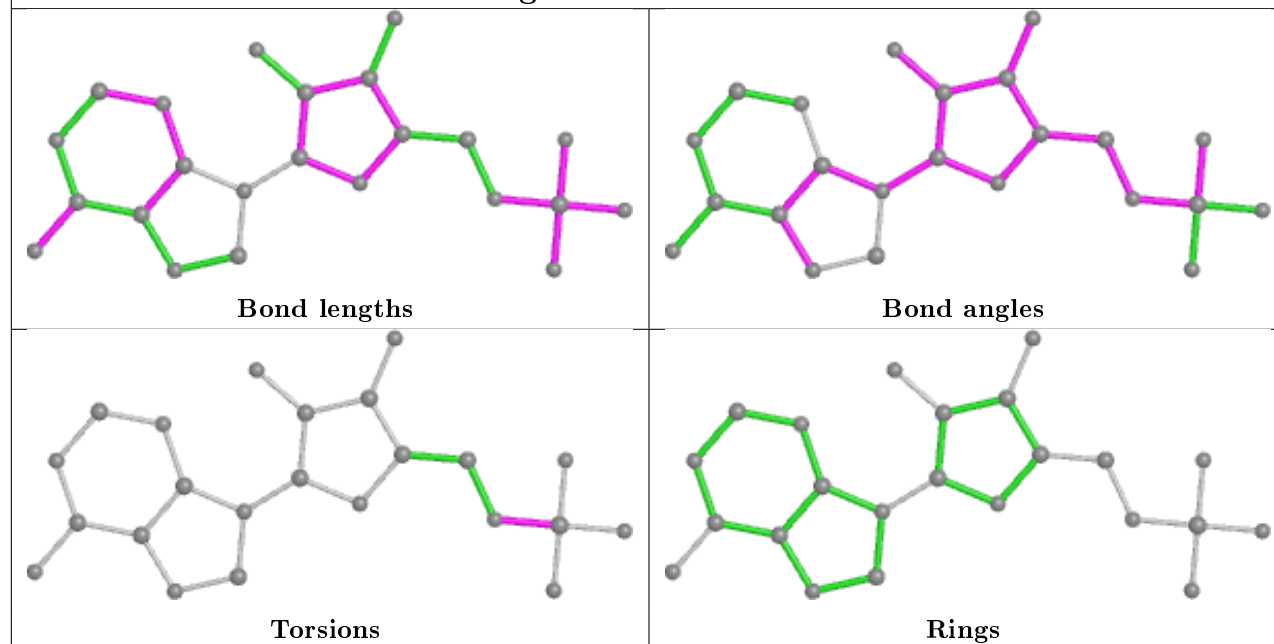
Ligand AMP W 7519



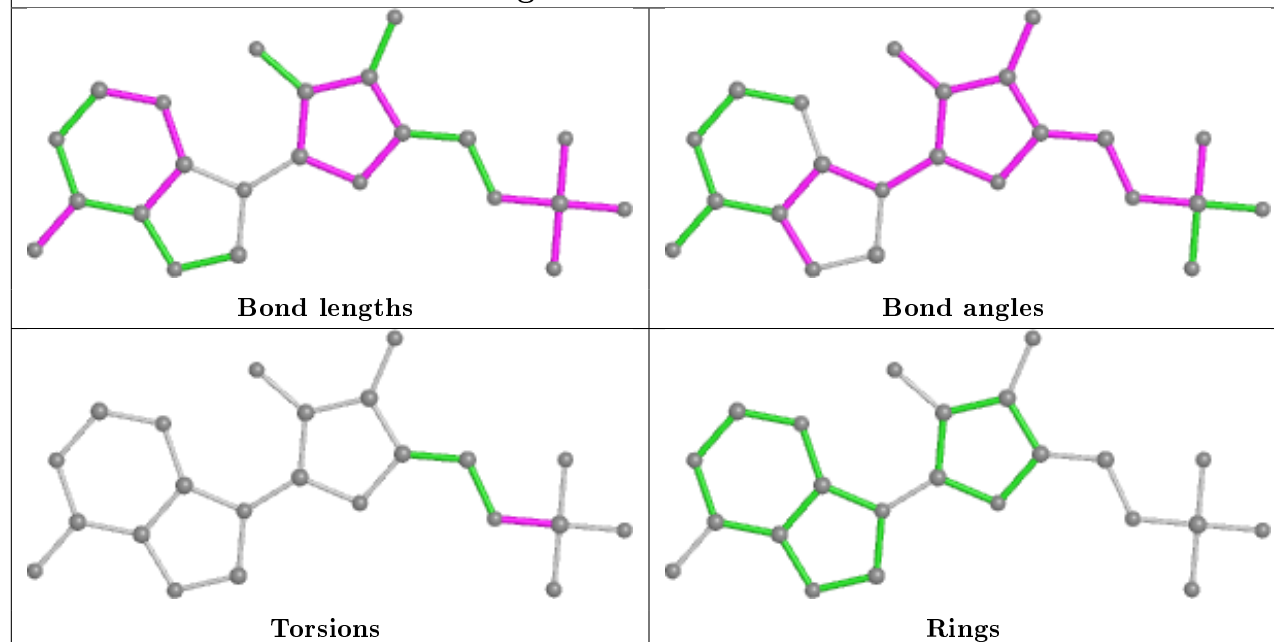
Ligand AMP J 7493



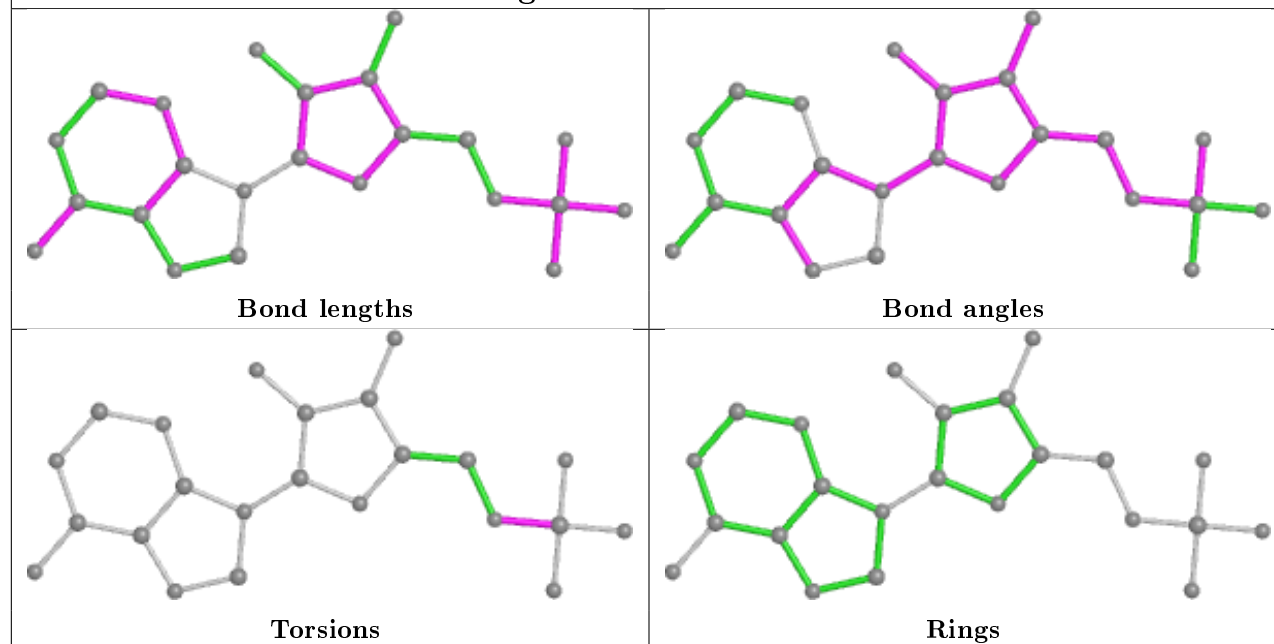
Ligand AMP F 7485

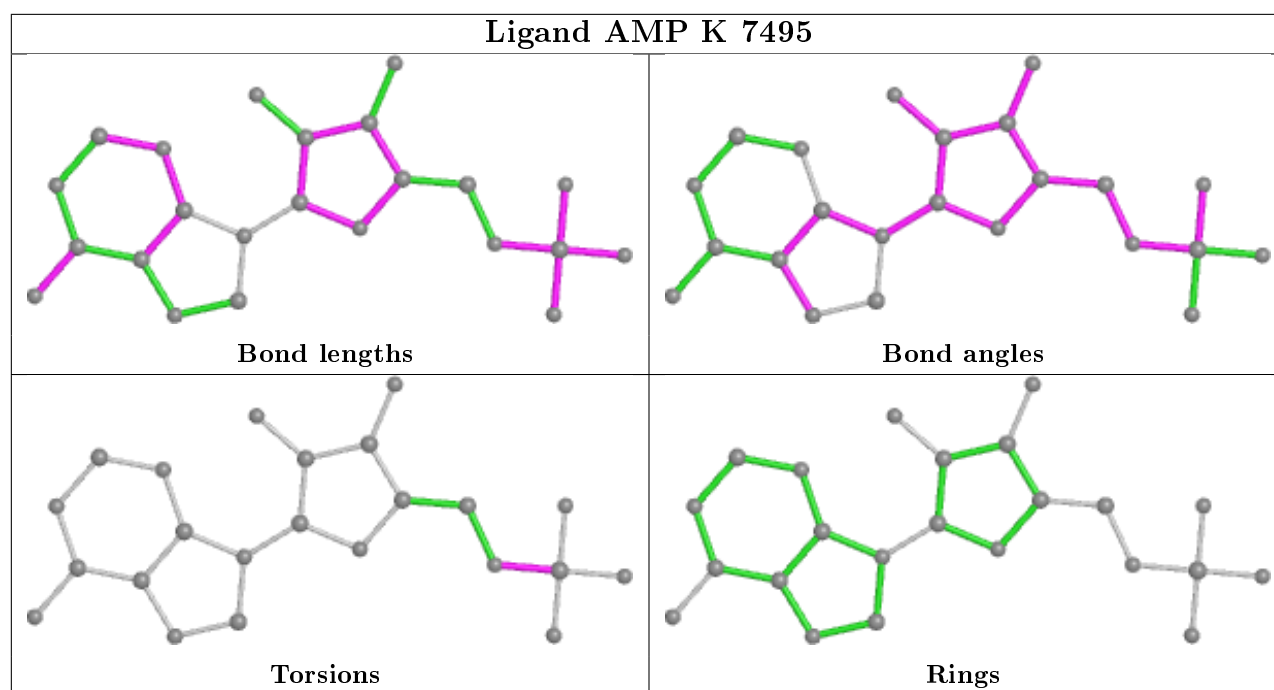


Ligand AMP D 7481



Ligand AMP T 7513





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	477/477 (100%)	0.15	31 (6%)	18 17	10, 26, 90, 100	0
1	B	477/477 (100%)	0.25	43 (9%)	9 8	10, 26, 90, 100	0
1	C	477/477 (100%)	0.26	43 (9%)	9 8	10, 26, 90, 100	0
1	D	477/477 (100%)	0.16	35 (7%)	15 13	10, 26, 90, 100	0
1	E	477/477 (100%)	0.24	41 (8%)	10 9	10, 26, 90, 100	0
1	F	477/477 (100%)	0.23	35 (7%)	15 13	10, 26, 90, 100	0
1	G	477/477 (100%)	0.30	39 (8%)	11 10	10, 26, 90, 100	0
1	H	477/477 (100%)	0.15	35 (7%)	15 13	10, 26, 90, 100	0
1	I	477/477 (100%)	0.29	50 (10%)	6 5	10, 26, 90, 100	0
1	J	477/477 (100%)	0.03	27 (5%)	23 22	10, 26, 90, 100	0
1	K	477/477 (100%)	0.15	38 (7%)	12 11	10, 26, 90, 100	0
1	L	477/477 (100%)	0.36	38 (7%)	12 11	10, 26, 90, 100	0
1	M	477/477 (100%)	0.23	33 (6%)	16 15	10, 26, 90, 100	0
1	N	477/477 (100%)	0.25	34 (7%)	16 14	10, 26, 90, 100	0
1	O	477/477 (100%)	0.25	32 (6%)	17 16	10, 26, 90, 100	0
1	P	477/477 (100%)	0.36	36 (7%)	14 13	10, 26, 90, 100	0
1	Q	477/477 (100%)	0.32	36 (7%)	14 13	10, 26, 90, 100	0
1	R	477/477 (100%)	0.29	32 (6%)	17 16	10, 26, 90, 100	0
1	S	477/477 (100%)	0.27	38 (7%)	12 11	10, 26, 90, 100	0
1	T	477/477 (100%)	0.18	34 (7%)	16 14	10, 26, 90, 100	0
1	U	477/477 (100%)	0.23	38 (7%)	12 11	10, 26, 90, 100	0
1	V	477/477 (100%)	0.09	34 (7%)	16 14	10, 26, 90, 100	0
1	W	477/477 (100%)	0.07	28 (5%)	22 21	10, 26, 90, 100	0
1	X	477/477 (100%)	0.31	39 (8%)	11 10	10, 26, 90, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	11448/11448 (100%)	0.23	869 (7%) 13 12	10, 26, 92, 100	0

All (869) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	61	HIS	16.1
1	W	60	ILE	15.8
1	R	53	SER	15.5
1	Q	54	ILE	15.5
1	V	61	HIS	15.4
1	Q	60	ILE	15.3
1	E	60	ILE	15.1
1	W	56	GLY	14.7
1	O	54	ILE	14.4
1	N	61	HIS	14.3
1	B	601	THR	14.1
1	E	53	SER	14.0
1	Q	53	SER	13.9
1	X	61	HIS	13.7
1	R	61	HIS	13.3
1	B	61	HIS	13.3
1	J	61	HIS	13.2
1	A	60	ILE	13.0
1	U	55	ARG	12.9
1	R	54	ILE	12.5
1	L	60	ILE	12.5
1	L	61	HIS	12.3
1	I	62	GLU	12.0
1	I	55	ARG	12.0
1	T	53	SER	11.9
1	C	54	ILE	11.8
1	B	54	ILE	11.8
1	J	53	SER	11.7
1	F	54	ILE	11.6
1	T	54	ILE	11.6
1	A	53	SER	11.6
1	J	56	GLY	11.5
1	L	53	SER	11.5
1	B	55	ARG	11.3
1	I	54	ILE	11.3
1	D	54	ILE	11.2
1	J	55	ARG	11.2

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Mol	Chain	Res	Type	RSRZ
1	G	54	ILE	11.2
1	C	61	HIS	11.2
1	S	62	GLU	11.1
1	H	53	SER	11.1
1	I	61	HIS	11.0
1	W	61	HIS	10.9
1	S	54	ILE	10.9
1	P	61	HIS	10.8
1	B	62	GLU	10.8
1	S	61	HIS	10.8
1	L	97	LEU	10.7
1	N	56	GLY	10.7
1	J	54	ILE	10.7
1	M	62	GLU	10.7
1	O	61	HIS	10.7
1	Q	61	HIS	10.6
1	P	62	GLU	10.6
1	O	53	SER	10.6
1	E	55	ARG	10.6
1	W	53	SER	10.6
1	C	53	SER	10.5
1	T	61	HIS	10.5
1	V	56	GLY	10.4
1	I	601	THR	10.4
1	L	96	THR	10.4
1	N	54	ILE	10.3
1	X	54	ILE	10.3
1	X	53	SER	10.3
1	E	62	GLU	10.3
1	F	53	SER	10.3
1	A	62	GLU	10.3
1	F	61	HIS	10.2
1	Q	601	THR	10.2
1	W	55	ARG	10.2
1	K	53	SER	10.2
1	A	61	HIS	10.1
1	U	54	ILE	10.1
1	V	54	ILE	10.1
1	W	59	SER	10.0
1	G	61	HIS	10.0
1	N	53	SER	10.0
1	A	56	GLY	10.0

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Mol	Chain	Res	Type	RSRZ
1	J	62	GLU	10.0
1	E	64	ASP	9.9
1	B	53	SER	9.9
1	C	601	THR	9.9
1	H	61	HIS	9.9
1	V	55	ARG	9.9
1	Q	59	SER	9.8
1	V	53	SER	9.8
1	K	55	ARG	9.8
1	B	57	PHE	9.8
1	M	57	PHE	9.7
1	F	55	ARG	9.7
1	L	62	GLU	9.7
1	Q	62	GLU	9.7
1	X	96	THR	9.7
1	X	95	PHE	9.6
1	A	54	ILE	9.6
1	H	60	ILE	9.5
1	M	54	ILE	9.5
1	N	55	ARG	9.4
1	S	53	SER	9.4
1	O	601	THR	9.4
1	X	97	LEU	9.4
1	M	601	THR	9.4
1	T	60	ILE	9.3
1	D	53	SER	9.3
1	N	62	GLU	9.3
1	C	57	PHE	9.3
1	X	64	ASP	9.3
1	X	60	ILE	9.3
1	L	59	SER	9.2
1	L	95	PHE	9.2
1	J	60	ILE	9.1
1	X	601	THR	9.1
1	Q	56	GLY	9.1
1	K	59	SER	9.0
1	O	57	PHE	9.0
1	G	95	PHE	9.0
1	R	57	PHE	8.9
1	P	601	THR	8.9
1	L	52	SER	8.8
1	O	56	GLY	8.8

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Mol	Chain	Res	Type	RSRZ
1	M	60	ILE	8.7
1	W	54	ILE	8.7
1	G	53	SER	8.7
1	K	397	TYR	8.7
1	X	55	ARG	8.7
1	R	55	ARG	8.7
1	M	53	SER	8.7
1	T	62	GLU	8.6
1	F	56	GLY	8.5
1	L	57	PHE	8.5
1	Q	55	ARG	8.5
1	V	60	ILE	8.5
1	K	54	ILE	8.5
1	B	56	GLY	8.5
1	T	56	GLY	8.5
1	D	61	HIS	8.5
1	N	60	ILE	8.5
1	P	54	ILE	8.5
1	Q	57	PHE	8.4
1	A	601	THR	8.4
1	T	57	PHE	8.4
1	M	55	ARG	8.4
1	F	62	GLU	8.4
1	K	62	GLU	8.4
1	R	62	GLU	8.4
1	L	54	ILE	8.3
1	C	62	GLU	8.3
1	A	55	ARG	8.3
1	L	601	THR	8.2
1	M	56	GLY	8.1
1	G	55	ARG	8.1
1	H	56	GLY	8.1
1	F	57	PHE	8.0
1	U	62	GLU	8.0
1	K	52	SER	8.0
1	H	54	ILE	8.0
1	T	397	TYR	8.0
1	U	61	HIS	7.9
1	E	61	HIS	7.9
1	M	61	HIS	7.9
1	C	55	ARG	7.9
1	L	55	ARG	7.9

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Mol	Chain	Res	Type	RSRZ
1	V	52	SER	7.8
1	N	601	THR	7.7
1	W	601	THR	7.7
1	T	55	ARG	7.7
1	O	62	GLU	7.7
1	S	55	ARG	7.6
1	O	59	SER	7.6
1	L	56	GLY	7.6
1	I	56	GLY	7.6
1	C	56	GLY	7.6
1	X	59	SER	7.6
1	M	59	SER	7.5
1	O	55	ARG	7.5
1	X	56	GLY	7.5
1	C	58	GLN	7.5
1	K	601	THR	7.4
1	F	601	THR	7.4
1	X	57	PHE	7.4
1	Q	52	SER	7.4
1	J	601	THR	7.3
1	E	56	GLY	7.3
1	V	57	PHE	7.3
1	A	59	SER	7.3
1	E	54	ILE	7.3
1	L	64	ASP	7.3
1	C	60	ILE	7.2
1	P	55	ARG	7.2
1	D	601	THR	7.2
1	B	397	TYR	7.1
1	K	56	GLY	7.1
1	H	397	TYR	7.0
1	H	63	SER	6.9
1	W	62	GLU	6.9
1	S	56	GLY	6.9
1	L	93	ASP	6.9
1	N	397	TYR	6.9
1	H	52	SER	6.9
1	V	601	THR	6.9
1	B	52	SER	6.9
1	I	59	SER	6.9
1	P	53	SER	6.9
1	W	57	PHE	6.8

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Mol	Chain	Res	Type	RSRZ
1	G	59	SER	6.8
1	T	59	SER	6.8
1	D	55	ARG	6.8
1	P	326	TYR	6.8
1	M	397	TYR	6.8
1	V	62	GLU	6.7
1	K	60	ILE	6.7
1	F	397	TYR	6.7
1	R	401	PRO	6.7
1	E	57	PHE	6.7
1	L	51	GLY	6.6
1	T	601	THR	6.6
1	J	57	PHE	6.6
1	L	397	TYR	6.6
1	R	601	THR	6.6
1	V	51	GLY	6.6
1	D	326	TYR	6.6
1	C	397	TYR	6.5
1	I	402	GLU	6.5
1	P	57	PHE	6.4
1	F	58	GLN	6.4
1	H	57	PHE	6.4
1	A	401	PRO	6.4
1	U	601	THR	6.4
1	W	397	TYR	6.4
1	D	58	GLN	6.4
1	N	52	SER	6.3
1	G	326	TYR	6.3
1	U	397	TYR	6.3
1	D	327	GLU	6.3
1	F	401	PRO	6.3
1	H	326	TYR	6.2
1	H	62	GLU	6.2
1	R	56	GLY	6.2
1	I	53	SER	6.2
1	X	62	GLU	6.2
1	P	56	GLY	6.2
1	H	602	GLU	6.2
1	E	52	SER	6.2
1	X	93	ASP	6.1
1	S	95	PHE	6.1
1	S	601	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	51	GLY	6.1
1	N	57	PHE	6.1
1	U	59	SER	6.0
1	B	602	GLU	6.0
1	J	397	TYR	6.0
1	U	53	SER	6.0
1	O	60	ILE	6.0
1	G	62	GLU	6.0
1	I	52	SER	6.0
1	R	52	SER	6.0
1	O	58	GLN	5.9
1	H	601	THR	5.9
1	D	56	GLY	5.9
1	I	51	GLY	5.9
1	M	51	GLY	5.9
1	P	402	GLU	5.9
1	L	63	SER	5.9
1	R	397	TYR	5.9
1	G	58	GLN	5.9
1	I	397	TYR	5.9
1	L	58	GLN	5.9
1	A	52	SER	5.9
1	U	402	GLU	5.8
1	I	60	ILE	5.8
1	N	59	SER	5.8
1	H	51	GLY	5.8
1	D	62	GLU	5.8
1	M	58	GLN	5.7
1	V	95	PHE	5.7
1	R	402	GLU	5.7
1	S	397	TYR	5.7
1	E	601	THR	5.7
1	D	602	GLU	5.7
1	S	57	PHE	5.7
1	X	94	PRO	5.7
1	E	58	GLN	5.6
1	R	59	SER	5.6
1	X	397	TYR	5.6
1	I	398	GLU	5.6
1	F	399	LEU	5.6
1	V	326	TYR	5.6
1	K	401	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	52	SER	5.6
1	B	59	SER	5.6
1	G	327	GLU	5.6
1	U	401	PRO	5.5
1	U	326	TYR	5.5
1	G	57	PHE	5.5
1	N	326	TYR	5.5
1	C	398	GLU	5.4
1	M	52	SER	5.4
1	L	94	PRO	5.4
1	O	401	PRO	5.4
1	T	58	GLN	5.4
1	M	63	SER	5.4
1	W	52	SER	5.3
1	W	58	GLN	5.3
1	D	401	PRO	5.3
1	N	401	PRO	5.3
1	I	403	GLU	5.3
1	G	601	THR	5.3
1	D	57	PHE	5.3
1	B	60	ILE	5.3
1	E	96	THR	5.2
1	A	58	GLN	5.2
1	M	399	LEU	5.2
1	B	283	TYR	5.2
1	S	326	TYR	5.2
1	F	402	GLU	5.2
1	T	52	SER	5.2
1	X	52	SER	5.2
1	G	397	TYR	5.2
1	G	56	GLY	5.2
1	H	58	GLN	5.2
1	B	58	GLN	5.2
1	R	399	LEU	5.2
1	A	326	TYR	5.1
1	J	63	SER	5.1
1	T	402	GLU	5.1
1	Q	401	PRO	5.1
1	H	55	ARG	5.1
1	X	58	GLN	5.0
1	I	401	PRO	5.0
1	V	401	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
1	K	402	GLU	5.0
1	P	327	GLU	5.0
1	F	403	GLU	5.0
1	U	57	PHE	5.0
1	T	398	GLU	5.0
1	S	51	GLY	5.0
1	Q	208	LYS	4.9
1	A	402	GLU	4.9
1	D	402	GLU	4.9
1	J	51	GLY	4.9
1	D	397	TYR	4.9
1	O	326	TYR	4.9
1	H	59	SER	4.9
1	E	59	SER	4.9
1	X	402	GLU	4.9
1	C	52	SER	4.9
1	E	97	LEU	4.8
1	B	95	PHE	4.8
1	F	60	ILE	4.8
1	G	347	ILE	4.8
1	J	602	GLU	4.8
1	X	63	SER	4.8
1	G	51	GLY	4.8
1	F	405	ALA	4.8
1	G	401	PRO	4.8
1	P	401	PRO	4.8
1	P	58	GLN	4.7
1	A	397	TYR	4.7
1	F	326	TYR	4.7
1	Q	397	TYR	4.7
1	P	52	SER	4.7
1	W	402	GLU	4.6
1	B	402	GLU	4.6
1	K	326	TYR	4.6
1	G	402	GLU	4.6
1	D	208	LYS	4.6
1	Q	405	ALA	4.6
1	P	179	TYR	4.6
1	J	402	GLU	4.6
1	I	602	GLU	4.5
1	Q	326	TYR	4.5
1	R	60	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	208	LYS	4.5
1	B	326	TYR	4.5
1	R	58	GLN	4.5
1	A	602	GLU	4.5
1	S	402	GLU	4.5
1	P	51	GLY	4.5
1	C	400	PRO	4.5
1	S	208	LYS	4.5
1	S	347	ILE	4.5
1	J	58	GLN	4.5
1	K	57	PHE	4.5
1	D	60	ILE	4.4
1	A	399	LEU	4.4
1	G	398	GLU	4.4
1	Q	63	SER	4.4
1	S	60	ILE	4.4
1	E	397	TYR	4.4
1	C	402	GLU	4.4
1	N	58	GLN	4.4
1	I	400	PRO	4.4
1	U	398	GLU	4.4
1	O	52	SER	4.4
1	A	57	PHE	4.4
1	F	51	GLY	4.4
1	X	51	GLY	4.4
1	C	602	GLU	4.4
1	E	63	SER	4.3
1	L	65	MET	4.3
1	U	602	GLU	4.3
1	D	63	SER	4.3
1	C	403	GLU	4.3
1	R	326	TYR	4.3
1	N	95	PHE	4.3
1	K	350	SER	4.3
1	X	326	TYR	4.3
1	X	405	ALA	4.3
1	M	401	PRO	4.2
1	E	41	SER	4.2
1	L	50	ASP	4.2
1	X	401	PRO	4.2
1	S	327	GLU	4.2
1	H	402	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	179	TYR	4.2
1	O	51	GLY	4.1
1	P	208	LYS	4.1
1	R	208	LYS	4.1
1	E	326	TYR	4.1
1	U	327	GLU	4.1
1	R	51	GLY	4.1
1	I	57	PHE	4.1
1	P	95	PHE	4.1
1	Q	96	THR	4.1
1	G	60	ILE	4.1
1	U	403	GLU	4.1
1	P	397	TYR	4.1
1	R	403	GLU	4.1
1	W	51	GLY	4.1
1	N	398	GLU	4.0
1	J	52	SER	4.0
1	G	96	THR	4.0
1	L	401	PRO	4.0
1	L	326	TYR	4.0
1	O	397	TYR	4.0
1	W	326	TYR	4.0
1	X	65	MET	4.0
1	M	602	GLU	4.0
1	B	403	GLU	4.0
1	J	95	PHE	4.0
1	M	326	TYR	4.0
1	T	326	TYR	4.0
1	E	602	GLU	4.0
1	P	602	GLU	4.0
1	J	326	TYR	3.9
1	B	401	PRO	3.9
1	C	59	SER	3.9
1	H	396	LEU	3.9
1	F	59	SER	3.9
1	N	602	GLU	3.9
1	L	402	GLU	3.9
1	N	402	GLU	3.9
1	Q	97	LEU	3.9
1	S	398	GLU	3.9
1	Q	64	ASP	3.9
1	W	399	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	P	60	ILE	3.8
1	K	399	LEU	3.8
1	V	397	TYR	3.8
1	L	49	PHE	3.8
1	W	63	SER	3.8
1	O	95	PHE	3.8
1	Q	58	GLN	3.7
1	O	208	LYS	3.7
1	T	96	THR	3.7
1	W	602	GLU	3.7
1	K	403	GLU	3.7
1	Q	402	GLU	3.7
1	V	63	SER	3.7
1	F	95	PHE	3.7
1	T	95	PHE	3.7
1	G	325	GLY	3.7
1	U	56	GLY	3.7
1	B	337	ARG	3.7
1	S	602	GLU	3.7
1	S	65	MET	3.6
1	H	95	PHE	3.6
1	V	59	SER	3.6
1	U	58	GLN	3.6
1	M	402	GLU	3.6
1	K	283	TYR	3.6
1	E	402	GLU	3.6
1	S	63	SER	3.6
1	S	400	PRO	3.6
1	R	400	PRO	3.6
1	V	208	LYS	3.6
1	M	95	PHE	3.5
1	P	347	ILE	3.5
1	B	398	GLU	3.5
1	H	97	LEU	3.5
1	R	396	LEU	3.5
1	B	63	SER	3.5
1	C	395	ASP	3.5
1	I	337	ARG	3.5
1	E	405	ALA	3.5
1	F	602	GLU	3.5
1	J	399	LEU	3.5
1	C	353	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	98	GLU	3.5
1	L	602	GLU	3.5
1	P	405	ALA	3.5
1	E	93	ASP	3.4
1	H	337	ARG	3.4
1	Q	95	PHE	3.4
1	V	58	GLN	3.4
1	V	325	GLY	3.4
1	H	398	GLU	3.4
1	W	403	GLU	3.4
1	O	63	SER	3.4
1	I	503	GLY	3.4
1	K	349	GLY	3.4
1	C	401	PRO	3.4
1	G	602	GLU	3.4
1	S	52	SER	3.4
1	U	283	TYR	3.4
1	A	166	ALA	3.4
1	F	208	LYS	3.4
1	S	58	GLN	3.4
1	S	50	ASP	3.4
1	C	399	LEU	3.3
1	C	406	SER	3.3
1	G	49	PHE	3.3
1	O	602	GLU	3.3
1	F	400	PRO	3.3
1	D	179	TYR	3.3
1	G	65	MET	3.3
1	X	403	GLU	3.3
1	H	401	PRO	3.3
1	E	395	ASP	3.3
1	U	52	SER	3.3
1	I	95	PHE	3.3
1	D	398	GLU	3.3
1	B	400	PRO	3.3
1	K	95	PHE	3.2
1	S	179	TYR	3.2
1	F	327	GLU	3.2
1	J	401	PRO	3.2
1	G	52	SER	3.2
1	K	63	SER	3.2
1	I	208	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	95	PHE	3.2
1	R	327	GLU	3.2
1	V	602	GLU	3.2
1	D	51	GLY	3.2
1	C	97	LEU	3.2
1	I	405	ALA	3.2
1	V	166	ALA	3.2
1	I	327	GLU	3.2
1	T	602	GLU	3.2
1	L	403	GLU	3.2
1	K	602	GLU	3.2
1	P	325	GLY	3.2
1	X	399	LEU	3.2
1	K	400	PRO	3.2
1	W	95	PHE	3.1
1	D	59	SER	3.1
1	K	58	GLN	3.1
1	L	208	LYS	3.1
1	I	326	TYR	3.1
1	J	64	ASP	3.1
1	R	405	ALA	3.1
1	S	98	GLU	3.1
1	S	401	PRO	3.1
1	F	394	LYS	3.1
1	U	399	LEU	3.1
1	V	399	LEU	3.1
1	A	327	GLU	3.1
1	R	63	SER	3.1
1	C	208	LYS	3.1
1	C	404	ALA	3.1
1	Q	347	ILE	3.1
1	W	400	PRO	3.1
1	C	326	TYR	3.1
1	S	49	PHE	3.0
1	E	403	GLU	3.0
1	Q	602	GLU	3.0
1	K	286	THR	3.0
1	P	59	SER	3.0
1	V	41	SER	3.0
1	W	401	PRO	3.0
1	N	403	GLU	3.0
1	B	399	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	400	PRO	3.0
1	T	401	PRO	3.0
1	C	503	GLY	3.0
1	O	286	THR	3.0
1	T	97	LEU	3.0
1	O	398	GLU	3.0
1	C	289	GLY	3.0
1	T	50	ASP	3.0
1	N	97	LEU	3.0
1	N	327	GLU	3.0
1	R	179	TYR	3.0
1	L	405	ALA	3.0
1	O	96	THR	3.0
1	R	394	LYS	3.0
1	X	208	LYS	2.9
1	F	396	LEU	2.9
1	K	97	LEU	2.9
1	N	51	GLY	2.9
1	E	45	ASP	2.9
1	N	208	LYS	2.9
1	O	347	ILE	2.9
1	U	386	ILE	2.9
1	N	339	ARG	2.9
1	J	398	GLU	2.9
1	C	95	PHE	2.9
1	D	347	ILE	2.9
1	A	64	ASP	2.9
1	C	277	ASP	2.9
1	E	44	ASP	2.9
1	E	401	PRO	2.9
1	D	52	SER	2.9
1	I	404	ALA	2.9
1	B	406	SER	2.9
1	K	405	ALA	2.9
1	N	337	ARG	2.9
1	A	404	ALA	2.9
1	C	1	THR	2.8
1	E	179	TYR	2.8
1	T	337	ARG	2.8
1	M	97	LEU	2.8
1	U	286	THR	2.8
1	O	402	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	V	402	GLU	2.8
1	V	64	ASP	2.8
1	C	350	SER	2.8
1	P	63	SER	2.8
1	P	398	GLU	2.8
1	H	404	ALA	2.8
1	E	51	GLY	2.8
1	W	64	ASP	2.8
1	I	406	SER	2.8
1	L	98	GLU	2.8
1	I	394	LYS	2.8
1	F	179	TYR	2.8
1	P	166	ALA	2.8
1	X	602	GLU	2.8
1	N	63	SER	2.8
1	J	208	LYS	2.8
1	F	337	ARG	2.8
1	Q	337	ARG	2.8
1	P	323	VAL	2.8
1	V	400	PRO	2.8
1	A	398	GLU	2.8
1	C	288	ALA	2.8
1	K	347	ILE	2.8
1	K	404	ALA	2.8
1	U	208	LYS	2.8
1	R	602	GLU	2.7
1	A	208	LYS	2.7
1	W	208	LYS	2.7
1	C	504	ASN	2.7
1	M	285	GLU	2.7
1	D	95	PHE	2.7
1	M	350	SER	2.7
1	G	50	ASP	2.7
1	X	50	ASP	2.7
1	K	208	LYS	2.7
1	C	63	SER	2.7
1	I	347	ILE	2.7
1	N	390	ALA	2.7
1	O	327	GLU	2.7
1	T	208	LYS	2.7
1	B	405	ALA	2.7
1	P	98	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	O	337	ARG	2.7
1	I	58	GLN	2.7
1	K	11	ASP	2.6
1	S	325	GLY	2.6
1	U	95	PHE	2.6
1	P	324	PRO	2.6
1	M	208	LYS	2.6
1	U	350	SER	2.6
1	H	64	ASP	2.6
1	B	327	GLU	2.6
1	Q	407	ILE	2.6
1	Q	51	GLY	2.6
1	T	395	ASP	2.6
1	E	95	PHE	2.6
1	M	403	GLU	2.6
1	V	398	GLU	2.6
1	P	328	ALA	2.6
1	E	49	PHE	2.6
1	B	51	GLY	2.6
1	B	339	ARG	2.6
1	U	63	SER	2.6
1	F	398	GLU	2.6
1	I	96	THR	2.5
1	U	60	ILE	2.5
1	S	59	SER	2.5
1	T	403	GLU	2.5
1	K	351	PRO	2.5
1	T	396	LEU	2.5
1	O	64	ASP	2.5
1	C	405	ALA	2.5
1	M	166	ALA	2.5
1	I	399	LEU	2.5
1	W	398	GLU	2.5
1	I	64	ASP	2.5
1	C	347	ILE	2.5
1	M	406	SER	2.5
1	I	324	PRO	2.5
1	O	405	ALA	2.5
1	V	283	TYR	2.5
1	A	50	ASP	2.5
1	H	40	LYS	2.5
1	G	93	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	96	THR	2.5
1	D	98	GLU	2.5
1	G	350	SER	2.5
1	G	208	LYS	2.5
1	G	94	PRO	2.5
1	L	431	GLY	2.5
1	I	385	LYS	2.5
1	N	50	ASP	2.5
1	E	285	GLU	2.5
1	X	398	GLU	2.5
1	A	403	GLU	2.4
1	N	176	LYS	2.4
1	U	51	GLY	2.4
1	C	283	TYR	2.4
1	H	325	GLY	2.4
1	B	348	THR	2.4
1	I	166	ALA	2.4
1	G	403	GLU	2.4
1	E	167	ASP	2.4
1	H	208	LYS	2.4
1	T	64	ASP	2.4
1	L	91	VAL	2.4
1	B	98	GLU	2.4
1	F	64	ASP	2.4
1	S	97	LEU	2.4
1	E	337	ARG	2.4
1	F	338	ASN	2.4
1	C	348	THR	2.4
1	H	395	ASP	2.4
1	Q	395	ASP	2.4
1	P	500	GLY	2.4
1	P	403	GLU	2.4
1	U	385	LYS	2.4
1	D	400	PRO	2.4
1	E	347	ILE	2.4
1	X	49	PHE	2.4
1	C	339	ARG	2.4
1	K	64	ASP	2.4
1	R	404	ALA	2.4
1	V	405	ALA	2.4
1	S	96	THR	2.4
1	H	403	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	324	PRO	2.3
1	Q	284	ASP	2.3
1	J	501	SER	2.3
1	M	96	THR	2.3
1	K	500	GLY	2.3
1	O	399	LEU	2.3
1	T	51	GLY	2.3
1	K	285	GLU	2.3
1	B	404	ALA	2.3
1	U	404	ALA	2.3
1	O	406	SER	2.3
1	E	398	GLU	2.3
1	L	92	HIS	2.3
1	G	323	VAL	2.3
1	C	394	LYS	2.3
1	T	40	LYS	2.3
1	B	286	THR	2.3
1	I	63	SER	2.3
1	I	287	TYR	2.3
1	V	350	SER	2.3
1	M	398	GLU	2.3
1	B	208	LYS	2.3
1	B	385	LYS	2.3
1	D	500	GLY	2.3
1	F	63	SER	2.3
1	R	338	ASN	2.3
1	H	285	GLU	2.3
1	N	39	ASP	2.3
1	U	277	ASP	2.3
1	L	398	GLU	2.3
1	Q	65	MET	2.3
1	B	288	ALA	2.3
1	D	166	ALA	2.3
1	G	63	SER	2.3
1	K	287	TYR	2.3
1	R	337	ARG	2.3
1	B	394	LYS	2.3
1	X	404	ALA	2.3
1	M	324	PRO	2.2
1	I	349	GLY	2.2
1	U	349	GLY	2.2
1	M	50	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	339	ARG	2.2
1	L	396	LEU	2.2
1	U	400	PRO	2.2
1	S	64	ASP	2.2
1	X	98	GLU	2.2
1	B	179	TYR	2.2
1	M	504	ASN	2.2
1	D	50	ASP	2.2
1	F	406	SER	2.2
1	X	91	VAL	2.2
1	L	99	PRO	2.2
1	V	97	LEU	2.2
1	J	325	GLY	2.2
1	E	396	LEU	2.2
1	H	400	PRO	2.2
1	I	284	ASP	2.2
1	I	117	SER	2.2
1	T	406	SER	2.2
1	N	347	ILE	2.2
1	Q	49	PHE	2.2
1	H	339	ARG	2.2
1	B	350	SER	2.2
1	C	285	GLU	2.2
1	P	350	SER	2.2
1	E	42	VAL	2.2
1	F	40	LYS	2.2
1	T	404	ALA	2.2
1	R	209	GLY	2.2
1	N	399	LEU	2.2
1	W	179	TYR	2.1
1	G	310	ALA	2.1
1	T	94	PRO	2.1
1	I	504	ASN	2.1
1	D	405	ALA	2.1
1	X	431	GLY	2.1
1	E	286	THR	2.1
1	B	349	GLY	2.1
1	O	182	VAL	2.1
1	Q	283	TYR	2.1
1	I	116	ILE	2.1
1	P	400	PRO	2.1
1	B	287	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	286	THR	2.1
1	S	286	THR	2.1
1	G	64	ASP	2.1
1	I	384	ASN	2.1
1	T	325	GLY	2.1
1	S	285	GLU	2.1
1	A	63	SER	2.1
1	I	350	SER	2.1
1	J	59	SER	2.1
1	H	503	GLY	2.1
1	U	285	GLU	2.1
1	V	285	GLU	2.1
1	G	166	ALA	2.1
1	Q	339	ARG	2.1
1	U	1	THR	2.1
1	I	179	TYR	2.1
1	K	284	ASP	2.1
1	U	347	ILE	2.1
1	U	396	LEU	2.1
1	J	339	ARG	2.1
1	S	339	ARG	2.1
1	W	347	ILE	2.0
1	X	350	SER	2.0
1	D	97	LEU	2.0
1	I	49	PHE	2.0
1	D	163	ALA	2.0
1	D	328	ALA	2.0
1	B	96	THR	2.0
1	X	286	THR	2.0
1	Q	385	LYS	2.0
1	S	324	PRO	2.0
1	Q	399	LEU	2.0
1	V	396	LEU	2.0
1	D	324	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	O	470	1/1	0.26	0.40	60,60,60,60	1
2	MN	N	470	1/1	0.39	0.23	60,60,60,60	1
2	MN	E	470	1/1	0.40	0.30	60,60,60,60	1
2	MN	M	470	1/1	0.42	0.31	60,60,60,60	1
2	MN	R	470	1/1	0.47	0.33	60,60,60,60	1
3	AMP	A	7475	23/23	0.48	0.71	2,16,71,83	23
3	AMP	U	7515	23/23	0.53	0.59	2,16,71,83	23
3	AMP	W	7519	23/23	0.54	0.62	2,16,71,83	23
3	AMP	S	7511	23/23	0.55	0.68	2,16,71,83	23
3	AMP	G	7487	23/23	0.55	0.66	2,16,71,83	23
2	MN	I	470	1/1	0.57	0.28	60,60,60,60	1
3	AMP	E	7483	23/23	0.59	0.60	2,16,71,83	23
2	MN	A	470	1/1	0.59	0.29	60,60,60,60	1
3	AMP	V	7517	23/23	0.59	0.62	2,16,71,83	23
3	AMP	J	7493	23/23	0.60	0.63	2,16,71,83	23
3	AMP	B	7477	23/23	0.60	0.56	2,16,71,83	23
3	AMP	R	7509	23/23	0.60	0.69	2,16,71,83	23
2	MN	W	470	1/1	0.61	0.17	60,60,60,60	1
3	AMP	F	7485	23/23	0.61	0.66	2,16,71,83	23
3	AMP	L	7497	23/23	0.61	0.65	2,16,71,83	23
3	AMP	O	7503	23/23	0.61	0.55	2,16,71,83	23
3	AMP	T	7513	23/23	0.62	0.59	2,16,71,83	23
3	AMP	D	7481	23/23	0.62	0.54	2,16,71,83	23
3	AMP	I	7491	23/23	0.62	0.56	2,16,71,83	23
3	AMP	P	7505	23/23	0.62	0.59	2,16,71,83	23
3	AMP	K	7495	23/23	0.62	0.62	2,16,71,83	23
3	AMP	N	7501	23/23	0.63	0.57	2,16,71,83	23
2	MN	C	470	1/1	0.64	0.27	60,60,60,60	1
3	AMP	M	7499	23/23	0.64	0.58	2,16,71,83	23
3	AMP	X	7521	23/23	0.65	0.57	2,16,71,83	23
2	MN	L	470	1/1	0.65	0.25	60,60,60,60	1

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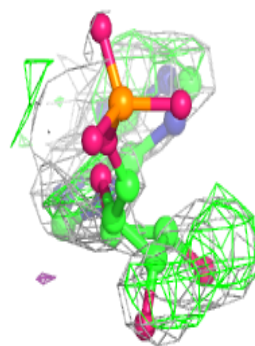
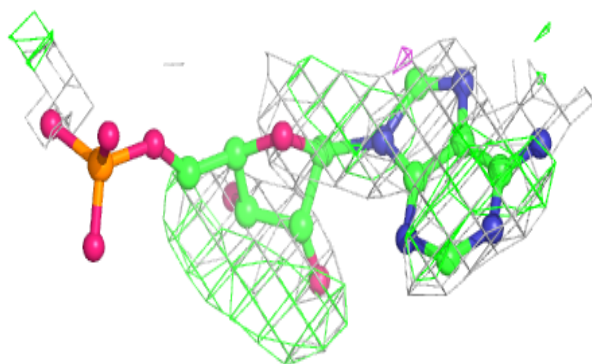
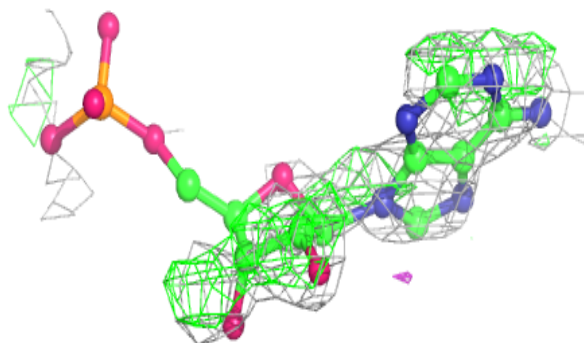
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	D	470	1/1	0.65	0.22	60,60,60,60	1
2	MN	Q	470	1/1	0.66	0.26	60,60,60,60	1
3	AMP	Q	7507	23/23	0.67	0.52	2,16,71,83	23
3	AMP	H	7489	23/23	0.67	0.54	2,16,71,83	23
3	AMP	C	7479	23/23	0.68	0.48	2,16,71,83	23
4	CIT	T	7514	13/13	0.69	0.36	41,62,79,84	0
4	CIT	Q	7508	13/13	0.71	0.40	41,62,79,84	0
2	MN	F	470	1/1	0.71	0.24	60,60,60,60	1
4	CIT	E	7484	13/13	0.72	0.38	41,62,79,84	0
4	CIT	R	7510	13/13	0.74	0.46	41,62,79,84	0
4	CIT	A	7476	13/13	0.76	0.29	41,62,79,84	0
4	CIT	F	7486	13/13	0.76	0.48	41,62,79,84	0
2	MN	G	470	1/1	0.76	0.18	60,60,60,60	1
4	CIT	N	7502	13/13	0.77	0.30	41,62,79,84	0
4	CIT	G	7488	13/13	0.77	0.42	41,62,79,84	0
4	CIT	K	7496	13/13	0.77	0.37	41,62,79,84	0
4	CIT	H	7490	13/13	0.78	0.34	41,62,79,84	0
2	MN	P	470	1/1	0.78	0.22	60,60,60,60	1
2	MN	B	470	1/1	0.78	0.16	60,60,60,60	1
4	CIT	X	7522	13/13	0.79	0.38	41,62,79,84	0
4	CIT	C	7480	13/13	0.79	0.28	41,62,79,84	0
4	CIT	P	7506	13/13	0.79	0.32	41,62,79,84	0
4	CIT	U	7516	13/13	0.79	0.28	41,62,79,84	0
4	CIT	V	7518	13/13	0.79	0.33	41,62,79,84	0
2	MN	X	470	1/1	0.80	0.25	60,60,60,60	1
4	CIT	B	7478	13/13	0.80	0.29	41,62,79,84	0
2	MN	S	470	1/1	0.80	0.19	60,60,60,60	1
4	CIT	J	7494	13/13	0.80	0.34	41,62,79,84	0
2	MN	J	470	1/1	0.80	0.20	60,60,60,60	1
4	CIT	O	7504	13/13	0.80	0.35	41,62,79,84	0
4	CIT	L	7498	13/13	0.80	0.39	41,62,79,84	0
2	MN	T	470	1/1	0.81	0.35	60,60,60,60	1
4	CIT	S	7512	13/13	0.82	0.39	41,62,79,84	0
2	MN	H	470	1/1	0.82	0.26	60,60,60,60	1
4	CIT	I	7492	13/13	0.82	0.26	41,62,79,84	0
4	CIT	D	7482	13/13	0.82	0.39	41,62,79,84	0
2	MN	V	470	1/1	0.84	0.19	60,60,60,60	1
2	MN	K	470	1/1	0.84	0.12	60,60,60,60	1
4	CIT	W	7520	13/13	0.84	0.33	41,62,79,84	0
4	CIT	M	7500	13/13	0.86	0.30	41,62,79,84	0
2	MN	U	470	1/1	0.86	0.20	60,60,60,60	1

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

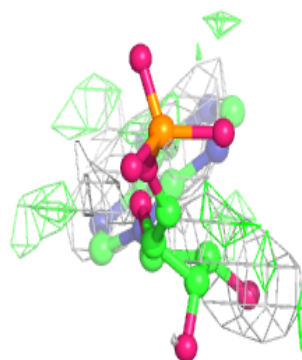
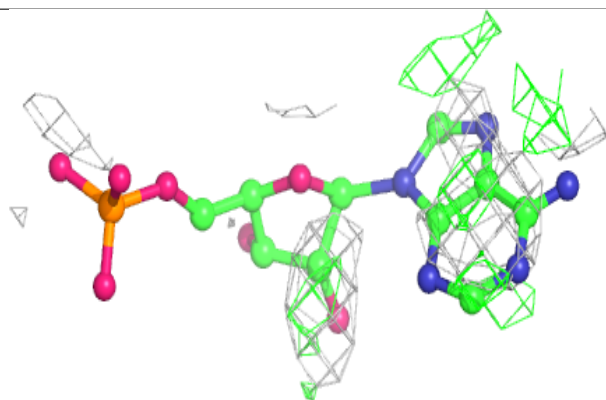
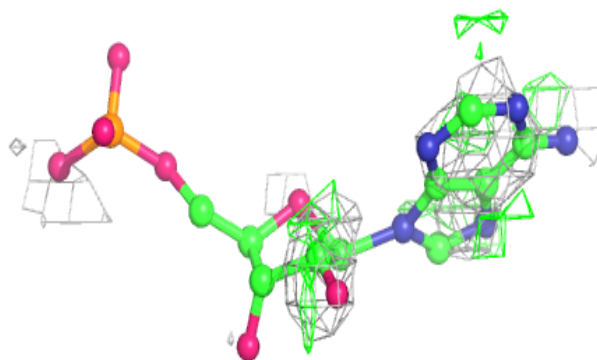
Electron density around AMP A 7475:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

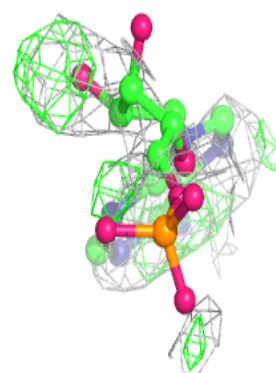
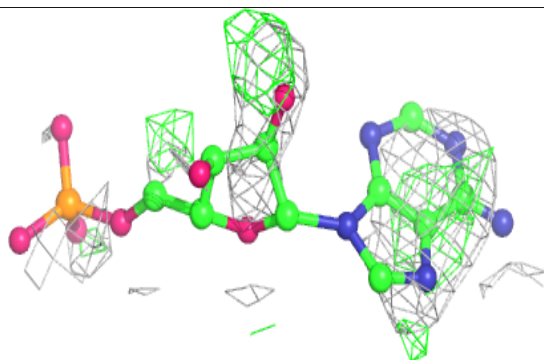
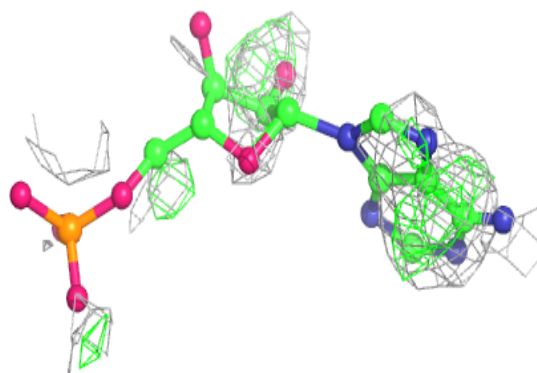


Electron density around AMP U 7515:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

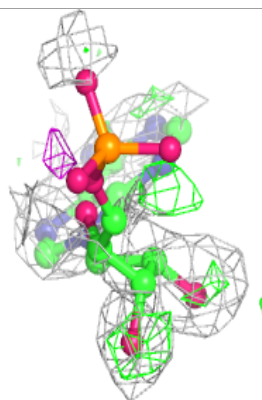
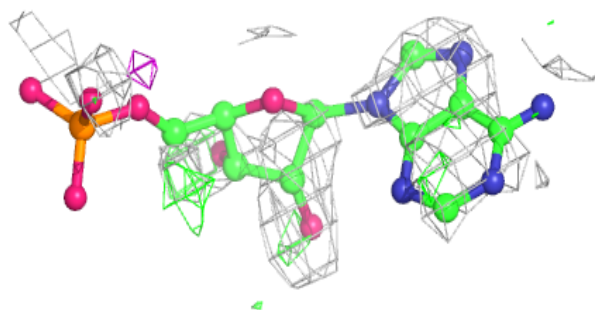
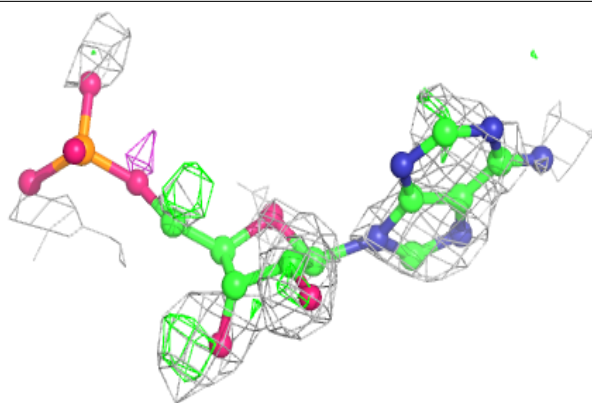
**Electron density around AMP W 7519:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

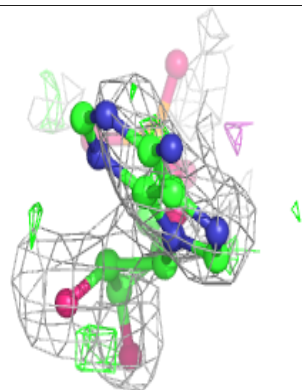
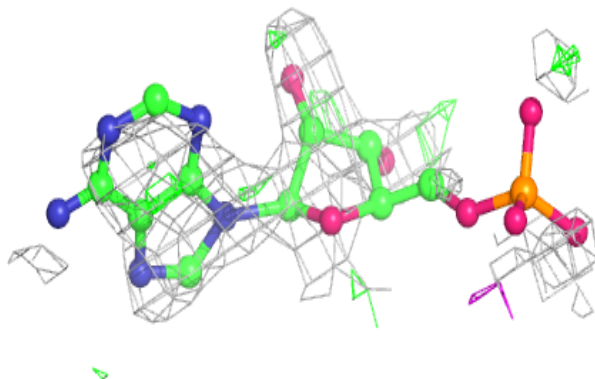
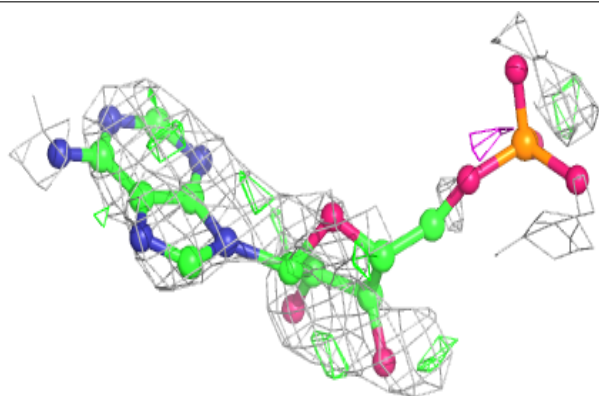


Electron density around AMP S 7511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

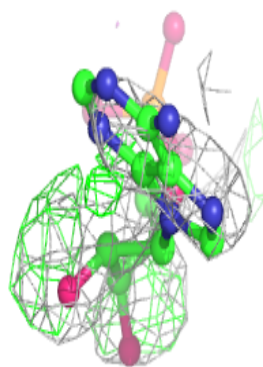
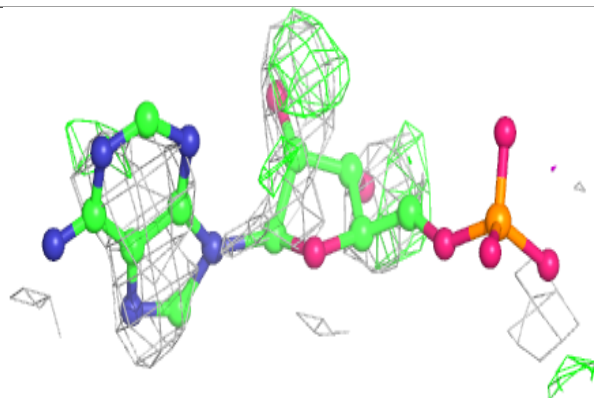
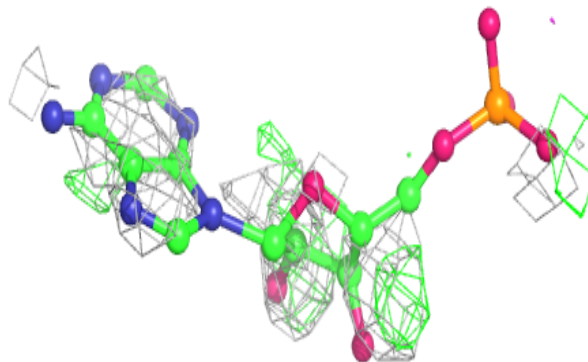
**Electron density around AMP G 7487:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

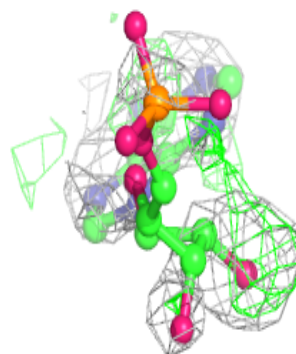
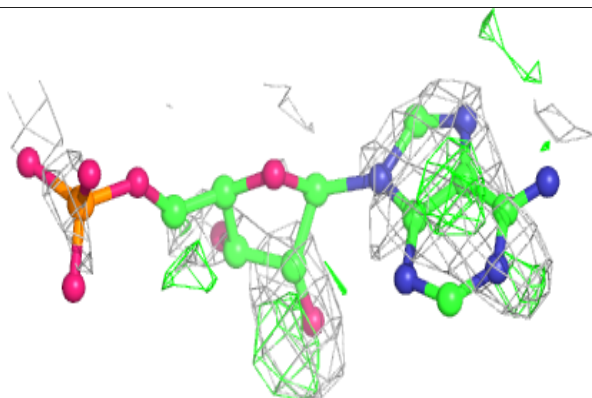
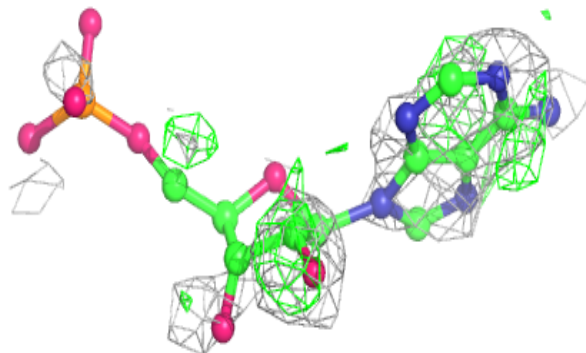


Electron density around AMP E 7483:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

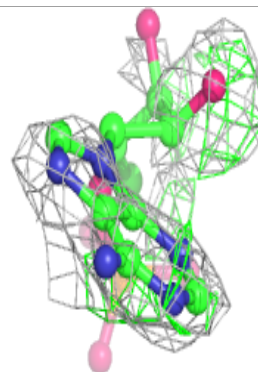
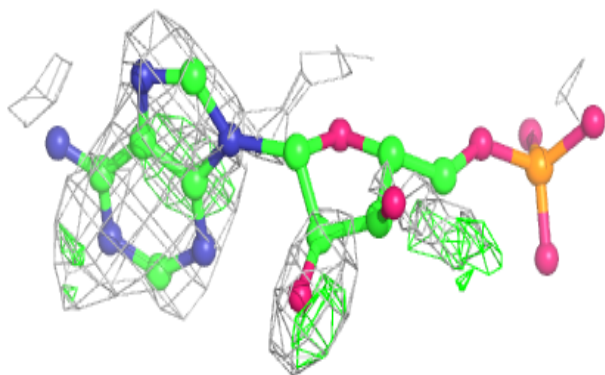
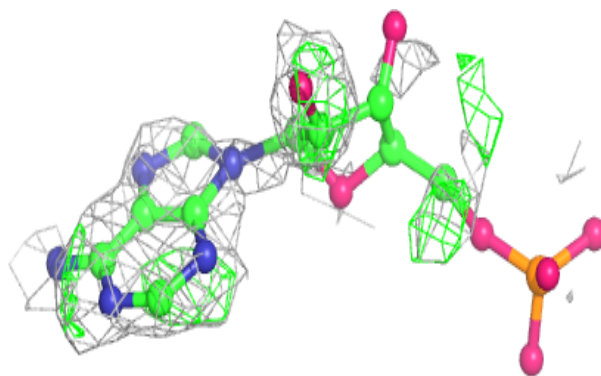
**Electron density around AMP V 7517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

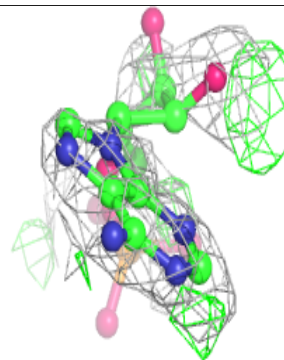
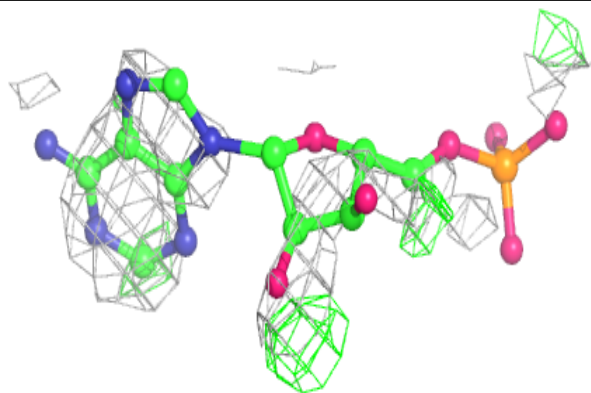
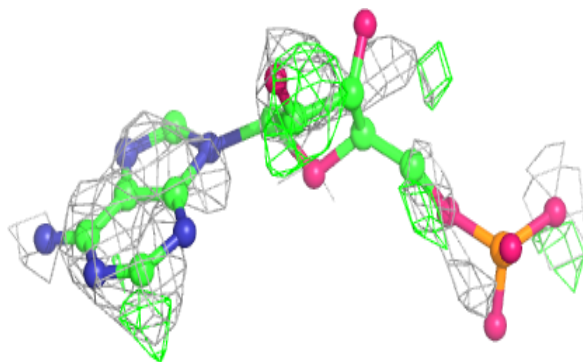


Electron density around AMP J 7493:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

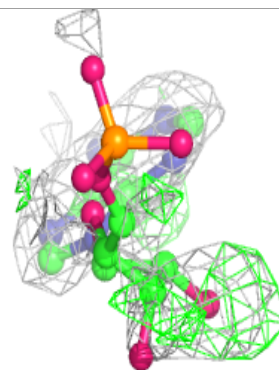
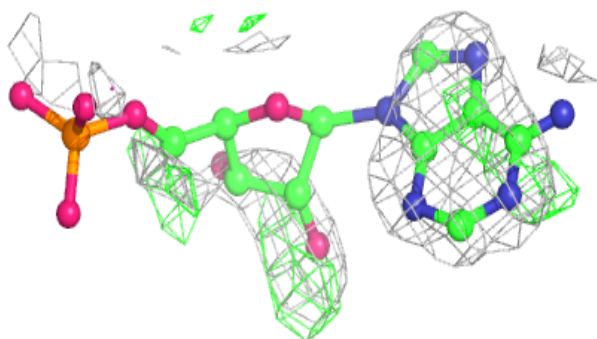
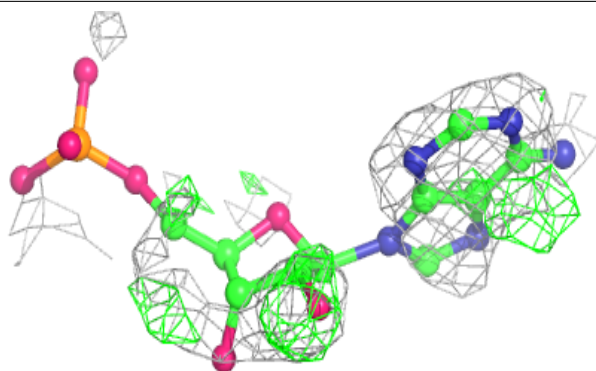
**Electron density around AMP B 7477:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

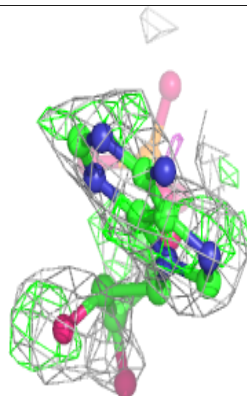
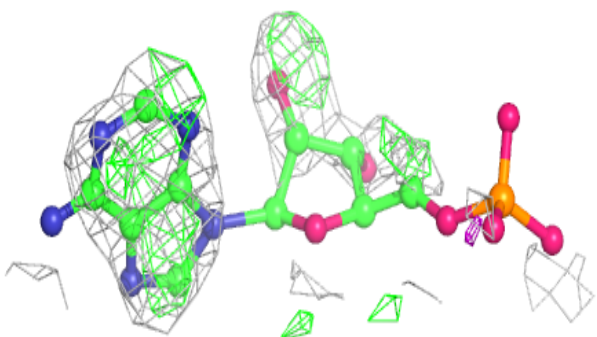
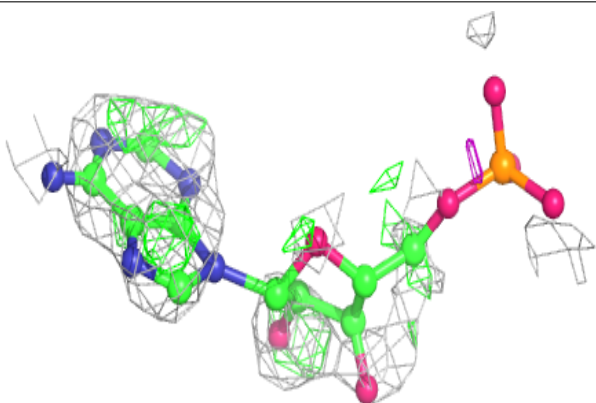


Electron density around AMP R 7509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

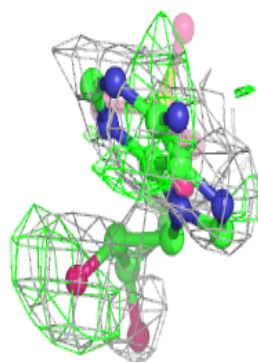
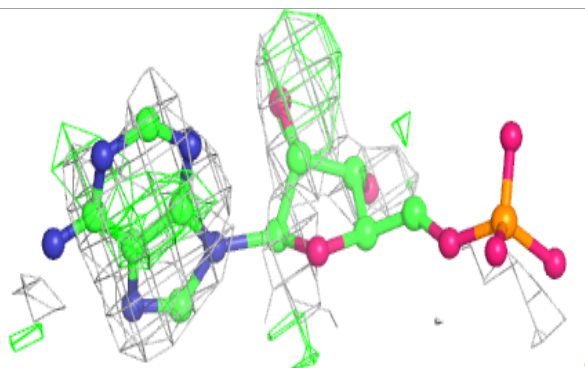
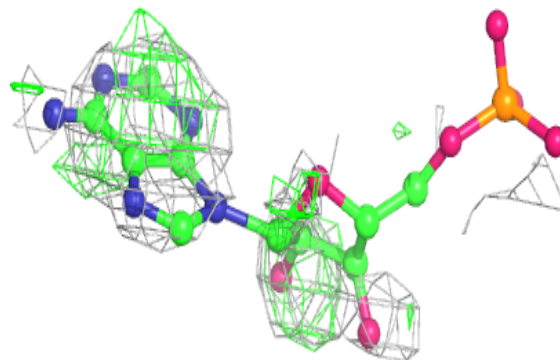
**Electron density around AMP F 7485:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

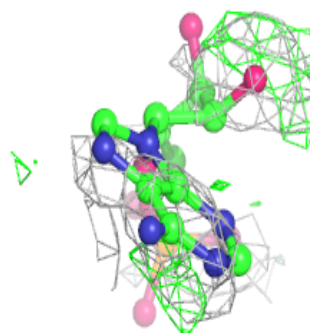
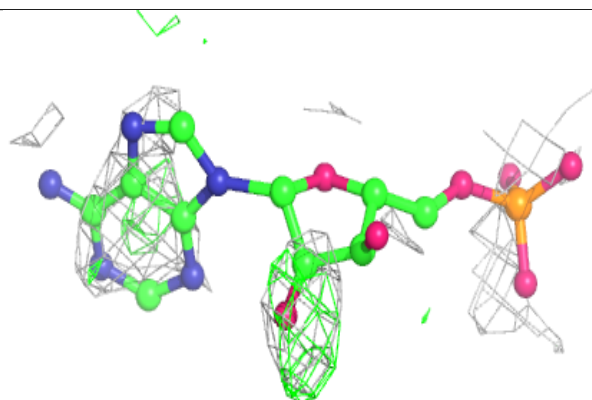
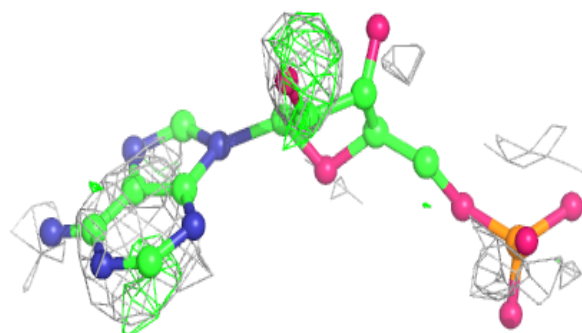


Electron density around AMP L 7497:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

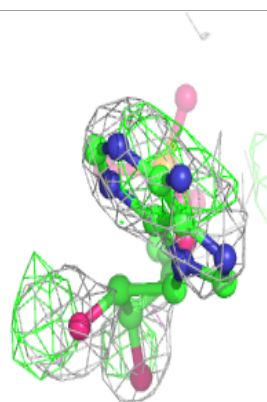
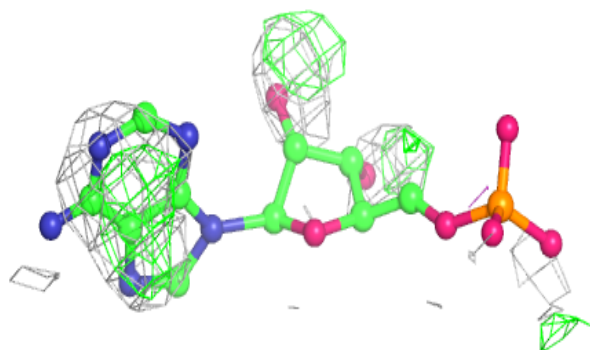
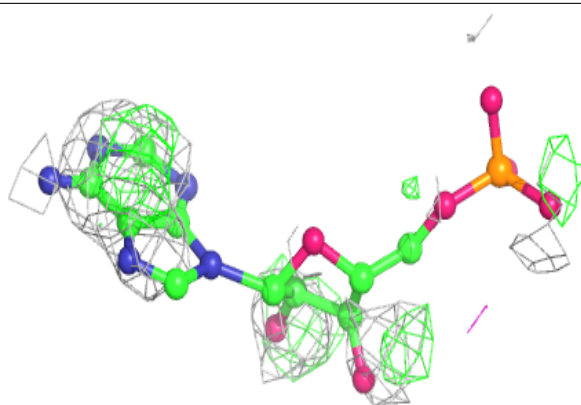
**Electron density around AMP O 7503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

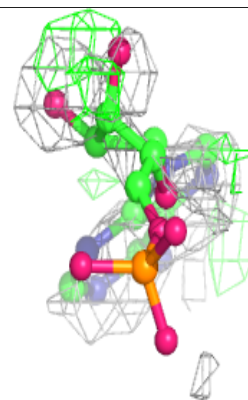
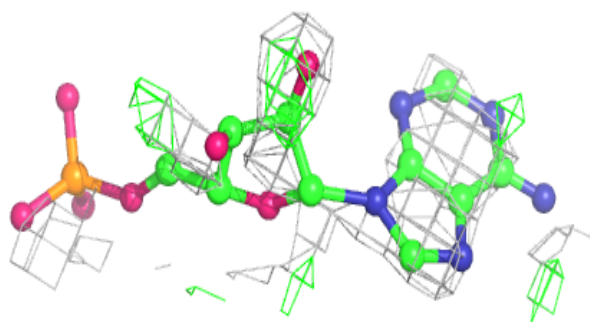
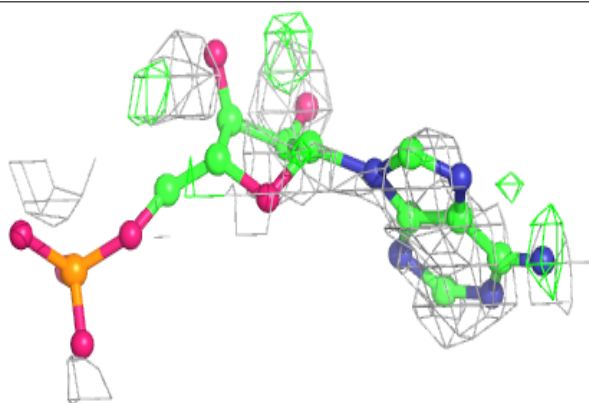


Electron density around AMP T 7513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

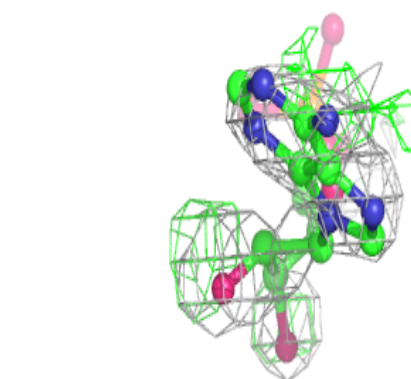
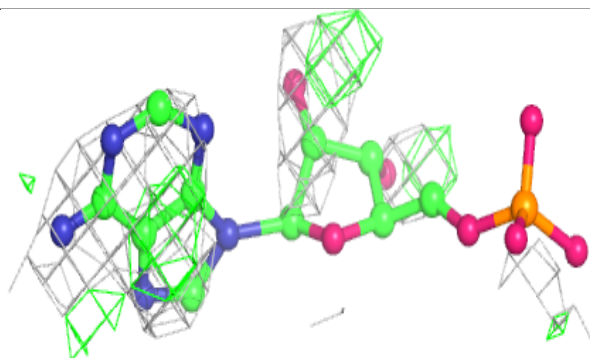
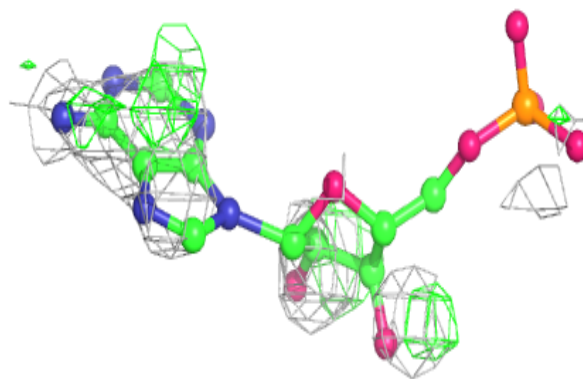
**Electron density around AMP D 7481:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

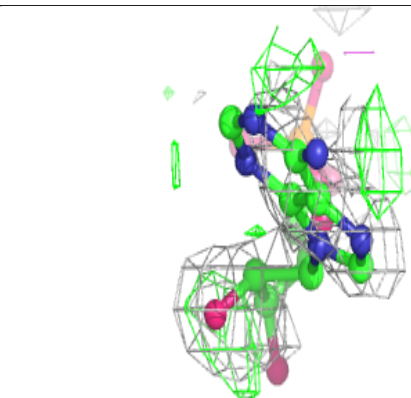
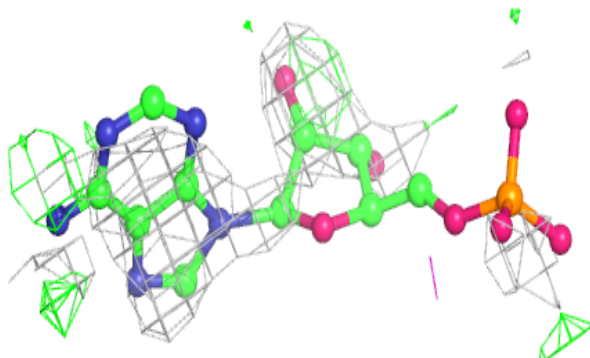
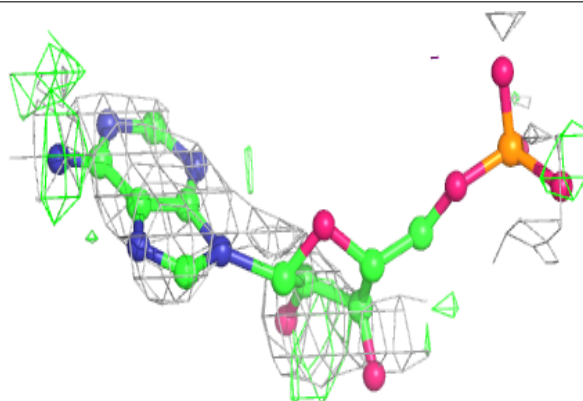


Electron density around AMP I 7491:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

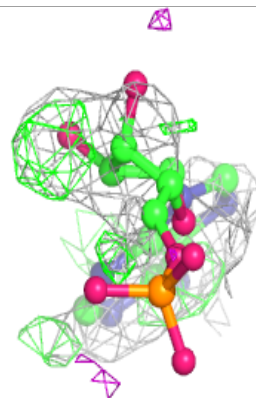
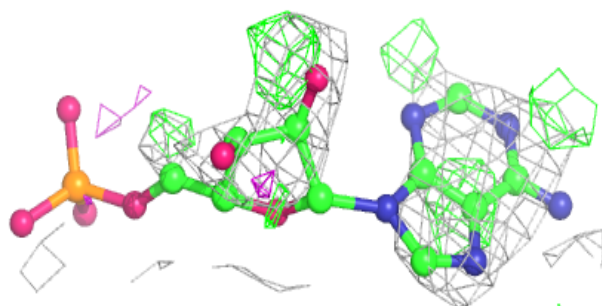
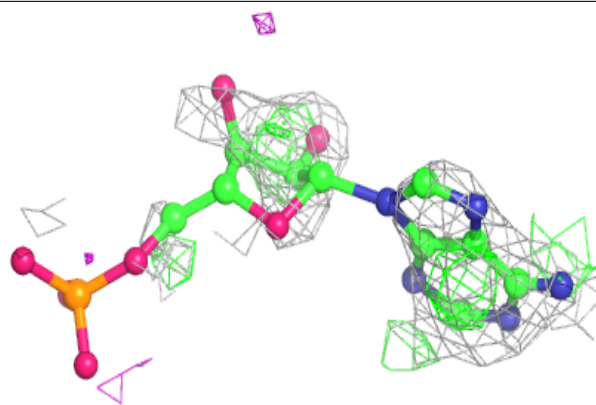
**Electron density around AMP P 7505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

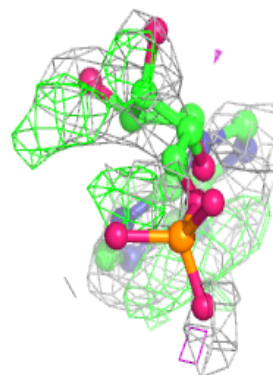
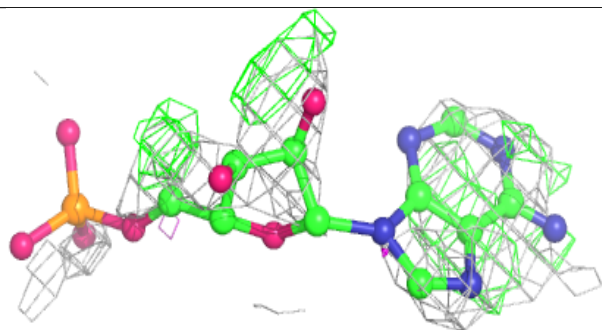
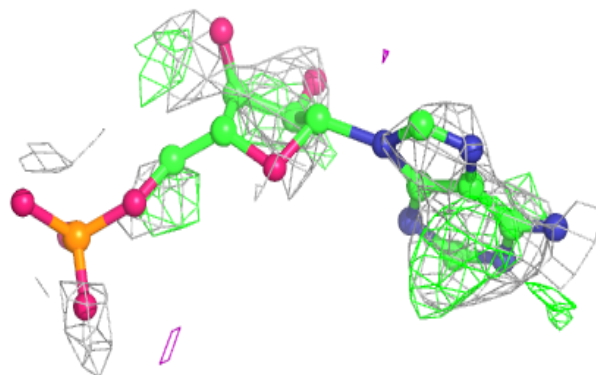


Electron density around AMP K 7495:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

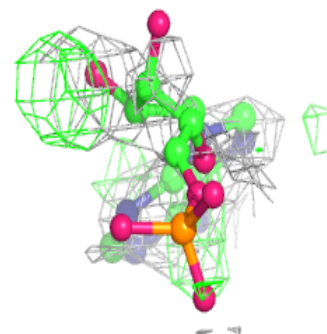
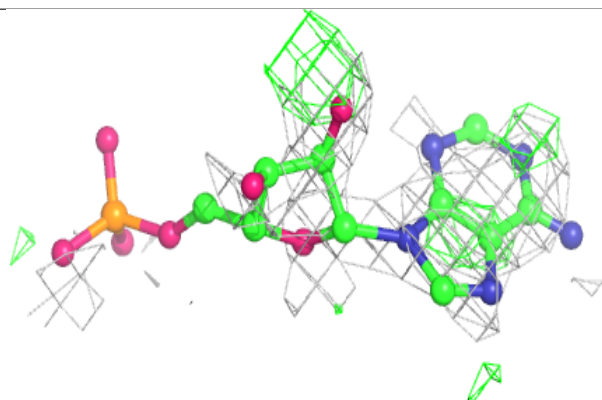
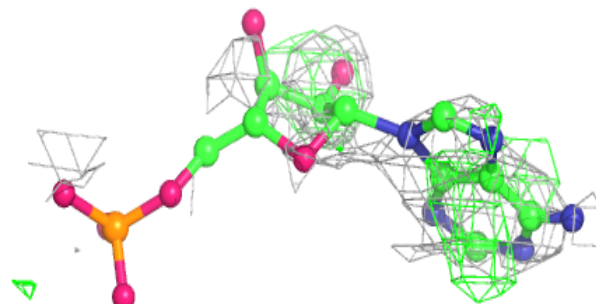
**Electron density around AMP N 7501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

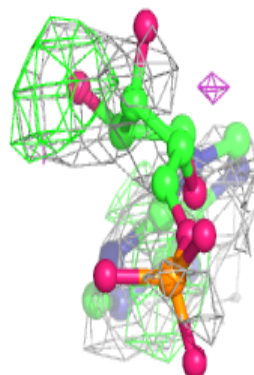
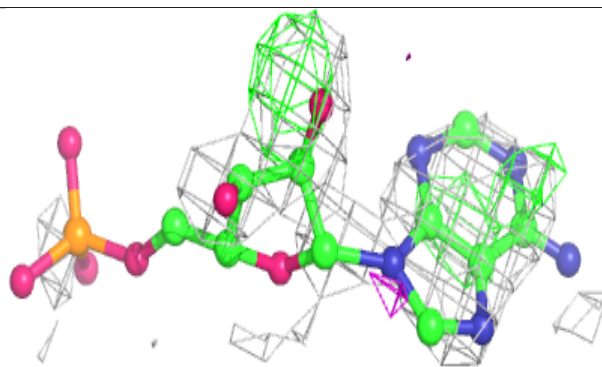
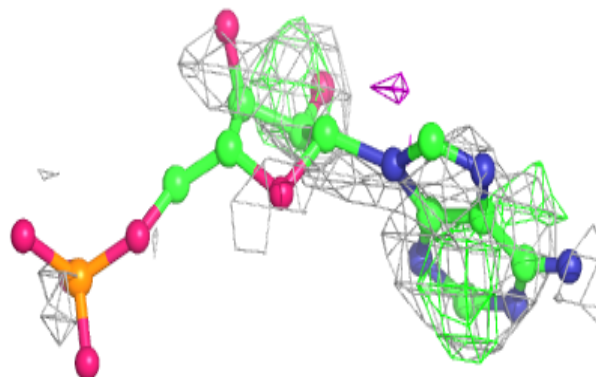


Electron density around AMP M 7499:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

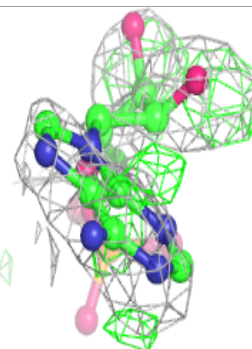
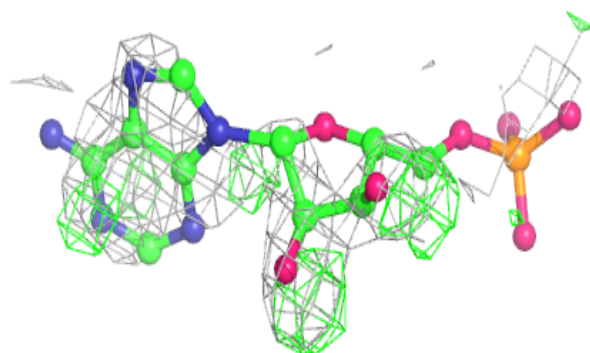
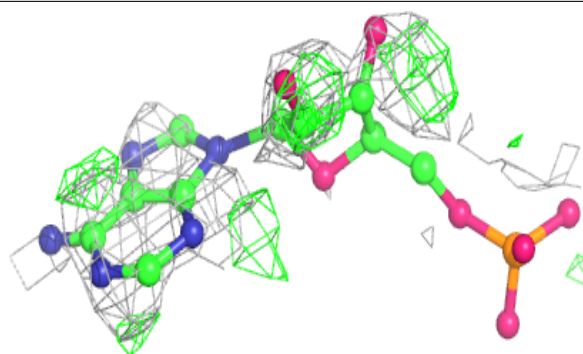
**Electron density around AMP X 7521:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

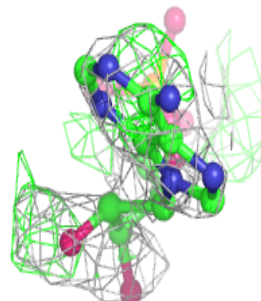
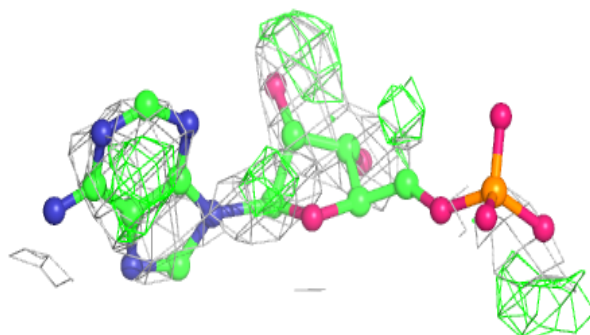
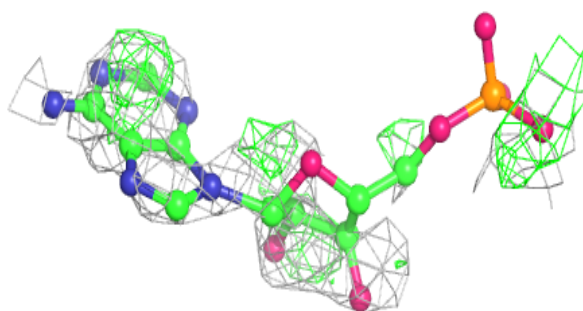


Electron density around AMP Q 7507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

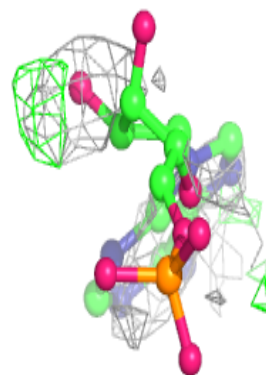
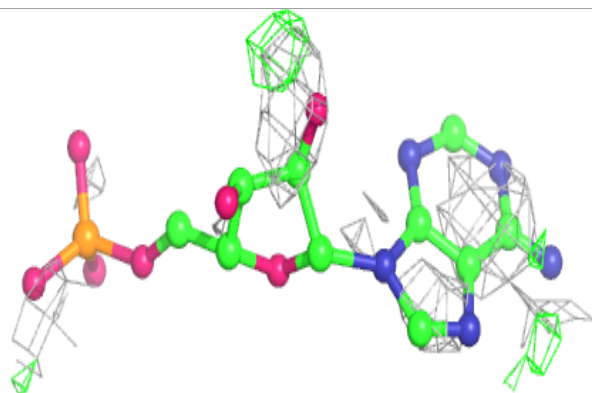
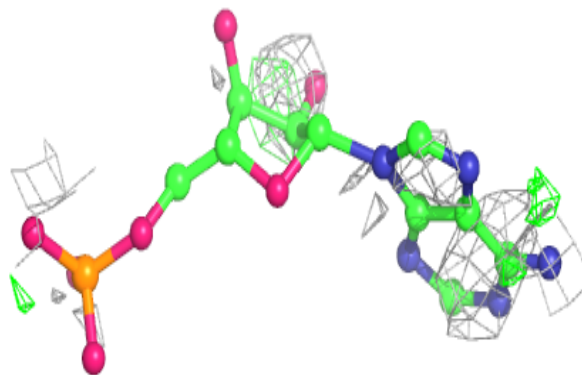
**Electron density around AMP H 7489:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AMP C 7479:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.