



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:31 am BST

PDB ID : 1F1H  
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM  
SALMONELLA TYPHIMURIUM WITH THALLIUM IONS  
Authors : Gill, H.S.; Eisenberg, D.  
Deposited on : 2000-05-19  
Resolution : 2.67 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (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

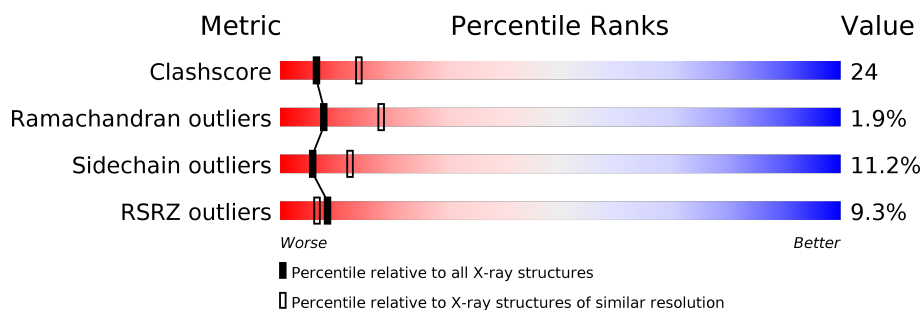
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.67 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	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	468	<div> <div>17%</div> <div>69%</div> <div>23%</div> <div>7%</div> </div>
1	B	468	<div> <div>11%</div> <div>71%</div> <div>21%</div> <div>7%</div> </div>
1	C	468	<div> <div>10%</div> <div>69%</div> <div>23%</div> <div>7%</div> </div>
1	D	468	<div> <div>7%</div> <div>70%</div> <div>22%</div> <div>7%</div> </div>
1	E	468	<div> <div>12%</div> <div>70%</div> <div>22%</div> <div>7%</div> </div>
1	F	468	<div> <div>9%</div> <div>70%</div> <div>23%</div> <div>7%</div> </div>
1	G	468	<div> <div>8%</div> <div>71%</div> <div>22%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	468	
1	I	468	
1	J	468	
1	K	468	
1	L	468	

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
3	ADP	B	1472	-	-	-	X
3	ADP	D	1474	-	-	-	X
3	ADP	F	1476	-	-	-	X
3	ADP	I	1479	-	-	-	X
3	ADP	K	1481	-	-	-	X
3	ADP	L	1482	-	-	-	X
5	MPD	A	1483	-	-	X	-
5	MPD	B	1484	-	-	X	X
5	MPD	C	1485	-	-	X	-
5	MPD	D	1486	-	-	X	-
5	MPD	E	1487	-	-	X	-
5	MPD	F	1488	-	-	X	-
5	MPD	G	1489	-	-	X	-
5	MPD	H	1490	-	-	X	-
5	MPD	I	1491	-	-	X	-
5	MPD	J	1492	-	-	X	-
5	MPD	K	1493	-	-	X	-
5	MPD	L	1494	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 45564 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 PROTEIN (GLUTAMINE SYNTHETASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	B	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	C	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	D	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	E	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	F	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	G	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	H	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	I	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	J	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	K	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			
1	L	468	Total	C	N	O	S	0	0	0
			3637	2301	624	692	20			

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

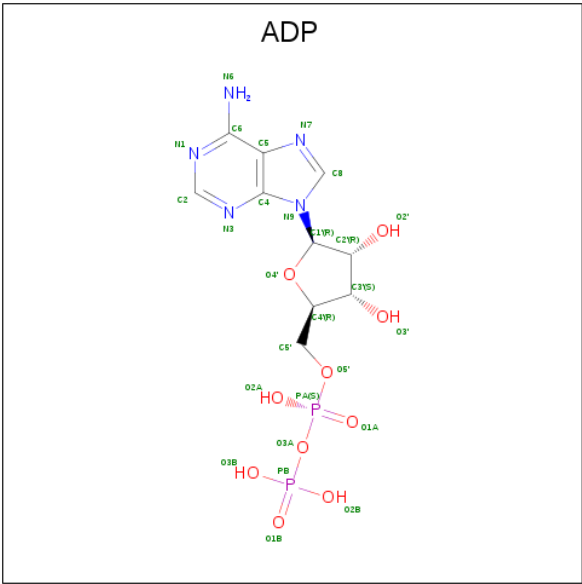
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Mn	0	0
			2	2		
2	K	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	H	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	I	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		
2	L	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	I	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	J	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	K	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	L	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is THALLIUM (I) ION (three-letter code: Tl) (formula: Tl).

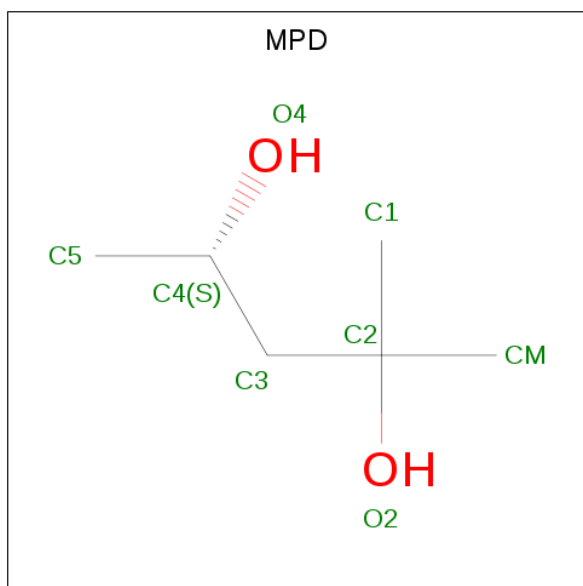
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total 2	Tl 2	0	0
4	J	2	Total 2	Tl 2	0	0
4	D	2	Total 2	Tl 2	0	0
4	K	2	Total 2	Tl 2	0	0
4	E	2	Total 2	Tl 2	0	0
4	H	2	Total 2	Tl 2	0	0
4	B	2	Total 2	Tl 2	0	0
4	I	2	Total 2	Tl 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	Tl 2	0	0
4	A	2	Total 2	Tl 2	0	0
4	L	2	Total 2	Tl 2	0	0
4	F	2	Total 2	Tl 2	0	0

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 8	C 6	O 2	0	0
5	B	1	Total 8	C 6	O 2	0	0
5	C	1	Total 8	C 6	O 2	0	0
5	D	1	Total 8	C 6	O 2	0	0
5	E	1	Total 8	C 6	O 2	0	0
5	F	1	Total 8	C 6	O 2	0	0
5	G	1	Total 8	C 6	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			8	6	2		
5	I	1	Total	C	O	0	0
			8	6	2		
5	J	1	Total	C	O	0	0
			8	6	2		
5	K	1	Total	C	O	0	0
			8	6	2		
5	L	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

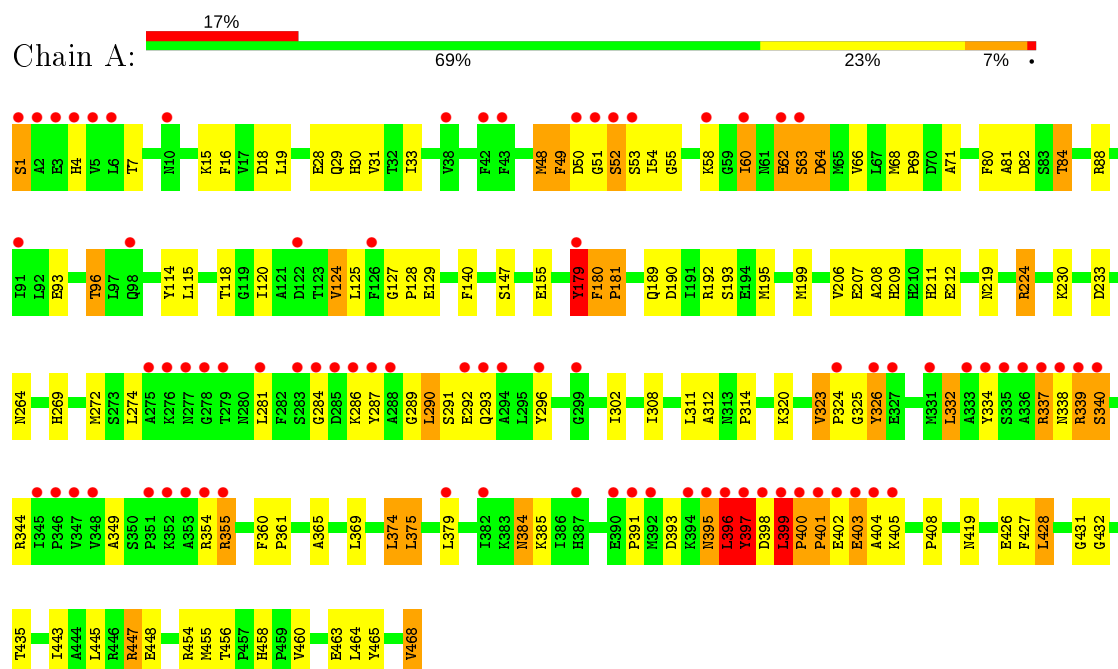
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		
6	B	121	Total	O	0	0
			121	121		
6	C	119	Total	O	0	0
			119	119		
6	D	122	Total	O	0	0
			122	122		
6	E	122	Total	O	0	0
			122	122		
6	F	121	Total	O	0	0
			121	121		
6	G	122	Total	O	0	0
			122	122		
6	H	121	Total	O	0	0
			121	121		
6	I	122	Total	O	0	0
			122	122		
6	J	120	Total	O	0	0
			120	120		
6	K	123	Total	O	0	0
			123	123		
6	L	119	Total	O	0	0
			119	119		



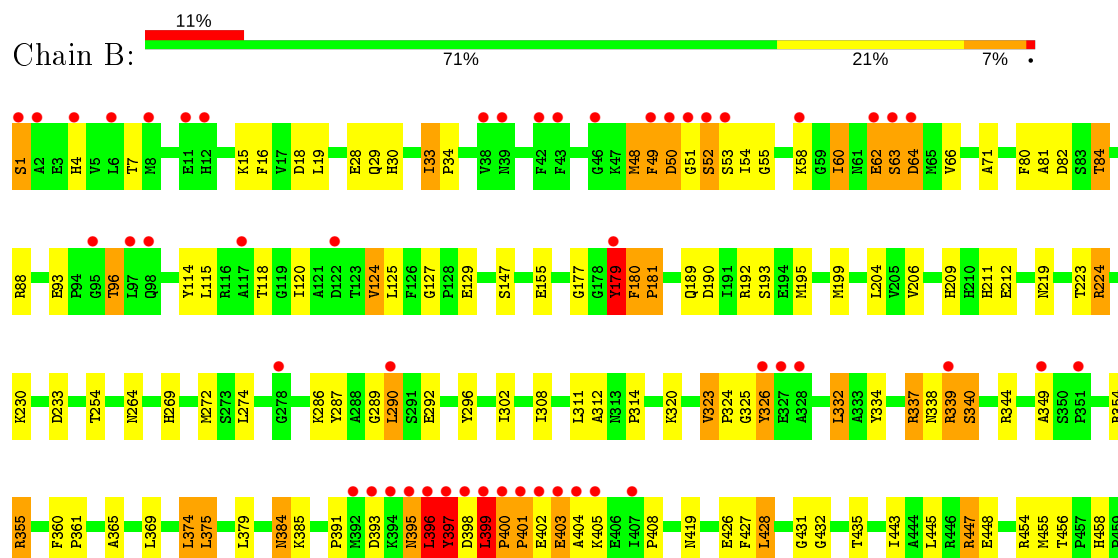
### 3 Residue-property plots [i](#)

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: PROTEIN (GLUTAMINE SYNTHETASE)

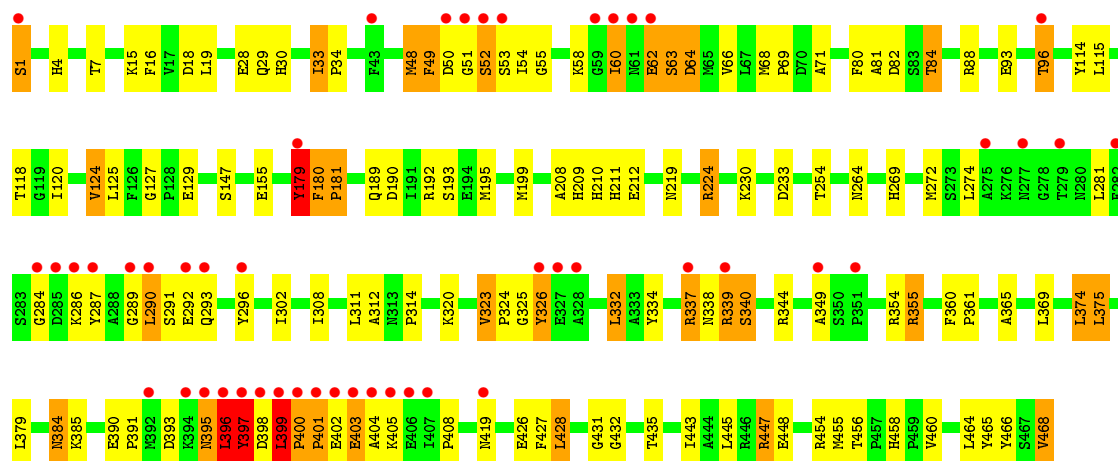


#### • Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

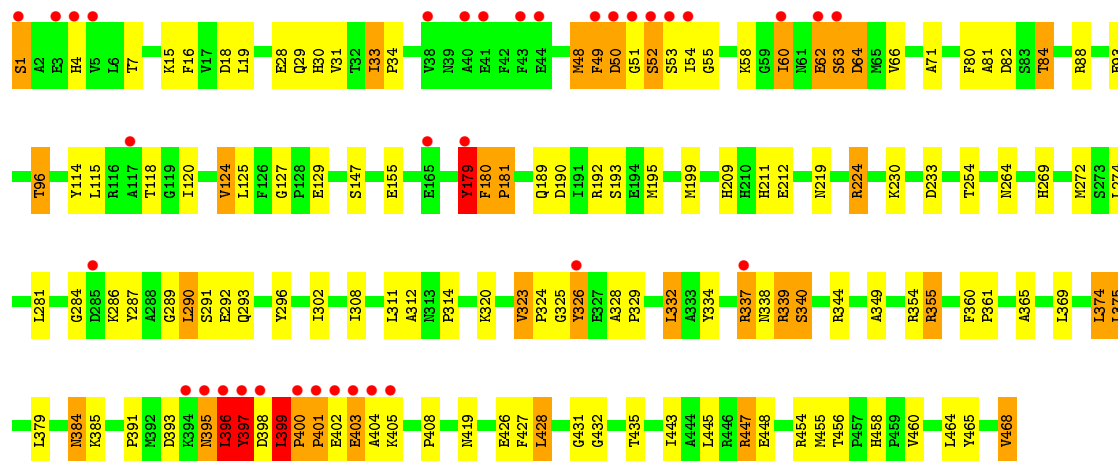




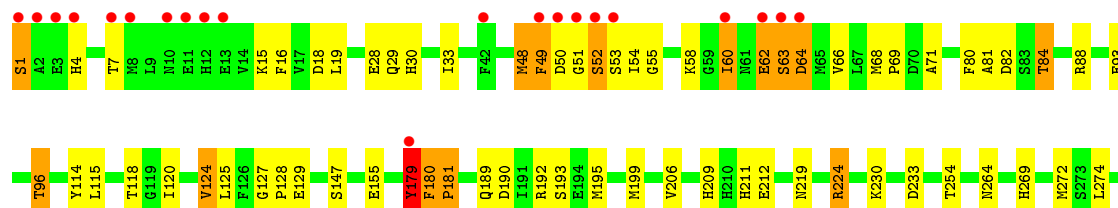
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

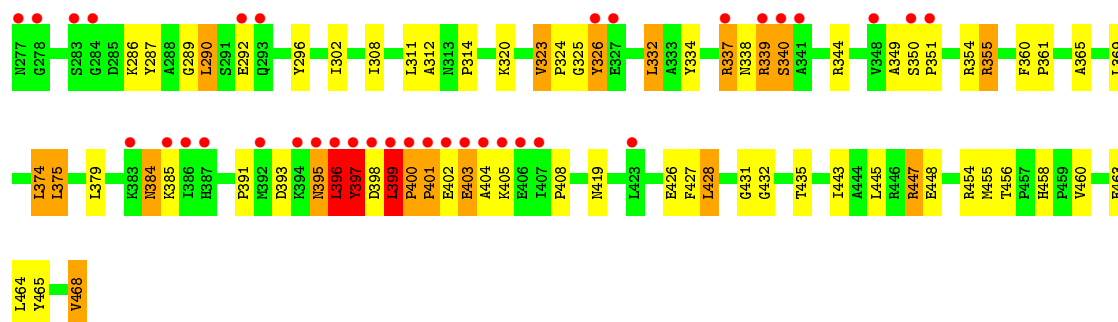


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

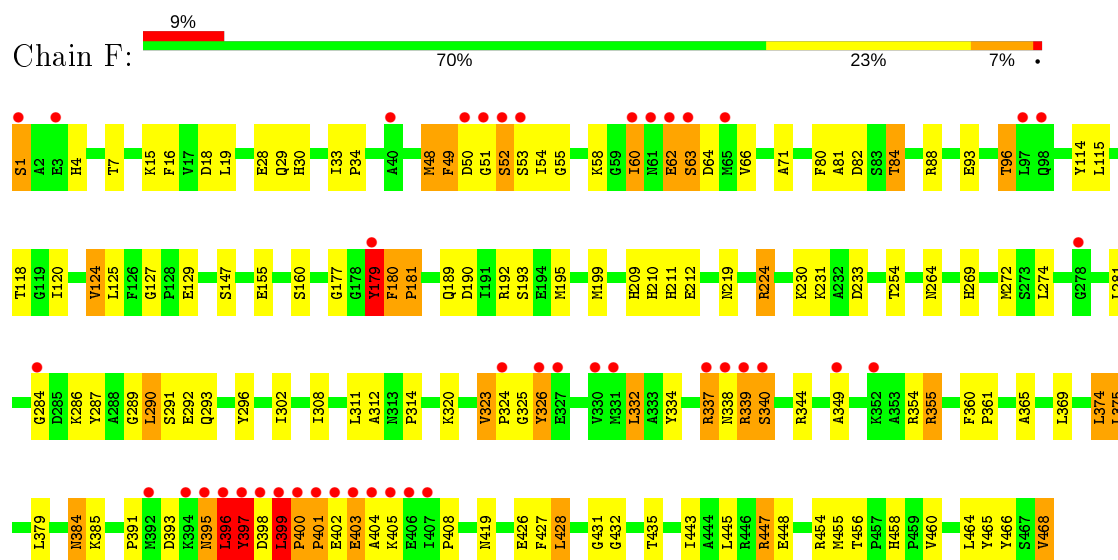


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

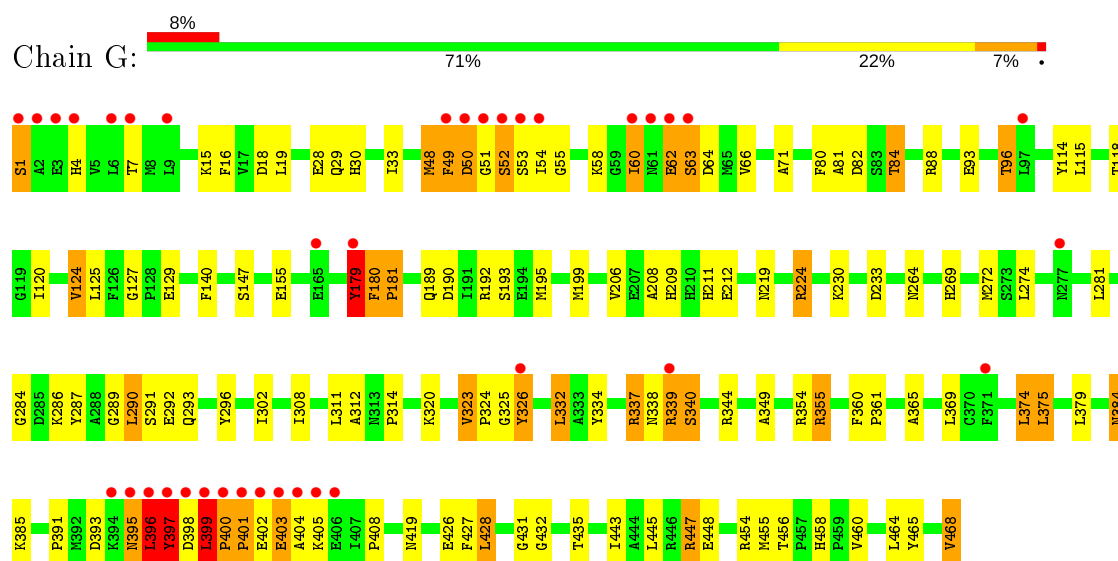




• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

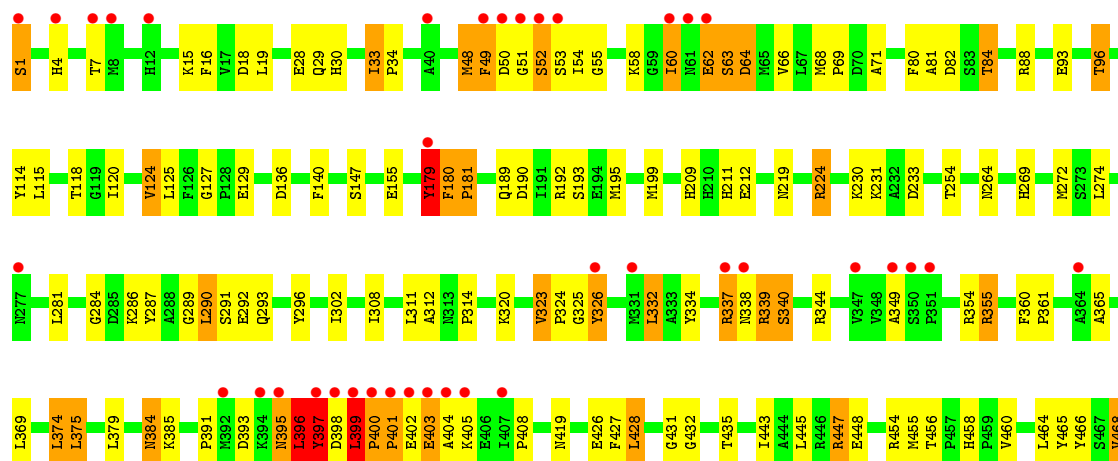


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

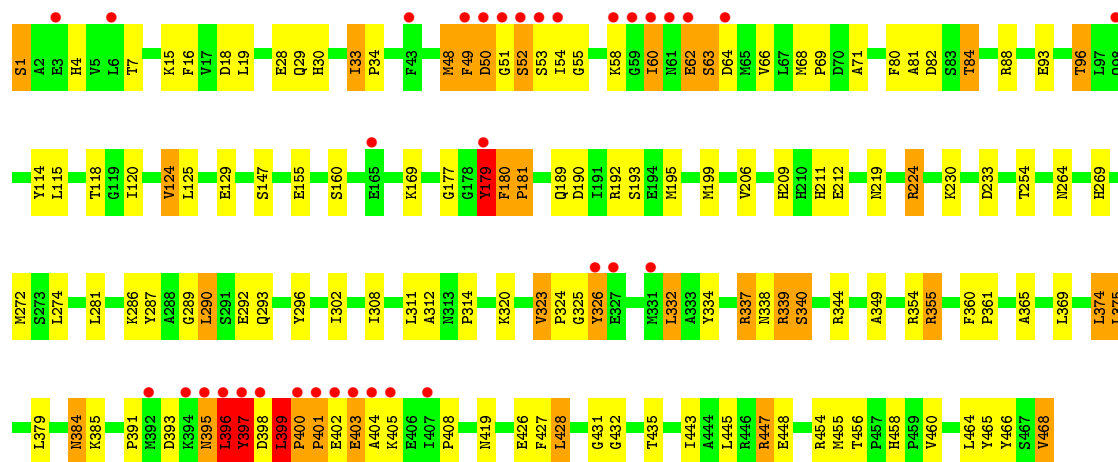


• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)

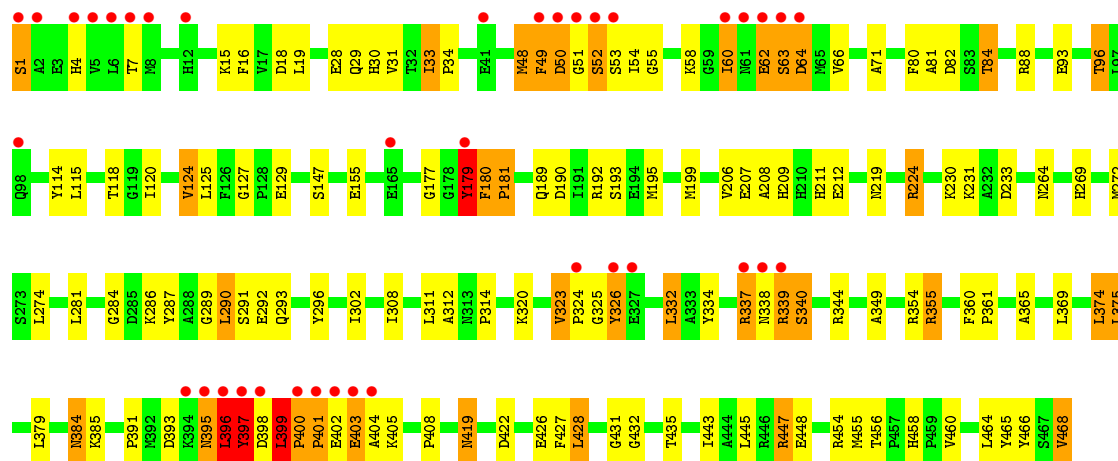




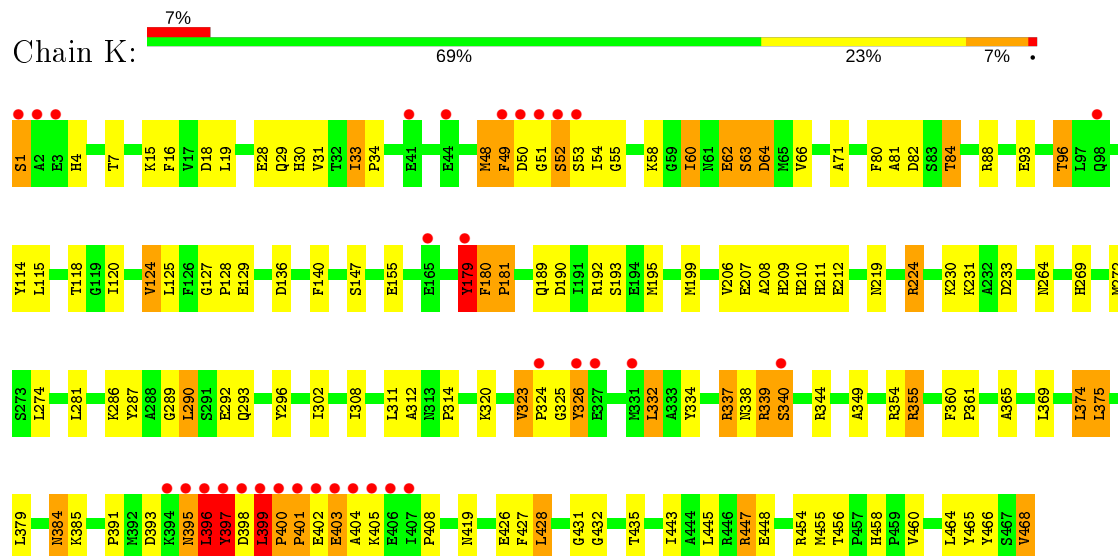
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



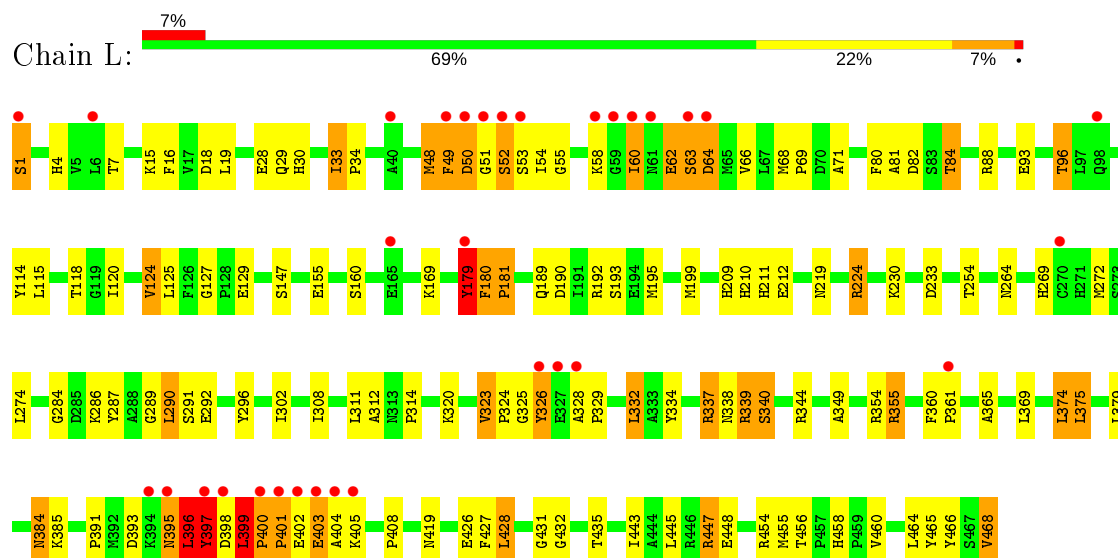
• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



• Molecule 1: PROTEIN (GLUTAMINE SYNTHETASE)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.13Å 132.79Å 196.78Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	32.00 – 2.67 36.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	82.0 (32.00-2.67) 82.0 (36.87-2.70)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.68Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.232 , 0.263 0.229 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	45564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPD, MN, TL, ADP

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	0.52	0/3724	0.85	4/5043 (0.1%)
1	B	0.52	0/3724	0.85	4/5043 (0.1%)
1	C	0.52	0/3724	0.85	4/5043 (0.1%)
1	D	0.52	0/3724	0.85	4/5043 (0.1%)
1	E	0.52	0/3724	0.85	4/5043 (0.1%)
1	F	0.52	0/3724	0.85	4/5043 (0.1%)
1	G	0.52	0/3724	0.85	4/5043 (0.1%)
1	H	0.52	0/3724	0.85	4/5043 (0.1%)
1	I	0.52	0/3724	0.85	4/5043 (0.1%)
1	J	0.52	0/3724	0.85	4/5043 (0.1%)
1	K	0.52	0/3724	0.85	4/5043 (0.1%)
1	L	0.52	0/3724	0.85	4/5043 (0.1%)
All	All	0.52	0/44688	0.85	48/60516 (0.1%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	TYR	CB-CG-CD1	6.17	124.70	121.00
1	K	179	TYR	CB-CG-CD1	6.14	124.69	121.00
1	J	179	TYR	CB-CG-CD1	6.12	124.67	121.00
1	D	179	TYR	CB-CG-CD1	6.11	124.67	121.00
1	I	179	TYR	CB-CG-CD1	6.10	124.66	121.00
1	B	179	TYR	CB-CG-CD1	6.10	124.66	121.00
1	L	179	TYR	CB-CG-CD1	6.09	124.66	121.00
1	A	179	TYR	CB-CG-CD1	6.08	124.65	121.00
1	C	179	TYR	CB-CG-CD1	6.05	124.63	121.00
1	H	179	TYR	CB-CG-CD1	6.04	124.62	121.00
1	E	179	TYR	CB-CG-CD1	6.02	124.61	121.00
1	G	179	TYR	CB-CG-CD1	5.96	124.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	J	179	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	I	179	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	K	179	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	E	179	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	F	399	LEU	O-C-N	5.44	131.44	121.10
1	D	179	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	B	179	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	K	399	LEU	O-C-N	5.43	131.41	121.10
1	A	179	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	399	LEU	O-C-N	5.42	131.39	121.10
1	E	399	LEU	O-C-N	5.42	131.39	121.10
1	H	179	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	J	399	LEU	O-C-N	5.42	131.39	121.10
1	B	399	LEU	O-C-N	5.42	131.39	121.10
1	L	399	LEU	O-C-N	5.42	131.39	121.10
1	H	399	LEU	O-C-N	5.41	131.38	121.10
1	D	399	LEU	O-C-N	5.40	131.37	121.10
1	C	399	LEU	O-C-N	5.40	131.37	121.10
1	I	399	LEU	O-C-N	5.39	131.35	121.10
1	G	399	LEU	O-C-N	5.39	131.35	121.10
1	C	179	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	L	179	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	G	179	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	F	397	TYR	CA-CB-CG	5.30	123.47	113.40
1	C	397	TYR	CA-CB-CG	5.30	123.46	113.40
1	I	397	TYR	CA-CB-CG	5.29	123.46	113.40
1	H	397	TYR	CA-CB-CG	5.29	123.45	113.40
1	J	397	TYR	CA-CB-CG	5.29	123.45	113.40
1	A	397	TYR	CA-CB-CG	5.29	123.45	113.40
1	E	397	TYR	CA-CB-CG	5.28	123.44	113.40
1	K	397	TYR	CA-CB-CG	5.28	123.44	113.40
1	B	397	TYR	CA-CB-CG	5.28	123.43	113.40
1	L	397	TYR	CA-CB-CG	5.28	123.42	113.40
1	D	397	TYR	CA-CB-CG	5.27	123.42	113.40
1	G	397	TYR	CA-CB-CG	5.27	123.41	113.40

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	3637	0	3542	186	0
1	B	3637	0	3543	185	0
1	C	3637	0	3543	188	0
1	D	3637	0	3542	180	0
1	E	3637	0	3543	175	0
1	F	3637	0	3543	176	0
1	G	3637	0	3542	176	0
1	H	3637	0	3543	180	0
1	I	3637	0	3542	189	0
1	J	3637	0	3543	193	0
1	K	3637	0	3543	189	0
1	L	3637	0	3543	179	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	27	0	10	4	0
3	B	27	0	10	4	0
3	C	27	0	10	4	0
3	D	27	0	10	4	0
3	E	27	0	10	4	0
3	F	27	0	10	4	0
3	G	27	0	10	4	0
3	H	27	0	10	4	0
3	I	27	0	10	3	0
3	J	27	0	10	4	0
3	K	27	0	10	4	0
3	L	27	0	10	4	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	8	0	14	29	0
5	B	8	0	14	34	0
5	C	8	0	14	33	0
5	D	8	0	14	34	0
5	E	8	0	14	29	0
5	F	8	0	14	34	0
5	G	8	0	14	31	0
5	H	8	0	14	33	0
5	I	8	0	14	35	0
5	J	8	0	14	34	0
5	K	8	0	14	33	0
5	L	8	0	14	32	0
6	A	120	0	0	6	0
6	B	121	0	0	6	0
6	C	119	0	0	5	0
6	D	122	0	0	6	0
6	E	122	0	0	6	0
6	F	121	0	0	5	0
6	G	122	0	0	6	0
6	H	121	0	0	5	0
6	I	122	0	0	6	0
6	J	120	0	0	6	0
6	K	123	0	0	6	0
6	L	119	0	0	6	0
All	All	45564	0	42800	2077	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 24.

All (2077) 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:K:1481:ADP:N9	3:K:1481:ADP:C1'	1.71	1.54
3:I:1479:ADP:N9	3:I:1479:ADP:C1'	1.71	1.54
3:B:1472:ADP:N9	3:B:1472:ADP:C1'	1.71	1.52
3:F:1476:ADP:N9	3:F:1476:ADP:C1'	1.71	1.52
3:E:1475:ADP:N9	3:E:1475:ADP:C1'	1.71	1.51
3:H:1478:ADP:N9	3:H:1478:ADP:C1'	1.71	1.51
3:G:1477:ADP:N9	3:G:1477:ADP:C1'	1.71	1.51
3:C:1473:ADP:C1'	3:C:1473:ADP:N9	1.71	1.50
3:J:1480:ADP:C1'	3:J:1480:ADP:N9	1.71	1.50
3:D:1474:ADP:C1'	3:D:1474:ADP:N9	1.71	1.50
3:L:1482:ADP:N9	3:L:1482:ADP:C1'	1.71	1.49
3:A:1471:ADP:N9	3:A:1471:ADP:C1'	1.71	1.47
1:E:398:ASP:O	1:E:400:PRO:HD3	1.29	1.33
1:J:398:ASP:O	1:J:400:PRO:HD3	1.29	1.33
1:A:398:ASP:O	1:A:400:PRO:HD3	1.29	1.33
1:B:398:ASP:O	1:B:400:PRO:HD3	1.29	1.31
1:D:398:ASP:O	1:D:400:PRO:HD3	1.29	1.30
1:L:398:ASP:O	1:L:400:PRO:HD3	1.29	1.29
1:H:398:ASP:O	1:H:400:PRO:HD3	1.29	1.27
1:K:398:ASP:O	1:K:400:PRO:HD3	1.29	1.27
1:I:398:ASP:O	1:I:400:PRO:HD3	1.29	1.26
1:C:398:ASP:O	1:C:400:PRO:HD3	1.29	1.26
1:F:398:ASP:O	1:F:400:PRO:HD3	1.29	1.24
1:G:398:ASP:O	1:G:400:PRO:HD3	1.29	1.23
1:I:395:ASN:HB3	1:I:399:LEU:CD1	1.69	1.23
1:B:395:ASN:HB3	1:B:399:LEU:CD1	1.69	1.22
1:E:395:ASN:HB3	1:E:399:LEU:CD1	1.69	1.22
1:C:395:ASN:HB3	1:C:399:LEU:CD1	1.69	1.22
1:K:395:ASN:HB3	1:K:399:LEU:CD1	1.69	1.22
1:L:395:ASN:HB3	1:L:399:LEU:CD1	1.69	1.22
1:F:395:ASN:HB3	1:F:399:LEU:CD1	1.70	1.22
1:A:395:ASN:HB3	1:A:399:LEU:CD1	1.69	1.21
1:D:395:ASN:HB3	1:D:399:LEU:CD1	1.69	1.21
1:J:395:ASN:HB3	1:J:399:LEU:CD1	1.69	1.21
1:H:395:ASN:HB3	1:H:399:LEU:CD1	1.69	1.20
1:G:395:ASN:HB3	1:G:399:LEU:CD1	1.70	1.20
1:C:360:PHE:CD2	1:C:361:PRO:HD3	1.78	1.19
1:A:360:PHE:CD2	1:A:361:PRO:HD3	1.78	1.19
1:I:360:PHE:CD2	1:I:361:PRO:HD3	1.78	1.19
1:H:360:PHE:CD2	1:H:361:PRO:HD3	1.78	1.18
1:E:51:GLY:O	1:E:53:SER:N	1.76	1.18
1:L:51:GLY:O	1:L:53:SER:N	1.76	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.78	1.18
1:I:51:GLY:O	1:I:53:SER:N	1.76	1.18
1:K:51:GLY:O	1:K:53:SER:N	1.76	1.18
1:L:360:PHE:CD2	1:L:361:PRO:HD3	1.78	1.18
1:F:360:PHE:CD2	1:F:361:PRO:HD3	1.78	1.18
1:F:51:GLY:O	1:F:53:SER:N	1.77	1.18
1:H:51:GLY:O	1:H:53:SER:N	1.76	1.18
1:K:360:PHE:CD2	1:K:361:PRO:HD3	1.78	1.18
1:A:51:GLY:O	1:A:53:SER:N	1.76	1.18
1:B:51:GLY:O	1:B:53:SER:N	1.76	1.17
1:D:360:PHE:CD2	1:D:361:PRO:HD3	1.78	1.17
1:G:51:GLY:O	1:G:53:SER:N	1.76	1.17
1:J:51:GLY:O	1:J:53:SER:N	1.76	1.17
1:D:51:GLY:O	1:D:53:SER:N	1.77	1.17
1:G:360:PHE:CD2	1:G:361:PRO:HD3	1.78	1.17
1:J:360:PHE:CD2	1:J:361:PRO:HD3	1.78	1.17
1:C:51:GLY:O	1:C:53:SER:N	1.77	1.17
1:B:360:PHE:CD2	1:B:361:PRO:HD3	1.78	1.16
1:I:60:ILE:CG2	1:J:395:ASN:HD21	1.58	1.14
1:G:60:ILE:CG2	1:H:395:ASN:HD21	1.63	1.12
1:A:395:ASN:HD21	1:B:60:ILE:HG21	1.15	1.10
1:A:395:ASN:HD21	1:B:60:ILE:CG2	1.65	1.08
1:I:60:ILE:HG21	1:J:395:ASN:HD21	1.10	1.08
1:C:395:ASN:HD21	1:D:60:ILE:CG2	1.67	1.07
1:L:395:ASN:HB3	1:L:399:LEU:HD11	1.36	1.06
1:F:82:ASP:H	5:F:1488:MPD:C1	1.69	1.06
1:G:60:ILE:HG21	1:H:395:ASN:HD21	1.19	1.06
1:J:395:ASN:HB3	1:J:399:LEU:HD11	1.36	1.06
1:H:82:ASP:H	5:H:1490:MPD:C1	1.69	1.06
1:B:82:ASP:H	5:B:1484:MPD:C1	1.69	1.06
1:E:82:ASP:H	5:E:1487:MPD:C1	1.69	1.06
1:D:82:ASP:H	5:D:1486:MPD:C1	1.69	1.05
1:K:82:ASP:H	5:K:1493:MPD:C1	1.69	1.05
1:C:82:ASP:H	5:C:1485:MPD:C1	1.69	1.05
1:G:82:ASP:H	5:G:1489:MPD:C1	1.69	1.05
1:C:395:ASN:HD21	1:D:60:ILE:HG21	1.20	1.05
1:H:395:ASN:HB3	1:H:399:LEU:HD11	1.36	1.05
1:J:82:ASP:H	5:J:1492:MPD:C1	1.69	1.05
1:B:395:ASN:HB3	1:B:399:LEU:HD11	1.36	1.05
1:I:82:ASP:H	5:I:1491:MPD:C1	1.69	1.04
1:I:395:ASN:HB3	1:I:399:LEU:HD11	1.36	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:82:ASP:H	5:L:1494:MPD:C1	1.69	1.04
1:D:395:ASN:HB3	1:D:399:LEU:HD11	1.36	1.04
1:A:82:ASP:H	5:A:1483:MPD:C1	1.69	1.04
1:C:395:ASN:HB3	1:C:399:LEU:HD11	1.36	1.03
1:F:395:ASN:HB3	1:F:399:LEU:HD11	1.36	1.03
1:K:395:ASN:HB3	1:K:399:LEU:HD11	1.36	1.03
1:A:395:ASN:HB3	1:A:399:LEU:HD11	1.36	1.03
1:G:395:ASN:HB3	1:G:399:LEU:HD11	1.36	1.02
1:E:395:ASN:HB3	1:E:399:LEU:HD11	1.36	1.02
1:J:60:ILE:CG2	1:K:395:ASN:HD21	1.74	1.00
1:K:51:GLY:C	1:K:53:SER:H	1.64	1.00
1:H:51:GLY:C	1:H:53:SER:H	1.65	0.99
1:J:51:GLY:C	1:J:53:SER:H	1.64	0.99
1:I:51:GLY:C	1:I:53:SER:H	1.65	0.97
1:E:51:GLY:C	1:E:53:SER:H	1.65	0.97
1:B:51:GLY:C	1:B:53:SER:H	1.65	0.97
1:D:395:ASN:HD21	1:E:60:ILE:CG2	1.77	0.97
1:L:51:GLY:C	1:L:53:SER:H	1.65	0.96
1:D:51:GLY:C	1:D:53:SER:H	1.64	0.95
1:G:395:ASN:HD21	1:L:60:ILE:HG21	1.28	0.95
1:A:51:GLY:C	1:A:53:SER:H	1.65	0.95
1:C:51:GLY:C	1:C:53:SER:H	1.65	0.94
1:C:82:ASP:O	1:C:84:THR:HG22	1.68	0.94
5:H:1490:MPD:H32	1:I:193:SER:CB	1.97	0.94
1:A:82:ASP:O	1:A:84:THR:HG22	1.68	0.94
1:E:82:ASP:O	1:E:84:THR:HG22	1.68	0.94
1:J:82:ASP:O	1:J:84:THR:HG22	1.68	0.94
1:G:82:ASP:O	1:G:84:THR:HG22	1.68	0.94
1:C:80:PHE:HB3	5:C:1485:MPD:H11	1.50	0.94
1:I:82:ASP:O	1:I:84:THR:HG22	1.68	0.94
1:L:82:ASP:O	1:L:84:THR:HG22	1.68	0.94
1:K:80:PHE:HB3	5:K:1493:MPD:H11	1.50	0.94
1:A:80:PHE:HB3	5:A:1483:MPD:H11	1.50	0.93
1:J:60:ILE:HG21	1:K:395:ASN:HD21	1.32	0.93
1:D:395:ASN:HD21	1:E:60:ILE:HG21	1.33	0.93
1:I:80:PHE:HB3	5:I:1491:MPD:H11	1.50	0.93
1:F:80:PHE:HB3	5:F:1488:MPD:H11	1.50	0.93
1:K:82:ASP:O	1:K:84:THR:HG22	1.68	0.93
1:D:80:PHE:HB3	5:D:1486:MPD:H11	1.50	0.93
1:H:80:PHE:HB3	5:H:1490:MPD:H11	1.50	0.93
1:J:80:PHE:HB3	5:J:1492:MPD:H11	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASN:HB3	1:A:399:LEU:HD12	1.50	0.93
1:C:395:ASN:HB3	1:C:399:LEU:HD12	1.50	0.92
1:G:80:PHE:HB3	5:G:1489:MPD:H11	1.50	0.92
1:H:82:ASP:O	1:H:84:THR:HG22	1.68	0.92
1:L:395:ASN:HB3	1:L:399:LEU:HD12	1.50	0.92
1:C:52:SER:HB3	1:C:63:SER:HB3	1.51	0.92
1:E:80:PHE:HB3	5:E:1487:MPD:H11	1.50	0.92
1:F:82:ASP:O	1:F:84:THR:HG22	1.68	0.92
1:I:395:ASN:HB3	1:I:399:LEU:HD12	1.50	0.92
1:J:52:SER:HB3	1:J:63:SER:HB3	1.51	0.92
1:B:82:ASP:O	1:B:84:THR:HG22	1.68	0.92
1:E:52:SER:HB3	1:E:63:SER:HB3	1.51	0.92
1:A:52:SER:HB3	1:A:63:SER:HB3	1.51	0.92
5:J:1492:MPD:H32	1:K:193:SER:CB	1.99	0.92
1:C:1:SER:HA	1:C:71:ALA:CB	2.00	0.92
1:H:52:SER:HB3	1:H:63:SER:HB3	1.51	0.92
1:L:52:SER:HB3	1:L:63:SER:HB3	1.51	0.92
1:L:80:PHE:HB3	5:L:1494:MPD:H11	1.50	0.92
1:C:82:ASP:H	5:C:1485:MPD:H13	1.34	0.92
1:D:1:SER:HA	1:D:71:ALA:CB	2.00	0.92
1:G:82:ASP:H	5:G:1489:MPD:H13	1.34	0.92
1:H:1:SER:HA	1:H:71:ALA:CB	2.00	0.92
1:L:1:SER:HA	1:L:71:ALA:CB	2.00	0.92
1:D:82:ASP:O	1:D:84:THR:HG22	1.68	0.91
1:K:1:SER:HA	1:K:71:ALA:CB	2.00	0.91
1:K:395:ASN:HB3	1:K:399:LEU:HD12	1.50	0.91
1:D:395:ASN:HB3	1:D:399:LEU:HD12	1.50	0.91
1:F:1:SER:HA	1:F:71:ALA:CB	2.00	0.91
1:G:395:ASN:HD21	1:L:60:ILE:CG2	1.82	0.91
1:B:395:ASN:HB3	1:B:399:LEU:HD12	1.50	0.91
1:B:52:SER:HB3	1:B:63:SER:HB3	1.51	0.91
1:B:80:PHE:HB3	5:B:1484:MPD:H11	1.50	0.91
1:F:395:ASN:HB3	1:F:399:LEU:HD12	1.50	0.91
1:G:51:GLY:C	1:G:53:SER:H	1.65	0.91
1:H:395:ASN:HB3	1:H:399:LEU:HD12	1.50	0.91
1:I:1:SER:HA	1:I:71:ALA:CB	2.00	0.91
1:F:51:GLY:C	1:F:53:SER:H	1.65	0.91
1:J:395:ASN:HB3	1:J:399:LEU:HD12	1.50	0.91
1:K:52:SER:HB3	1:K:63:SER:HB3	1.51	0.91
1:B:1:SER:HA	1:B:71:ALA:CB	2.00	0.91
5:I:1491:MPD:H32	1:J:193:SER:CB	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1:SER:HA	1:J:71:ALA:CB	2.00	0.91
1:L:82:ASP:H	5:L:1494:MPD:H13	1.34	0.91
1:B:82:ASP:H	5:B:1484:MPD:H13	1.34	0.91
1:A:1:SER:HA	1:A:71:ALA:CB	2.00	0.90
1:B:193:SER:CB	5:C:1485:MPD:H32	2.00	0.90
1:D:52:SER:HB3	1:D:63:SER:HB3	1.51	0.90
1:G:52:SER:HB3	1:G:63:SER:HB3	1.51	0.90
1:D:82:ASP:H	5:D:1486:MPD:H13	1.34	0.90
1:H:82:ASP:H	5:H:1490:MPD:H13	1.34	0.90
1:E:1:SER:HA	1:E:71:ALA:CB	2.00	0.90
1:G:395:ASN:HB3	1:G:399:LEU:HD12	1.50	0.90
1:G:1:SER:HA	1:G:71:ALA:CB	2.00	0.90
1:F:458:HIS:HD2	1:F:460:VAL:H	1.20	0.90
1:G:193:SER:CB	5:L:1494:MPD:H32	2.02	0.90
1:E:458:HIS:HD2	1:E:460:VAL:H	1.20	0.89
1:C:458:HIS:HD2	1:C:460:VAL:H	1.20	0.89
1:F:82:ASP:H	5:F:1488:MPD:H13	1.34	0.89
1:J:458:HIS:HD2	1:J:460:VAL:H	1.20	0.89
1:A:82:ASP:H	5:A:1483:MPD:H13	1.34	0.89
1:E:193:SER:CB	5:F:1488:MPD:H32	2.01	0.89
1:E:395:ASN:HB3	1:E:399:LEU:HD12	1.50	0.89
1:A:60:ILE:CG2	1:F:395:ASN:HD21	1.85	0.89
1:J:82:ASP:H	5:J:1492:MPD:H13	1.34	0.89
1:E:82:ASP:H	5:E:1487:MPD:H13	1.34	0.89
1:H:458:HIS:HD2	1:H:460:VAL:H	1.20	0.89
1:I:82:ASP:H	5:I:1491:MPD:H13	1.34	0.89
1:K:82:ASP:H	5:K:1493:MPD:H13	1.34	0.89
1:L:458:HIS:HD2	1:L:460:VAL:H	1.20	0.89
1:G:458:HIS:HD2	1:G:460:VAL:H	1.20	0.89
1:B:458:HIS:HD2	1:B:460:VAL:H	1.20	0.89
1:I:52:SER:HB3	1:I:63:SER:HB3	1.51	0.89
1:D:401:PRO:HB3	1:D:404:ALA:HA	1.56	0.88
1:F:52:SER:HB3	1:F:63:SER:HB3	1.51	0.88
1:A:401:PRO:HB3	1:A:404:ALA:HA	1.56	0.88
1:I:401:PRO:HB3	1:I:404:ALA:HA	1.56	0.87
1:K:401:PRO:HB3	1:K:404:ALA:HA	1.56	0.87
1:I:458:HIS:HD2	1:I:460:VAL:H	1.20	0.87
1:A:193:SER:CB	5:B:1484:MPD:H32	2.05	0.87
1:K:458:HIS:HD2	1:K:460:VAL:H	1.20	0.87
1:B:401:PRO:HB3	1:B:404:ALA:HA	1.56	0.86
1:B:395:ASN:HD21	1:C:60:ILE:CG2	1.88	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1490:MPD:HM3	1:I:190:ASP:OD2	1.75	0.86
1:D:458:HIS:HD2	1:D:460:VAL:H	1.20	0.86
1:G:401:PRO:HB3	1:G:404:ALA:HA	1.56	0.86
1:C:401:PRO:HB3	1:C:404:ALA:HA	1.56	0.86
1:H:401:PRO:HB3	1:H:404:ALA:HA	1.56	0.86
1:E:401:PRO:HB3	1:E:404:ALA:HA	1.56	0.86
1:L:401:PRO:HB3	1:L:404:ALA:HA	1.56	0.86
1:A:224:ARG:HG2	1:A:224:ARG:HH21	1.41	0.85
1:A:458:HIS:HD2	1:A:460:VAL:H	1.20	0.85
1:G:190:ASP:OD2	5:L:1494:MPD:HM3	1.76	0.85
1:L:224:ARG:HG2	1:L:224:ARG:HH21	1.41	0.85
1:H:224:ARG:HH21	1:H:224:ARG:HG2	1.41	0.85
5:K:1493:MPD:HM3	1:L:190:ASP:OD2	1.74	0.85
1:J:401:PRO:HB3	1:J:404:ALA:HA	1.56	0.85
1:J:16:PHE:CD1	5:J:1492:MPD:H52	2.12	0.85
1:B:224:ARG:HH21	1:B:224:ARG:HG2	1.42	0.85
1:E:16:PHE:CD1	5:E:1487:MPD:H52	2.12	0.85
1:F:16:PHE:CD1	5:F:1488:MPD:H52	2.12	0.85
1:F:224:ARG:HH21	1:F:224:ARG:HG2	1.41	0.85
1:L:16:PHE:CD1	5:L:1494:MPD:H52	2.12	0.85
1:D:16:PHE:CD1	5:D:1486:MPD:H52	2.12	0.85
1:I:398:ASP:O	1:I:400:PRO:CD	2.22	0.85
1:I:60:ILE:HG21	1:J:395:ASN:ND2	1.89	0.85
1:B:16:PHE:CD1	5:B:1484:MPD:H52	2.12	0.85
1:E:224:ARG:HG2	1:E:224:ARG:HH21	1.41	0.85
1:G:224:ARG:HH21	1:G:224:ARG:HG2	1.41	0.85
1:C:224:ARG:HH21	1:C:224:ARG:HG2	1.41	0.84
1:F:398:ASP:O	1:F:400:PRO:CD	2.22	0.84
1:G:16:PHE:CD1	5:G:1489:MPD:H52	2.12	0.84
1:J:224:ARG:HG2	1:J:224:ARG:HH21	1.42	0.84
1:H:16:PHE:CD1	5:H:1490:MPD:H52	2.12	0.84
1:C:16:PHE:CD1	5:C:1485:MPD:H52	2.12	0.84
1:D:224:ARG:HH21	1:D:224:ARG:HG2	1.42	0.84
1:A:398:ASP:O	1:A:400:PRO:CD	2.22	0.84
1:F:401:PRO:HB3	1:F:404:ALA:HA	1.56	0.84
1:J:51:GLY:C	1:J:53:SER:N	2.26	0.84
1:K:16:PHE:CD1	5:K:1493:MPD:H52	2.12	0.84
1:A:16:PHE:CD1	5:A:1483:MPD:H52	2.12	0.84
1:I:224:ARG:HG2	1:I:224:ARG:HH21	1.41	0.84
1:E:51:GLY:C	1:E:53:SER:N	2.26	0.83
1:A:60:ILE:HG21	1:F:395:ASN:HD21	1.39	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:16:PHE:CD1	5:I:1491:MPD:H52	2.12	0.83
1:E:398:ASP:O	1:E:400:PRO:CD	2.22	0.83
1:L:51:GLY:C	1:L:53:SER:N	2.26	0.83
1:K:224:ARG:HH21	1:K:224:ARG:HG2	1.41	0.83
1:K:398:ASP:O	1:K:400:PRO:CD	2.22	0.83
1:H:82:ASP:H	5:H:1490:MPD:H12	1.44	0.83
1:L:398:ASP:O	1:L:400:PRO:CD	2.22	0.83
5:A:1483:MPD:HM3	1:F:190:ASP:OD2	1.78	0.83
1:B:398:ASP:O	1:B:400:PRO:CD	2.22	0.83
1:A:395:ASN:ND2	1:B:60:ILE:HG21	1.94	0.82
1:A:82:ASP:H	5:A:1483:MPD:H12	1.44	0.82
1:G:398:ASP:O	1:G:400:PRO:CD	2.22	0.82
1:J:398:ASP:O	1:J:400:PRO:CD	2.22	0.82
5:H:1490:MPD:H32	1:I:193:SER:HB2	1.61	0.82
1:E:323:VAL:HG21	1:K:455:MET:HG2	1.60	0.82
1:D:398:ASP:O	1:D:400:PRO:CD	2.22	0.82
5:K:1493:MPD:H32	1:L:193:SER:CB	2.08	0.82
1:K:340:SER:HB3	1:K:396:LEU:HB3	1.62	0.82
1:G:340:SER:HB3	1:G:396:LEU:HB3	1.62	0.81
1:A:340:SER:HB3	1:A:396:LEU:HB3	1.62	0.81
1:A:81:ALA:N	5:A:1483:MPD:H13	1.96	0.81
1:D:395:ASN:CB	1:D:399:LEU:HD11	2.11	0.81
1:G:395:ASN:CB	1:G:399:LEU:HD11	2.11	0.81
1:E:340:SER:HB3	1:E:396:LEU:HB3	1.62	0.81
1:I:82:ASP:H	5:I:1491:MPD:H12	1.44	0.81
1:K:395:ASN:CB	1:K:399:LEU:HD11	2.10	0.81
1:C:81:ALA:N	5:C:1485:MPD:H13	1.96	0.81
1:J:81:ALA:N	5:J:1492:MPD:H13	1.96	0.81
5:J:1492:MPD:O2	1:K:190:ASP:HA	1.80	0.81
1:L:82:ASP:H	5:L:1494:MPD:H12	1.44	0.81
1:A:395:ASN:CB	1:A:399:LEU:HD11	2.10	0.81
1:E:81:ALA:N	5:E:1487:MPD:H13	1.96	0.81
1:G:82:ASP:H	5:G:1489:MPD:H12	1.44	0.81
1:K:81:ALA:N	5:K:1493:MPD:H13	1.96	0.81
1:E:190:ASP:HA	5:F:1488:MPD:O2	1.81	0.81
1:H:81:ALA:N	5:H:1490:MPD:H13	1.96	0.81
1:J:395:ASN:CB	1:J:399:LEU:HD11	2.10	0.81
1:K:82:ASP:H	5:K:1493:MPD:H12	1.44	0.81
1:H:340:SER:HB3	1:H:396:LEU:HB3	1.62	0.81
1:I:81:ALA:N	5:I:1491:MPD:H13	1.96	0.81
1:L:340:SER:HB3	1:L:396:LEU:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:395:ASN:CB	1:H:399:LEU:HD11	2.10	0.81
1:J:82:ASP:H	5:J:1492:MPD:H12	1.44	0.81
1:F:395:ASN:CB	1:F:399:LEU:HD11	2.10	0.81
1:H:398:ASP:O	1:H:400:PRO:CD	2.22	0.81
1:I:395:ASN:CB	1:I:399:LEU:HD11	2.10	0.81
5:J:1492:MPD:H32	1:K:193:SER:HB2	1.62	0.81
1:F:455:MET:HG2	1:L:323:VAL:HG21	1.62	0.81
1:C:395:ASN:CB	1:C:399:LEU:HD11	2.10	0.81
1:C:398:ASP:O	1:C:400:PRO:CD	2.22	0.80
1:C:193:SER:CB	5:D:1486:MPD:H32	2.10	0.80
1:L:81:ALA:N	5:L:1494:MPD:H13	1.96	0.80
1:F:82:ASP:H	5:F:1488:MPD:H12	1.44	0.80
1:C:340:SER:HB3	1:C:396:LEU:HB3	1.62	0.80
1:L:395:ASN:CB	1:L:399:LEU:HD11	2.10	0.80
1:D:82:ASP:H	5:D:1486:MPD:H12	1.44	0.80
1:C:190:ASP:OD2	5:D:1486:MPD:HM3	1.81	0.80
1:B:81:ALA:N	5:B:1484:MPD:H13	1.96	0.80
1:B:395:ASN:CB	1:B:399:LEU:HD11	2.10	0.80
1:F:340:SER:HB3	1:F:396:LEU:HB3	1.62	0.80
1:F:81:ALA:N	5:F:1488:MPD:H13	1.96	0.80
1:G:190:ASP:HA	5:L:1494:MPD:O2	1.81	0.80
1:I:340:SER:HB3	1:I:396:LEU:HB3	1.62	0.80
1:B:340:SER:HB3	1:B:396:LEU:HB3	1.62	0.80
1:D:340:SER:HB3	1:D:396:LEU:HB3	1.62	0.80
1:D:81:ALA:N	5:D:1486:MPD:H13	1.96	0.80
1:E:82:ASP:H	5:E:1487:MPD:H12	1.44	0.80
1:F:402:GLU:HB2	1:F:405:LYS:HD3	1.64	0.80
1:C:82:ASP:H	5:C:1485:MPD:H12	1.44	0.79
1:G:193:SER:HB2	5:L:1494:MPD:H32	1.62	0.79
1:L:402:GLU:HB2	1:L:405:LYS:HD3	1.64	0.79
1:A:402:GLU:HB2	1:A:405:LYS:HD3	1.64	0.79
1:B:82:ASP:H	5:B:1484:MPD:H12	1.44	0.79
1:E:395:ASN:CB	1:E:399:LEU:HD11	2.10	0.79
1:G:81:ALA:N	5:G:1489:MPD:H13	1.96	0.79
1:J:340:SER:HB3	1:J:396:LEU:HB3	1.62	0.79
1:G:402:GLU:HB2	1:G:405:LYS:HD3	1.64	0.78
1:A:323:VAL:HG21	1:G:455:MET:HG2	1.64	0.78
1:I:60:ILE:CG2	1:J:395:ASN:ND2	2.42	0.78
1:A:51:GLY:C	1:A:53:SER:N	2.26	0.78
5:I:1491:MPD:H32	1:J:193:SER:HB2	1.65	0.78
1:J:402:GLU:HB2	1:J:405:LYS:HD3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:402:GLU:HB2	1:K:405:LYS:HD3	1.64	0.78
1:L:52:SER:CB	1:L:63:SER:HB3	2.13	0.78
1:D:52:SER:CB	1:D:63:SER:HB3	2.13	0.78
1:J:52:SER:CB	1:J:63:SER:HB3	2.13	0.78
1:K:52:SER:CB	1:K:63:SER:HB3	2.13	0.78
1:K:60:ILE:CG2	1:L:395:ASN:HD21	1.96	0.78
1:B:52:SER:CB	1:B:63:SER:HB3	2.13	0.78
1:H:60:ILE:CG2	1:I:395:ASN:HD21	1.96	0.78
1:H:395:ASN:CB	1:H:399:LEU:CD1	2.60	0.78
1:I:402:GLU:HB2	1:I:405:LYS:HD3	1.64	0.78
1:I:52:SER:CB	1:I:63:SER:HB3	2.13	0.78
1:K:51:GLY:C	1:K:53:SER:N	2.26	0.78
1:B:190:ASP:HA	5:C:1485:MPD:O2	1.84	0.77
1:K:1:SER:HA	1:K:71:ALA:HB1	1.66	0.77
1:C:402:GLU:HB2	1:C:405:LYS:HD3	1.64	0.77
1:D:402:GLU:HB2	1:D:405:LYS:HD3	1.64	0.77
1:A:1:SER:HA	1:A:71:ALA:HB1	1.66	0.77
1:E:402:GLU:HB2	1:E:405:LYS:HD3	1.64	0.77
1:F:395:ASN:CB	1:F:399:LEU:CD1	2.60	0.77
1:G:52:SER:CB	1:G:63:SER:HB3	2.13	0.77
5:J:1492:MPD:HM3	1:K:190:ASP:OD2	1.82	0.77
1:F:1:SER:HA	1:F:71:ALA:HB1	1.66	0.77
1:F:52:SER:CB	1:F:63:SER:HB3	2.13	0.77
1:E:395:ASN:HD21	1:F:60:ILE:CG2	1.98	0.77
1:B:402:GLU:HB2	1:B:405:LYS:HD3	1.64	0.77
1:B:395:ASN:HD21	1:C:60:ILE:HG21	1.48	0.77
1:B:323:VAL:HG21	1:H:455:MET:HG2	1.66	0.77
1:A:52:SER:CB	1:A:63:SER:HB3	2.13	0.77
1:B:51:GLY:C	1:B:53:SER:N	2.26	0.77
1:H:402:GLU:HB2	1:H:405:LYS:HD3	1.64	0.77
1:H:52:SER:CB	1:H:63:SER:HB3	2.13	0.77
1:H:1:SER:HA	1:H:71:ALA:HB1	1.66	0.77
1:I:1:SER:HA	1:I:71:ALA:HB3	1.67	0.77
1:A:190:ASP:HA	5:B:1484:MPD:O2	1.84	0.77
1:E:1:SER:HA	1:E:71:ALA:HB1	1.66	0.77
1:I:1:SER:HA	1:I:71:ALA:HB1	1.66	0.77
1:B:1:SER:HA	1:B:71:ALA:HB3	1.67	0.77
1:E:52:SER:CB	1:E:63:SER:HB3	2.13	0.77
1:J:395:ASN:CB	1:J:399:LEU:CD1	2.60	0.77
1:G:1:SER:HA	1:G:71:ALA:HB3	1.67	0.76
1:J:1:SER:HA	1:J:71:ALA:HB1	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1:SER:HA	1:L:71:ALA:HB3	1.67	0.76
1:C:52:SER:CB	1:C:63:SER:HB3	2.13	0.76
5:G:1489:MPD:H32	1:H:193:SER:CB	2.14	0.76
1:I:395:ASN:CB	1:I:399:LEU:CD1	2.60	0.76
1:L:1:SER:HA	1:L:71:ALA:HB1	1.66	0.76
1:A:52:SER:HB3	1:A:63:SER:CB	2.16	0.76
1:C:455:MET:HG2	1:I:323:VAL:HG21	1.66	0.76
1:B:395:ASN:CB	1:B:399:LEU:CD1	2.60	0.76
1:B:1:SER:HA	1:B:71:ALA:HB1	1.66	0.76
1:C:52:SER:HB3	1:C:63:SER:CB	2.16	0.76
1:E:395:ASN:CB	1:E:399:LEU:CD1	2.60	0.76
1:G:1:SER:HA	1:G:71:ALA:HB1	1.66	0.76
1:J:1:SER:HA	1:J:71:ALA:HB3	1.67	0.76
1:G:52:SER:HB3	1:G:63:SER:CB	2.16	0.76
1:K:52:SER:HB3	1:K:63:SER:CB	2.16	0.76
1:C:1:SER:HA	1:C:71:ALA:HB3	1.67	0.76
1:E:52:SER:HB3	1:E:63:SER:CB	2.16	0.76
1:B:190:ASP:OD2	5:C:1485:MPD:HM3	1.86	0.76
1:B:193:SER:HB2	5:C:1485:MPD:H32	1.67	0.76
1:D:323:VAL:HG21	1:J:455:MET:HG2	1.68	0.76
1:D:1:SER:HA	1:D:71:ALA:HB1	1.66	0.76
1:C:395:ASN:ND2	1:D:60:ILE:HG21	2.00	0.76
1:E:189:GLN:HG3	5:F:1488:MPD:HM1	1.68	0.76
1:A:189:GLN:HG3	5:B:1484:MPD:HM1	1.68	0.75
1:C:1:SER:HA	1:C:71:ALA:HB1	1.66	0.75
3:A:1471:ADP:H1'	3:A:1471:ADP:N9	1.99	0.75
1:G:60:ILE:HG21	1:H:395:ASN:ND2	1.97	0.75
3:H:1478:ADP:N9	3:H:1478:ADP:H1'	1.99	0.75
1:K:80:PHE:HB3	5:K:1493:MPD:C1	2.17	0.75
5:I:1491:MPD:O2	1:J:190:ASP:HA	1.85	0.75
1:A:80:PHE:HB3	5:A:1483:MPD:C1	2.17	0.75
1:F:52:SER:HB3	1:F:63:SER:CB	2.16	0.75
1:I:52:SER:HB3	1:I:63:SER:CB	2.16	0.75
3:K:1481:ADP:N9	3:K:1481:ADP:H1'	1.98	0.75
1:B:52:SER:HB3	1:B:63:SER:CB	2.16	0.75
1:D:1:SER:HA	1:D:71:ALA:HB3	1.67	0.75
1:F:1:SER:HA	1:F:71:ALA:HB3	1.67	0.75
1:G:323:VAL:O	1:G:325:GLY:N	2.20	0.75
1:L:52:SER:HB3	1:L:63:SER:CB	2.16	0.75
1:A:395:ASN:ND2	1:B:60:ILE:CG2	2.48	0.75
1:F:80:PHE:HB3	5:F:1488:MPD:C1	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1491:MPD:HM3	1:J:190:ASP:OD2	1.87	0.75
1:J:52:SER:HB3	1:J:63:SER:CB	2.16	0.75
1:L:80:PHE:HB3	5:L:1494:MPD:C1	2.17	0.75
1:A:323:VAL:O	1:A:325:GLY:N	2.20	0.75
1:C:323:VAL:O	1:C:325:GLY:N	2.20	0.75
1:D:190:ASP:OD2	5:E:1487:MPD:HM3	1.85	0.75
1:E:193:SER:HB2	5:F:1488:MPD:H32	1.67	0.75
1:I:80:PHE:HB3	5:I:1491:MPD:C1	2.17	0.75
1:A:1:SER:HA	1:A:71:ALA:HB3	1.67	0.75
1:D:323:VAL:O	1:D:325:GLY:N	2.20	0.75
1:D:80:PHE:HB3	5:D:1486:MPD:C1	2.17	0.75
1:E:1:SER:HA	1:E:71:ALA:HB3	1.67	0.75
1:C:80:PHE:HB3	5:C:1485:MPD:C1	2.17	0.74
1:D:52:SER:HB3	1:D:63:SER:CB	2.16	0.74
1:I:323:VAL:O	1:I:325:GLY:N	2.20	0.74
5:K:1493:MPD:H32	1:L:193:SER:HB2	1.69	0.74
1:B:189:GLN:HG3	5:C:1485:MPD:HM1	1.69	0.74
1:H:52:SER:HB3	1:H:63:SER:CB	2.16	0.74
1:K:1:SER:HA	1:K:71:ALA:HB3	1.67	0.74
1:B:80:PHE:HB3	5:B:1484:MPD:C1	2.17	0.74
3:C:1473:ADP:H1'	3:C:1473:ADP:N9	1.99	0.74
1:C:190:ASP:HA	5:D:1486:MPD:O2	1.87	0.74
1:H:80:PHE:HB3	5:H:1490:MPD:C1	2.17	0.74
1:J:323:VAL:O	1:J:325:GLY:N	2.20	0.74
1:K:323:VAL:O	1:K:325:GLY:N	2.20	0.74
1:L:323:VAL:O	1:L:325:GLY:N	2.20	0.74
1:H:179:TYR:O	1:H:181:PRO:CD	2.36	0.74
1:H:323:VAL:O	1:H:325:GLY:N	2.20	0.74
1:K:395:ASN:CB	1:K:399:LEU:CD1	2.60	0.74
1:E:179:TYR:O	1:E:181:PRO:CD	2.36	0.74
1:E:323:VAL:O	1:E:325:GLY:N	2.20	0.74
1:G:60:ILE:CG2	1:H:395:ASN:ND2	2.47	0.74
1:L:179:TYR:O	1:L:181:PRO:CD	2.36	0.74
1:A:179:TYR:O	1:A:181:PRO:CD	2.36	0.74
1:H:1:SER:HA	1:H:71:ALA:HB3	1.67	0.74
1:B:455:MET:HG2	1:H:323:VAL:HG21	1.69	0.74
1:J:80:PHE:HB3	5:J:1492:MPD:C1	2.17	0.74
1:E:190:ASP:OD2	5:F:1488:MPD:HM3	1.86	0.74
1:D:179:TYR:O	1:D:181:PRO:CD	2.36	0.73
1:F:323:VAL:O	1:F:325:GLY:N	2.20	0.73
1:G:179:TYR:O	1:G:181:PRO:CD	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:TYR:O	1:C:181:PRO:CD	2.36	0.73
1:E:80:PHE:HB3	5:E:1487:MPD:C1	2.17	0.73
1:F:51:GLY:C	1:F:53:SER:N	2.26	0.73
1:A:455:MET:HG2	1:G:323:VAL:HG21	1.69	0.73
1:H:60:ILE:HG21	1:I:395:ASN:HD21	1.53	0.73
1:I:179:TYR:O	1:I:181:PRO:CD	2.36	0.73
1:A:340:SER:CB	1:A:396:LEU:HB3	2.19	0.73
1:K:179:TYR:O	1:K:181:PRO:CD	2.36	0.73
5:K:1493:MPD:O2	1:L:190:ASP:HA	1.87	0.73
1:B:323:VAL:O	1:B:325:GLY:N	2.20	0.73
5:G:1489:MPD:HM1	1:H:189:GLN:HG3	1.71	0.73
1:B:179:TYR:O	1:B:181:PRO:CD	2.36	0.73
3:E:1475:ADP:H1'	3:E:1475:ADP:N9	1.98	0.73
1:B:340:SER:CB	1:B:396:LEU:HB3	2.19	0.73
1:E:189:GLN:HG3	5:F:1488:MPD:CM	2.19	0.73
1:E:340:SER:CB	1:E:396:LEU:HB3	2.19	0.73
1:H:340:SER:CB	1:H:396:LEU:HB3	2.19	0.73
1:K:340:SER:CB	1:K:396:LEU:HB3	2.19	0.73
1:C:51:GLY:C	1:C:53:SER:N	2.26	0.73
1:G:80:PHE:HB3	5:G:1489:MPD:C1	2.17	0.73
1:F:323:VAL:HG21	1:L:455:MET:HG2	1.71	0.73
1:A:395:ASN:CB	1:A:399:LEU:CD1	2.60	0.72
1:J:179:TYR:O	1:J:181:PRO:CD	2.36	0.72
1:D:340:SER:CB	1:D:396:LEU:HB3	2.19	0.72
1:F:179:TYR:O	1:F:181:PRO:CD	2.36	0.72
5:H:1490:MPD:O2	1:I:190:ASP:HA	1.87	0.72
1:C:180:PHE:HB3	1:D:29:GLN:HB3	1.72	0.72
1:C:340:SER:CB	1:C:396:LEU:HB3	2.19	0.72
1:A:193:SER:HB2	5:B:1484:MPD:H32	1.70	0.72
1:I:29:GLN:HB3	1:J:180:PHE:HB3	1.71	0.72
1:E:395:ASN:HD21	1:F:60:ILE:HG21	1.55	0.72
1:L:395:ASN:CB	1:L:399:LEU:CD1	2.60	0.72
1:A:189:GLN:HG3	5:B:1484:MPD:CM	2.20	0.72
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.25	0.72
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.25	0.72
1:F:340:SER:CB	1:F:396:LEU:HB3	2.19	0.72
1:G:340:SER:CB	1:G:396:LEU:HB3	2.19	0.72
1:I:340:SER:CB	1:I:396:LEU:HB3	2.19	0.72
1:B:189:GLN:HG3	5:C:1485:MPD:CM	2.20	0.71
1:L:340:SER:CB	1:L:396:LEU:HB3	2.19	0.71
3:J:1480:ADP:H1'	3:J:1480:ADP:N9	1.99	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.25	0.71
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.25	0.71
1:C:395:ASN:CB	1:C:399:LEU:CD1	2.60	0.71
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.25	0.71
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.25	0.71
1:C:323:VAL:HG21	1:I:455:MET:HG2	1.70	0.71
1:C:193:SER:HB2	5:D:1486:MPD:H32	1.72	0.71
5:I:1491:MPD:HM1	1:J:189:GLN:HG3	1.71	0.71
1:J:340:SER:CB	1:J:396:LEU:HB3	2.19	0.71
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.25	0.71
1:K:60:ILE:HG21	1:L:395:ASN:HD21	1.55	0.71
5:J:1492:MPD:HM1	1:K:189:GLN:HG3	1.73	0.71
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.25	0.71
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.25	0.71
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.25	0.71
1:G:395:ASN:CB	1:G:399:LEU:CD1	2.60	0.71
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.25	0.70
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.25	0.70
5:I:1491:MPD:CM	1:J:189:GLN:HG3	2.21	0.70
1:A:190:ASP:OD2	5:B:1484:MPD:HM3	1.89	0.70
1:D:455:MET:HG2	1:J:323:VAL:HG21	1.73	0.70
5:G:1489:MPD:HM3	1:H:190:ASP:OD2	1.91	0.70
5:G:1489:MPD:O2	1:H:190:ASP:HA	1.90	0.70
3:I:1479:ADP:H1'	3:I:1479:ADP:N9	1.99	0.70
1:D:190:ASP:HA	5:E:1487:MPD:O2	1.91	0.70
3:F:1476:ADP:H1'	3:F:1476:ADP:N9	1.98	0.70
1:E:455:MET:HG2	1:K:323:VAL:HG21	1.72	0.69
1:A:398:ASP:C	1:A:400:PRO:HD3	2.13	0.69
1:D:1:SER:CA	1:D:71:ALA:HB1	2.23	0.69
5:A:1483:MPD:O2	1:F:190:ASP:HA	1.92	0.69
1:F:1:SER:CA	1:F:71:ALA:HB1	2.23	0.69
1:A:1:SER:CA	1:A:71:ALA:HB1	2.23	0.69
1:A:211:HIS:HD2	1:A:212:GLU:O	1.76	0.69
1:B:1:SER:CA	1:B:71:ALA:HB1	2.23	0.69
1:J:211:HIS:HD2	1:J:212:GLU:O	1.76	0.69
5:A:1483:MPD:H32	1:F:193:SER:CB	2.23	0.69
1:G:211:HIS:HD2	1:G:212:GLU:O	1.76	0.69
1:H:1:SER:CA	1:H:71:ALA:HB1	2.23	0.69
3:B:1472:ADP:H1'	3:B:1472:ADP:N9	1.99	0.69
1:E:211:HIS:HD2	1:E:212:GLU:O	1.76	0.69
5:J:1492:MPD:CM	1:K:189:GLN:HG3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:HIS:HD2	1:F:212:GLU:O	1.76	0.69
1:H:211:HIS:HD2	1:H:212:GLU:O	1.76	0.69
1:I:398:ASP:C	1:I:400:PRO:HD3	2.13	0.69
1:J:1:SER:CA	1:J:71:ALA:HB1	2.23	0.69
1:K:211:HIS:HD2	1:K:212:GLU:O	1.76	0.69
1:C:1:SER:CA	1:C:71:ALA:HB1	2.23	0.68
1:K:1:SER:CA	1:K:71:ALA:HB1	2.23	0.68
1:L:1:SER:CA	1:L:71:ALA:HB1	2.23	0.68
1:C:398:ASP:C	1:C:400:PRO:HD3	2.13	0.68
1:G:1:SER:CA	1:G:71:ALA:HB1	2.23	0.68
1:I:1:SER:CA	1:I:71:ALA:HB1	2.23	0.68
1:A:397:TYR:CE1	1:A:401:PRO:HD3	2.29	0.68
1:C:211:HIS:HD2	1:C:212:GLU:O	1.76	0.68
1:J:397:TYR:CE1	1:J:401:PRO:HD3	2.29	0.68
1:B:211:HIS:HD2	1:B:212:GLU:O	1.76	0.68
1:C:397:TYR:CE1	1:C:401:PRO:HD3	2.29	0.68
1:D:193:SER:CB	5:E:1487:MPD:H32	2.22	0.68
1:D:395:ASN:CB	1:D:399:LEU:CD1	2.60	0.68
1:D:397:TYR:CE1	1:D:401:PRO:HD3	2.29	0.68
1:E:224:ARG:CG	1:E:224:ARG:HH21	2.07	0.68
1:G:397:TYR:CE1	1:G:401:PRO:HD3	2.29	0.68
1:I:211:HIS:HD2	1:I:212:GLU:O	1.76	0.68
1:I:397:TYR:CE1	1:I:401:PRO:HD3	2.29	0.68
1:K:458:HIS:CD2	1:K:460:VAL:H	2.09	0.68
1:L:211:HIS:HD2	1:L:212:GLU:O	1.76	0.68
1:K:224:ARG:HH21	1:K:224:ARG:CG	2.07	0.68
1:L:398:ASP:C	1:L:400:PRO:HD3	2.13	0.68
1:E:398:ASP:C	1:E:400:PRO:HD3	2.13	0.68
5:G:1489:MPD:CM	1:H:189:GLN:HG3	2.24	0.68
1:K:397:TYR:CE1	1:K:401:PRO:HD3	2.29	0.68
1:E:1:SER:CA	1:E:71:ALA:HB1	2.23	0.67
1:L:397:TYR:CE1	1:L:401:PRO:HD3	2.29	0.67
1:D:129:GLU:OE2	1:D:269:HIS:HB2	1.95	0.67
1:D:211:HIS:HD2	1:D:212:GLU:O	1.76	0.67
3:L:1482:ADP:N9	3:L:1482:ADP:H1'	1.99	0.67
1:L:458:HIS:CD2	1:L:460:VAL:H	2.09	0.67
1:E:397:TYR:CE1	1:E:401:PRO:HD3	2.29	0.67
1:F:398:ASP:C	1:F:400:PRO:HD3	2.13	0.67
1:K:129:GLU:OE2	1:K:269:HIS:HB2	1.95	0.67
1:J:398:ASP:C	1:J:400:PRO:HD3	2.13	0.67
3:D:1474:ADP:H1'	3:D:1474:ADP:N9	1.99	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:129:GLU:OE2	1:I:269:HIS:HB2	1.95	0.67
1:A:224:ARG:CG	1:A:224:ARG:HH21	2.07	0.67
1:B:224:ARG:HH21	1:B:224:ARG:CG	2.07	0.67
1:G:129:GLU:OE2	1:G:269:HIS:HB2	1.95	0.67
1:B:129:GLU:OE2	1:B:269:HIS:HB2	1.95	0.67
1:F:397:TYR:CE1	1:F:401:PRO:HD3	2.29	0.67
1:F:1:SER:C	1:F:71:ALA:HB1	2.15	0.67
1:G:458:HIS:CD2	1:G:460:VAL:H	2.10	0.67
1:J:129:GLU:OE2	1:J:269:HIS:HB2	1.95	0.67
1:J:224:ARG:HH21	1:J:224:ARG:CG	2.07	0.67
1:L:129:GLU:OE2	1:L:269:HIS:HB2	1.95	0.67
1:D:224:ARG:HH21	1:D:224:ARG:CG	2.07	0.67
1:F:129:GLU:OE2	1:F:269:HIS:HB2	1.95	0.67
1:F:224:ARG:HH21	1:F:224:ARG:CG	2.07	0.67
1:H:224:ARG:HH21	1:H:224:ARG:CG	2.07	0.67
1:H:82:ASP:HB2	5:H:1490:MPD:H12	1.77	0.67
1:A:1:SER:C	1:A:71:ALA:HB1	2.15	0.67
1:C:129:GLU:OE2	1:C:269:HIS:HB2	1.95	0.67
1:E:1:SER:C	1:E:71:ALA:HB1	2.15	0.67
1:G:1:SER:C	1:G:71:ALA:HB1	2.15	0.67
1:H:1:SER:C	1:H:71:ALA:HB1	2.15	0.67
1:H:397:TYR:CE1	1:H:401:PRO:HD3	2.29	0.67
1:J:82:ASP:HB2	5:J:1492:MPD:H12	1.77	0.67
1:E:129:GLU:OE2	1:E:269:HIS:HB2	1.95	0.66
1:H:458:HIS:CD2	1:H:460:VAL:H	2.09	0.66
1:B:82:ASP:HB2	5:B:1484:MPD:H12	1.77	0.66
1:D:82:ASP:HB2	5:D:1486:MPD:H12	1.77	0.66
1:I:1:SER:C	1:I:71:ALA:HB1	2.15	0.66
1:B:397:TYR:CE1	1:B:401:PRO:HD3	2.29	0.66
1:C:458:HIS:CD2	1:C:460:VAL:H	2.09	0.66
1:F:82:ASP:HB2	5:F:1488:MPD:H12	1.77	0.66
1:H:129:GLU:OE2	1:H:269:HIS:HB2	1.95	0.66
1:L:1:SER:C	1:L:71:ALA:HB1	2.15	0.66
1:G:180:PHE:HB3	1:L:29:GLN:HB3	1.77	0.66
1:B:398:ASP:C	1:B:400:PRO:HD3	2.13	0.66
1:C:224:ARG:HH21	1:C:224:ARG:CG	2.07	0.66
1:E:458:HIS:CD2	1:E:460:VAL:H	2.10	0.66
3:G:1477:ADP:N9	3:G:1477:ADP:H1'	1.98	0.66
1:L:403:GLU:HG2	1:L:403:GLU:O	1.96	0.66
1:A:129:GLU:OE2	1:A:269:HIS:HB2	1.95	0.66
1:B:1:SER:C	1:B:71:ALA:HB1	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:29:GLN:HB3	1:K:180:PHE:HB3	1.77	0.66
1:D:1:SER:C	1:D:71:ALA:HB1	2.15	0.66
1:G:224:ARG:CG	1:G:224:ARG:HH21	2.07	0.66
1:E:82:ASP:HB2	5:E:1487:MPD:H12	1.77	0.66
1:J:1:SER:C	1:J:71:ALA:HB1	2.15	0.66
1:K:1:SER:C	1:K:71:ALA:HB1	2.15	0.66
1:C:82:ASP:HB2	5:C:1485:MPD:H12	1.77	0.66
1:F:458:HIS:CD2	1:F:460:VAL:H	2.10	0.66
1:I:397:TYR:HE1	1:I:401:PRO:HD3	1.61	0.66
1:J:397:TYR:HE1	1:J:401:PRO:HD3	1.61	0.66
1:L:224:ARG:HH21	1:L:224:ARG:CG	2.07	0.66
1:L:397:TYR:HE1	1:L:401:PRO:HD3	1.61	0.66
1:B:397:TYR:HE1	1:B:401:PRO:HD3	1.61	0.66
1:C:1:SER:C	1:C:71:ALA:HB1	2.15	0.66
1:F:397:TYR:HE1	1:F:401:PRO:HD3	1.61	0.66
1:I:82:ASP:HB2	5:I:1491:MPD:H12	1.77	0.66
1:F:403:GLU:HG2	1:F:403:GLU:O	1.96	0.65
1:D:403:GLU:HG2	1:D:403:GLU:O	1.96	0.65
1:I:224:ARG:HH21	1:I:224:ARG:CG	2.07	0.65
1:L:82:ASP:HB2	5:L:1494:MPD:H12	1.77	0.65
1:I:403:GLU:HG2	1:I:403:GLU:O	1.96	0.65
1:A:82:ASP:HB2	5:A:1483:MPD:H12	1.77	0.65
1:B:403:GLU:HG2	1:B:403:GLU:O	1.96	0.65
1:J:60:ILE:HG21	1:K:395:ASN:ND2	2.08	0.65
1:D:84:THR:HG21	5:D:1486:MPD:O4	1.97	0.65
1:E:403:GLU:HG2	1:E:403:GLU:O	1.96	0.65
1:A:403:GLU:O	1:A:403:GLU:HG2	1.96	0.65
1:I:84:THR:HG21	5:I:1491:MPD:O4	1.97	0.65
1:J:403:GLU:O	1:J:403:GLU:HG2	1.96	0.65
1:C:397:TYR:HE1	1:C:401:PRO:HD3	1.61	0.65
1:C:403:GLU:O	1:C:403:GLU:HG2	1.96	0.65
1:G:155:GLU:OE1	1:G:211:HIS:HE1	1.80	0.65
1:H:403:GLU:O	1:H:403:GLU:HG2	1.96	0.65
1:K:82:ASP:HB2	5:K:1493:MPD:H12	1.77	0.65
1:B:84:THR:HG21	5:B:1484:MPD:O4	1.97	0.65
1:H:397:TYR:HE1	1:H:401:PRO:HD3	1.61	0.65
1:C:180:PHE:O	1:D:29:GLN:HA	1.97	0.64
1:D:398:ASP:C	1:D:400:PRO:HD3	2.13	0.64
1:E:84:THR:HG21	5:E:1487:MPD:O4	1.97	0.64
1:C:155:GLU:OE1	1:C:211:HIS:HE1	1.80	0.64
1:D:189:GLN:HG3	5:E:1487:MPD:HM1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:84:THR:HG21	5:L:1494:MPD:O4	1.97	0.64
1:B:193:SER:OG	5:C:1485:MPD:H32	1.97	0.64
1:D:155:GLU:OE1	1:D:211:HIS:HE1	1.80	0.64
1:D:397:TYR:HE1	1:D:401:PRO:HD3	1.61	0.64
1:G:84:THR:HG21	5:G:1489:MPD:O4	1.97	0.64
1:G:395:ASN:ND2	1:L:60:ILE:HG21	2.07	0.64
1:A:84:THR:HG21	5:A:1483:MPD:O4	1.97	0.64
1:A:180:PHE:HB3	1:B:29:GLN:HB3	1.80	0.64
1:G:398:ASP:C	1:G:400:PRO:HD3	2.13	0.64
1:G:403:GLU:O	1:G:403:GLU:HG2	1.96	0.64
1:G:82:ASP:HB2	5:G:1489:MPD:H12	1.77	0.64
1:G:360:PHE:CD2	1:G:361:PRO:CD	2.71	0.64
1:J:84:THR:HG21	5:J:1492:MPD:O4	1.97	0.64
1:A:155:GLU:OE1	1:A:211:HIS:HE1	1.80	0.64
1:A:397:TYR:HE1	1:A:401:PRO:HD3	1.61	0.64
1:B:458:HIS:CD2	1:B:460:VAL:H	2.10	0.64
1:C:189:GLN:HG3	5:D:1486:MPD:HM1	1.79	0.64
1:F:84:THR:HG21	5:F:1488:MPD:O4	1.97	0.64
1:I:155:GLU:OE1	1:I:211:HIS:HE1	1.80	0.64
1:F:155:GLU:OE1	1:F:211:HIS:HE1	1.80	0.64
1:J:155:GLU:OE1	1:J:211:HIS:HE1	1.80	0.64
1:C:84:THR:HG21	5:C:1485:MPD:O4	1.97	0.64
1:F:179:TYR:C	1:F:181:PRO:HD2	2.19	0.64
1:H:84:THR:HG21	5:H:1490:MPD:O4	1.97	0.64
1:H:29:GLN:HB3	1:I:180:PHE:HB3	1.79	0.64
1:K:84:THR:HG21	5:K:1493:MPD:O4	1.97	0.64
1:K:397:TYR:HE1	1:K:401:PRO:HD3	1.61	0.64
1:D:179:TYR:C	1:D:181:PRO:HD2	2.19	0.63
1:E:155:GLU:OE1	1:E:211:HIS:HE1	1.80	0.63
1:H:398:ASP:C	1:H:400:PRO:HD3	2.13	0.63
1:C:395:ASN:ND2	1:D:60:ILE:CG2	2.51	0.63
1:L:360:PHE:CD2	1:L:361:PRO:CD	2.71	0.63
1:B:155:GLU:OE1	1:B:211:HIS:HE1	1.80	0.63
1:G:397:TYR:HE1	1:G:401:PRO:HD3	1.61	0.63
1:G:29:GLN:HB3	1:H:180:PHE:HB3	1.78	0.63
1:H:179:TYR:C	1:H:181:PRO:HD2	2.19	0.63
1:D:458:HIS:CD2	1:D:460:VAL:H	2.09	0.63
5:G:1489:MPD:H32	1:H:193:SER:HB2	1.78	0.63
1:K:403:GLU:HG2	1:K:403:GLU:O	1.96	0.63
1:E:360:PHE:CD2	1:E:361:PRO:CD	2.71	0.63
1:H:155:GLU:OE1	1:H:211:HIS:HE1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:HIS:CD2	1:A:460:VAL:H	2.10	0.63
1:A:384:ASN:HD22	1:A:384:ASN:N	1.97	0.63
1:D:384:ASN:N	1:D:384:ASN:HD22	1.97	0.63
1:D:51:GLY:C	1:D:53:SER:N	2.26	0.63
1:E:384:ASN:HD22	1:E:384:ASN:N	1.97	0.63
1:G:179:TYR:C	1:G:181:PRO:HD2	2.19	0.63
1:K:179:TYR:C	1:K:181:PRO:HD2	2.19	0.63
1:K:155:GLU:OE1	1:K:211:HIS:HE1	1.80	0.63
1:B:179:TYR:C	1:B:181:PRO:HD2	2.19	0.63
1:E:397:TYR:HE1	1:E:401:PRO:HD3	1.61	0.63
1:A:29:GLN:HB3	1:F:180:PHE:HB3	1.81	0.63
1:J:179:TYR:C	1:J:181:PRO:HD2	2.19	0.63
1:J:51:GLY:O	1:J:52:SER:C	2.37	0.63
1:L:179:TYR:C	1:L:181:PRO:HD2	2.19	0.63
1:C:179:TYR:C	1:C:181:PRO:HD2	2.19	0.63
1:F:384:ASN:N	1:F:384:ASN:HD22	1.97	0.63
1:G:189:GLN:HG3	5:L:1494:MPD:CM	2.28	0.63
1:G:189:GLN:HG3	5:L:1494:MPD:HM1	1.79	0.63
1:H:384:ASN:HD22	1:H:384:ASN:N	1.97	0.63
1:K:384:ASN:HD22	1:K:384:ASN:N	1.97	0.63
1:E:51:GLY:O	1:E:52:SER:C	2.37	0.62
1:I:179:TYR:C	1:I:181:PRO:HD2	2.19	0.62
1:B:384:ASN:N	1:B:384:ASN:HD22	1.97	0.62
1:E:179:TYR:C	1:E:181:PRO:HD2	2.19	0.62
1:I:384:ASN:N	1:I:384:ASN:HD22	1.97	0.62
1:C:179:TYR:O	1:C:181:PRO:HD2	2.00	0.62
1:E:396:LEU:O	1:E:399:LEU:HB2	2.00	0.62
1:I:29:GLN:HA	1:J:180:PHE:O	1.98	0.62
1:I:360:PHE:CD2	1:I:361:PRO:CD	2.71	0.62
1:K:396:LEU:O	1:K:399:LEU:HB2	2.00	0.62
1:L:155:GLU:OE1	1:L:211:HIS:HE1	1.80	0.62
1:C:384:ASN:N	1:C:384:ASN:HD22	1.97	0.62
1:A:179:TYR:C	1:A:181:PRO:HD2	2.19	0.62
1:A:396:LEU:O	1:A:399:LEU:HB2	2.00	0.62
1:I:396:LEU:O	1:I:399:LEU:HB2	2.00	0.62
1:K:398:ASP:C	1:K:400:PRO:HD3	2.13	0.62
1:K:29:GLN:HB3	1:L:180:PHE:HB3	1.81	0.62
1:C:396:LEU:O	1:C:399:LEU:HB2	2.00	0.62
1:D:396:LEU:O	1:D:399:LEU:HB2	2.00	0.62
1:E:193:SER:OG	5:F:1488:MPD:H32	1.99	0.62
1:F:179:TYR:O	1:F:181:PRO:HD2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:TYR:O	1:J:181:PRO:HD2	2.00	0.62
1:K:51:GLY:O	1:K:52:SER:C	2.37	0.62
1:D:360:PHE:CD2	1:D:361:PRO:CD	2.71	0.62
1:F:179:TYR:O	1:F:181:PRO:HD3	2.00	0.62
1:G:179:TYR:O	1:G:181:PRO:HD3	2.00	0.62
1:G:384:ASN:N	1:G:384:ASN:HD22	1.97	0.62
5:H:1490:MPD:HM1	1:I:189:GLN:HG3	1.81	0.62
1:J:60:ILE:CG2	1:K:395:ASN:ND2	2.57	0.62
1:C:189:GLN:HG3	5:D:1486:MPD:CM	2.30	0.62
1:F:396:LEU:O	1:F:399:LEU:HB2	2.00	0.62
1:H:396:LEU:O	1:H:399:LEU:HB2	2.00	0.62
1:K:179:TYR:O	1:K:181:PRO:HD3	2.00	0.62
1:C:179:TYR:O	1:C:181:PRO:HD3	2.00	0.62
1:G:179:TYR:O	1:G:181:PRO:HD2	2.00	0.62
1:L:384:ASN:N	1:L:384:ASN:HD22	1.97	0.62
1:A:179:TYR:O	1:A:181:PRO:HD3	2.00	0.61
1:J:384:ASN:N	1:J:384:ASN:HD22	1.97	0.61
1:B:51:GLY:O	1:B:52:SER:C	2.37	0.61
5:A:1483:MPD:H32	1:F:193:SER:HB2	1.82	0.61
1:H:51:GLY:C	1:H:53:SER:N	2.26	0.61
1:G:396:LEU:O	1:G:399:LEU:HB2	2.00	0.61
1:J:396:LEU:O	1:J:399:LEU:HB2	2.00	0.61
1:L:396:LEU:O	1:L:399:LEU:HB2	2.00	0.61
1:B:396:LEU:O	1:B:399:LEU:HB2	2.00	0.61
1:G:224:ARG:NH2	1:G:224:ARG:HG2	2.15	0.61
1:I:179:TYR:O	1:I:181:PRO:HD3	2.00	0.61
5:H:1490:MPD:C3	1:I:193:SER:CB	2.77	0.61
1:J:179:TYR:O	1:J:181:PRO:HD3	2.00	0.61
5:A:1483:MPD:CM	1:F:190:ASP:OD2	2.48	0.61
1:E:48:MET:CE	1:E:66:VAL:HG22	2.31	0.61
1:F:360:PHE:CD2	1:F:361:PRO:CD	2.71	0.61
1:F:48:MET:CE	1:F:66:VAL:HG22	2.31	0.61
3:H:1478:ADP:C1'	3:H:1478:ADP:C8	2.81	0.61
1:L:48:MET:CE	1:L:66:VAL:HG22	2.31	0.61
1:B:179:TYR:O	1:B:181:PRO:HD2	2.00	0.61
5:I:1491:MPD:H32	1:J:193:SER:OG	2.00	0.61
1:D:179:TYR:O	1:D:181:PRO:HD2	2.00	0.61
1:D:48:MET:CE	1:D:66:VAL:HG22	2.31	0.61
1:H:48:MET:CE	1:H:66:VAL:HG22	2.31	0.61
1:B:193:SER:OG	5:C:1485:MPD:C3	2.48	0.61
1:C:82:ASP:N	5:C:1485:MPD:H13	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:MET:CE	1:C:66:VAL:HG22	2.31	0.61
1:E:179:TYR:O	1:E:181:PRO:HD3	2.00	0.61
1:H:179:TYR:O	1:H:181:PRO:HD2	2.00	0.61
1:H:51:GLY:O	1:H:52:SER:C	2.37	0.61
1:A:179:TYR:O	1:A:181:PRO:HD2	2.00	0.60
1:A:48:MET:CE	1:A:66:VAL:HG22	2.31	0.60
1:D:179:TYR:O	1:D:181:PRO:HD3	2.00	0.60
1:D:180:PHE:HB3	1:E:29:GLN:HB3	1.83	0.60
1:I:179:TYR:O	1:I:181:PRO:HD2	2.00	0.60
5:H:1490:MPD:CM	1:I:189:GLN:HG3	2.31	0.60
1:I:48:MET:CE	1:I:66:VAL:HG22	2.31	0.60
1:K:179:TYR:O	1:K:181:PRO:HD2	2.00	0.60
1:L:179:TYR:O	1:L:181:PRO:HD3	2.00	0.60
1:D:193:SER:HB2	5:E:1487:MPD:H32	1.84	0.60
1:E:179:TYR:O	1:E:181:PRO:HD2	2.00	0.60
1:H:179:TYR:O	1:H:181:PRO:HD3	2.00	0.60
1:I:395:ASN:CB	1:I:399:LEU:HD12	2.29	0.60
1:B:179:TYR:O	1:B:181:PRO:HD3	2.00	0.60
1:B:48:MET:CE	1:B:66:VAL:HG22	2.31	0.60
1:G:48:MET:CE	1:G:66:VAL:HG22	2.31	0.60
1:G:82:ASP:CB	5:G:1489:MPD:H12	2.32	0.60
1:A:82:ASP:CB	5:A:1483:MPD:H12	2.32	0.60
1:B:82:ASP:CB	5:B:1484:MPD:H12	2.32	0.60
1:G:82:ASP:N	5:G:1489:MPD:H12	2.17	0.60
1:I:458:HIS:CD2	1:I:460:VAL:H	2.09	0.60
1:J:82:ASP:CB	5:J:1492:MPD:H12	2.32	0.60
1:L:179:TYR:O	1:L:181:PRO:HD2	2.00	0.60
1:A:82:ASP:N	5:A:1483:MPD:H13	2.13	0.60
1:F:82:ASP:CB	5:F:1488:MPD:H12	2.32	0.60
1:J:29:GLN:HA	1:K:180:PHE:O	2.01	0.60
5:K:1493:MPD:HM1	1:L:189:GLN:HG3	1.84	0.60
1:L:51:GLY:O	1:L:52:SER:C	2.37	0.60
1:D:395:ASN:ND2	1:E:60:ILE:HG21	2.11	0.60
1:F:51:GLY:O	1:F:52:SER:C	2.37	0.60
5:I:1491:MPD:C3	1:J:193:SER:OG	2.49	0.60
1:F:82:ASP:N	5:F:1488:MPD:H12	2.17	0.60
1:H:82:ASP:N	5:H:1490:MPD:C1	2.54	0.60
5:H:1490:MPD:C3	1:I:193:SER:OG	2.50	0.60
1:J:48:MET:CE	1:J:66:VAL:HG22	2.31	0.60
1:H:360:PHE:CD2	1:H:361:PRO:CD	2.71	0.60
3:L:1482:ADP:C1'	3:L:1482:ADP:C8	2.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ASP:CB	5:C:1485:MPD:H12	2.32	0.59
1:E:82:ASP:N	5:E:1487:MPD:H12	2.17	0.59
1:I:82:ASP:CB	5:I:1491:MPD:H12	2.32	0.59
1:F:82:ASP:N	5:F:1488:MPD:H13	2.13	0.59
1:K:224:ARG:NH2	1:K:224:ARG:HG2	2.15	0.59
1:L:395:ASN:CB	1:L:399:LEU:HD12	2.30	0.59
1:B:180:PHE:N	1:B:180:PHE:CD1	2.70	0.59
1:D:180:PHE:CD1	1:D:180:PHE:N	2.70	0.59
1:D:82:ASP:CB	5:D:1486:MPD:H12	2.32	0.59
1:D:189:GLN:HG3	5:E:1487:MPD:CM	2.32	0.59
1:E:193:SER:OG	5:F:1488:MPD:C3	2.50	0.59
1:J:82:ASP:N	5:J:1492:MPD:H12	2.17	0.59
1:K:48:MET:CE	1:K:66:VAL:HG22	2.31	0.59
1:D:456:THR:O	1:J:458:HIS:HE1	1.86	0.59
1:E:82:ASP:CB	5:E:1487:MPD:H12	2.32	0.59
1:C:82:ASP:N	5:C:1485:MPD:C1	2.54	0.59
1:E:180:PHE:CD1	1:E:180:PHE:N	2.70	0.59
1:F:180:PHE:N	1:F:180:PHE:CD1	2.70	0.59
1:K:82:ASP:N	5:K:1493:MPD:H13	2.13	0.59
1:K:180:PHE:N	1:K:180:PHE:CD1	2.70	0.59
1:L:82:ASP:CB	5:L:1494:MPD:H12	2.32	0.59
1:L:58:LYS:HZ1	1:L:60:ILE:HD11	1.67	0.59
1:K:48:MET:HE2	1:K:66:VAL:HG22	1.83	0.59
1:E:179:TYR:HB2	6:E:1524:HOH:O	2.03	0.59
5:J:1492:MPD:H32	1:K:193:SER:OG	2.01	0.59
3:D:1474:ADP:C1'	3:D:1474:ADP:C8	2.81	0.59
1:K:179:TYR:HB2	6:K:1534:HOH:O	2.03	0.59
5:J:1492:MPD:C3	1:K:193:SER:OG	2.50	0.59
1:B:179:TYR:HB2	6:B:1521:HOH:O	2.03	0.59
1:H:82:ASP:N	5:H:1490:MPD:H12	2.17	0.59
1:D:82:ASP:N	5:D:1486:MPD:H13	2.13	0.59
1:H:82:ASP:CB	5:H:1490:MPD:H12	2.32	0.59
1:A:179:TYR:HB2	6:A:1514:HOH:O	2.03	0.58
3:C:1473:ADP:C8	3:C:1473:ADP:C1'	2.81	0.58
1:C:180:PHE:CD1	1:C:180:PHE:N	2.70	0.58
1:D:51:GLY:O	1:D:52:SER:C	2.37	0.58
1:F:82:ASP:N	5:F:1488:MPD:C1	2.54	0.58
1:H:179:TYR:HB2	6:H:1528:HOH:O	2.03	0.58
1:J:458:HIS:CD2	1:J:460:VAL:H	2.10	0.58
1:L:82:ASP:N	5:L:1494:MPD:H12	2.17	0.58
1:A:193:SER:OG	5:B:1484:MPD:H32	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ASP:N	5:G:1489:MPD:C1	2.54	0.58
1:H:180:PHE:CD1	1:H:180:PHE:N	2.70	0.58
1:K:82:ASP:CB	5:K:1493:MPD:H12	2.32	0.58
1:D:179:TYR:HB2	6:D:1525:HOH:O	2.03	0.58
1:E:82:ASP:N	5:E:1487:MPD:C1	2.54	0.58
1:E:308:ILE:HG21	1:E:374:LEU:HD13	1.86	0.58
1:G:180:PHE:N	1:G:180:PHE:CD1	2.70	0.58
1:H:82:ASP:N	5:H:1490:MPD:H13	2.13	0.58
1:A:308:ILE:HG21	1:A:374:LEU:HD13	1.86	0.58
1:A:29:GLN:HA	1:F:180:PHE:O	2.02	0.58
1:G:308:ILE:HG21	1:G:374:LEU:HD13	1.86	0.58
1:K:308:ILE:HG21	1:K:374:LEU:HD13	1.86	0.58
1:K:360:PHE:CD2	1:K:361:PRO:CD	2.71	0.58
1:A:16:PHE:HB2	5:A:1483:MPD:H51	1.86	0.58
1:I:63:SER:HB2	1:J:339:ARG:HH22	1.69	0.58
1:B:48:MET:HE2	1:B:66:VAL:HG22	1.85	0.58
1:B:224:ARG:NH2	1:B:224:ARG:HG2	2.15	0.58
1:G:326:TYR:N	1:G:326:TYR:CD2	2.72	0.58
1:I:180:PHE:CD1	1:I:180:PHE:N	2.70	0.58
1:F:179:TYR:HB2	6:F:1527:HOH:O	2.03	0.58
5:H:1490:MPD:C3	1:I:193:SER:HB2	2.32	0.58
1:J:179:TYR:HB2	6:J:1530:HOH:O	2.03	0.58
3:A:1471:ADP:C8	3:A:1471:ADP:C1'	2.81	0.58
1:D:16:PHE:HB2	5:D:1486:MPD:H51	1.86	0.58
1:F:16:PHE:CD1	5:F:1488:MPD:C5	2.87	0.57
1:F:395:ASN:CB	1:F:399:LEU:HD12	2.30	0.57
1:I:51:GLY:O	1:I:52:SER:C	2.37	0.57
1:A:395:ASN:CB	1:A:399:LEU:HD12	2.30	0.57
1:B:308:ILE:HG21	1:B:374:LEU:HD13	1.86	0.57
1:G:29:GLN:HA	1:H:180:PHE:O	2.03	0.57
1:K:326:TYR:CD2	1:K:326:TYR:N	2.72	0.57
1:G:180:PHE:O	1:L:29:GLN:HA	2.03	0.57
1:C:308:ILE:HG21	1:C:374:LEU:HD13	1.86	0.57
1:C:326:TYR:CD2	1:C:326:TYR:N	2.72	0.57
1:A:82:ASP:N	5:A:1483:MPD:H12	2.17	0.57
1:C:179:TYR:HB2	6:C:1523:HOH:O	2.03	0.57
1:G:179:TYR:HB2	6:G:1528:HOH:O	2.03	0.57
1:H:308:ILE:HG21	1:H:374:LEU:HD13	1.86	0.57
1:H:29:GLN:HA	1:I:180:PHE:O	2.03	0.57
1:K:16:PHE:HB2	5:K:1493:MPD:H51	1.86	0.57
1:I:16:PHE:HB2	5:I:1491:MPD:H51	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:180:PHE:N	1:J:180:PHE:CD1	2.70	0.57
1:L:16:PHE:CD1	5:L:1494:MPD:C5	2.87	0.57
1:B:82:ASP:N	5:B:1484:MPD:H12	2.17	0.57
1:F:308:ILE:HG21	1:F:374:LEU:HD13	1.86	0.57
1:L:179:TYR:HB2	6:L:1365:HOH:O	2.03	0.57
1:B:180:PHE:HB3	1:C:29:GLN:HB3	1.85	0.57
1:C:224:ARG:NH2	1:C:224:ARG:HG2	2.15	0.57
1:D:326:TYR:N	1:D:326:TYR:CD2	2.72	0.57
1:F:192:ARG:HD3	1:F:219:ASN:HD22	1.70	0.57
5:H:1490:MPD:H32	1:I:193:SER:OG	2.04	0.57
1:L:16:PHE:HB2	5:L:1494:MPD:H51	1.86	0.57
5:K:1493:MPD:CM	1:L:190:ASP:OD2	2.49	0.57
5:A:1483:MPD:HM1	1:F:189:GLN:HG3	1.86	0.57
1:C:51:GLY:O	1:C:52:SER:C	2.37	0.57
1:D:180:PHE:O	1:E:29:GLN:HA	2.05	0.57
1:E:326:TYR:CD2	1:E:326:TYR:N	2.72	0.57
1:E:395:ASN:CB	1:E:399:LEU:HD12	2.30	0.57
1:E:48:MET:HE2	1:E:66:VAL:HG22	1.86	0.57
1:G:192:ARG:HD3	1:G:219:ASN:HD22	1.70	0.57
1:I:82:ASP:N	5:I:1491:MPD:H13	2.13	0.57
1:I:308:ILE:HG21	1:I:374:LEU:HD13	1.86	0.57
1:K:82:ASP:N	5:K:1493:MPD:C1	2.54	0.57
1:A:193:SER:OG	5:B:1484:MPD:C3	2.53	0.57
1:C:395:ASN:CB	1:C:399:LEU:HD12	2.30	0.57
1:E:16:PHE:CD1	5:E:1487:MPD:C5	2.87	0.57
1:E:1:SER:CA	1:E:71:ALA:CB	2.80	0.57
1:I:179:TYR:HB2	6:I:1530:HOH:O	2.03	0.57
1:I:192:ARG:HD3	1:I:219:ASN:HD22	1.70	0.57
3:J:1480:ADP:C8	3:J:1480:ADP:C1'	2.81	0.57
1:J:16:PHE:HB2	5:J:1492:MPD:H51	1.86	0.57
3:K:1481:ADP:C1'	3:K:1481:ADP:C8	2.81	0.57
1:L:180:PHE:N	1:L:180:PHE:CD1	2.70	0.57
1:K:29:GLN:HA	1:L:180:PHE:O	2.04	0.57
1:A:16:PHE:CD1	5:A:1483:MPD:C5	2.87	0.57
3:B:1472:ADP:C8	3:B:1472:ADP:C1'	2.81	0.57
1:D:458:HIS:HE1	1:J:456:THR:O	1.87	0.57
1:A:82:ASP:N	5:A:1483:MPD:C1	2.54	0.56
1:A:326:TYR:CD2	1:A:326:TYR:N	2.72	0.56
1:H:16:PHE:HB2	5:H:1490:MPD:H51	1.86	0.56
1:J:308:ILE:HG21	1:J:374:LEU:HD13	1.86	0.56
1:J:58:LYS:HZ1	1:J:60:ILE:HD11	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:MET:HE2	1:L:66:VAL:HG22	1.86	0.56
1:B:360:PHE:CD2	1:B:361:PRO:CD	2.71	0.56
3:E:1475:ADP:C8	3:E:1475:ADP:C1'	2.81	0.56
3:G:1477:ADP:C1'	3:G:1477:ADP:C8	2.81	0.56
1:H:16:PHE:CD1	5:H:1490:MPD:C5	2.87	0.56
1:L:308:ILE:HG21	1:L:374:LEU:HD13	1.86	0.56
1:A:180:PHE:N	1:A:180:PHE:CD1	2.70	0.56
1:B:82:ASP:N	5:B:1484:MPD:H13	2.13	0.56
1:C:82:ASP:N	5:C:1485:MPD:H12	2.17	0.56
1:D:82:ASP:N	5:D:1486:MPD:H12	2.17	0.56
5:K:1493:MPD:CM	1:L:189:GLN:HG3	2.35	0.56
1:C:192:ARG:HD3	1:C:219:ASN:HD22	1.70	0.56
1:D:308:ILE:HG21	1:D:374:LEU:HD13	1.86	0.56
1:I:63:SER:OG	1:J:339:ARG:NH2	2.39	0.56
1:J:326:TYR:CD2	1:J:326:TYR:N	2.72	0.56
1:B:16:PHE:HB2	5:B:1484:MPD:H51	1.86	0.56
1:C:16:PHE:HB2	5:C:1485:MPD:H51	1.86	0.56
1:E:16:PHE:HB2	5:E:1487:MPD:H51	1.86	0.56
1:G:82:ASP:N	5:G:1489:MPD:H13	2.13	0.56
1:G:16:PHE:HB2	5:G:1489:MPD:H51	1.86	0.56
1:G:193:SER:CB	5:L:1494:MPD:C3	2.82	0.56
1:A:360:PHE:CD2	1:A:361:PRO:CD	2.71	0.56
1:D:399:LEU:O	1:D:400:PRO:O	2.24	0.56
1:D:48:MET:HE2	1:D:66:VAL:HG22	1.87	0.56
1:F:48:MET:HE2	1:F:66:VAL:HG22	1.86	0.56
1:H:192:ARG:HD3	1:H:219:ASN:HD22	1.70	0.56
1:I:48:MET:HE2	1:I:66:VAL:HG22	1.87	0.56
1:G:193:SER:HB2	5:L:1494:MPD:C3	2.35	0.56
1:B:399:LEU:O	1:B:400:PRO:O	2.24	0.56
1:B:456:THR:O	1:H:458:HIS:HE1	1.88	0.56
1:F:399:LEU:O	1:F:400:PRO:O	2.24	0.56
1:I:82:ASP:N	5:I:1491:MPD:C1	2.54	0.56
1:L:1:SER:CA	1:L:71:ALA:CB	2.80	0.56
1:A:58:LYS:HZ1	1:A:60:ILE:HD11	1.70	0.56
1:J:16:PHE:CD1	5:J:1492:MPD:C5	2.87	0.56
1:K:399:LEU:O	1:K:400:PRO:O	2.24	0.56
1:L:192:ARG:HD3	1:L:219:ASN:HD22	1.70	0.56
1:C:48:MET:HE2	1:C:66:VAL:HG22	1.86	0.56
1:E:118:THR:OG1	1:E:120:ILE:HG13	2.06	0.56
1:K:82:ASP:N	5:K:1493:MPD:H12	2.17	0.56
1:B:192:ARG:HD3	1:B:219:ASN:HD22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:HIS:HE1	1:H:456:THR:O	1.89	0.56
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.70	0.56
1:E:224:ARG:HG2	1:E:224:ARG:NH2	2.15	0.56
1:G:16:PHE:CD1	5:G:1489:MPD:C5	2.87	0.56
1:G:51:GLY:O	1:G:52:SER:C	2.37	0.56
1:H:399:LEU:O	1:H:400:PRO:O	2.24	0.56
1:K:192:ARG:HD3	1:K:219:ASN:HD22	1.70	0.56
1:F:16:PHE:HB2	5:F:1488:MPD:H51	1.86	0.55
1:H:118:THR:OG1	1:H:120:ILE:HG13	2.06	0.55
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.70	0.55
1:K:16:PHE:CD1	5:K:1493:MPD:C5	2.87	0.55
1:C:118:THR:OG1	1:C:120:ILE:HG13	2.06	0.55
1:F:326:TYR:CD2	1:F:326:TYR:N	2.72	0.55
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.70	0.55
1:F:1:SER:CA	1:F:71:ALA:CB	2.80	0.55
1:H:395:ASN:CB	1:H:399:LEU:HD12	2.30	0.55
1:J:118:THR:OG1	1:J:120:ILE:HG13	2.06	0.55
1:L:224:ARG:HG2	1:L:224:ARG:NH2	2.15	0.55
1:A:180:PHE:O	1:B:29:GLN:HA	2.06	0.55
1:D:16:PHE:CD1	5:D:1486:MPD:C5	2.87	0.55
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.70	0.55
1:G:395:ASN:CB	1:G:399:LEU:HD12	2.30	0.55
1:B:118:THR:OG1	1:B:120:ILE:HG13	2.06	0.55
1:C:400:PRO:CB	1:C:401:PRO:HD2	2.37	0.55
1:I:326:TYR:CD2	1:I:326:TYR:N	2.72	0.55
1:B:326:TYR:CD2	1:B:326:TYR:N	2.72	0.55
1:B:395:ASN:CB	1:B:399:LEU:HD12	2.29	0.55
1:C:16:PHE:CD1	5:C:1485:MPD:C5	2.87	0.55
1:J:1:SER:CA	1:J:71:ALA:CB	2.80	0.55
1:L:118:THR:OG1	1:L:120:ILE:HG13	2.06	0.55
1:E:399:LEU:O	1:E:400:PRO:O	2.24	0.55
1:J:82:ASP:N	5:J:1492:MPD:H13	2.13	0.55
1:L:399:LEU:O	1:L:400:PRO:O	2.24	0.55
1:A:118:THR:OG1	1:A:120:ILE:HG13	2.06	0.55
1:D:397:TYR:C	1:D:399:LEU:N	2.60	0.55
1:F:400:PRO:CB	1:F:401:PRO:HD2	2.37	0.55
1:G:400:PRO:CB	1:G:401:PRO:HD2	2.37	0.55
3:I:1479:ADP:C8	3:I:1479:ADP:C1'	2.81	0.55
1:I:397:TYR:C	1:I:399:LEU:N	2.60	0.55
1:I:50:ASP:CG	6:I:1613:HOH:O	2.44	0.55
1:J:360:PHE:CD2	1:J:361:PRO:CD	2.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:395:ASN:CB	1:J:399:LEU:HD12	2.30	0.55
1:K:395:ASN:CB	1:K:399:LEU:HD12	2.29	0.55
1:K:397:TYR:C	1:K:399:LEU:N	2.60	0.55
1:G:193:SER:OG	5:L:1494:MPD:C3	2.55	0.55
1:L:326:TYR:N	1:L:326:TYR:CD2	2.72	0.55
1:L:400:PRO:CB	1:L:401:PRO:HD2	2.37	0.55
1:G:395:ASN:ND2	1:L:60:ILE:CG2	2.63	0.55
1:B:180:PHE:O	1:C:29:GLN:HA	2.06	0.55
1:D:118:THR:OG1	1:D:120:ILE:HG13	2.06	0.55
1:D:400:PRO:CB	1:D:401:PRO:HD2	2.37	0.55
1:G:118:THR:OG1	1:G:120:ILE:HG13	2.06	0.55
1:H:326:TYR:N	1:H:326:TYR:CD2	2.72	0.55
1:I:118:THR:OG1	1:I:120:ILE:HG13	2.06	0.55
1:I:400:PRO:CB	1:I:401:PRO:HD2	2.37	0.55
1:J:399:LEU:O	1:J:400:PRO:O	2.24	0.55
1:C:399:LEU:O	1:C:400:PRO:O	2.24	0.55
1:E:400:PRO:CB	1:E:401:PRO:HD2	2.37	0.55
1:G:399:LEU:O	1:G:400:PRO:O	2.24	0.55
1:K:400:PRO:CB	1:K:401:PRO:HD2	2.37	0.55
1:A:399:LEU:O	1:A:400:PRO:O	2.24	0.54
1:G:48:MET:HE2	1:G:66:VAL:HG22	1.89	0.54
1:J:82:ASP:N	5:J:1492:MPD:C1	2.54	0.54
1:J:400:PRO:CB	1:J:401:PRO:HD2	2.37	0.54
1:L:397:TYR:C	1:L:399:LEU:N	2.60	0.54
1:C:360:PHE:CD2	1:C:361:PRO:CD	2.71	0.54
1:I:399:LEU:O	1:I:400:PRO:O	2.24	0.54
1:K:118:THR:OG1	1:K:120:ILE:HG13	2.06	0.54
1:D:360:PHE:CE2	1:D:361:PRO:HD3	2.39	0.54
1:F:58:LYS:HZ1	1:F:60:ILE:HD11	1.73	0.54
1:I:16:PHE:CD1	5:I:1491:MPD:C5	2.87	0.54
1:A:51:GLY:O	1:A:52:SER:C	2.37	0.54
1:B:400:PRO:CB	1:B:401:PRO:HD2	2.37	0.54
1:D:82:ASP:N	5:D:1486:MPD:C1	2.54	0.54
3:F:1476:ADP:C8	3:F:1476:ADP:C1'	2.81	0.54
5:I:1491:MPD:C3	1:J:193:SER:HB2	2.37	0.54
1:G:190:ASP:OD2	5:L:1494:MPD:CM	2.53	0.54
1:B:82:ASP:N	5:B:1484:MPD:C1	2.54	0.54
1:C:458:HIS:HE1	1:I:456:THR:O	1.90	0.54
5:J:1492:MPD:C3	1:K:193:SER:HB2	2.36	0.54
1:A:400:PRO:CB	1:A:401:PRO:HD2	2.37	0.54
1:F:360:PHE:CE2	1:F:361:PRO:HD3	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:458:HIS:HE1	1:L:456:THR:O	1.90	0.54
1:I:82:ASP:N	5:I:1491:MPD:H12	2.17	0.54
1:C:58:LYS:HZ1	1:C:60:ILE:HD11	1.73	0.53
1:F:118:THR:OG1	1:F:120:ILE:HG13	2.06	0.53
1:B:16:PHE:CD1	5:B:1484:MPD:C5	2.87	0.53
1:B:193:SER:CB	5:C:1485:MPD:C3	2.81	0.53
5:H:1490:MPD:CM	1:I:190:ASP:OD2	2.53	0.53
1:E:454:ARG:O	1:K:320:LYS:HG2	2.08	0.53
1:A:360:PHE:CE2	1:A:361:PRO:HD3	2.39	0.53
1:E:397:TYR:C	1:E:399:LEU:N	2.60	0.53
1:H:400:PRO:CB	1:H:401:PRO:HD2	2.37	0.53
1:H:48:MET:HE1	1:H:66:VAL:HG22	1.90	0.53
1:C:456:THR:O	1:I:458:HIS:HE1	1.91	0.53
1:D:302:ILE:HG23	1:D:332:LEU:HB3	1.91	0.53
1:E:58:LYS:HZ1	1:E:60:ILE:HD11	1.73	0.53
1:J:397:TYR:C	1:J:399:LEU:N	2.60	0.53
1:A:397:TYR:C	1:A:399:LEU:N	2.60	0.53
1:G:427:PHE:CE1	1:G:428:LEU:HD13	2.44	0.53
1:I:58:LYS:HZ1	1:I:60:ILE:HD11	1.74	0.53
5:I:1491:MPD:C3	1:J:193:SER:CB	2.80	0.53
1:E:82:ASP:N	5:E:1487:MPD:H13	2.13	0.53
5:A:1483:MPD:CM	1:F:189:GLN:HG3	2.39	0.53
1:B:360:PHE:CE2	1:B:361:PRO:HD3	2.39	0.53
1:G:337:ARG:HG2	1:G:338:ASN:H	1.74	0.53
1:H:302:ILE:HG23	1:H:332:LEU:HB3	1.91	0.53
1:D:80:PHE:CG	5:D:1486:MPD:HM2	2.44	0.53
1:H:427:PHE:CE1	1:H:428:LEU:HD13	2.44	0.53
1:I:224:ARG:NH2	1:I:224:ARG:HG2	2.15	0.53
1:I:337:ARG:HG2	1:I:338:ASN:H	1.74	0.53
1:J:427:PHE:CE1	1:J:428:LEU:HD13	2.44	0.53
1:L:80:PHE:CG	5:L:1494:MPD:HM2	2.44	0.53
1:A:80:PHE:CG	5:A:1483:MPD:HM2	2.44	0.53
1:B:397:TYR:C	1:B:399:LEU:N	2.60	0.53
1:D:395:ASN:CB	1:D:399:LEU:HD12	2.30	0.53
1:E:312:ALA:HB1	1:E:361:PRO:HG3	1.91	0.53
1:H:337:ARG:HG2	1:H:338:ASN:H	1.74	0.53
1:J:360:PHE:CE2	1:J:361:PRO:HD3	2.39	0.53
1:K:80:PHE:CG	5:K:1493:MPD:HM2	2.44	0.53
1:B:337:ARG:HG2	1:B:338:ASN:H	1.74	0.53
1:C:427:PHE:CE1	1:C:428:LEU:HD13	2.44	0.53
1:F:337:ARG:HG2	1:F:338:ASN:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:PHE:CG	5:F:1488:MPD:HM2	2.44	0.53
1:G:80:PHE:CG	5:G:1489:MPD:HM2	2.44	0.53
1:I:427:PHE:CE1	1:I:428:LEU:HD13	2.44	0.53
1:J:312:ALA:HB1	1:J:361:PRO:HG3	1.91	0.53
5:J:1492:MPD:C3	1:K:193:SER:CB	2.81	0.53
1:K:58:LYS:HZ1	1:K:60:ILE:HD11	1.73	0.53
1:A:302:ILE:HG23	1:A:332:LEU:HB3	1.91	0.52
1:C:312:ALA:HB1	1:C:361:PRO:HG3	1.91	0.52
1:C:339:ARG:NH2	1:D:63:SER:OG	2.42	0.52
1:D:427:PHE:CE1	1:D:428:LEU:HD13	2.44	0.52
1:H:80:PHE:CG	5:H:1490:MPD:HM2	2.44	0.52
1:J:302:ILE:HG23	1:J:332:LEU:HB3	1.91	0.52
1:G:193:SER:OG	5:L:1494:MPD:H32	2.08	0.52
1:L:427:PHE:CE1	1:L:428:LEU:HD13	2.44	0.52
1:A:312:ALA:HB1	1:A:361:PRO:HG3	1.91	0.52
1:B:427:PHE:CE1	1:B:428:LEU:HD13	2.44	0.52
1:C:1:SER:CA	1:C:71:ALA:CB	2.80	0.52
1:F:427:PHE:CE1	1:F:428:LEU:HD13	2.44	0.52
1:L:312:ALA:HB1	1:L:361:PRO:HG3	1.91	0.52
1:A:48:MET:HE1	1:A:66:VAL:HG22	1.91	0.52
1:C:124:VAL:HG11	1:C:375:LEU:HG	1.92	0.52
1:E:80:PHE:CG	5:E:1487:MPD:HM2	2.44	0.52
1:E:180:PHE:HB3	1:F:29:GLN:HB3	1.92	0.52
1:E:427:PHE:CE1	1:E:428:LEU:HD13	2.44	0.52
1:F:124:VAL:HG11	1:F:375:LEU:HG	1.92	0.52
1:K:337:ARG:HG2	1:K:338:ASN:H	1.74	0.52
1:E:320:LYS:HG2	1:K:454:ARG:O	2.09	0.52
1:B:80:PHE:CG	5:B:1484:MPD:HM2	2.44	0.52
1:C:337:ARG:HG2	1:C:338:ASN:H	1.74	0.52
1:C:397:TYR:C	1:C:399:LEU:N	2.60	0.52
1:D:312:ALA:HB1	1:D:361:PRO:HG3	1.91	0.52
1:F:80:PHE:CD1	5:F:1488:MPD:O4	2.63	0.52
1:H:80:PHE:CD1	5:H:1490:MPD:O4	2.63	0.52
1:H:360:PHE:CE2	1:H:361:PRO:HD3	2.39	0.52
1:K:427:PHE:CE1	1:K:428:LEU:HD13	2.44	0.52
1:L:302:ILE:HG23	1:L:332:LEU:HB3	1.91	0.52
1:B:302:ILE:HG23	1:B:332:LEU:HB3	1.91	0.52
1:B:80:PHE:CD1	5:B:1484:MPD:O4	2.63	0.52
1:F:302:ILE:HG23	1:F:332:LEU:HB3	1.91	0.52
1:G:124:VAL:HG11	1:G:375:LEU:HG	1.92	0.52
1:H:312:ALA:HB1	1:H:361:PRO:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:PHE:CG	5:I:1491:MPD:HM2	2.44	0.52
1:J:48:MET:HE1	1:J:66:VAL:HG22	1.91	0.52
1:J:80:PHE:CG	5:J:1492:MPD:HM2	2.44	0.52
1:A:80:PHE:CD1	5:A:1483:MPD:O4	2.63	0.52
1:A:465:TYR:O	1:A:468:VAL:HB	2.10	0.52
1:B:465:TYR:O	1:B:468:VAL:HB	2.10	0.52
1:C:80:PHE:CD1	5:C:1485:MPD:O4	2.63	0.52
1:C:465:TYR:O	1:C:468:VAL:HB	2.10	0.52
1:E:124:VAL:HG11	1:E:375:LEU:HG	1.92	0.52
1:G:80:PHE:CD1	5:G:1489:MPD:O4	2.63	0.52
1:H:397:TYR:C	1:H:399:LEU:N	2.60	0.52
1:I:465:TYR:O	1:I:468:VAL:HB	2.10	0.52
1:K:80:PHE:CD1	5:K:1493:MPD:O4	2.63	0.52
1:L:124:VAL:HG11	1:L:375:LEU:HG	1.92	0.52
1:L:82:ASP:N	5:L:1494:MPD:H13	2.13	0.52
1:B:124:VAL:HG11	1:B:375:LEU:HG	1.92	0.52
1:C:302:ILE:HG23	1:C:332:LEU:HB3	1.91	0.52
1:E:16:PHE:HB2	1:E:84:THR:HB	1.92	0.52
1:F:456:THR:O	1:L:458:HIS:HE1	1.93	0.52
1:G:360:PHE:CE2	1:G:361:PRO:HD3	2.39	0.52
1:I:124:VAL:HG11	1:I:375:LEU:HG	1.92	0.52
1:L:82:ASP:N	5:L:1494:MPD:C1	2.54	0.52
1:A:60:ILE:HG21	1:F:395:ASN:ND2	2.18	0.52
1:B:312:ALA:HB1	1:B:361:PRO:HG3	1.91	0.52
1:F:312:ALA:HB1	1:F:361:PRO:HG3	1.91	0.52
1:I:312:ALA:HB1	1:I:361:PRO:HG3	1.91	0.52
1:I:302:ILE:HG23	1:I:332:LEU:HB3	1.91	0.52
1:J:340:SER:OG	1:J:396:LEU:HB3	2.10	0.52
1:K:16:PHE:HB2	1:K:84:THR:HB	1.92	0.52
1:L:180:PHE:HD1	1:L:180:PHE:N	2.08	0.52
1:A:337:ARG:HG2	1:A:338:ASN:H	1.74	0.52
1:C:80:PHE:CG	5:C:1485:MPD:HM2	2.44	0.52
1:D:337:ARG:HG2	1:D:338:ASN:H	1.74	0.52
1:D:465:TYR:O	1:D:468:VAL:HB	2.10	0.52
1:E:337:ARG:HG2	1:E:338:ASN:H	1.74	0.52
1:F:340:SER:OG	1:F:396:LEU:HB3	2.10	0.52
1:H:136:ASP:O	1:I:169:LYS:NZ	2.35	0.52
1:K:124:VAL:HG11	1:K:375:LEU:HG	1.92	0.52
1:L:340:SER:OG	1:L:396:LEU:HB3	2.10	0.52
1:L:80:PHE:CD1	5:L:1494:MPD:O4	2.63	0.52
1:F:465:TYR:O	1:F:468:VAL:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:397:TYR:C	1:G:399:LEU:N	2.60	0.52
1:I:80:PHE:CD1	5:I:1491:MPD:O4	2.63	0.52
1:J:180:PHE:HD1	1:J:180:PHE:N	2.08	0.52
1:K:360:PHE:CE2	1:K:361:PRO:HD3	2.39	0.52
1:D:340:SER:OG	1:D:396:LEU:HB3	2.10	0.51
1:D:80:PHE:CD1	5:D:1486:MPD:O4	2.63	0.51
1:J:337:ARG:HG2	1:J:338:ASN:H	1.74	0.51
1:K:312:ALA:HB1	1:K:361:PRO:HG3	1.91	0.51
1:K:302:ILE:HG23	1:K:332:LEU:HB3	1.91	0.51
1:K:465:TYR:O	1:K:468:VAL:HB	2.10	0.51
1:B:340:SER:OG	1:B:396:LEU:HB3	2.10	0.51
1:B:16:PHE:HB2	1:B:84:THR:HB	1.92	0.51
1:E:465:TYR:O	1:E:468:VAL:HB	2.10	0.51
1:E:80:PHE:CD1	5:E:1487:MPD:O4	2.63	0.51
1:H:124:VAL:HG11	1:H:375:LEU:HG	1.92	0.51
1:H:180:PHE:HD1	1:H:180:PHE:N	2.08	0.51
5:G:1489:MPD:H32	1:H:193:SER:OG	2.09	0.51
1:J:80:PHE:CD1	5:J:1492:MPD:O4	2.63	0.51
1:G:312:ALA:HB1	1:G:361:PRO:HG3	1.91	0.51
1:H:16:PHE:HB2	1:H:84:THR:HB	1.92	0.51
1:A:340:SER:OG	1:A:396:LEU:HB3	2.10	0.51
1:A:427:PHE:CE1	1:A:428:LEU:HD13	2.44	0.51
1:C:180:PHE:HD1	1:C:180:PHE:N	2.08	0.51
1:C:340:SER:OG	1:C:396:LEU:HB3	2.10	0.51
1:E:360:PHE:CE2	1:E:361:PRO:HD3	2.39	0.51
1:G:302:ILE:HG23	1:G:332:LEU:HB3	1.91	0.51
1:J:465:TYR:O	1:J:468:VAL:HB	2.10	0.51
1:L:337:ARG:HG2	1:L:338:ASN:H	1.74	0.51
1:L:465:TYR:O	1:L:468:VAL:HB	2.10	0.51
1:B:193:SER:HB2	5:C:1485:MPD:C3	2.39	0.51
1:D:50:ASP:CG	6:D:1493:HOH:O	2.48	0.51
1:G:16:PHE:HB2	1:G:84:THR:HB	1.92	0.51
1:G:465:TYR:O	1:G:468:VAL:HB	2.10	0.51
1:H:465:TYR:O	1:H:468:VAL:HB	2.10	0.51
1:I:375:LEU:HD22	1:I:379:LEU:HG	1.93	0.51
1:A:224:ARG:HG2	1:A:224:ARG:NH2	2.15	0.51
1:F:124:VAL:HG13	1:F:274:LEU:CD2	2.41	0.51
1:F:49:PHE:CD2	1:F:49:PHE:N	2.79	0.51
1:I:16:PHE:HB2	1:I:84:THR:HB	1.92	0.51
1:I:124:VAL:HG13	1:I:274:LEU:CD2	2.41	0.51
1:I:340:SER:OG	1:I:396:LEU:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:49:PHE:CD2	1:K:49:PHE:N	2.79	0.51
1:A:180:PHE:N	1:A:180:PHE:HD1	2.08	0.51
1:H:58:LYS:HZ1	1:H:60:ILE:HD11	1.74	0.51
1:L:49:PHE:N	1:L:49:PHE:CD2	2.79	0.51
1:A:16:PHE:HB2	1:A:84:THR:HB	1.92	0.51
1:A:124:VAL:HG11	1:A:375:LEU:HG	1.92	0.51
1:G:124:VAL:HG13	1:G:274:LEU:CD2	2.41	0.51
1:I:180:PHE:HD1	1:I:180:PHE:N	2.08	0.51
1:J:124:VAL:HG11	1:J:375:LEU:HG	1.92	0.51
1:L:360:PHE:CE2	1:L:361:PRO:HD3	2.39	0.51
1:A:48:MET:HE2	1:A:66:VAL:HG22	1.93	0.51
1:B:180:PHE:N	1:B:180:PHE:HD1	2.08	0.51
1:C:16:PHE:HB2	1:C:84:THR:HB	1.92	0.51
1:C:124:VAL:HG13	1:C:274:LEU:CD2	2.41	0.51
1:D:360:PHE:CG	1:D:361:PRO:HD3	2.42	0.51
1:F:397:TYR:C	1:F:399:LEU:N	2.60	0.51
1:G:340:SER:OG	1:G:396:LEU:HB3	2.10	0.51
1:H:49:PHE:CD2	1:H:49:PHE:N	2.79	0.51
1:K:124:VAL:HG13	1:K:274:LEU:CD2	2.41	0.51
1:D:375:LEU:HD22	1:D:379:LEU:HG	1.93	0.51
1:E:302:ILE:HG23	1:E:332:LEU:HB3	1.91	0.51
1:G:180:PHE:N	1:G:180:PHE:HD1	2.08	0.51
1:J:124:VAL:HG13	1:J:274:LEU:CD2	2.41	0.51
1:D:124:VAL:HG13	1:D:274:LEU:CD2	2.41	0.50
1:E:49:PHE:N	1:E:49:PHE:CD2	2.79	0.50
1:F:375:LEU:HD22	1:F:379:LEU:HG	1.93	0.50
1:J:16:PHE:HB2	1:J:84:THR:HB	1.92	0.50
1:J:58:LYS:O	1:J:58:LYS:HG2	2.12	0.50
5:K:1493:MPD:C3	1:L:193:SER:HB2	2.41	0.50
1:A:124:VAL:HG13	1:A:274:LEU:CD2	2.41	0.50
1:A:49:PHE:N	1:A:49:PHE:CD2	2.79	0.50
1:A:339:ARG:HH22	1:B:63:SER:HB2	1.76	0.50
1:E:124:VAL:HG13	1:E:274:LEU:CD2	2.41	0.50
1:F:16:PHE:HB2	1:F:84:THR:HB	1.92	0.50
1:F:360:PHE:CG	1:F:361:PRO:HD3	2.43	0.50
1:H:124:VAL:HG13	1:H:274:LEU:CD2	2.41	0.50
1:L:124:VAL:HG13	1:L:274:LEU:CD2	2.41	0.50
1:B:375:LEU:HD22	1:B:379:LEU:HG	1.93	0.50
1:D:124:VAL:HG11	1:D:375:LEU:HG	1.92	0.50
1:B:49:PHE:CD2	1:B:49:PHE:N	2.79	0.50
1:H:340:SER:OG	1:H:396:LEU:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:LYS:O	1:H:58:LYS:HG2	2.12	0.50
1:I:49:PHE:N	1:I:49:PHE:CD2	2.79	0.50
1:D:16:PHE:HB2	1:D:84:THR:HB	1.92	0.50
1:E:58:LYS:HG2	1:E:58:LYS:O	2.12	0.50
1:G:375:LEU:HD22	1:G:379:LEU:HG	1.93	0.50
1:G:49:PHE:CD2	1:G:49:PHE:N	2.79	0.50
1:K:375:LEU:HD22	1:K:379:LEU:HG	1.93	0.50
1:A:360:PHE:CG	1:A:361:PRO:HD3	2.43	0.50
1:B:124:VAL:HG13	1:B:274:LEU:CD2	2.41	0.50
1:B:49:PHE:HD2	1:B:49:PHE:N	2.10	0.50
1:D:401:PRO:CB	1:D:404:ALA:HA	2.37	0.50
1:E:189:GLN:OE1	5:F:1488:MPD:H4	2.12	0.50
1:F:224:ARG:HG2	1:F:224:ARG:NH2	2.15	0.50
1:L:16:PHE:HB2	1:L:84:THR:HB	1.92	0.50
1:L:58:LYS:O	1:L:58:LYS:HG2	2.12	0.50
1:A:454:ARG:O	1:G:320:LYS:HG2	2.11	0.50
1:G:84:THR:HG21	5:G:1489:MPD:C5	2.42	0.50
1:I:84:THR:HG21	5:I:1491:MPD:C5	2.42	0.50
1:K:340:SER:OG	1:K:396:LEU:HB3	2.10	0.50
1:K:435:THR:HG23	6:K:1518:HOH:O	2.12	0.50
1:B:58:LYS:HG2	1:B:58:LYS:O	2.12	0.50
1:B:395:ASN:ND2	1:C:60:ILE:HG21	2.22	0.50
1:D:49:PHE:CD2	1:D:49:PHE:N	2.79	0.50
1:D:84:THR:HG21	5:D:1486:MPD:C5	2.42	0.50
1:D:395:ASN:ND2	1:E:60:ILE:CG2	2.61	0.50
1:H:49:PHE:HD2	1:H:49:PHE:N	2.10	0.50
1:J:49:PHE:CD2	1:J:49:PHE:N	2.79	0.50
1:K:84:THR:HG21	5:K:1493:MPD:C5	2.42	0.50
1:A:49:PHE:N	1:A:49:PHE:HD2	2.10	0.50
1:C:360:PHE:CE2	1:C:361:PRO:HD3	2.39	0.50
1:C:375:LEU:HD22	1:C:379:LEU:HG	1.93	0.50
1:C:49:PHE:CD2	1:C:49:PHE:N	2.79	0.50
1:E:340:SER:OG	1:E:396:LEU:HB3	2.10	0.50
1:J:48:MET:HE2	1:J:66:VAL:HG22	1.93	0.50
1:D:180:PHE:N	1:D:180:PHE:HD1	2.08	0.49
1:E:84:THR:HG21	5:E:1487:MPD:C5	2.42	0.49
1:F:49:PHE:N	1:F:49:PHE:HD2	2.10	0.49
5:G:1489:MPD:H4	1:H:189:GLN:OE1	2.12	0.49
1:H:375:LEU:HD22	1:H:379:LEU:HG	1.93	0.49
1:K:49:PHE:HD2	1:K:49:PHE:N	2.10	0.49
1:A:58:LYS:HG2	1:A:58:LYS:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ARG:NH2	1:B:63:SER:OG	2.46	0.49
1:I:179:TYR:C	1:I:181:PRO:CD	2.81	0.49
1:J:375:LEU:HD22	1:J:379:LEU:HG	1.93	0.49
1:J:435:THR:HG23	6:J:1514:HOH:O	2.12	0.49
1:F:84:THR:HG21	5:F:1488:MPD:C5	2.42	0.49
5:G:1489:MPD:C3	1:H:193:SER:OG	2.60	0.49
1:I:34:PRO:HG2	1:J:206:VAL:O	2.12	0.49
5:K:1493:MPD:C3	1:L:193:SER:CB	2.88	0.49
1:L:375:LEU:HD22	1:L:379:LEU:HG	1.93	0.49
1:A:435:THR:HG23	6:A:1498:HOH:O	2.12	0.49
1:B:435:THR:HG23	6:B:1505:HOH:O	2.12	0.49
1:E:375:LEU:HD22	1:E:379:LEU:HG	1.93	0.49
1:F:180:PHE:N	1:F:180:PHE:HD1	2.08	0.49
1:I:29:GLN:HB3	1:J:180:PHE:CB	2.41	0.49
1:L:84:THR:HG21	5:L:1494:MPD:C5	2.42	0.49
1:A:375:LEU:HD22	1:A:379:LEU:HG	1.93	0.49
1:A:84:THR:HG21	5:A:1483:MPD:C5	2.42	0.49
1:C:190:ASP:OD2	5:D:1486:MPD:CM	2.54	0.49
1:C:193:SER:OG	5:D:1486:MPD:H32	2.13	0.49
1:G:58:LYS:O	1:G:58:LYS:HG2	2.12	0.49
1:I:49:PHE:N	1:I:49:PHE:HD2	2.10	0.49
1:I:33:ILE:CD1	1:J:208:ALA:HB2	2.42	0.49
1:B:84:THR:HG21	5:B:1484:MPD:C5	2.42	0.49
1:D:1:SER:CA	1:D:71:ALA:CB	2.80	0.49
1:G:179:TYR:C	1:G:181:PRO:CD	2.81	0.49
1:I:33:ILE:HD11	1:J:208:ALA:HB2	1.94	0.49
1:I:1:SER:CA	1:I:71:ALA:CB	2.80	0.49
1:L:49:PHE:N	1:L:49:PHE:HD2	2.10	0.49
1:B:58:LYS:HZ1	1:B:60:ILE:HD11	1.77	0.49
1:D:190:ASP:OD2	5:E:1487:MPD:CM	2.55	0.49
1:D:49:PHE:HD2	1:D:49:PHE:N	2.10	0.49
1:E:179:TYR:C	1:E:181:PRO:CD	2.81	0.49
1:E:49:PHE:N	1:E:49:PHE:HD2	2.10	0.49
1:H:48:MET:HE2	1:H:66:VAL:HG22	1.94	0.49
1:J:49:PHE:N	1:J:49:PHE:HD2	2.10	0.49
1:C:84:THR:HG21	5:C:1485:MPD:C5	2.42	0.49
1:D:58:LYS:HG2	1:D:58:LYS:O	2.12	0.49
1:A:192:ARG:HH21	1:A:219:ASN:ND2	2.11	0.49
1:G:48:MET:HE1	1:G:66:VAL:HG22	1.95	0.49
1:I:401:PRO:CB	1:I:404:ALA:HA	2.37	0.49
1:I:435:THR:HG23	6:I:1514:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:58:LYS:O	1:K:58:LYS:HG2	2.12	0.49
1:C:193:SER:OG	5:D:1486:MPD:C3	2.61	0.49
1:F:435:THR:HG23	6:F:1511:HOH:O	2.12	0.49
1:J:192:ARG:HH21	1:J:219:ASN:ND2	2.11	0.49
1:J:60:ILE:HA	1:J:60:ILE:HD13	1.62	0.49
1:D:435:THR:HG23	6:D:1509:HOH:O	2.12	0.48
1:F:179:TYR:C	1:F:181:PRO:CD	2.81	0.48
1:H:435:THR:HG23	6:H:1512:HOH:O	2.12	0.48
1:H:84:THR:HG21	5:H:1490:MPD:C5	2.42	0.48
1:I:192:ARG:HH21	1:I:219:ASN:ND2	2.11	0.48
1:C:454:ARG:O	1:I:320:LYS:HG2	2.13	0.48
1:J:84:THR:HG21	5:J:1492:MPD:C5	2.42	0.48
1:K:401:PRO:CB	1:K:404:ALA:HA	2.37	0.48
1:B:189:GLN:OE1	5:C:1485:MPD:H4	2.13	0.48
1:C:192:ARG:HH21	1:C:219:ASN:ND2	2.11	0.48
1:D:58:LYS:HZ1	1:D:60:ILE:HD11	1.78	0.48
1:F:287:TYR:O	1:F:290:LEU:HB2	2.14	0.48
1:G:435:THR:HG23	6:G:1512:HOH:O	2.12	0.48
1:K:192:ARG:HH21	1:K:219:ASN:ND2	2.11	0.48
1:L:360:PHE:CG	1:L:361:PRO:HD3	2.43	0.48
1:L:435:THR:HG23	6:L:1348:HOH:O	2.12	0.48
1:A:320:LYS:HG2	1:G:454:ARG:O	2.13	0.48
1:C:435:THR:HG23	6:C:1507:HOH:O	2.12	0.48
1:D:287:TYR:O	1:D:290:LEU:HB2	2.14	0.48
1:E:180:PHE:O	1:F:29:GLN:HA	2.13	0.48
1:E:435:THR:HG23	6:E:1508:HOH:O	2.12	0.48
1:F:58:LYS:HG2	1:F:58:LYS:O	2.12	0.48
5:K:1493:MPD:H32	1:L:193:SER:OG	2.13	0.48
1:L:287:TYR:O	1:L:290:LEU:HB2	2.14	0.48
1:A:193:SER:CB	5:B:1484:MPD:C3	2.86	0.48
1:C:49:PHE:HD2	1:C:49:PHE:N	2.10	0.48
1:G:287:TYR:O	1:G:290:LEU:HB2	2.14	0.48
1:G:49:PHE:N	1:G:49:PHE:HD2	2.10	0.48
1:I:287:TYR:O	1:I:290:LEU:HB2	2.14	0.48
1:D:192:ARG:HH21	1:D:219:ASN:ND2	2.11	0.48
1:G:58:LYS:HZ1	1:G:60:ILE:HD11	1.78	0.48
1:J:224:ARG:HG2	1:J:224:ARG:NH2	2.15	0.48
1:K:179:TYR:C	1:K:181:PRO:CD	2.81	0.48
1:L:192:ARG:HH21	1:L:219:ASN:ND2	2.11	0.48
1:C:58:LYS:HG2	1:C:58:LYS:O	2.12	0.48
1:F:332:LEU:HB2	1:F:408:PRO:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:LYS:O	1:I:58:LYS:HG2	2.12	0.48
1:J:287:TYR:O	1:J:290:LEU:HB2	2.14	0.48
1:K:136:ASP:O	1:L:169:LYS:NZ	2.42	0.48
1:B:179:TYR:C	1:B:181:PRO:CD	2.81	0.48
1:H:192:ARG:HH21	1:H:219:ASN:ND2	2.11	0.48
1:I:332:LEU:HB2	1:I:408:PRO:O	2.14	0.48
1:K:1:SER:CA	1:K:71:ALA:CB	2.80	0.48
5:K:1493:MPD:C3	1:L:193:SER:OG	2.61	0.48
1:B:1:SER:CA	1:B:71:ALA:CB	2.80	0.48
1:C:287:TYR:O	1:C:290:LEU:HB2	2.14	0.48
1:C:332:LEU:HB2	1:C:408:PRO:O	2.14	0.48
1:B:192:ARG:HH21	1:B:219:ASN:ND2	2.11	0.48
1:C:179:TYR:C	1:C:181:PRO:CD	2.81	0.48
1:E:180:PHE:HD1	1:E:180:PHE:N	2.08	0.48
1:L:332:LEU:HB2	1:L:408:PRO:O	2.14	0.48
1:D:443:ILE:O	1:D:447:ARG:HB2	2.14	0.48
1:E:287:TYR:O	1:E:290:LEU:HB2	2.14	0.48
1:G:332:LEU:HB2	1:G:408:PRO:O	2.14	0.48
1:G:60:ILE:HA	1:G:60:ILE:HD13	1.62	0.48
1:H:332:LEU:HB2	1:H:408:PRO:O	2.14	0.48
1:A:332:LEU:HB2	1:A:408:PRO:O	2.14	0.47
1:B:287:TYR:O	1:B:290:LEU:HB2	2.14	0.47
1:D:395:ASN:HD22	1:D:395:ASN:HA	1.53	0.47
1:E:332:LEU:HB2	1:E:408:PRO:O	2.14	0.47
1:F:192:ARG:HH21	1:F:219:ASN:ND2	2.11	0.47
1:K:180:PHE:N	1:K:180:PHE:HD1	2.08	0.47
1:C:339:ARG:HH22	1:D:63:SER:HB2	1.78	0.47
1:E:395:ASN:ND2	1:F:60:ILE:HG21	2.28	0.47
1:J:311:LEU:HD22	1:J:369:LEU:HB3	1.97	0.47
1:A:189:GLN:OE1	5:B:1484:MPD:H4	2.13	0.47
1:A:443:ILE:O	1:A:447:ARG:HB2	2.14	0.47
1:D:189:GLN:OE1	5:E:1487:MPD:H4	2.13	0.47
1:D:224:ARG:NH2	1:D:224:ARG:HG2	2.15	0.47
1:D:332:LEU:HB2	1:D:408:PRO:O	2.14	0.47
1:G:63:SER:HB2	1:H:339:ARG:HH22	1.79	0.47
1:A:287:TYR:O	1:A:290:LEU:HB2	2.14	0.47
1:C:397:TYR:OH	1:C:404:ALA:O	2.29	0.47
1:F:18:ASP:OD2	1:F:30:HIS:HD2	1.98	0.47
1:G:311:LEU:HD22	1:G:369:LEU:HB3	1.97	0.47
1:G:63:SER:OG	1:H:339:ARG:NH2	2.47	0.47
1:I:48:MET:HE1	1:I:66:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:443:ILE:O	1:L:447:ARG:HB2	2.14	0.47
1:A:179:TYR:C	1:A:181:PRO:CD	2.81	0.47
1:A:53:SER:HB2	1:F:179:TYR:HE2	1.79	0.47
1:G:18:ASP:OD2	1:G:30:HIS:HD2	1.98	0.47
1:G:401:PRO:CB	1:G:404:ALA:HA	2.37	0.47
1:I:443:ILE:O	1:I:447:ARG:HB2	2.14	0.47
1:J:18:ASP:OD2	1:J:30:HIS:HD2	1.98	0.47
1:J:34:PRO:HG2	1:K:206:VAL:O	2.14	0.47
1:L:401:PRO:CB	1:L:404:ALA:HA	2.37	0.47
1:A:339:ARG:HD3	1:A:339:ARG:HA	1.71	0.47
1:F:443:ILE:O	1:F:447:ARG:HB2	2.14	0.47
1:H:287:TYR:O	1:H:290:LEU:HB2	2.14	0.47
1:J:332:LEU:HB2	1:J:408:PRO:O	2.14	0.47
1:J:443:ILE:O	1:J:447:ARG:HB2	2.14	0.47
1:K:332:LEU:HB2	1:K:408:PRO:O	2.14	0.47
1:L:179:TYR:C	1:L:181:PRO:CD	2.81	0.47
1:B:443:ILE:O	1:B:447:ARG:HB2	2.14	0.47
1:D:179:TYR:C	1:D:181:PRO:CD	2.81	0.47
1:F:311:LEU:HD22	1:F:369:LEU:HB3	1.97	0.47
1:G:443:ILE:O	1:G:447:ARG:HB2	2.14	0.47
1:G:50:ASP:CG	6:G:1609:HOH:O	2.53	0.47
1:H:1:SER:CA	1:H:71:ALA:CB	2.81	0.47
1:K:60:ILE:HD13	1:K:60:ILE:HA	1.62	0.47
1:C:18:ASP:OD2	1:C:30:HIS:HD2	1.98	0.47
1:D:18:ASP:OD2	1:D:30:HIS:HD2	1.98	0.47
1:E:193:SER:CB	5:F:1488:MPD:C3	2.84	0.47
1:B:360:PHE:CG	1:B:361:PRO:HD3	2.43	0.47
1:C:193:SER:HB2	5:D:1486:MPD:C3	2.44	0.47
1:E:456:THR:O	1:K:458:HIS:HE1	1.97	0.47
1:G:192:ARG:HH21	1:G:219:ASN:ND2	2.11	0.47
1:B:18:ASP:OD2	1:B:30:HIS:HD2	1.98	0.47
1:B:311:LEU:HD22	1:B:369:LEU:HB3	1.97	0.47
1:B:332:LEU:HB2	1:B:408:PRO:O	2.14	0.47
1:A:400:PRO:HB3	1:A:401:PRO:HD2	1.97	0.47
1:C:208:ALA:HB2	1:D:33:ILE:HD11	1.97	0.47
1:C:311:LEU:HD22	1:C:369:LEU:HB3	1.97	0.47
1:C:443:ILE:O	1:C:447:ARG:HB2	2.15	0.47
1:C:180:PHE:CB	1:D:29:GLN:HB3	2.43	0.47
1:E:192:ARG:HH21	1:E:219:ASN:ND2	2.11	0.47
1:A:53:SER:HB2	1:F:179:TYR:CE2	2.50	0.47
1:F:401:PRO:CB	1:F:404:ALA:HA	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:1492:MPD:H4	1:K:189:GLN:OE1	2.15	0.47
1:K:287:TYR:O	1:K:290:LEU:HB2	2.14	0.47
1:E:401:PRO:CB	1:E:404:ALA:HA	2.37	0.46
1:E:443:ILE:O	1:E:447:ARG:HB2	2.14	0.46
1:G:81:ALA:H	5:G:1489:MPD:H13	1.80	0.46
1:G:360:PHE:CG	1:G:361:PRO:HD3	2.43	0.46
1:H:179:TYR:C	1:H:181:PRO:CD	2.80	0.46
1:K:443:ILE:O	1:K:447:ARG:HB2	2.14	0.46
1:A:456:THR:O	1:G:458:HIS:HE1	1.98	0.46
1:D:397:TYR:OH	1:D:404:ALA:O	2.29	0.46
1:E:311:LEU:HD22	1:E:369:LEU:HB3	1.96	0.46
1:I:18:ASP:OD2	1:I:30:HIS:HD2	1.98	0.46
1:I:286:LYS:HE2	1:I:292:GLU:HB3	1.98	0.46
1:I:360:PHE:CE2	1:I:361:PRO:HD3	2.39	0.46
1:K:311:LEU:HD22	1:K:369:LEU:HB3	1.97	0.46
1:C:286:LYS:HE2	1:C:292:GLU:HB3	1.98	0.46
1:F:337:ARG:HD3	1:F:393:ASP:OD2	2.15	0.46
1:H:443:ILE:O	1:H:447:ARG:HB2	2.14	0.46
1:I:337:ARG:HD3	1:I:393:ASP:OD2	2.15	0.46
1:K:360:PHE:CG	1:K:361:PRO:HD3	2.43	0.46
1:L:311:LEU:HD22	1:L:369:LEU:HB3	1.97	0.46
1:C:400:PRO:HB3	1:C:401:PRO:HD2	1.97	0.46
1:F:286:LYS:HE2	1:F:292:GLU:HB3	1.98	0.46
1:G:286:LYS:HE2	1:G:292:GLU:HB3	1.98	0.46
1:I:311:LEU:HD22	1:I:369:LEU:HB3	1.97	0.46
1:K:18:ASP:OD2	1:K:30:HIS:HD2	1.98	0.46
1:A:18:ASP:OD2	1:A:30:HIS:HD2	1.98	0.46
1:D:286:LYS:HE2	1:D:292:GLU:HB3	1.98	0.46
1:E:48:MET:HE1	1:E:66:VAL:HG22	1.98	0.46
1:G:124:VAL:HG13	1:G:274:LEU:HD21	1.98	0.46
5:I:1491:MPD:O4	5:I:1491:MPD:HM2	2.16	0.46
1:J:395:ASN:HD22	1:J:395:ASN:HA	1.53	0.46
1:F:454:ARG:O	1:L:320:LYS:HG2	2.15	0.46
1:L:400:PRO:HB3	1:L:401:PRO:HD2	1.97	0.46
1:B:60:ILE:HA	1:B:60:ILE:HD13	1.62	0.46
1:B:395:ASN:ND2	1:C:60:ILE:CG2	2.69	0.46
1:E:400:PRO:HB3	1:E:401:PRO:HD2	1.97	0.46
1:G:400:PRO:HB3	1:G:401:PRO:HD2	1.97	0.46
1:I:33:ILE:HG13	1:J:207:GLU:O	2.14	0.46
1:I:400:PRO:HB3	1:I:401:PRO:HD2	1.97	0.46
1:K:296:TYR:CE2	1:K:385:LYS:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:ASP:OD2	1:L:30:HIS:HD2	1.98	0.46
1:L:28:GLU:OE1	1:L:88:ARG:NH1	2.48	0.46
1:B:337:ARG:HD3	1:B:393:ASP:OD2	2.16	0.46
1:C:124:VAL:HG13	1:C:274:LEU:HD21	1.98	0.46
1:H:18:ASP:OD2	1:H:30:HIS:HD2	1.98	0.46
1:J:179:TYR:C	1:J:181:PRO:CD	2.81	0.46
1:L:296:TYR:CE2	1:L:385:LYS:HD3	2.51	0.46
5:A:1483:MPD:O4	5:A:1483:MPD:HM2	2.16	0.46
1:C:296:TYR:CE2	1:C:385:LYS:HD3	2.51	0.46
5:E:1487:MPD:HM2	5:E:1487:MPD:O4	2.16	0.46
1:E:18:ASP:OD2	1:E:30:HIS:HD2	1.98	0.46
1:F:466:TYR:CE1	1:L:254:THR:HB	2.51	0.46
1:H:296:TYR:CE2	1:H:385:LYS:HD3	2.51	0.46
1:J:286:LYS:HE2	1:J:292:GLU:HB3	1.98	0.46
1:L:48:MET:HE1	1:L:66:VAL:HG22	1.98	0.46
1:A:311:LEU:HD22	1:A:369:LEU:HB3	1.97	0.46
1:C:337:ARG:HD3	1:C:393:ASP:OD2	2.15	0.46
5:D:1486:MPD:O4	5:D:1486:MPD:HM2	2.16	0.46
1:D:311:LEU:HD22	1:D:369:LEU:HB3	1.97	0.46
1:D:93:GLU:HB3	1:D:96:THR:HG23	1.98	0.46
1:E:193:SER:HB2	5:F:1488:MPD:C3	2.40	0.46
1:G:1:SER:CA	1:G:71:ALA:CB	2.80	0.46
1:A:296:TYR:CE2	1:A:385:LYS:HD3	2.51	0.46
1:B:296:TYR:CE2	1:B:385:LYS:HD3	2.51	0.46
1:C:401:PRO:CB	1:C:404:ALA:HA	2.37	0.46
5:F:1488:MPD:HM2	5:F:1488:MPD:O4	2.16	0.46
1:F:48:MET:HE1	1:F:66:VAL:HG22	1.98	0.46
1:A:463:GLU:HA	1:G:140:PHE:CE1	2.51	0.46
5:G:1489:MPD:O4	5:G:1489:MPD:HM2	2.16	0.46
1:I:296:TYR:CE2	1:I:385:LYS:HD3	2.51	0.46
1:I:93:GLU:HB3	1:I:96:THR:HG23	1.98	0.46
1:L:286:LYS:HE2	1:L:292:GLU:HB3	1.98	0.46
1:A:286:LYS:HE2	1:A:292:GLU:HB3	1.98	0.45
1:A:337:ARG:HD3	1:A:393:ASP:OD2	2.15	0.45
1:A:93:GLU:HB3	1:A:96:THR:HG23	1.98	0.45
5:B:1484:MPD:HM2	5:B:1484:MPD:O4	2.16	0.45
1:B:320:LYS:HG2	1:H:454:ARG:O	2.16	0.45
1:B:206:VAL:O	1:C:34:PRO:HG2	2.16	0.45
1:F:296:TYR:CE2	1:F:385:LYS:HD3	2.51	0.45
1:I:397:TYR:OH	1:I:404:ALA:O	2.29	0.45
1:J:296:TYR:CE2	1:J:385:LYS:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:124:VAL:HG13	1:K:274:LEU:HD21	1.98	0.45
1:K:337:ARG:HD3	1:K:393:ASP:OD2	2.15	0.45
1:L:337:ARG:HD3	1:L:393:ASP:OD2	2.15	0.45
1:A:124:VAL:HG13	1:A:274:LEU:HD21	1.98	0.45
1:B:401:PRO:CB	1:B:404:ALA:HA	2.37	0.45
1:F:400:PRO:HB3	1:F:401:PRO:HD2	1.97	0.45
5:H:1490:MPD:HM2	5:H:1490:MPD:O4	2.16	0.45
1:I:124:VAL:HG13	1:I:274:LEU:HD21	1.98	0.45
1:J:337:ARG:HD3	1:J:393:ASP:OD2	2.16	0.45
1:K:400:PRO:HB3	1:K:401:PRO:HD2	1.97	0.45
1:K:93:GLU:HB3	1:K:96:THR:HG23	1.98	0.45
1:G:339:ARG:NH2	1:L:63:SER:OG	2.49	0.45
1:D:124:VAL:HG13	1:D:274:LEU:HD21	1.98	0.45
1:D:432:GLY:HA2	6:D:1602:HOH:O	2.17	0.45
1:E:124:VAL:HG13	1:E:274:LEU:HD21	1.98	0.45
1:E:296:TYR:CE2	1:E:385:LYS:HD3	2.51	0.45
1:H:286:LYS:HE2	1:H:292:GLU:HB3	1.98	0.45
1:I:60:ILE:HA	1:I:60:ILE:HD13	1.62	0.45
1:J:401:PRO:CB	1:J:404:ALA:HA	2.37	0.45
5:C:1485:MPD:HM2	5:C:1485:MPD:O4	2.16	0.45
1:E:286:LYS:HE2	1:E:292:GLU:HB3	1.98	0.45
1:G:337:ARG:HD3	1:G:393:ASP:OD2	2.15	0.45
1:J:33:ILE:HD11	1:K:208:ALA:HB2	1.98	0.45
1:L:195:MET:O	1:L:199:MET:HG3	2.17	0.45
1:L:339:ARG:HA	1:L:339:ARG:HD3	1.71	0.45
1:F:124:VAL:HG13	1:F:274:LEU:HD21	1.98	0.45
1:H:311:LEU:HD22	1:H:369:LEU:HB3	1.97	0.45
5:I:1491:MPD:H4	1:J:189:GLN:OE1	2.17	0.45
1:J:400:PRO:HB3	1:J:401:PRO:HD2	1.98	0.45
1:L:432:GLY:HA2	6:L:1452:HOH:O	2.17	0.45
1:A:195:MET:O	1:A:199:MET:HG3	2.17	0.45
1:C:48:MET:HE1	1:C:66:VAL:HG22	1.98	0.45
5:J:1492:MPD:O4	5:J:1492:MPD:HM2	2.16	0.45
1:K:395:ASN:HA	1:K:395:ASN:HD22	1.53	0.45
1:A:289:GLY:O	1:A:354:ARG:HD2	2.17	0.45
1:B:50:ASP:CG	6:B:1490:HOH:O	2.54	0.45
1:D:195:MET:O	1:D:199:MET:HG3	2.17	0.45
1:D:289:GLY:O	1:D:354:ARG:HD2	2.17	0.45
1:D:337:ARG:HD3	1:D:393:ASP:OD2	2.15	0.45
1:G:93:GLU:HB3	1:G:96:THR:HG23	1.98	0.45
1:H:337:ARG:HD3	1:H:393:ASP:OD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:395:ASN:HD22	1:H:395:ASN:HA	1.53	0.45
1:I:195:MET:O	1:I:199:MET:HG3	2.17	0.45
1:I:432:GLY:HA2	6:I:1606:HOH:O	2.17	0.45
5:L:1494:MPD:HM2	5:L:1494:MPD:O4	2.16	0.45
1:A:206:VAL:O	1:B:34:PRO:HG2	2.17	0.45
1:B:84:THR:CG2	5:B:1484:MPD:C5	2.95	0.45
1:B:124:VAL:HG13	1:B:274:LEU:HD21	1.98	0.45
1:C:193:SER:CB	5:D:1486:MPD:C3	2.90	0.45
1:D:272:MET:O	1:D:355:ARG:HB2	2.17	0.45
1:D:339:ARG:HA	1:D:339:ARG:HD3	1.71	0.45
1:D:296:TYR:CE2	1:D:385:LYS:HD3	2.51	0.45
1:G:289:GLY:O	1:G:354:ARG:HD2	2.17	0.45
1:H:124:VAL:HG13	1:H:274:LEU:HD21	1.98	0.45
1:H:272:MET:O	1:H:355:ARG:HB2	2.17	0.45
1:J:289:GLY:O	1:J:354:ARG:HD2	2.17	0.45
1:J:432:GLY:HA2	6:J:1605:HOH:O	2.17	0.45
1:J:33:ILE:CD1	1:K:208:ALA:HB2	2.47	0.45
1:K:272:MET:O	1:K:355:ARG:HB2	2.17	0.45
1:B:432:GLY:HA2	6:B:1597:HOH:O	2.17	0.45
1:C:93:GLU:HB3	1:C:96:THR:HG23	1.98	0.45
1:E:289:GLY:O	1:E:354:ARG:HD2	2.17	0.45
1:F:254:THR:HB	1:L:466:TYR:CE1	2.52	0.45
1:F:432:GLY:HA2	6:F:1604:HOH:O	2.17	0.45
1:A:432:GLY:HA2	6:A:1590:HOH:O	2.17	0.45
1:B:289:GLY:O	1:B:354:ARG:HD2	2.17	0.45
1:B:93:GLU:HB3	1:B:96:THR:HG23	1.98	0.45
1:D:400:PRO:HB3	1:D:401:PRO:HD2	1.97	0.45
1:G:190:ASP:N	5:L:1494:MPD:HM1	2.32	0.45
1:G:296:TYR:CE2	1:G:385:LYS:HD3	2.51	0.45
1:H:339:ARG:HD3	6:H:1602:HOH:O	2.17	0.45
1:H:400:PRO:HB3	1:H:401:PRO:HD2	1.97	0.45
1:I:84:THR:CG2	5:I:1491:MPD:C5	2.95	0.45
1:J:396:LEU:HG	1:J:396:LEU:H	1.54	0.45
5:K:1493:MPD:HM2	5:K:1493:MPD:O4	2.16	0.45
1:K:289:GLY:O	1:K:354:ARG:HD2	2.17	0.45
1:L:93:GLU:HB3	1:L:96:THR:HG23	1.98	0.45
1:D:28:GLU:OE1	1:D:88:ARG:NH1	2.48	0.44
1:E:84:THR:CG2	5:E:1487:MPD:C5	2.95	0.44
1:E:337:ARG:HD3	1:E:393:ASP:OD2	2.16	0.44
1:F:195:MET:O	1:F:199:MET:HG3	2.17	0.44
1:G:339:ARG:HD3	6:G:1602:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:PRO:HG2	1:I:206:VAL:O	2.17	0.44
1:D:84:THR:CG2	5:D:1486:MPD:C5	2.95	0.44
1:E:339:ARG:HD3	6:E:1597:HOH:O	2.17	0.44
1:G:84:THR:CG2	5:G:1489:MPD:C5	2.95	0.44
1:H:93:GLU:HB3	1:H:96:THR:HG23	1.98	0.44
1:I:289:GLY:O	1:I:354:ARG:HD2	2.17	0.44
1:I:405:LYS:HA	1:I:405:LYS:HD2	1.84	0.44
1:K:28:GLU:OE1	1:K:88:ARG:NH1	2.48	0.44
1:K:286:LYS:HE2	1:K:292:GLU:HB3	1.98	0.44
1:L:124:VAL:HG13	1:L:274:LEU:HD21	1.98	0.44
1:A:114:TYR:CD2	1:A:431:GLY:HA3	2.53	0.44
1:A:458:HIS:HE1	1:G:456:THR:O	2.00	0.44
1:B:195:MET:O	1:B:199:MET:HG3	2.17	0.44
1:B:286:LYS:HE2	1:B:292:GLU:HB3	1.98	0.44
1:E:272:MET:O	1:E:355:ARG:HB2	2.17	0.44
1:E:458:HIS:HE1	1:K:456:THR:O	2.00	0.44
1:F:114:TYR:CD2	1:F:431:GLY:HA3	2.53	0.44
1:A:140:PHE:CE1	1:F:160:SER:HB2	2.53	0.44
1:H:432:GLY:HA2	6:H:1604:HOH:O	2.17	0.44
1:B:114:TYR:CD2	1:B:431:GLY:HA3	2.53	0.44
1:B:230:LYS:O	1:B:233:ASP:HB2	2.18	0.44
1:B:54:ILE:HG22	1:B:55:GLY:N	2.33	0.44
1:B:4:HIS:O	1:B:7:THR:HB	2.18	0.44
1:C:432:GLY:HA2	6:C:1597:HOH:O	2.17	0.44
1:E:360:PHE:CG	1:E:361:PRO:HD3	2.42	0.44
1:F:272:MET:O	1:F:355:ARG:HB2	2.17	0.44
1:G:272:MET:O	1:G:355:ARG:HB2	2.17	0.44
1:G:405:LYS:HD2	1:G:405:LYS:HA	1.84	0.44
1:H:54:ILE:HG22	1:H:55:GLY:N	2.33	0.44
1:L:54:ILE:HG22	1:L:55:GLY:N	2.33	0.44
1:A:84:THR:CG2	5:A:1483:MPD:C5	2.95	0.44
1:B:28:GLU:OE1	1:B:88:ARG:NH1	2.48	0.44
1:B:272:MET:O	1:B:355:ARG:HB2	2.17	0.44
1:E:54:ILE:HG22	1:E:55:GLY:N	2.33	0.44
1:F:84:THR:CG2	5:F:1488:MPD:C5	2.95	0.44
1:B:454:ARG:O	1:H:320:LYS:HG2	2.17	0.44
1:H:289:GLY:O	1:H:354:ARG:HD2	2.17	0.44
1:J:114:TYR:CD2	1:J:431:GLY:HA3	2.53	0.44
5:J:1492:MPD:HM1	1:K:190:ASP:N	2.33	0.44
1:J:4:HIS:O	1:J:7:THR:HB	2.18	0.44
1:K:195:MET:O	1:K:199:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:400:PRO:CB	1:L:401:PRO:CD	2.96	0.44
1:A:272:MET:O	1:A:355:ARG:HB2	2.17	0.44
1:A:28:GLU:OE1	1:A:88:ARG:NH1	2.48	0.44
1:C:400:PRO:CB	1:C:401:PRO:CD	2.96	0.44
1:F:54:ILE:HG22	1:F:55:GLY:N	2.33	0.44
1:G:28:GLU:OE1	1:G:88:ARG:NH1	2.48	0.44
5:G:1489:MPD:CM	1:H:190:ASP:OD2	2.64	0.44
1:H:360:PHE:CG	1:H:361:PRO:HD3	2.43	0.44
1:J:54:ILE:HG22	1:J:55:GLY:N	2.33	0.44
1:J:84:THR:CG2	5:J:1492:MPD:C5	2.95	0.44
1:K:54:ILE:HG22	1:K:55:GLY:N	2.33	0.44
1:L:114:TYR:CD2	1:L:431:GLY:HA3	2.53	0.44
1:L:68:MET:HA	1:L:69:PRO:HD2	1.89	0.44
1:B:400:PRO:CB	1:B:401:PRO:CD	2.96	0.44
1:B:400:PRO:HB3	1:B:401:PRO:HD2	1.97	0.44
1:C:114:TYR:CD2	1:C:431:GLY:HA3	2.53	0.44
1:C:195:MET:O	1:C:199:MET:HG3	2.17	0.44
1:C:54:ILE:HG22	1:C:55:GLY:N	2.33	0.44
1:D:81:ALA:H	5:D:1486:MPD:H13	1.79	0.44
1:D:339:ARG:HD3	6:D:1600:HOH:O	2.17	0.44
1:D:4:HIS:O	1:D:7:THR:HB	2.18	0.44
1:F:230:LYS:O	1:F:233:ASP:HB2	2.18	0.44
1:G:195:MET:O	1:G:199:MET:HG3	2.17	0.44
1:G:230:LYS:O	1:G:233:ASP:HB2	2.18	0.44
1:I:51:GLY:C	1:I:53:SER:N	2.26	0.44
1:J:195:MET:O	1:J:199:MET:HG3	2.17	0.44
1:J:93:GLU:HB3	1:J:96:THR:HG23	1.98	0.44
1:K:230:LYS:O	1:K:233:ASP:HB2	2.18	0.44
1:K:339:ARG:HD3	6:K:1607:HOH:O	2.17	0.44
1:L:84:THR:CG2	5:L:1494:MPD:C5	2.95	0.44
1:D:114:TYR:CD2	1:D:431:GLY:HA3	2.53	0.44
1:E:195:MET:O	1:E:199:MET:HG3	2.17	0.44
1:G:114:TYR:CD2	1:G:431:GLY:HA3	2.53	0.44
1:H:224:ARG:NH2	1:H:224:ARG:HG2	2.15	0.44
1:I:400:PRO:CB	1:I:401:PRO:CD	2.96	0.44
1:J:400:PRO:CB	1:J:401:PRO:CD	2.96	0.44
1:L:289:GLY:O	1:L:354:ARG:HD2	2.17	0.44
1:L:339:ARG:HD3	6:L:1450:HOH:O	2.17	0.44
1:A:4:HIS:O	1:A:7:THR:HB	2.18	0.44
1:B:339:ARG:HD3	6:B:1595:HOH:O	2.17	0.44
1:D:230:LYS:O	1:D:233:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:TYR:CD2	1:E:431:GLY:HA3	2.53	0.44
1:E:93:GLU:HB3	1:E:96:THR:HG23	1.98	0.44
1:F:289:GLY:O	1:F:354:ARG:HD2	2.17	0.44
1:F:339:ARG:HD3	6:F:1602:HOH:O	2.17	0.44
1:F:60:ILE:HA	1:F:60:ILE:HD13	1.62	0.44
1:F:4:HIS:O	1:F:7:THR:HB	2.18	0.44
1:G:432:GLY:HA2	6:G:1604:HOH:O	2.17	0.44
1:H:195:MET:O	1:H:199:MET:HG3	2.17	0.44
1:I:230:LYS:O	1:I:233:ASP:HB2	2.18	0.44
1:I:272:MET:O	1:I:355:ARG:HB2	2.17	0.44
1:I:337:ARG:HG2	1:I:338:ASN:N	2.33	0.44
1:I:51:GLY:O	1:I:54:ILE:N	2.51	0.44
1:I:80:PHE:CE2	1:J:189:GLN:HG2	2.53	0.44
1:J:124:VAL:HG13	1:J:274:LEU:HD21	1.98	0.44
1:K:53:SER:HB2	1:L:179:TYR:HE2	1.83	0.44
1:K:84:THR:CG2	5:K:1493:MPD:C5	2.95	0.44
1:F:320:LYS:HG2	1:L:454:ARG:O	2.17	0.44
1:C:4:HIS:O	1:C:7:THR:HB	2.18	0.43
1:C:84:THR:CG2	5:C:1485:MPD:C5	2.95	0.43
1:D:54:ILE:HG22	1:D:55:GLY:N	2.33	0.43
1:E:432:GLY:HA2	6:E:1599:HOH:O	2.17	0.43
1:E:463:GLU:HA	1:K:140:PHE:CE1	2.53	0.43
1:F:93:GLU:HB3	1:F:96:THR:HG23	1.98	0.43
1:G:4:HIS:O	1:G:7:THR:HB	2.18	0.43
1:I:54:ILE:HG22	1:I:55:GLY:N	2.33	0.43
1:K:432:GLY:HA2	6:K:1609:HOH:O	2.17	0.43
1:L:272:MET:O	1:L:355:ARG:HB2	2.17	0.43
1:L:337:ARG:HG2	1:L:338:ASN:N	2.33	0.43
1:L:398:ASP:C	1:L:400:PRO:CD	2.82	0.43
1:L:4:HIS:O	1:L:7:THR:HB	2.18	0.43
1:L:51:GLY:O	1:L:54:ILE:N	2.51	0.43
1:A:400:PRO:CB	1:A:401:PRO:CD	2.96	0.43
1:B:395:ASN:HA	1:B:395:ASN:HD22	1.53	0.43
1:C:289:GLY:O	1:C:354:ARG:HD2	2.17	0.43
1:D:337:ARG:HG2	1:D:338:ASN:N	2.33	0.43
1:D:48:MET:HE1	1:D:66:VAL:HG22	1.96	0.43
1:H:84:THR:CG2	5:H:1490:MPD:C5	2.95	0.43
1:I:339:ARG:HD3	6:I:1604:HOH:O	2.17	0.43
1:I:398:ASP:C	1:I:400:PRO:CD	2.82	0.43
1:J:272:MET:O	1:J:355:ARG:HB2	2.17	0.43
1:A:230:LYS:O	1:A:233:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:N	1:A:384:ASN:ND2	2.66	0.43
1:C:254:THR:HB	1:I:466:TYR:CE1	2.54	0.43
1:C:339:ARG:HD3	6:C:1595:HOH:O	2.17	0.43
1:F:337:ARG:HG2	1:F:338:ASN:N	2.33	0.43
1:C:320:LYS:HG2	1:I:454:ARG:O	2.18	0.43
1:I:4:HIS:O	1:I:7:THR:HB	2.18	0.43
1:J:339:ARG:HD3	6:J:1603:HOH:O	2.17	0.43
1:L:230:LYS:O	1:L:233:ASP:HB2	2.18	0.43
1:C:210:HIS:HB3	1:D:31:VAL:HG23	2.01	0.43
1:C:189:GLN:OE1	5:D:1486:MPD:H4	2.18	0.43
1:D:33:ILE:HA	1:D:34:PRO:HD3	1.92	0.43
1:G:445:LEU:O	1:G:448:GLU:HG2	2.19	0.43
1:H:28:GLU:OE1	1:H:88:ARG:NH1	2.48	0.43
1:J:33:ILE:HG13	1:K:207:GLU:O	2.19	0.43
1:K:400:PRO:CB	1:K:401:PRO:CD	2.96	0.43
1:A:445:LEU:O	1:A:448:GLU:HG2	2.19	0.43
1:C:272:MET:O	1:C:355:ARG:HB2	2.17	0.43
1:E:230:LYS:O	1:E:233:ASP:HB2	2.18	0.43
1:E:4:HIS:O	1:E:7:THR:HB	2.18	0.43
1:G:337:ARG:HG2	1:G:338:ASN:N	2.33	0.43
1:G:400:PRO:CB	1:G:401:PRO:CD	2.96	0.43
1:H:4:HIS:O	1:H:7:THR:HB	2.18	0.43
1:J:81:ALA:H	5:J:1492:MPD:H13	1.79	0.43
1:G:54:ILE:HG22	1:G:55:GLY:N	2.33	0.43
1:H:114:TYR:CD2	1:H:431:GLY:HA3	2.53	0.43
1:H:400:PRO:CB	1:H:401:PRO:CD	2.96	0.43
1:J:230:LYS:O	1:J:233:ASP:HB2	2.18	0.43
1:J:28:GLU:OE1	1:J:88:ARG:NH1	2.48	0.43
1:J:360:PHE:CG	1:J:361:PRO:HD3	2.43	0.43
1:K:81:ALA:H	5:K:1493:MPD:H13	1.79	0.43
1:A:193:SER:HB2	5:B:1484:MPD:C3	2.43	0.43
1:A:54:ILE:HG22	1:A:55:GLY:N	2.33	0.43
1:B:337:ARG:HG2	1:B:338:ASN:N	2.33	0.43
1:B:339:ARG:HA	1:B:339:ARG:HD3	1.71	0.43
1:C:360:PHE:CG	1:C:361:PRO:HD3	2.43	0.43
1:D:445:LEU:O	1:D:448:GLU:HG2	2.19	0.43
1:E:337:ARG:HG2	1:E:338:ASN:N	2.33	0.43
1:F:445:LEU:O	1:F:448:GLU:HG2	2.19	0.43
1:H:230:LYS:O	1:H:233:ASP:HB2	2.18	0.43
1:H:401:PRO:CB	1:H:404:ALA:HA	2.37	0.43
5:I:1491:MPD:HM2	1:J:189:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ALA:HB2	1:B:33:ILE:HD11	2.01	0.43
1:B:445:LEU:O	1:B:448:GLU:HG2	2.19	0.43
1:C:384:ASN:ND2	1:C:384:ASN:N	2.66	0.43
1:E:189:GLN:HG3	5:F:1488:MPD:HM2	2.00	0.43
1:E:384:ASN:N	1:E:384:ASN:ND2	2.66	0.43
1:F:400:PRO:CB	1:F:401:PRO:CD	2.96	0.43
1:I:445:LEU:O	1:I:448:GLU:HG2	2.19	0.43
1:K:314:PRO:HG3	1:K:365:ALA:HA	2.01	0.43
1:L:445:LEU:O	1:L:448:GLU:HG2	2.19	0.43
1:A:339:ARG:HD3	6:A:1588:HOH:O	2.17	0.43
1:D:400:PRO:CB	1:D:401:PRO:CD	2.96	0.43
1:E:396:LEU:O	1:E:399:LEU:CB	2.67	0.43
1:E:400:PRO:CB	1:E:401:PRO:CD	2.96	0.43
1:E:398:ASP:C	1:E:400:PRO:CD	2.82	0.43
1:H:445:LEU:O	1:H:448:GLU:HG2	2.19	0.43
1:I:114:TYR:CD2	1:I:431:GLY:HA3	2.53	0.43
1:D:454:ARG:O	1:J:320:LYS:HG2	2.19	0.43
1:K:114:TYR:CD2	1:K:431:GLY:HA3	2.53	0.43
1:K:445:LEU:O	1:K:448:GLU:HG2	2.19	0.43
1:K:4:HIS:O	1:K:7:THR:HB	2.18	0.43
5:A:1483:MPD:H4	1:F:189:GLN:OE1	2.19	0.43
1:A:208:ALA:HB2	1:B:33:ILE:CD1	2.49	0.43
1:A:337:ARG:HG2	1:A:338:ASN:N	2.33	0.43
1:A:398:ASP:C	1:A:400:PRO:CD	2.82	0.43
1:C:337:ARG:HG2	1:C:338:ASN:N	2.33	0.43
1:E:28:GLU:OE1	1:E:88:ARG:NH1	2.48	0.43
1:E:339:ARG:HD3	1:E:339:ARG:HA	1.71	0.43
1:E:206:VAL:O	1:F:34:PRO:HG2	2.19	0.43
1:G:339:ARG:HA	1:G:339:ARG:HD3	1.71	0.43
1:H:33:ILE:HA	1:H:34:PRO:HD3	1.92	0.43
1:A:426:GLU:HG2	6:A:1563:HOH:O	2.20	0.42
1:B:396:LEU:O	1:B:399:LEU:CB	2.67	0.42
1:C:445:LEU:O	1:C:448:GLU:HG2	2.19	0.42
1:F:231:LYS:HA	1:F:231:LYS:HD2	1.82	0.42
1:G:314:PRO:HG3	1:G:365:ALA:HA	2.01	0.42
1:H:314:PRO:HG3	1:H:365:ALA:HA	2.01	0.42
1:J:405:LYS:HA	1:J:405:LYS:HD2	1.84	0.42
1:K:337:ARG:HG2	1:K:338:ASN:N	2.34	0.42
1:G:208:ALA:HB2	1:L:33:ILE:HD11	2.01	0.42
1:A:51:GLY:O	1:A:54:ILE:N	2.51	0.42
1:E:314:PRO:HG3	1:E:365:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:LYS:HD2	1:F:405:LYS:HA	1.85	0.42
1:H:140:PHE:CE1	1:I:160:SER:HB2	2.54	0.42
1:H:426:GLU:HG2	6:H:1577:HOH:O	2.20	0.42
1:I:63:SER:CB	1:J:339:ARG:NH2	2.82	0.42
1:E:254:THR:HB	1:K:466:TYR:CE1	2.54	0.42
1:K:48:MET:HE1	1:K:66:VAL:HG22	2.01	0.42
1:B:314:PRO:HG3	1:B:365:ALA:HA	2.01	0.42
1:K:53:SER:HB2	1:L:179:TYR:CE2	2.55	0.42
1:C:28:GLU:OE1	1:C:88:ARG:NH1	2.48	0.42
1:E:68:MET:HA	1:E:69:PRO:HD2	1.89	0.42
1:F:397:TYR:OH	1:F:404:ALA:O	2.29	0.42
1:H:58:LYS:NZ	1:H:60:ILE:HD11	2.35	0.42
1:J:314:PRO:HG3	1:J:365:ALA:HA	2.01	0.42
1:K:398:ASP:C	1:K:400:PRO:CD	2.82	0.42
1:A:405:LYS:HD2	1:A:405:LYS:HA	1.84	0.42
1:C:81:ALA:H	5:C:1485:MPD:H13	1.79	0.42
1:C:208:ALA:HB2	1:D:33:ILE:CD1	2.50	0.42
1:C:33:ILE:HA	1:C:34:PRO:HD3	1.92	0.42
1:F:28:GLU:OE1	1:F:88:ARG:NH1	2.48	0.42
5:I:1491:MPD:CM	1:J:190:ASP:OD2	2.63	0.42
1:K:231:LYS:HD2	1:K:231:LYS:HA	1.82	0.42
1:K:458:HIS:HD2	1:K:460:VAL:N	2.02	0.42
1:C:396:LEU:O	1:C:399:LEU:CB	2.67	0.42
1:D:398:ASP:C	1:D:400:PRO:CD	2.82	0.42
1:D:426:GLU:HG2	6:D:1575:HOH:O	2.20	0.42
1:E:426:GLU:HG2	6:E:1572:HOH:O	2.19	0.42
1:K:397:TYR:OH	1:K:404:ALA:O	2.29	0.42
1:B:48:MET:HE1	1:B:66:VAL:HG22	1.99	0.42
1:C:230:LYS:O	1:C:233:ASP:HB2	2.18	0.42
1:D:320:LYS:HG2	1:J:454:ARG:O	2.18	0.42
1:D:58:LYS:HZ2	1:D:60:ILE:HD13	1.84	0.42
1:E:127:GLY:HA3	3:E:1475:ADP:H1'	2.02	0.42
1:F:396:LEU:O	1:F:399:LEU:CB	2.67	0.42
1:A:401:PRO:CB	1:A:404:ALA:HA	2.37	0.42
1:C:68:MET:HA	1:C:69:PRO:HD2	1.89	0.42
1:E:58:LYS:NZ	1:E:60:ILE:HD11	2.35	0.42
1:H:337:ARG:HG2	1:H:338:ASN:N	2.33	0.42
1:L:426:GLU:HG2	6:L:1421:HOH:O	2.20	0.42
1:A:190:ASP:OD2	5:B:1484:MPD:CM	2.65	0.42
1:C:426:GLU:HG2	6:C:1571:HOH:O	2.20	0.42
1:G:403:GLU:O	1:G:404:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:28:GLU:OE1	1:I:88:ARG:NH1	2.48	0.42
1:J:339:ARG:HA	1:J:339:ARG:HD3	1.71	0.42
1:J:445:LEU:O	1:J:448:GLU:HG2	2.19	0.42
1:K:127:GLY:HA3	3:K:1481:ADP:H1'	2.02	0.42
1:K:384:ASN:N	1:K:384:ASN:ND2	2.66	0.42
1:K:403:GLU:C	1:K:405:LYS:H	2.23	0.42
1:A:230:LYS:HB2	1:A:230:LYS:HE3	1.89	0.42
1:B:127:GLY:HA3	3:B:1472:ADP:H1'	2.02	0.42
1:C:58:LYS:NZ	1:C:60:ILE:HD11	2.35	0.42
1:E:445:LEU:O	1:E:448:GLU:HG2	2.19	0.42
1:A:31:VAL:HG23	1:F:210:HIS:HB3	2.02	0.42
1:F:426:GLU:HG2	6:F:1577:HOH:O	2.19	0.42
1:H:68:MET:HA	1:H:69:PRO:HD2	1.89	0.42
1:H:80:PHE:CZ	1:I:189:GLN:HG2	2.55	0.42
1:I:314:PRO:HG3	1:I:365:ALA:HA	2.01	0.42
1:J:403:GLU:O	1:J:404:ALA:HB3	2.20	0.42
1:K:426:GLU:HG2	6:K:1582:HOH:O	2.20	0.42
1:L:405:LYS:HD2	1:L:405:LYS:HA	1.84	0.42
1:A:314:PRO:HG3	1:A:365:ALA:HA	2.01	0.41
1:A:82:ASP:O	1:A:84:THR:CG2	2.55	0.41
1:B:81:ALA:H	5:B:1484:MPD:H13	1.79	0.41
1:C:339:ARG:HA	1:C:339:ARG:HD3	1.71	0.41
1:C:314:PRO:HG3	1:C:365:ALA:HA	2.01	0.41
1:D:328:ALA:HA	1:D:329:PRO:HD2	1.93	0.41
1:D:396:LEU:O	1:D:399:LEU:CB	2.67	0.41
1:A:53:SER:CB	1:F:179:TYR:CE2	3.03	0.41
1:G:426:GLU:HG2	6:G:1577:HOH:O	2.19	0.41
1:G:58:LYS:NZ	1:G:60:ILE:HD11	2.35	0.41
1:H:127:GLY:HA3	3:H:1478:ADP:H1'	2.02	0.41
1:H:51:GLY:O	1:H:54:ILE:N	2.51	0.41
5:J:1492:MPD:CM	1:K:190:ASP:OD2	2.59	0.41
1:K:58:LYS:NZ	1:K:60:ILE:HD11	2.35	0.41
1:A:396:LEU:O	1:A:399:LEU:CB	2.67	0.41
1:B:403:GLU:C	1:B:405:LYS:H	2.24	0.41
1:C:390:GLU:HA	1:C:391:PRO:HD3	1.95	0.41
1:C:403:GLU:O	1:C:404:ALA:HB3	2.20	0.41
1:D:58:LYS:NZ	1:D:60:ILE:HD11	2.35	0.41
1:G:396:LEU:O	1:G:399:LEU:CB	2.67	0.41
1:J:51:GLY:O	1:J:54:ILE:N	2.51	0.41
1:L:230:LYS:HB2	1:L:230:LYS:HE3	1.89	0.41
1:A:127:GLY:HA3	3:A:1471:ADP:H1'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLN:HG3	5:C:1485:MPD:HM2	2.00	0.41
1:F:340:SER:OG	1:F:396:LEU:CB	2.69	0.41
1:F:403:GLU:C	1:F:405:LYS:H	2.23	0.41
1:G:127:GLY:HA3	3:G:1477:ADP:H1'	2.02	0.41
1:J:337:ARG:HG2	1:J:338:ASN:N	2.33	0.41
1:J:426:GLU:HG2	6:J:1578:HOH:O	2.20	0.41
1:J:80:PHE:CE2	1:K:189:GLN:HG2	2.55	0.41
1:K:31:VAL:HG23	1:L:210:HIS:HB3	2.03	0.41
1:L:328:ALA:HA	1:L:329:PRO:HD2	1.93	0.41
1:A:58:LYS:NZ	1:A:60:ILE:HD11	2.35	0.41
1:F:339:ARG:HA	1:F:339:ARG:HD3	1.71	0.41
1:G:340:SER:OG	1:G:396:LEU:CB	2.69	0.41
1:G:58:LYS:HZ2	1:G:60:ILE:HD13	1.84	0.41
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.82	0.41
1:I:81:ALA:H	5:I:1491:MPD:H13	1.79	0.41
1:I:58:LYS:NZ	1:I:60:ILE:HD11	2.35	0.41
1:K:339:ARG:HA	1:K:339:ARG:HD3	1.71	0.41
1:K:403:GLU:O	1:K:404:ALA:HB3	2.20	0.41
1:B:254:THR:HB	1:H:466:TYR:CE1	2.55	0.41
1:B:426:GLU:HG2	6:B:1570:HOH:O	2.20	0.41
1:D:16:PHE:CG	5:D:1486:MPD:H52	2.55	0.41
1:E:51:GLY:O	1:E:54:ILE:N	2.51	0.41
1:D:179:TYR:HE2	1:E:53:SER:HB2	1.86	0.41
1:F:398:ASP:C	1:F:400:PRO:CD	2.82	0.41
1:H:49:PHE:O	1:H:64:ASP:OD2	2.39	0.41
5:H:1490:MPD:HM1	1:I:190:ASP:N	2.35	0.41
1:J:340:SER:OG	1:J:396:LEU:CB	2.69	0.41
1:K:405:LYS:HD2	1:K:405:LYS:HA	1.84	0.41
1:L:49:PHE:O	1:L:64:ASP:OD2	2.39	0.41
1:A:16:PHE:CG	5:A:1483:MPD:H52	2.55	0.41
1:A:49:PHE:O	1:A:64:ASP:OD2	2.39	0.41
1:A:1:SER:CA	1:A:71:ALA:CB	2.80	0.41
1:B:403:GLU:O	1:B:404:ALA:HB3	2.20	0.41
1:C:127:GLY:HA3	3:C:1473:ADP:H1'	2.02	0.41
1:D:314:PRO:HG3	1:D:365:ALA:HA	2.01	0.41
1:H:403:GLU:O	1:H:404:ALA:HB3	2.20	0.41
1:H:405:LYS:HA	1:H:405:LYS:HD2	1.85	0.41
1:J:396:LEU:O	1:J:399:LEU:CB	2.67	0.41
1:B:384:ASN:N	1:B:384:ASN:ND2	2.66	0.41
1:B:51:GLY:O	1:B:54:ILE:N	2.51	0.41
1:C:340:SER:OG	1:C:396:LEU:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:PHE:O	1:C:64:ASP:OD2	2.39	0.41
1:C:82:ASP:O	1:C:84:THR:CG2	2.55	0.41
1:F:284:GLY:HA3	1:F:291:SER:HA	2.03	0.41
1:F:314:PRO:HG3	1:F:365:ALA:HA	2.01	0.41
1:G:206:VAL:O	1:L:34:PRO:HG2	2.21	0.41
1:I:396:LEU:H	1:I:396:LEU:HG	1.54	0.41
1:J:49:PHE:O	1:J:64:ASP:OD2	2.39	0.41
1:K:396:LEU:HG	1:K:396:LEU:H	1.54	0.41
1:K:140:PHE:CE1	1:L:160:SER:HB2	2.56	0.41
1:B:177:GLY:C	1:B:179:TYR:H	2.25	0.41
1:C:396:LEU:H	1:C:396:LEU:HG	1.54	0.41
1:C:466:TYR:CE1	1:I:254:THR:HB	2.56	0.41
1:C:51:GLY:O	1:C:54:ILE:N	2.51	0.41
1:D:284:GLY:HA3	1:D:291:SER:HA	2.03	0.41
1:E:81:ALA:H	5:E:1487:MPD:H13	1.79	0.41
1:E:190:ASP:N	5:F:1488:MPD:HM1	2.36	0.41
1:G:403:GLU:C	1:G:405:LYS:H	2.23	0.41
1:H:384:ASN:ND2	1:H:384:ASN:N	2.66	0.41
1:I:426:GLU:HG2	6:I:1579:HOH:O	2.20	0.41
1:J:403:GLU:C	1:J:405:LYS:H	2.23	0.41
1:L:314:PRO:HG3	1:L:365:ALA:HA	2.01	0.41
1:A:281:LEU:HD23	1:A:293:GLN:OE1	2.21	0.41
1:A:68:MET:HA	1:A:69:PRO:HD2	1.89	0.41
1:C:403:GLU:C	1:C:405:LYS:H	2.23	0.41
1:D:49:PHE:O	1:D:64:ASP:OD2	2.39	0.41
1:F:177:GLY:C	1:F:179:TYR:H	2.25	0.41
1:F:403:GLU:O	1:F:404:ALA:HB3	2.20	0.41
1:F:58:LYS:NZ	1:F:60:ILE:HD11	2.35	0.41
1:G:284:GLY:HA3	1:G:291:SER:HA	2.03	0.41
1:H:281:LEU:HD23	1:H:293:GLN:OE1	2.21	0.41
1:H:398:ASP:C	1:H:400:PRO:CD	2.82	0.41
1:I:396:LEU:O	1:I:399:LEU:CB	2.67	0.41
1:L:403:GLU:O	1:L:404:ALA:HB3	2.20	0.41
1:A:403:GLU:O	1:A:404:ALA:HB3	2.20	0.41
1:B:58:LYS:NZ	1:B:60:ILE:HD11	2.35	0.41
1:B:58:LYS:HZ2	1:B:60:ILE:HD13	1.85	0.41
1:B:49:PHE:O	1:B:64:ASP:OD2	2.39	0.41
1:C:179:TYR:HE2	1:D:53:SER:HB2	1.86	0.41
1:C:398:ASP:C	1:C:400:PRO:CD	2.82	0.41
1:C:458:HIS:HD2	1:C:460:VAL:N	2.02	0.41
1:E:340:SER:OG	1:E:396:LEU:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:SER:HA	1:E:351:PRO:HD3	1.98	0.41
1:F:51:GLY:O	1:F:54:ILE:N	2.51	0.41
1:I:177:GLY:C	1:I:179:TYR:H	2.25	0.41
1:H:80:PHE:CE2	1:I:189:GLN:HG2	2.55	0.41
1:I:340:SER:OG	1:I:396:LEU:CB	2.69	0.41
1:I:403:GLU:O	1:I:404:ALA:HB3	2.20	0.41
1:I:68:MET:HA	1:I:69:PRO:HD2	1.89	0.41
1:J:177:GLY:C	1:J:179:TYR:H	2.24	0.41
1:J:31:VAL:HG23	1:K:210:HIS:HB3	2.03	0.41
1:K:128:PRO:HD2	6:K:1507:HOH:O	2.21	0.41
1:L:127:GLY:HA3	3:L:1482:ADP:H1'	2.02	0.41
1:A:403:GLU:C	1:A:405:LYS:H	2.23	0.41
1:A:207:GLU:O	1:B:33:ILE:HG13	2.20	0.41
1:B:340:SER:OG	1:B:396:LEU:CB	2.69	0.41
1:C:281:LEU:HD23	1:C:293:GLN:OE1	2.21	0.41
1:C:284:GLY:HA3	1:C:291:SER:HA	2.03	0.41
1:D:127:GLY:HA3	3:D:1474:ADP:H1'	2.02	0.41
1:E:403:GLU:C	1:E:405:LYS:H	2.24	0.41
1:E:403:GLU:O	1:E:404:ALA:HB3	2.20	0.41
1:F:384:ASN:N	1:F:384:ASN:ND2	2.66	0.41
1:G:281:LEU:HD23	1:G:293:GLN:OE1	2.21	0.41
1:H:16:PHE:CG	5:H:1490:MPD:H52	2.55	0.41
1:I:16:PHE:CG	5:I:1491:MPD:H52	2.55	0.41
1:I:360:PHE:CG	1:I:361:PRO:HD3	2.43	0.41
1:J:284:GLY:HA3	1:J:291:SER:HA	2.03	0.41
1:L:284:GLY:HA3	1:L:291:SER:HA	2.03	0.41
1:B:466:TYR:CE1	1:H:254:THR:HB	2.56	0.40
1:F:16:PHE:CG	5:F:1488:MPD:H52	2.55	0.40
1:I:281:LEU:HD23	1:I:293:GLN:OE1	2.21	0.40
1:J:231:LYS:HA	1:J:231:LYS:HD2	1.82	0.40
1:J:33:ILE:HA	1:J:34:PRO:HD3	1.92	0.40
1:J:50:ASP:CG	6:J:1612:HOH:O	2.59	0.40
1:K:33:ILE:HA	1:K:34:PRO:HD3	1.92	0.40
1:K:396:LEU:O	1:K:399:LEU:CB	2.67	0.40
1:K:51:GLY:O	1:K:54:ILE:N	2.51	0.40
1:L:50:ASP:CG	6:L:838:HOH:O	2.60	0.40
1:A:128:PRO:HD2	6:A:1487:HOH:O	2.21	0.40
1:B:16:PHE:CG	5:B:1484:MPD:H52	2.55	0.40
1:B:189:GLN:HG2	1:C:80:PHE:CE2	2.57	0.40
1:D:403:GLU:O	1:D:404:ALA:HB3	2.20	0.40
1:E:128:PRO:HD2	6:E:1497:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:PHE:O	1:E:64:ASP:OD2	2.39	0.40
1:F:127:GLY:HA3	3:F:1476:ADP:H1'	2.02	0.40
1:H:340:SER:OG	1:H:396:LEU:CB	2.69	0.40
1:J:127:GLY:HA3	3:J:1480:ADP:H1'	2.02	0.40
1:L:340:SER:OG	1:L:396:LEU:CB	2.69	0.40
1:B:204:LEU:HD23	1:B:223:THR:HG21	2.04	0.40
1:D:82:ASP:O	1:D:84:THR:CG2	2.55	0.40
1:G:189:GLN:HG2	1:L:80:PHE:CE2	2.57	0.40
1:H:339:ARG:HA	1:H:339:ARG:HD3	1.71	0.40
1:H:396:LEU:O	1:H:399:LEU:CB	2.67	0.40
1:H:53:SER:HB2	1:I:179:TYR:HE2	1.86	0.40
1:I:230:LYS:HB2	1:I:230:LYS:HE3	1.89	0.40
1:K:281:LEU:HD23	1:K:293:GLN:OE1	2.21	0.40
1:A:284:GLY:HA3	1:A:291:SER:HA	2.03	0.40
1:D:230:LYS:HE3	1:D:230:LYS:HB2	1.89	0.40
1:D:281:LEU:HD23	1:D:293:GLN:OE1	2.21	0.40
1:F:281:LEU:HD23	1:F:293:GLN:OE1	2.21	0.40
1:J:281:LEU:HD23	1:J:293:GLN:OE1	2.21	0.40
5:K:1493:MPD:H4	1:L:189:GLN:OE1	2.21	0.40
1:A:180:PHE:CB	1:B:29:GLN:HB3	2.50	0.40
1:H:284:GLY:HA3	1:H:291:SER:HA	2.03	0.40
1:I:403:GLU:C	1:I:405:LYS:H	2.24	0.40
1:J:419:ASN:O	1:J:422:ASP:HB3	2.22	0.40
1:D:254:THR:HB	1:J:466:TYR:CE1	2.57	0.40
1:K:49:PHE:O	1:K:64:ASP:OD2	2.39	0.40
1:L:384:ASN:ND2	1:L:384:ASN:N	2.66	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	B	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	C	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	D	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	E	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	F	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	G	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	H	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	I	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	J	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	K	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
1	L	466/468 (100%)	429 (92%)	28 (6%)	9 (2%)	8	18
All	All	5592/5616 (100%)	5148 (92%)	336 (6%)	108 (2%)	8	18

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	62	GLU
1	A	180	PHE
1	A	399	LEU
1	A	400	PRO
1	A	401	PRO
1	B	52	SER
1	B	62	GLU
1	B	180	PHE
1	B	399	LEU
1	B	400	PRO
1	B	401	PRO
1	C	52	SER
1	C	62	GLU
1	C	180	PHE
1	C	399	LEU
1	C	400	PRO
1	C	401	PRO
1	D	52	SER
1	D	62	GLU
1	D	180	PHE
1	D	399	LEU

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Mol	Chain	Res	Type
1	D	400	PRO
1	D	401	PRO
1	E	52	SER
1	E	62	GLU
1	E	180	PHE
1	E	399	LEU
1	E	400	PRO
1	E	401	PRO
1	F	52	SER
1	F	62	GLU
1	F	180	PHE
1	F	399	LEU
1	F	400	PRO
1	F	401	PRO
1	G	52	SER
1	G	62	GLU
1	G	180	PHE
1	G	399	LEU
1	G	400	PRO
1	G	401	PRO
1	H	52	SER
1	H	62	GLU
1	H	180	PHE
1	H	399	LEU
1	H	400	PRO
1	H	401	PRO
1	I	52	SER
1	I	62	GLU
1	I	180	PHE
1	I	399	LEU
1	I	400	PRO
1	I	401	PRO
1	J	52	SER
1	J	62	GLU
1	J	180	PHE
1	J	399	LEU
1	J	400	PRO
1	J	401	PRO
1	K	52	SER
1	K	62	GLU
1	K	180	PHE
1	K	399	LEU

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Mol	Chain	Res	Type
1	K	400	PRO
1	K	401	PRO
1	L	52	SER
1	L	62	GLU
1	L	180	PHE
1	L	399	LEU
1	L	400	PRO
1	L	401	PRO
1	A	324	PRO
1	A	396	LEU
1	B	324	PRO
1	B	396	LEU
1	C	324	PRO
1	C	396	LEU
1	D	324	PRO
1	D	396	LEU
1	E	324	PRO
1	E	396	LEU
1	F	324	PRO
1	F	396	LEU
1	G	324	PRO
1	G	396	LEU
1	H	324	PRO
1	H	396	LEU
1	I	324	PRO
1	I	396	LEU
1	J	324	PRO
1	J	396	LEU
1	K	324	PRO
1	K	396	LEU
1	L	324	PRO
1	L	396	LEU
1	A	349	ALA
1	B	349	ALA
1	C	349	ALA
1	D	349	ALA
1	E	349	ALA
1	F	349	ALA
1	G	349	ALA
1	H	349	ALA
1	I	349	ALA
1	J	349	ALA

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Mol	Chain	Res	Type
1	K	349	ALA
1	L	349	ALA

### 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	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	B	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	C	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	D	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	E	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	F	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	G	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	H	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	I	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	J	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	K	384/384 (100%)	341 (89%)	43 (11%)	6	12
1	L	384/384 (100%)	341 (89%)	43 (11%)	6	12
All	All	4608/4608 (100%)	4092 (89%)	516 (11%)	6	12

All (516) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	15	LYS
1	A	19	LEU
1	A	33	ILE
1	A	48	MET
1	A	49	PHE
1	A	50	ASP
1	A	60	ILE

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Mol	Chain	Res	Type
1	A	62	GLU
1	A	63	SER
1	A	64	ASP
1	A	84	THR
1	A	96	THR
1	A	115	LEU
1	A	124	VAL
1	A	125	LEU
1	A	147	SER
1	A	179	TYR
1	A	181	PRO
1	A	209	HIS
1	A	224	ARG
1	A	264	ASN
1	A	290	LEU
1	A	323	VAL
1	A	326	TYR
1	A	332	LEU
1	A	337	ARG
1	A	339	ARG
1	A	340	SER
1	A	344	ARG
1	A	355	ARG
1	A	374	LEU
1	A	375	LEU
1	A	384	ASN
1	A	395	ASN
1	A	396	LEU
1	A	397	TYR
1	A	403	GLU
1	A	419	ASN
1	A	428	LEU
1	A	447	ARG
1	A	464	LEU
1	A	468	VAL
1	B	1	SER
1	B	15	LYS
1	B	19	LEU
1	B	33	ILE
1	B	48	MET
1	B	49	PHE
1	B	50	ASP

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Mol	Chain	Res	Type
1	B	60	ILE
1	B	62	GLU
1	B	63	SER
1	B	64	ASP
1	B	84	THR
1	B	96	THR
1	B	115	LEU
1	B	124	VAL
1	B	125	LEU
1	B	147	SER
1	B	179	TYR
1	B	181	PRO
1	B	209	HIS
1	B	224	ARG
1	B	264	ASN
1	B	290	LEU
1	B	323	VAL
1	B	326	TYR
1	B	332	LEU
1	B	337	ARG
1	B	339	ARG
1	B	340	SER
1	B	344	ARG
1	B	355	ARG
1	B	374	LEU
1	B	375	LEU
1	B	384	ASN
1	B	395	ASN
1	B	396	LEU
1	B	397	TYR
1	B	403	GLU
1	B	419	ASN
1	B	428	LEU
1	B	447	ARG
1	B	464	LEU
1	B	468	VAL
1	C	1	SER
1	C	15	LYS
1	C	19	LEU
1	C	33	ILE
1	C	48	MET
1	C	49	PHE

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Mol	Chain	Res	Type
1	C	50	ASP
1	C	60	ILE
1	C	62	GLU
1	C	63	SER
1	C	64	ASP
1	C	84	THR
1	C	96	THR
1	C	115	LEU
1	C	124	VAL
1	C	125	LEU
1	C	147	SER
1	C	179	TYR
1	C	181	PRO
1	C	209	HIS
1	C	224	ARG
1	C	264	ASN
1	C	290	LEU
1	C	323	VAL
1	C	326	TYR
1	C	332	LEU
1	C	337	ARG
1	C	339	ARG
1	C	340	SER
1	C	344	ARG
1	C	355	ARG
1	C	374	LEU
1	C	375	LEU
1	C	384	ASN
1	C	395	ASN
1	C	396	LEU
1	C	397	TYR
1	C	403	GLU
1	C	419	ASN
1	C	428	LEU
1	C	447	ARG
1	C	464	LEU
1	C	468	VAL
1	D	1	SER
1	D	15	LYS
1	D	19	LEU
1	D	33	ILE
1	D	48	MET

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Mol	Chain	Res	Type
1	D	49	PHE
1	D	50	ASP
1	D	60	ILE
1	D	62	GLU
1	D	63	SER
1	D	64	ASP
1	D	84	THR
1	D	96	THR
1	D	115	LEU
1	D	124	VAL
1	D	125	LEU
1	D	147	SER
1	D	179	TYR
1	D	181	PRO
1	D	209	HIS
1	D	224	ARG
1	D	264	ASN
1	D	290	LEU
1	D	323	VAL
1	D	326	TYR
1	D	332	LEU
1	D	337	ARG
1	D	339	ARG
1	D	340	SER
1	D	344	ARG
1	D	355	ARG
1	D	374	LEU
1	D	375	LEU
1	D	384	ASN
1	D	395	ASN
1	D	396	LEU
1	D	397	TYR
1	D	403	GLU
1	D	419	ASN
1	D	428	LEU
1	D	447	ARG
1	D	464	LEU
1	D	468	VAL
1	E	1	SER
1	E	15	LYS
1	E	19	LEU
1	E	33	ILE

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Mol	Chain	Res	Type
1	E	48	MET
1	E	49	PHE
1	E	50	ASP
1	E	60	ILE
1	E	62	GLU
1	E	63	SER
1	E	64	ASP
1	E	84	THR
1	E	96	THR
1	E	115	LEU
1	E	124	VAL
1	E	125	LEU
1	E	147	SER
1	E	179	TYR
1	E	181	PRO
1	E	209	HIS
1	E	224	ARG
1	E	264	ASN
1	E	290	LEU
1	E	323	VAL
1	E	326	TYR
1	E	332	LEU
1	E	337	ARG
1	E	339	ARG
1	E	340	SER
1	E	344	ARG
1	E	355	ARG
1	E	374	LEU
1	E	375	LEU
1	E	384	ASN
1	E	395	ASN
1	E	396	LEU
1	E	397	TYR
1	E	403	GLU
1	E	419	ASN
1	E	428	LEU
1	E	447	ARG
1	E	464	LEU
1	E	468	VAL
1	F	1	SER
1	F	15	LYS
1	F	19	LEU

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Mol	Chain	Res	Type
1	F	33	ILE
1	F	48	MET
1	F	49	PHE
1	F	50	ASP
1	F	60	ILE
1	F	62	GLU
1	F	63	SER
1	F	64	ASP
1	F	84	THR
1	F	96	THR
1	F	115	LEU
1	F	124	VAL
1	F	125	LEU
1	F	147	SER
1	F	179	TYR
1	F	181	PRO
1	F	209	HIS
1	F	224	ARG
1	F	264	ASN
1	F	290	LEU
1	F	323	VAL
1	F	326	TYR
1	F	332	LEU
1	F	337	ARG
1	F	339	ARG
1	F	340	SER
1	F	344	ARG
1	F	355	ARG
1	F	374	LEU
1	F	375	LEU
1	F	384	ASN
1	F	395	ASN
1	F	396	LEU
1	F	397	TYR
1	F	403	GLU
1	F	419	ASN
1	F	428	LEU
1	F	447	ARG
1	F	464	LEU
1	F	468	VAL
1	G	1	SER
1	G	15	LYS

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Mol	Chain	Res	Type
1	G	19	LEU
1	G	33	ILE
1	G	48	MET
1	G	49	PHE
1	G	50	ASP
1	G	60	ILE
1	G	62	GLU
1	G	63	SER
1	G	64	ASP
1	G	84	THR
1	G	96	THR
1	G	115	LEU
1	G	124	VAL
1	G	125	LEU
1	G	147	SER
1	G	179	TYR
1	G	181	PRO
1	G	209	HIS
1	G	224	ARG
1	G	264	ASN
1	G	290	LEU
1	G	323	VAL
1	G	326	TYR
1	G	332	LEU
1	G	337	ARG
1	G	339	ARG
1	G	340	SER
1	G	344	ARG
1	G	355	ARG
1	G	374	LEU
1	G	375	LEU
1	G	384	ASN
1	G	395	ASN
1	G	396	LEU
1	G	397	TYR
1	G	403	GLU
1	G	419	ASN
1	G	428	LEU
1	G	447	ARG
1	G	464	LEU
1	G	468	VAL
1	H	1	SER

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Mol	Chain	Res	Type
1	H	15	LYS
1	H	19	LEU
1	H	33	ILE
1	H	48	MET
1	H	49	PHE
1	H	50	ASP
1	H	60	ILE
1	H	62	GLU
1	H	63	SER
1	H	64	ASP
1	H	84	THR
1	H	96	THR
1	H	115	LEU
1	H	124	VAL
1	H	125	LEU
1	H	147	SER
1	H	179	TYR
1	H	181	PRO
1	H	209	HIS
1	H	224	ARG
1	H	264	ASN
1	H	290	LEU
1	H	323	VAL
1	H	326	TYR
1	H	332	LEU
1	H	337	ARG
1	H	339	ARG
1	H	340	SER
1	H	344	ARG
1	H	355	ARG
1	H	374	LEU
1	H	375	LEU
1	H	384	ASN
1	H	395	ASN
1	H	396	LEU
1	H	397	TYR
1	H	403	GLU
1	H	419	ASN
1	H	428	LEU
1	H	447	ARG
1	H	464	LEU
1	H	468	VAL

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Mol	Chain	Res	Type
1	I	1	SER
1	I	15	LYS
1	I	19	LEU
1	I	33	ILE
1	I	48	MET
1	I	49	PHE
1	I	50	ASP
1	I	60	ILE
1	I	62	GLU
1	I	63	SER
1	I	64	ASP
1	I	84	THR
1	I	96	THR
1	I	115	LEU
1	I	124	VAL
1	I	125	LEU
1	I	147	SER
1	I	179	TYR
1	I	181	PRO
1	I	209	HIS
1	I	224	ARG
1	I	264	ASN
1	I	290	LEU
1	I	323	VAL
1	I	326	TYR
1	I	332	LEU
1	I	337	ARG
1	I	339	ARG
1	I	340	SER
1	I	344	ARG
1	I	355	ARG
1	I	374	LEU
1	I	375	LEU
1	I	384	ASN
1	I	395	ASN
1	I	396	LEU
1	I	397	TYR
1	I	403	GLU
1	I	419	ASN
1	I	428	LEU
1	I	447	ARG
1	I	464	LEU

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Mol	Chain	Res	Type
1	I	468	VAL
1	J	1	SER
1	J	15	LYS
1	J	19	LEU
1	J	33	ILE
1	J	48	MET
1	J	49	PHE
1	J	50	ASP
1	J	60	ILE
1	J	62	GLU
1	J	63	SER
1	J	64	ASP
1	J	84	THR
1	J	96	THR
1	J	115	LEU
1	J	124	VAL
1	J	125	LEU
1	J	147	SER
1	J	179	TYR
1	J	181	PRO
1	J	209	HIS
1	J	224	ARG
1	J	264	ASN
1	J	290	LEU
1	J	323	VAL
1	J	326	TYR
1	J	332	LEU
1	J	337	ARG
1	J	339	ARG
1	J	340	SER
1	J	344	ARG
1	J	355	ARG
1	J	374	LEU
1	J	375	LEU
1	J	384	ASN
1	J	395	ASN
1	J	396	LEU
1	J	397	TYR
1	J	403	GLU
1	J	419	ASN
1	J	428	LEU
1	J	447	ARG

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Mol	Chain	Res	Type
1	J	464	LEU
1	J	468	VAL
1	K	1	SER
1	K	15	LYS
1	K	19	LEU
1	K	33	ILE
1	K	48	MET
1	K	49	PHE
1	K	50	ASP
1	K	60	ILE
1	K	62	GLU
1	K	63	SER
1	K	64	ASP
1	K	84	THR
1	K	96	THR
1	K	115	LEU
1	K	124	VAL
1	K	125	LEU
1	K	147	SER
1	K	179	TYR
1	K	181	PRO
1	K	209	HIS
1	K	224	ARG
1	K	264	ASN
1	K	290	LEU
1	K	323	VAL
1	K	326	TYR
1	K	332	LEU
1	K	337	ARG
1	K	339	ARG
1	K	340	SER
1	K	344	ARG
1	K	355	ARG
1	K	374	LEU
1	K	375	LEU
1	K	384	ASN
1	K	395	ASN
1	K	396	LEU
1	K	397	TYR
1	K	403	GLU
1	K	419	ASN
1	K	428	LEU

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Mol	Chain	Res	Type
1	K	447	ARG
1	K	464	LEU
1	K	468	VAL
1	L	1	SER
1	L	15	LYS
1	L	19	LEU
1	L	33	ILE
1	L	48	MET
1	L	49	PHE
1	L	50	ASP
1	L	60	ILE
1	L	62	GLU
1	L	63	SER
1	L	64	ASP
1	L	84	THR
1	L	96	THR
1	L	115	LEU
1	L	124	VAL
1	L	125	LEU
1	L	147	SER
1	L	179	TYR
1	L	181	PRO
1	L	209	HIS
1	L	224	ARG
1	L	264	ASN
1	L	290	LEU
1	L	323	VAL
1	L	326	TYR
1	L	332	LEU
1	L	337	ARG
1	L	339	ARG
1	L	340	SER
1	L	344	ARG
1	L	355	ARG
1	L	374	LEU
1	L	375	LEU
1	L	384	ASN
1	L	395	ASN
1	L	396	LEU
1	L	397	TYR
1	L	403	GLU
1	L	419	ASN

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Mol	Chain	Res	Type
1	L	428	LEU
1	L	447	ARG
1	L	464	LEU
1	L	468	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	211	HIS
1	A	218	GLN
1	A	219	ASN
1	A	244	ASN
1	A	313	ASN
1	A	338	ASN
1	A	384	ASN
1	A	395	ASN
1	A	409	GLN
1	A	458	HIS
1	B	61	ASN
1	B	211	HIS
1	B	218	GLN
1	B	219	ASN
1	B	244	ASN
1	B	313	ASN
1	B	338	ASN
1	B	384	ASN
1	B	395	ASN
1	B	409	GLN
1	B	458	HIS
1	C	61	ASN
1	C	211	HIS
1	C	218	GLN
1	C	219	ASN
1	C	236	GLN
1	C	244	ASN
1	C	313	ASN
1	C	338	ASN
1	C	384	ASN
1	C	395	ASN
1	C	409	GLN
1	C	458	HIS

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Mol	Chain	Res	Type
1	D	61	ASN
1	D	211	HIS
1	D	218	GLN
1	D	219	ASN
1	D	244	ASN
1	D	313	ASN
1	D	338	ASN
1	D	384	ASN
1	D	395	ASN
1	D	409	GLN
1	D	458	HIS
1	E	61	ASN
1	E	211	HIS
1	E	218	GLN
1	E	219	ASN
1	E	236	GLN
1	E	244	ASN
1	E	313	ASN
1	E	338	ASN
1	E	384	ASN
1	E	395	ASN
1	E	409	GLN
1	E	458	HIS
1	F	61	ASN
1	F	211	HIS
1	F	218	GLN
1	F	219	ASN
1	F	236	GLN
1	F	244	ASN
1	F	313	ASN
1	F	338	ASN
1	F	384	ASN
1	F	395	ASN
1	F	409	GLN
1	F	458	HIS
1	G	61	ASN
1	G	211	HIS
1	G	218	GLN
1	G	219	ASN
1	G	244	ASN
1	G	313	ASN
1	G	338	ASN

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Mol	Chain	Res	Type
1	G	384	ASN
1	G	395	ASN
1	G	409	GLN
1	G	458	HIS
1	H	61	ASN
1	H	211	HIS
1	H	218	GLN
1	H	219	ASN
1	H	236	GLN
1	H	244	ASN
1	H	313	ASN
1	H	338	ASN
1	H	384	ASN
1	H	395	ASN
1	H	409	GLN
1	H	458	HIS
1	I	61	ASN
1	I	211	HIS
1	I	218	GLN
1	I	219	ASN
1	I	244	ASN
1	I	313	ASN
1	I	338	ASN
1	I	384	ASN
1	I	395	ASN
1	I	409	GLN
1	I	458	HIS
1	J	61	ASN
1	J	211	HIS
1	J	218	GLN
1	J	219	ASN
1	J	244	ASN
1	J	313	ASN
1	J	338	ASN
1	J	384	ASN
1	J	395	ASN
1	J	409	GLN
1	J	458	HIS
1	K	61	ASN
1	K	211	HIS
1	K	218	GLN
1	K	219	ASN

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Mol	Chain	Res	Type
1	K	236	GLN
1	K	244	ASN
1	K	313	ASN
1	K	338	ASN
1	K	384	ASN
1	K	395	ASN
1	K	409	GLN
1	K	458	HIS
1	L	61	ASN
1	L	211	HIS
1	L	218	GLN
1	L	219	ASN
1	L	236	GLN
1	L	244	ASN
1	L	313	ASN
1	L	338	ASN
1	L	384	ASN
1	L	395	ASN
1	L	409	GLN
1	L	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, 48 are monoatomic - leaving 24 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
3	ADP	L	1482	-	24,29,29	2.63	7 (29%)	29,45,45	3.50	11 (37%)
5	MPD	D	1486	-	7,7,7	1.12	0	9,10,10	0.72	0
5	MPD	I	1491	-	7,7,7	1.13	0	9,10,10	0.72	0
3	ADP	F	1476	-	24,29,29	2.62	7 (29%)	29,45,45	3.50	10 (34%)
3	ADP	D	1474	-	24,29,29	2.63	7 (29%)	29,45,45	3.50	10 (34%)
3	ADP	B	1472	-	24,29,29	2.63	7 (29%)	29,45,45	3.50	10 (34%)
5	MPD	C	1485	-	7,7,7	1.14	0	9,10,10	0.72	0
3	ADP	A	1471	-	24,29,29	2.63	7 (29%)	29,45,45	3.50	10 (34%)
5	MPD	K	1493	-	7,7,7	1.12	0	9,10,10	0.72	0
3	ADP	K	1481	-	24,29,29	2.64	7 (29%)	29,45,45	3.50	10 (34%)
5	MPD	J	1492	-	7,7,7	1.12	0	9,10,10	0.72	0
3	ADP	H	1478	-	24,29,29	2.63	7 (29%)	29,45,45	3.50	11 (37%)
5	MPD	F	1488	-	7,7,7	1.13	0	9,10,10	0.73	0
3	ADP	E	1475	-	24,29,29	2.63	7 (29%)	29,45,45	3.50	10 (34%)
5	MPD	H	1490	-	7,7,7	1.13	0	9,10,10	0.73	0
5	MPD	B	1484	-	7,7,7	1.13	0	9,10,10	0.72	0
5	MPD	A	1483	-	7,7,7	1.13	0	9,10,10	0.73	0
3	ADP	C	1473	-	24,29,29	2.63	7 (29%)	29,45,45	3.50	11 (37%)
3	ADP	I	1479	-	24,29,29	2.63	7 (29%)	29,45,45	3.50	10 (34%)
5	MPD	L	1494	-	7,7,7	1.13	0	9,10,10	0.73	0
5	MPD	G	1489	-	7,7,7	1.12	0	9,10,10	0.72	0
5	MPD	E	1487	-	7,7,7	1.12	0	9,10,10	0.73	0
3	ADP	G	1477	-	24,29,29	2.63	7 (29%)	29,45,45	3.50	10 (34%)
3	ADP	J	1480	-	24,29,29	2.63	7 (29%)	29,45,45	3.50	10 (34%)

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
3	ADP	L	1482	-	-	4/12/32/32	0/3/3/3
5	MPD	D	1486	-	-	2/5/5/5	-
5	MPD	I	1491	-	-	1/5/5/5	-
3	ADP	F	1476	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	D	1474	-	-	4/12/32/32	0/3/3/3
3	ADP	B	1472	-	-	4/12/32/32	0/3/3/3
5	MPD	C	1485	-	-	2/5/5/5	-
3	ADP	A	1471	-	-	4/12/32/32	0/3/3/3
5	MPD	K	1493	-	-	2/5/5/5	-
3	ADP	K	1481	-	-	4/12/32/32	0/3/3/3
5	MPD	J	1492	-	-	2/5/5/5	-
3	ADP	H	1478	-	-	4/12/32/32	0/3/3/3
5	MPD	F	1488	-	-	1/5/5/5	-
3	ADP	E	1475	-	-	4/12/32/32	0/3/3/3
5	MPD	H	1490	-	-	1/5/5/5	-
5	MPD	B	1484	-	-	2/5/5/5	-
5	MPD	A	1483	-	-	1/5/5/5	-
3	ADP	C	1473	-	-	4/12/32/32	0/3/3/3
3	ADP	I	1479	-	-	4/12/32/32	0/3/3/3
5	MPD	L	1494	-	-	1/5/5/5	-
5	MPD	G	1489	-	-	1/5/5/5	-
5	MPD	E	1487	-	-	1/5/5/5	-
3	ADP	G	1477	-	-	4/12/32/32	0/3/3/3
3	ADP	J	1480	-	-	4/12/32/32	0/3/3/3

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1481	ADP	O4'-C1'	7.68	1.51	1.41
3	G	1477	ADP	O4'-C1'	7.68	1.51	1.41
3	H	1478	ADP	O4'-C1'	7.67	1.51	1.41
3	I	1479	ADP	O4'-C1'	7.67	1.51	1.41
3	L	1482	ADP	O4'-C1'	7.66	1.51	1.41
3	E	1475	ADP	O4'-C1'	7.65	1.51	1.41
3	B	1472	ADP	O4'-C1'	7.65	1.51	1.41
3	D	1474	ADP	O4'-C1'	7.65	1.51	1.41
3	A	1471	ADP	O4'-C1'	7.65	1.51	1.41
3	J	1480	ADP	O4'-C1'	7.63	1.51	1.41
3	C	1473	ADP	O4'-C1'	7.62	1.51	1.41
3	F	1476	ADP	O4'-C1'	7.60	1.51	1.41
3	L	1482	ADP	C4-N3	5.46	1.43	1.35
3	K	1481	ADP	C4-N3	5.42	1.43	1.35
3	B	1472	ADP	C4-N3	5.42	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1474	ADP	C4-N3	5.41	1.43	1.35
3	A	1471	ADP	C4-N3	5.40	1.43	1.35
3	H	1478	ADP	C4-N3	5.40	1.43	1.35
3	E	1475	ADP	C4-N3	5.38	1.43	1.35
3	G	1477	ADP	C4-N3	5.38	1.43	1.35
3	F	1476	ADP	C4-N3	5.37	1.43	1.35
3	C	1473	ADP	C4-N3	5.37	1.43	1.35
3	J	1480	ADP	C4-N3	5.37	1.43	1.35
3	I	1479	ADP	C4-N3	5.36	1.43	1.35
3	J	1480	ADP	C2-N3	4.20	1.38	1.32
3	K	1481	ADP	C2-N3	4.20	1.38	1.32
3	E	1475	ADP	C2-N3	4.19	1.38	1.32
3	I	1479	ADP	C2-N3	4.18	1.38	1.32
3	C	1473	ADP	C2-N3	4.18	1.38	1.32
3	F	1476	ADP	C2-N3	4.17	1.38	1.32
3	G	1477	ADP	C2-N3	4.17	1.38	1.32
3	A	1471	ADP	C2-N3	4.17	1.38	1.32
3	L	1482	ADP	C2-N3	4.17	1.38	1.32
3	B	1472	ADP	C2-N3	4.17	1.38	1.32
3	H	1478	ADP	C2-N3	4.16	1.38	1.32
3	D	1474	ADP	C2-N3	4.15	1.38	1.32
3	B	1472	ADP	O4'-C4'	4.03	1.54	1.45
3	C	1473	ADP	O4'-C4'	4.02	1.54	1.45
3	I	1479	ADP	O4'-C4'	4.02	1.54	1.45
3	J	1480	ADP	O4'-C4'	4.02	1.54	1.45
3	K	1481	ADP	O4'-C4'	4.01	1.54	1.45
3	F	1476	ADP	O4'-C4'	4.01	1.54	1.45
3	H	1478	ADP	O4'-C4'	4.00	1.53	1.45
3	A	1471	ADP	O4'-C4'	4.00	1.53	1.45
3	G	1477	ADP	O4'-C4'	4.00	1.53	1.45
3	E	1475	ADP	O4'-C4'	3.99	1.53	1.45
3	L	1482	ADP	O4'-C4'	3.99	1.53	1.45
3	D	1474	ADP	O4'-C4'	3.97	1.53	1.45
3	G	1477	ADP	PB-O3B	3.47	1.68	1.54
3	J	1480	ADP	PB-O3B	3.46	1.68	1.54
3	B	1472	ADP	PB-O3B	3.44	1.68	1.54
3	A	1471	ADP	PB-O3B	3.44	1.68	1.54
3	F	1476	ADP	PB-O3B	3.44	1.68	1.54
3	K	1481	ADP	PB-O3B	3.44	1.68	1.54
3	D	1474	ADP	PB-O3B	3.44	1.68	1.54
3	L	1482	ADP	PB-O3B	3.44	1.68	1.54
3	H	1478	ADP	PB-O3B	3.44	1.68	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1479	ADP	PB-O3B	3.43	1.68	1.54
3	C	1473	ADP	PB-O3B	3.43	1.68	1.54
3	E	1475	ADP	PB-O3B	3.43	1.68	1.54
3	K	1481	ADP	C6-N6	-2.88	1.23	1.34
3	I	1479	ADP	C6-N6	-2.88	1.23	1.34
3	D	1474	ADP	C6-N6	-2.88	1.23	1.34
3	G	1477	ADP	C6-N6	-2.88	1.23	1.34
3	C	1473	ADP	C6-N6	-2.87	1.23	1.34
3	A	1471	ADP	C6-N6	-2.87	1.23	1.34
3	J	1480	ADP	C6-N6	-2.86	1.23	1.34
3	H	1478	ADP	C6-N6	-2.86	1.23	1.34
3	E	1475	ADP	C6-N6	-2.86	1.23	1.34
3	L	1482	ADP	C6-N6	-2.86	1.23	1.34
3	B	1472	ADP	C6-N6	-2.85	1.23	1.34
3	F	1476	ADP	C6-N6	-2.85	1.23	1.34
3	H	1478	ADP	C3'-C4'	-2.72	1.46	1.53
3	J	1480	ADP	C3'-C4'	-2.72	1.46	1.53
3	K	1481	ADP	C3'-C4'	-2.72	1.46	1.53
3	G	1477	ADP	C3'-C4'	-2.72	1.46	1.53
3	L	1482	ADP	C3'-C4'	-2.71	1.46	1.53
3	E	1475	ADP	C3'-C4'	-2.71	1.46	1.53
3	F	1476	ADP	C3'-C4'	-2.71	1.46	1.53
3	A	1471	ADP	C3'-C4'	-2.71	1.46	1.53
3	I	1479	ADP	C3'-C4'	-2.70	1.46	1.53
3	D	1474	ADP	C3'-C4'	-2.70	1.46	1.53
3	B	1472	ADP	C3'-C4'	-2.69	1.46	1.53
3	C	1473	ADP	C3'-C4'	-2.68	1.46	1.53

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1474	ADP	O4'-C1'-C2'	-12.02	89.36	106.93
3	G	1477	ADP	O4'-C1'-C2'	-12.01	89.38	106.93
3	K	1481	ADP	O4'-C1'-C2'	-12.00	89.38	106.93
3	B	1472	ADP	O4'-C1'-C2'	-12.00	89.39	106.93
3	E	1475	ADP	O4'-C1'-C2'	-12.00	89.40	106.93
3	I	1479	ADP	O4'-C1'-C2'	-11.99	89.40	106.93
3	J	1480	ADP	O4'-C1'-C2'	-11.99	89.40	106.93
3	F	1476	ADP	O4'-C1'-C2'	-11.99	89.41	106.93
3	A	1471	ADP	O4'-C1'-C2'	-11.98	89.41	106.93
3	C	1473	ADP	O4'-C1'-C2'	-11.98	89.42	106.93
3	H	1478	ADP	O4'-C1'-C2'	-11.98	89.42	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1482	ADP	O4'-C1'-C2'	-11.97	89.43	106.93
3	K	1481	ADP	O5'-C5'-C4'	8.02	136.58	108.99
3	J	1480	ADP	O5'-C5'-C4'	8.01	136.56	108.99
3	E	1475	ADP	O5'-C5'-C4'	8.01	136.56	108.99
3	D	1474	ADP	O5'-C5'-C4'	8.01	136.56	108.99
3	L	1482	ADP	O5'-C5'-C4'	8.01	136.56	108.99
3	A	1471	ADP	O5'-C5'-C4'	8.00	136.54	108.99
3	H	1478	ADP	O5'-C5'-C4'	8.00	136.53	108.99
3	C	1473	ADP	O5'-C5'-C4'	8.00	136.53	108.99
3	I	1479	ADP	O5'-C5'-C4'	8.00	136.52	108.99
3	F	1476	ADP	O5'-C5'-C4'	8.00	136.52	108.99
3	B	1472	ADP	O5'-C5'-C4'	8.00	136.51	108.99
3	G	1477	ADP	O5'-C5'-C4'	7.99	136.50	108.99
3	L	1482	ADP	C1'-N9-C4	5.50	136.30	126.64
3	C	1473	ADP	C1'-N9-C4	5.49	136.29	126.64
3	G	1477	ADP	C1'-N9-C4	5.49	136.29	126.64
3	H	1478	ADP	C1'-N9-C4	5.49	136.28	126.64
3	J	1480	ADP	C1'-N9-C4	5.48	136.26	126.64
3	D	1474	ADP	C1'-N9-C4	5.48	136.26	126.64
3	B	1472	ADP	C1'-N9-C4	5.48	136.26	126.64
3	K	1481	ADP	C1'-N9-C4	5.47	136.26	126.64
3	E	1475	ADP	C1'-N9-C4	5.47	136.25	126.64
3	A	1471	ADP	C1'-N9-C4	5.47	136.25	126.64
3	I	1479	ADP	C1'-N9-C4	5.46	136.24	126.64
3	F	1476	ADP	C1'-N9-C4	5.44	136.21	126.64
3	D	1474	ADP	O4'-C4'-C5'	4.83	125.27	109.37
3	C	1473	ADP	O4'-C4'-C5'	4.83	125.25	109.37
3	E	1475	ADP	O4'-C4'-C5'	4.82	125.25	109.37
3	F	1476	ADP	O4'-C4'-C5'	4.82	125.24	109.37
3	B	1472	ADP	O4'-C4'-C5'	4.82	125.22	109.37
3	A	1471	ADP	O4'-C4'-C5'	4.82	125.22	109.37
3	G	1477	ADP	O4'-C4'-C5'	4.82	125.22	109.37
3	J	1480	ADP	O4'-C4'-C5'	4.81	125.20	109.37
3	K	1481	ADP	O4'-C4'-C5'	4.81	125.19	109.37
3	L	1482	ADP	O4'-C4'-C5'	4.81	125.19	109.37
3	I	1479	ADP	O4'-C4'-C5'	4.81	125.18	109.37
3	H	1478	ADP	O4'-C4'-C5'	4.80	125.18	109.37
3	H	1478	ADP	C4-C5-N7	4.67	114.26	109.40
3	B	1472	ADP	C4-C5-N7	4.66	114.25	109.40
3	J	1480	ADP	C4-C5-N7	4.65	114.24	109.40
3	I	1479	ADP	C4-C5-N7	4.65	114.24	109.40
3	C	1473	ADP	C4-C5-N7	4.63	114.23	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1471	ADP	C4-C5-N7	4.63	114.22	109.40
3	G	1477	ADP	C4-C5-N7	4.63	114.22	109.40
3	D	1474	ADP	C4-C5-N7	4.63	114.22	109.40
3	F	1476	ADP	C4-C5-N7	4.63	114.22	109.40
3	L	1482	ADP	C4-C5-N7	4.61	114.20	109.40
3	E	1475	ADP	C4-C5-N7	4.60	114.19	109.40
3	K	1481	ADP	C4-C5-N7	4.60	114.19	109.40
3	I	1479	ADP	C5'-C4'-C3'	-3.78	101.00	115.18
3	G	1477	ADP	C5'-C4'-C3'	-3.78	101.01	115.18
3	A	1471	ADP	C5'-C4'-C3'	-3.78	101.02	115.18
3	L	1482	ADP	C5'-C4'-C3'	-3.78	101.03	115.18
3	B	1472	ADP	C5'-C4'-C3'	-3.78	101.03	115.18
3	F	1476	ADP	C5'-C4'-C3'	-3.78	101.03	115.18
3	H	1478	ADP	C5'-C4'-C3'	-3.78	101.03	115.18
3	J	1480	ADP	C5'-C4'-C3'	-3.77	101.04	115.18
3	D	1474	ADP	C5'-C4'-C3'	-3.77	101.05	115.18
3	C	1473	ADP	C5'-C4'-C3'	-3.77	101.05	115.18
3	E	1475	ADP	C5'-C4'-C3'	-3.76	101.08	115.18
3	K	1481	ADP	C5'-C4'-C3'	-3.76	101.08	115.18
3	C	1473	ADP	O2'-C2'-C1'	3.07	122.20	110.85
3	G	1477	ADP	O2'-C2'-C1'	3.07	122.19	110.85
3	B	1472	ADP	O2'-C2'-C1'	3.07	122.19	110.85
3	H	1478	ADP	O2'-C2'-C1'	3.07	122.19	110.85
3	L	1482	ADP	O2'-C2'-C1'	3.07	122.19	110.85
3	A	1471	ADP	O2'-C2'-C1'	3.07	122.19	110.85
3	I	1479	ADP	O2'-C2'-C1'	3.07	122.18	110.85
3	J	1480	ADP	O2'-C2'-C1'	3.07	122.17	110.85
3	D	1474	ADP	O2'-C2'-C1'	3.06	122.17	110.85
3	K	1481	ADP	O2'-C2'-C1'	3.06	122.16	110.85
3	F	1476	ADP	O2'-C2'-C1'	3.06	122.15	110.85
3	E	1475	ADP	O2'-C2'-C1'	3.06	122.14	110.85
3	J	1480	ADP	O3'-C3'-C2'	2.95	121.38	111.82
3	E	1475	ADP	O3'-C3'-C2'	2.95	121.36	111.82
3	K	1481	ADP	O3'-C3'-C2'	2.95	121.36	111.82
3	I	1479	ADP	O3'-C3'-C2'	2.95	121.35	111.82
3	D	1474	ADP	O3'-C3'-C2'	2.95	121.35	111.82
3	F	1476	ADP	O3'-C3'-C2'	2.95	121.35	111.82
3	L	1482	ADP	O3'-C3'-C2'	2.94	121.34	111.82
3	B	1472	ADP	O3'-C3'-C2'	2.94	121.34	111.82
3	C	1473	ADP	O3'-C3'-C2'	2.94	121.33	111.82
3	A	1471	ADP	O3'-C3'-C2'	2.94	121.33	111.82
3	J	1480	ADP	O2B-PB-O3A	2.93	114.47	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1472	ADP	O2B-PB-O3A	2.93	114.46	104.64
3	L	1482	ADP	O2B-PB-O3A	2.93	114.46	104.64
3	G	1477	ADP	O3'-C3'-C2'	2.93	121.30	111.82
3	H	1478	ADP	O3'-C3'-C2'	2.93	121.29	111.82
3	C	1473	ADP	O2B-PB-O3A	2.93	114.45	104.64
3	G	1477	ADP	O2B-PB-O3A	2.92	114.44	104.64
3	D	1474	ADP	O2B-PB-O3A	2.92	114.44	104.64
3	E	1475	ADP	O2B-PB-O3A	2.92	114.44	104.64
3	K	1481	ADP	O2B-PB-O3A	2.92	114.44	104.64
3	A	1471	ADP	O2B-PB-O3A	2.92	114.43	104.64
3	I	1479	ADP	O2B-PB-O3A	2.92	114.43	104.64
3	H	1478	ADP	O2B-PB-O3A	2.92	114.42	104.64
3	F	1476	ADP	O2B-PB-O3A	2.90	114.36	104.64
3	J	1480	ADP	PA-O5'-C5'	2.82	138.20	121.68
3	I	1479	ADP	PA-O5'-C5'	2.82	138.19	121.68
3	K	1481	ADP	PA-O5'-C5'	2.82	138.19	121.68
3	B	1472	ADP	PA-O5'-C5'	2.81	138.18	121.68
3	F	1476	ADP	PA-O5'-C5'	2.81	138.18	121.68
3	D	1474	ADP	PA-O5'-C5'	2.81	138.18	121.68
3	A	1471	ADP	PA-O5'-C5'	2.81	138.18	121.68
3	E	1475	ADP	PA-O5'-C5'	2.81	138.17	121.68
3	C	1473	ADP	PA-O5'-C5'	2.81	138.17	121.68
3	G	1477	ADP	PA-O5'-C5'	2.81	138.16	121.68
3	L	1482	ADP	PA-O5'-C5'	2.81	138.15	121.68
3	H	1478	ADP	PA-O5'-C5'	2.81	138.14	121.68
3	C	1473	ADP	C3'-C2'-C1'	-2.02	97.94	100.98
3	L	1482	ADP	C3'-C2'-C1'	-2.01	97.96	100.98
3	H	1478	ADP	C3'-C2'-C1'	-2.00	97.97	100.98

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L	1482	ADP	PA-O3A-PB-O3B
3	D	1474	ADP	PA-O3A-PB-O3B
3	I	1479	ADP	PA-O3A-PB-O3B
3	K	1481	ADP	PA-O3A-PB-O3B
3	F	1476	ADP	PA-O3A-PB-O3B
3	B	1472	ADP	PA-O3A-PB-O3B
3	E	1475	ADP	PA-O3A-PB-O3B
3	C	1473	ADP	PA-O3A-PB-O3B
3	H	1478	ADP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	A	1471	ADP	PA-O3A-PB-O3B
3	G	1477	ADP	PA-O3A-PB-O3B
3	J	1480	ADP	PA-O3A-PB-O3B
3	L	1482	ADP	C5'-O5'-PA-O3A
3	D	1474	ADP	C5'-O5'-PA-O3A
3	I	1479	ADP	C5'-O5'-PA-O3A
3	K	1481	ADP	C5'-O5'-PA-O3A
3	F	1476	ADP	C5'-O5'-PA-O3A
3	B	1472	ADP	C5'-O5'-PA-O3A
3	E	1475	ADP	C5'-O5'-PA-O3A
3	C	1473	ADP	C5'-O5'-PA-O3A
3	H	1478	ADP	C5'-O5'-PA-O3A
3	A	1471	ADP	C5'-O5'-PA-O3A
3	G	1477	ADP	C5'-O5'-PA-O3A
3	J	1480	ADP	C5'-O5'-PA-O3A
3	L	1482	ADP	C5'-O5'-PA-O1A
3	D	1474	ADP	C5'-O5'-PA-O1A
3	I	1479	ADP	C5'-O5'-PA-O1A
3	K	1481	ADP	C5'-O5'-PA-O1A
3	F	1476	ADP	C5'-O5'-PA-O1A
3	B	1472	ADP	C5'-O5'-PA-O1A
3	E	1475	ADP	C5'-O5'-PA-O1A
3	C	1473	ADP	C5'-O5'-PA-O1A
3	H	1478	ADP	C5'-O5'-PA-O1A
3	A	1471	ADP	C5'-O5'-PA-O1A
3	G	1477	ADP	C5'-O5'-PA-O1A
3	J	1480	ADP	C5'-O5'-PA-O1A
3	L	1482	ADP	PA-O3A-PB-O1B
3	D	1474	ADP	PA-O3A-PB-O1B
3	I	1479	ADP	PA-O3A-PB-O1B
3	K	1481	ADP	PA-O3A-PB-O1B
3	F	1476	ADP	PA-O3A-PB-O1B
3	B	1472	ADP	PA-O3A-PB-O1B
3	E	1475	ADP	PA-O3A-PB-O1B
3	C	1473	ADP	PA-O3A-PB-O1B
3	H	1478	ADP	PA-O3A-PB-O1B
3	A	1471	ADP	PA-O3A-PB-O1B
3	G	1477	ADP	PA-O3A-PB-O1B
3	J	1480	ADP	PA-O3A-PB-O1B
5	D	1486	MPD	C2-C3-C4-C5
5	C	1485	MPD	C2-C3-C4-C5
5	J	1492	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	K	1493	MPD	C2-C3-C4-C5
5	B	1484	MPD	C2-C3-C4-C5
5	I	1491	MPD	C2-C3-C4-O4
5	E	1487	MPD	C2-C3-C4-O4
5	D	1486	MPD	C2-C3-C4-O4
5	C	1485	MPD	C2-C3-C4-O4
5	H	1490	MPD	C2-C3-C4-O4
5	J	1492	MPD	C2-C3-C4-O4
5	K	1493	MPD	C2-C3-C4-O4
5	F	1488	MPD	C2-C3-C4-O4
5	B	1484	MPD	C2-C3-C4-O4
5	A	1483	MPD	C2-C3-C4-O4
5	L	1494	MPD	C2-C3-C4-O4
5	G	1489	MPD	C2-C3-C4-O4

There are no ring outliers.

24 monomers are involved in 438 short contacts:

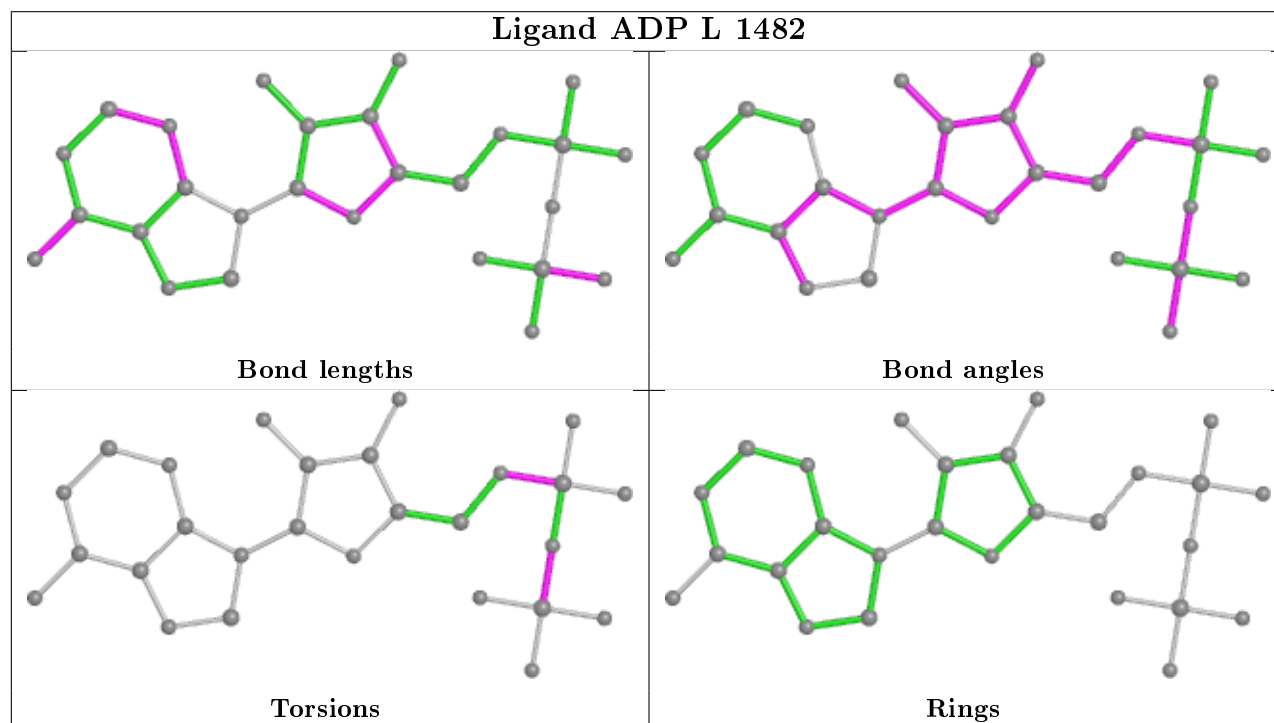
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1482	ADP	4	0
5	D	1486	MPD	34	0
5	I	1491	MPD	35	0
3	F	1476	ADP	4	0
3	D	1474	ADP	4	0
3	B	1472	ADP	4	0
5	C	1485	MPD	33	0
3	A	1471	ADP	4	0
5	K	1493	MPD	33	0
3	K	1481	ADP	4	0
5	J	1492	MPD	34	0
3	H	1478	ADP	4	0
5	F	1488	MPD	34	0
3	E	1475	ADP	4	0
5	H	1490	MPD	33	0
5	B	1484	MPD	34	0
5	A	1483	MPD	29	0
3	C	1473	ADP	4	0
3	I	1479	ADP	3	0
5	L	1494	MPD	32	0
5	G	1489	MPD	31	0
5	E	1487	MPD	29	0
3	G	1477	ADP	4	0

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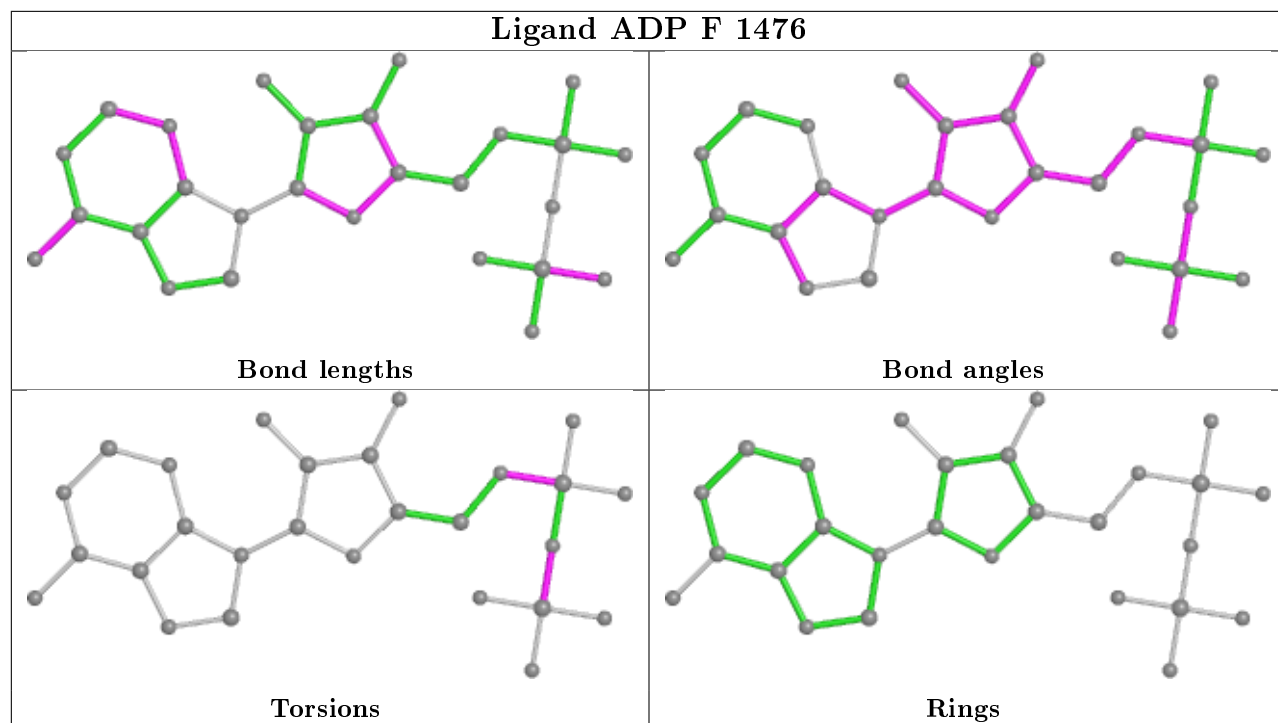
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1480	ADP	4	0

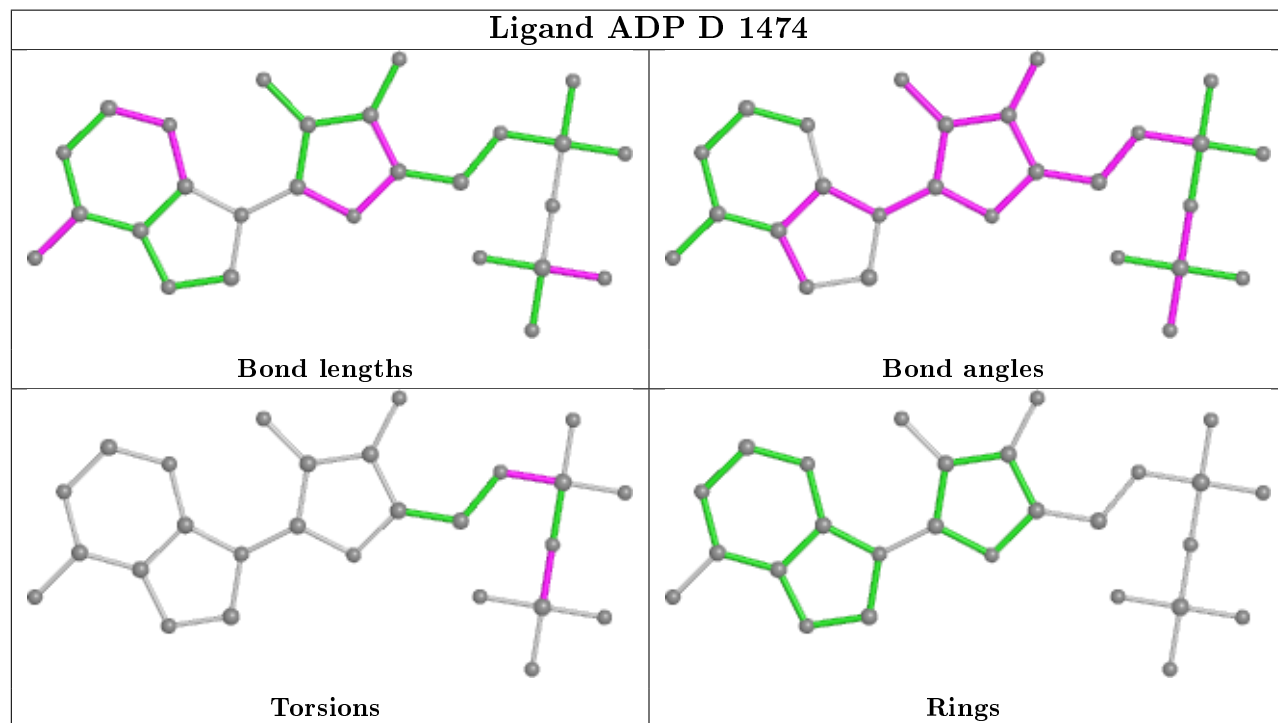
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



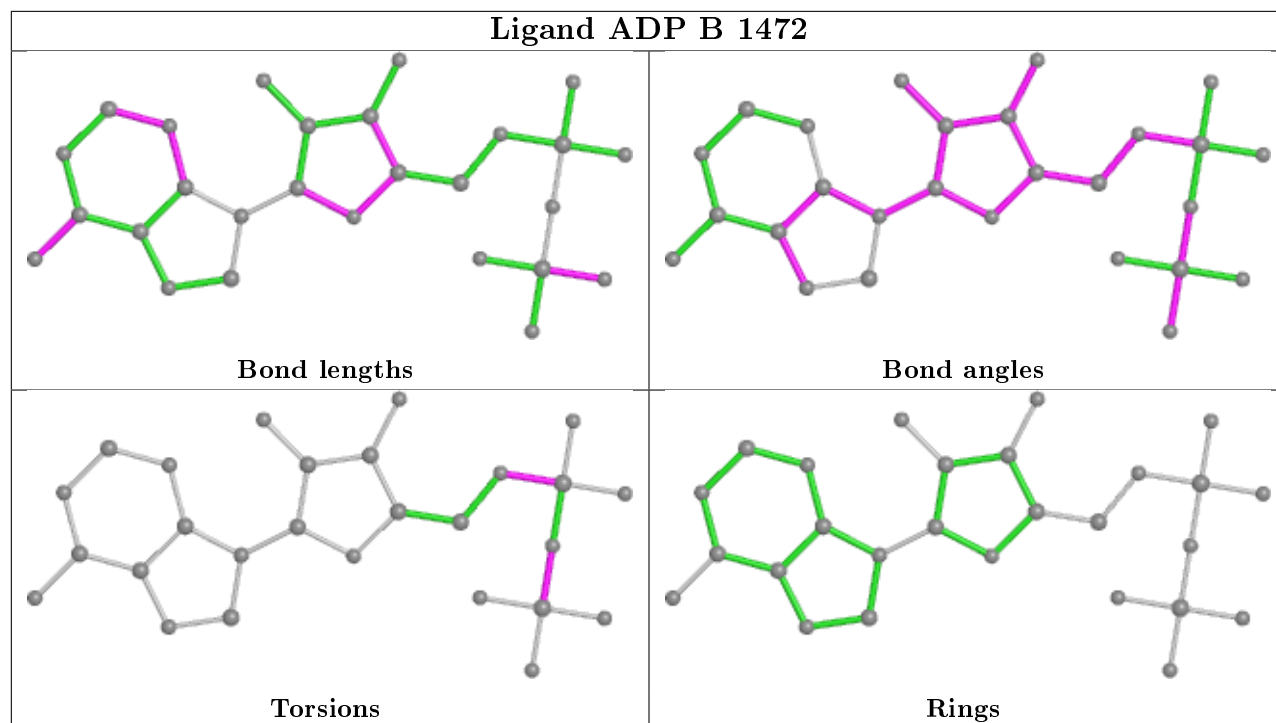
## Ligand ADP F 1476



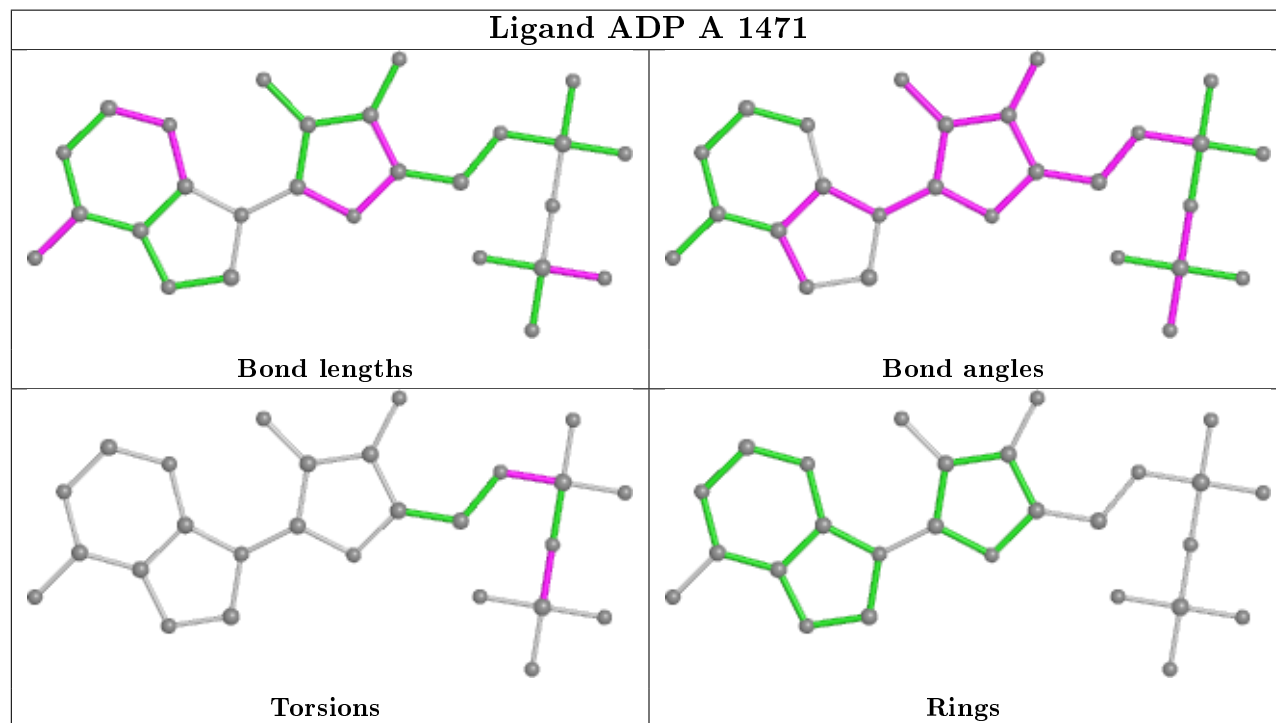
## Ligand ADP D 1474



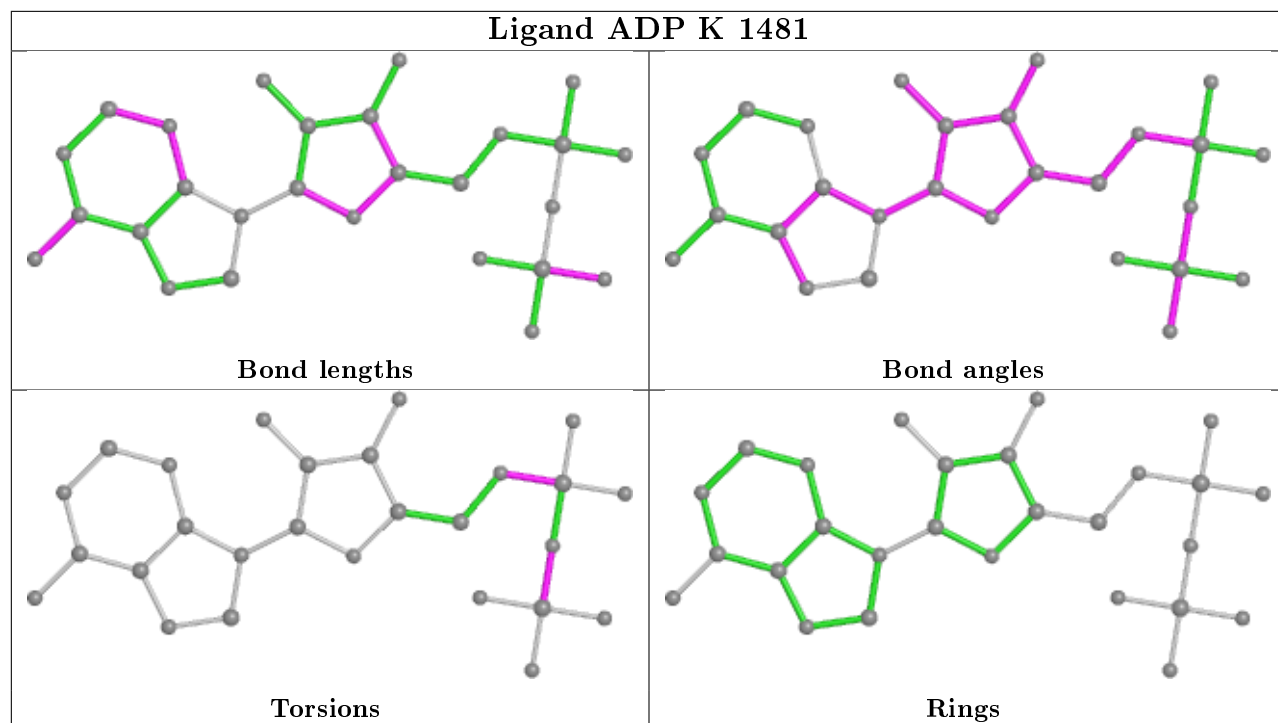
## Ligand ADP B 1472



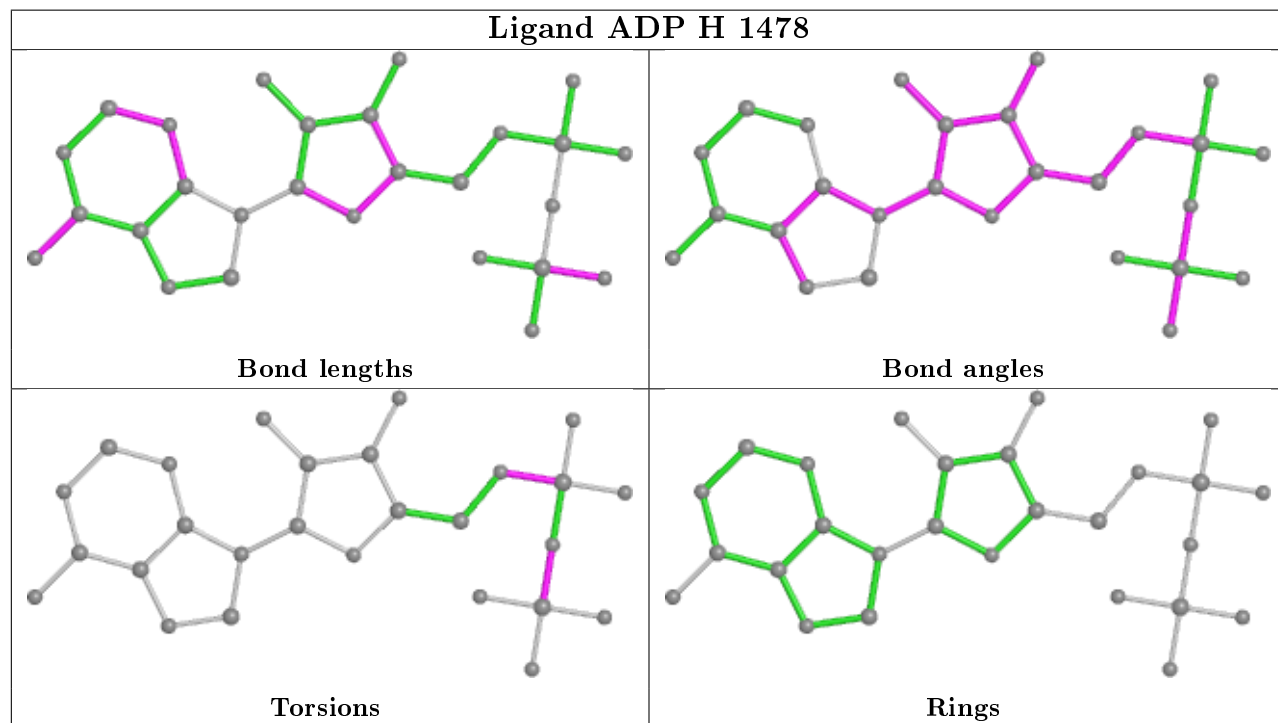
## Ligand ADP A 1471



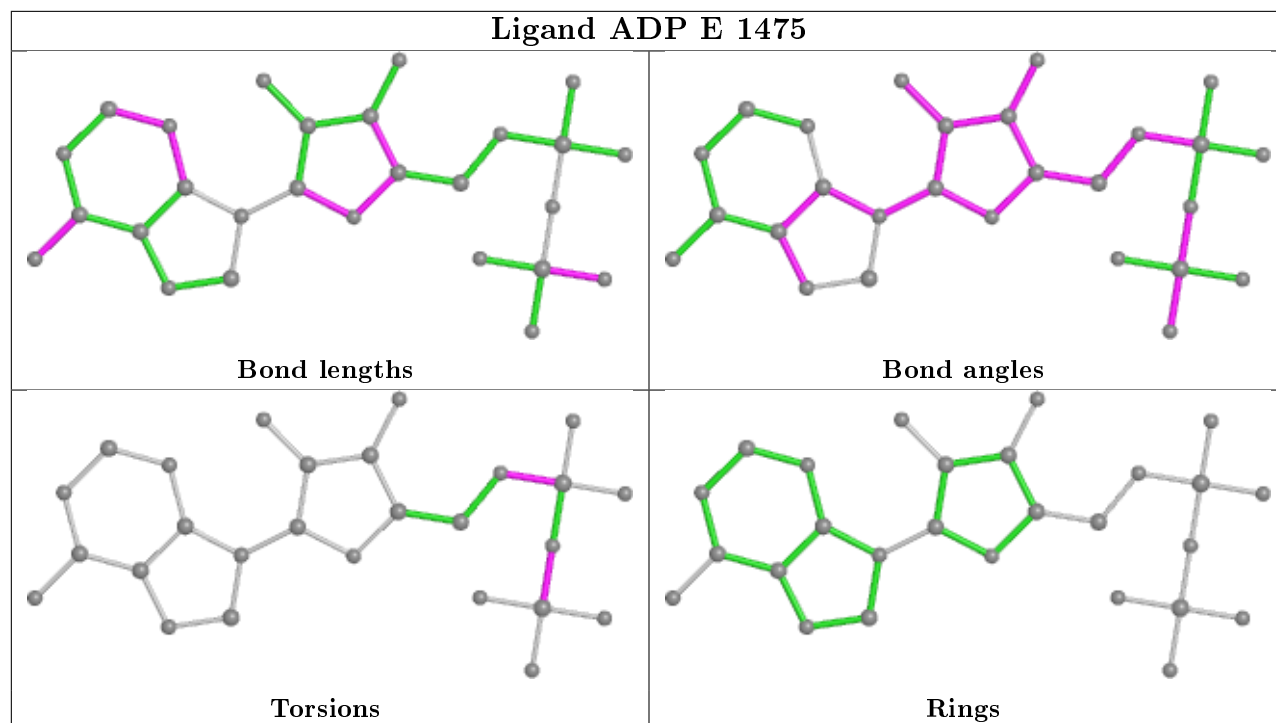
## Ligand ADP K 1481



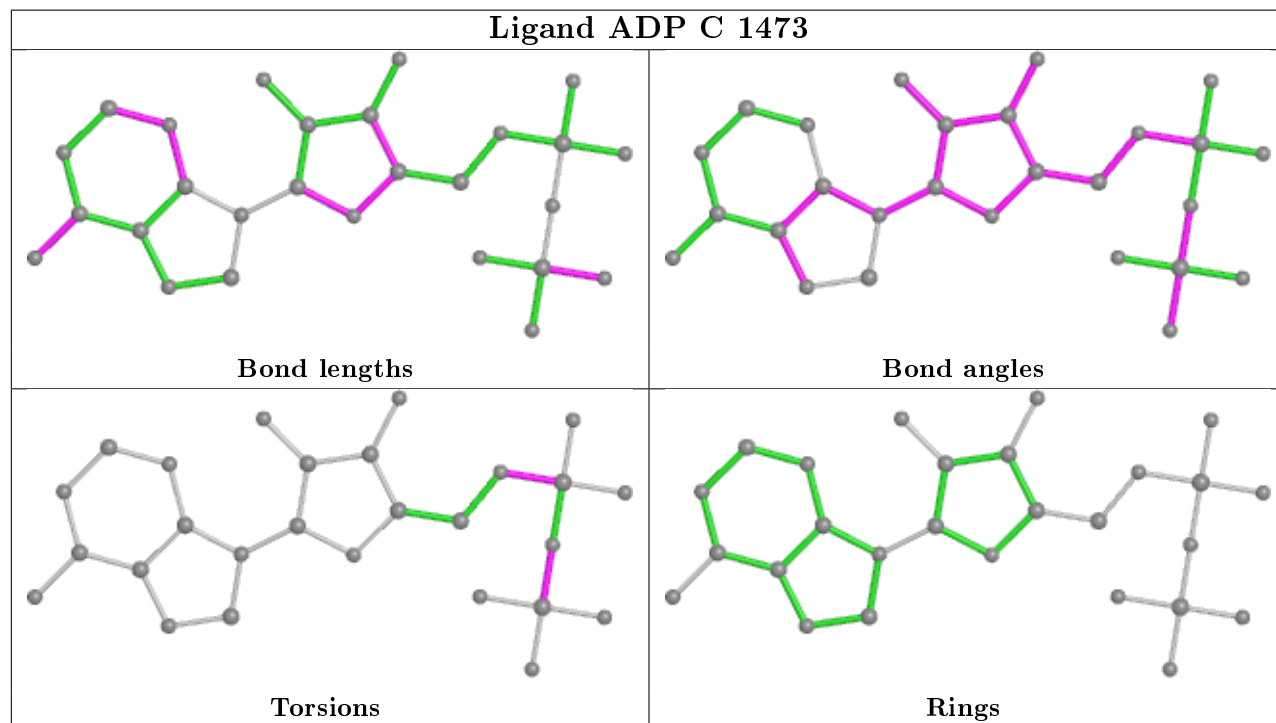
## Ligand ADP H 1478

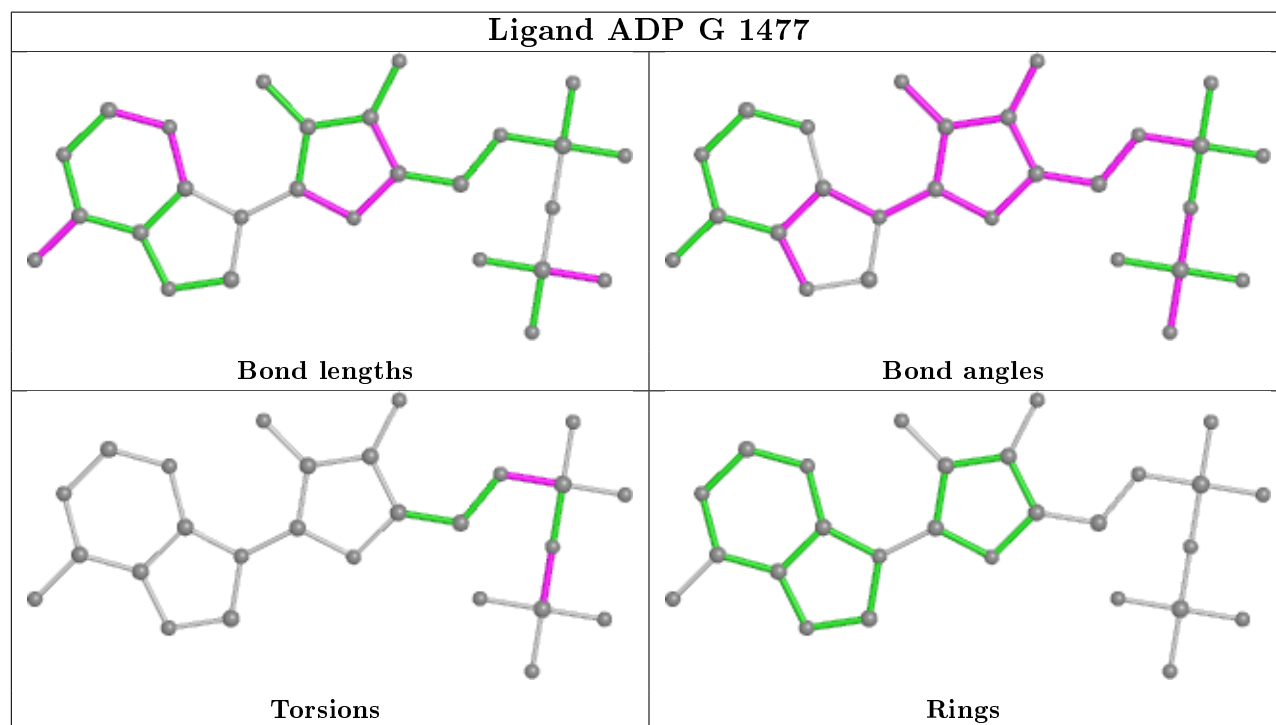
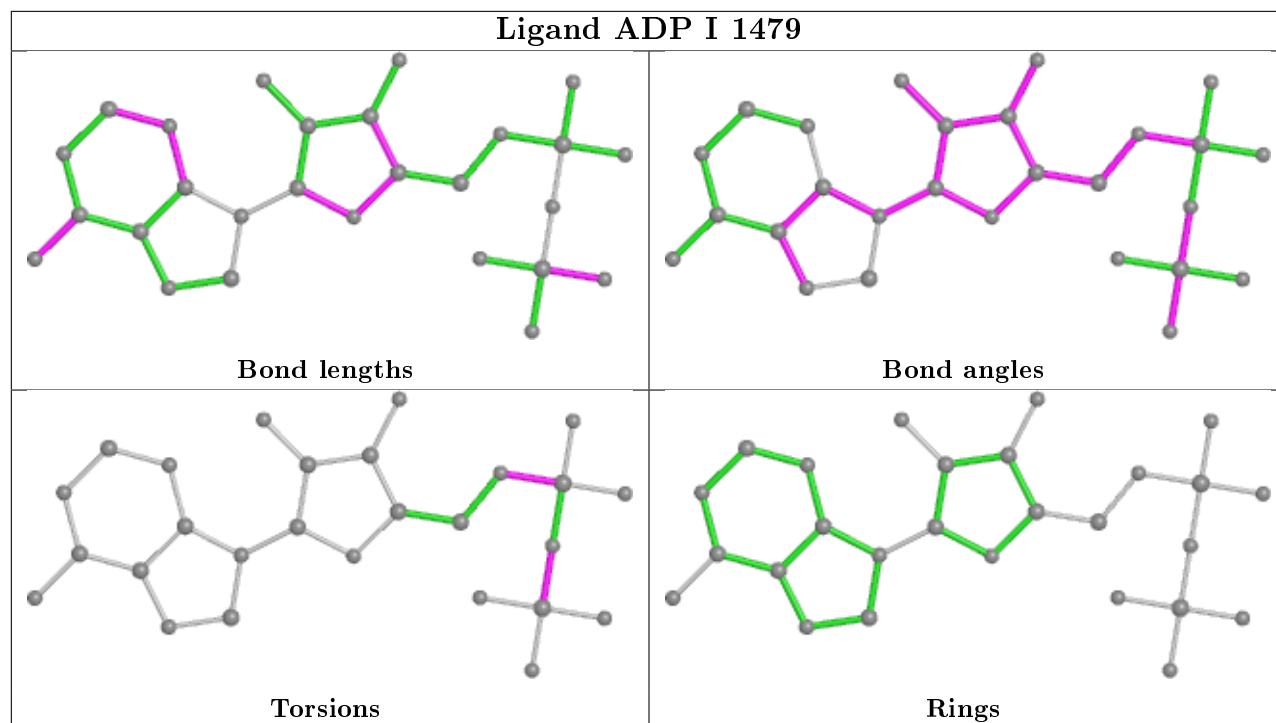


## Ligand ADP E 1475

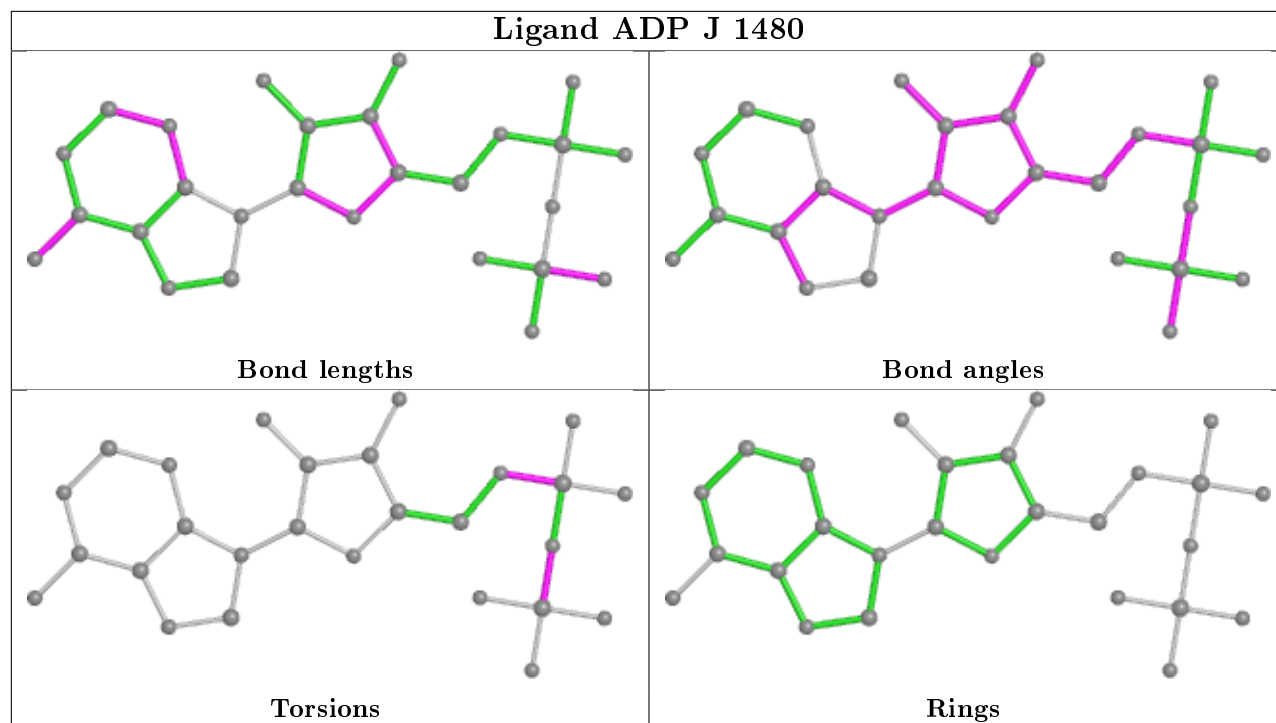


## Ligand ADP C 1473









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	468/468 (100%)	0.64	79 (16%) 1 1	18, 39, 91, 100	29 (6%)
1	B	468/468 (100%)	0.40	50 (10%) 6 4	18, 39, 91, 100	29 (6%)
1	C	468/468 (100%)	0.30	48 (10%) 6 5	18, 39, 91, 100	29 (6%)
1	D	468/468 (100%)	0.14	35 (7%) 14 12	18, 39, 91, 100	29 (6%)
1	E	468/468 (100%)	0.35	56 (11%) 4 3	18, 39, 91, 100	29 (6%)
1	F	468/468 (100%)	0.31	43 (9%) 9 7	18, 39, 91, 100	29 (6%)
1	G	468/468 (100%)	0.25	37 (7%) 12 10	18, 39, 91, 100	29 (6%)
1	H	468/468 (100%)	0.32	38 (8%) 12 10	18, 39, 91, 100	29 (6%)
1	I	468/468 (100%)	0.15	34 (7%) 15 12	18, 39, 91, 100	29 (6%)
1	J	468/468 (100%)	0.24	38 (8%) 12 10	18, 39, 91, 100	29 (6%)
1	K	468/468 (100%)	0.22	32 (6%) 17 15	18, 39, 91, 100	29 (6%)
1	L	468/468 (100%)	0.31	32 (6%) 17 15	18, 39, 91, 100	29 (6%)
All	All	5616/5616 (100%)	0.30	522 (9%) 8 6	18, 39, 92, 100	348 (6%)

All (522) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	397	TYR	13.1
1	K	397	TYR	12.7
1	H	402	GLU	12.5
1	B	397	TYR	12.3
1	L	51	GLY	11.9
1	K	326	TYR	11.5
1	J	397	TYR	11.4
1	F	400	PRO	11.3
1	K	398	ASP	10.5
1	C	397	TYR	10.4
1	A	397	TYR	10.2

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Mol	Chain	Res	Type	RSRZ
1	E	397	TYR	10.1
1	J	62	GLU	9.8
1	E	51	GLY	9.7
1	F	397	TYR	9.4
1	A	395	ASN	9.4
1	F	398	ASP	9.3
1	B	400	PRO	9.2
1	H	395	ASN	8.9
1	H	397	TYR	8.9
1	D	51	GLY	8.8
1	K	400	PRO	8.6
1	A	51	GLY	8.6
1	G	397	TYR	8.4
1	J	51	GLY	8.2
1	E	395	ASN	8.0
1	L	50	ASP	8.0
1	G	51	GLY	7.9
1	H	51	GLY	7.9
1	B	398	ASP	7.6
1	D	326	TYR	7.6
1	A	52	SER	7.4
1	F	326	TYR	7.4
1	H	403	GLU	7.4
1	F	51	GLY	7.3
1	G	401	PRO	7.3
1	K	402	GLU	7.2
1	C	403	GLU	7.2
1	K	394	LYS	7.1
1	F	401	PRO	7.1
1	K	51	GLY	7.1
1	L	52	SER	7.0
1	B	404	ALA	6.9
1	L	400	PRO	6.8
1	C	51	GLY	6.8
1	A	326	TYR	6.7
1	B	51	GLY	6.7
1	E	50	ASP	6.7
1	G	52	SER	6.6
1	G	50	ASP	6.6
1	H	62	GLU	6.4
1	H	50	ASP	6.4
1	F	61	ASN	6.4

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Mol	Chain	Res	Type	RSRZ
1	H	52	SER	6.3
1	D	403	GLU	6.3
1	G	402	GLU	6.2
1	J	403	GLU	6.2
1	B	326	TYR	6.2
1	E	394	LYS	6.2
1	F	52	SER	6.2
1	K	401	PRO	6.2
1	A	285	ASP	6.1
1	A	394	LYS	6.1
1	J	326	TYR	6.1
1	F	403	GLU	6.1
1	E	400	PRO	6.0
1	I	51	GLY	6.0
1	F	50	ASP	6.0
1	A	296	TYR	6.0
1	A	396	LEU	6.0
1	A	334	TYR	6.0
1	I	405	LYS	5.9
1	A	398	ASP	5.9
1	J	50	ASP	5.9
1	C	52	SER	5.9
1	G	60	ILE	5.9
1	K	396	LEU	5.9
1	G	400	PRO	5.8
1	L	394	LYS	5.8
1	J	398	ASP	5.8
1	C	400	PRO	5.8
1	G	395	ASN	5.7
1	D	394	LYS	5.7
1	K	395	ASN	5.7
1	D	60	ILE	5.5
1	K	52	SER	5.5
1	C	404	ALA	5.5
1	I	50	ASP	5.5
1	L	401	PRO	5.5
1	E	399	LEU	5.5
1	H	394	LYS	5.4
1	D	1	SER	5.4
1	C	326	TYR	5.4
1	K	403	GLU	5.4
1	B	396	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	398	ASP	5.4
1	F	399	LEU	5.4
1	A	354	ARG	5.4
1	L	179	TYR	5.4
1	L	60	ILE	5.3
1	J	394	LYS	5.3
1	K	50	ASP	5.3
1	G	398	ASP	5.3
1	J	400	PRO	5.3
1	I	394	LYS	5.3
1	H	179	TYR	5.2
1	B	405	LYS	5.2
1	D	52	SER	5.2
1	J	53	SER	5.2
1	K	399	LEU	5.1
1	F	62	GLU	5.1
1	I	397	TYR	5.1
1	C	405	LYS	5.1
1	H	398	ASP	5.1
1	B	52	SER	5.1
1	B	1	SER	5.1
1	A	345	ILE	5.0
1	J	60	ILE	5.0
1	G	61	ASN	5.0
1	A	392	MET	5.0
1	B	53	SER	5.0
1	D	405	LYS	5.0
1	B	403	GLU	5.0
1	I	404	ALA	5.0
1	I	53	SER	5.0
1	A	277	ASN	5.0
1	L	402	GLU	5.0
1	A	53	SER	4.9
1	G	1	SER	4.9
1	L	398	ASP	4.9
1	E	7	THR	4.9
1	E	1	SER	4.9
1	B	399	LEU	4.9
1	A	404	ALA	4.9
1	L	53	SER	4.9
1	J	395	ASN	4.8
1	I	52	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	J	63	SER	4.8
1	C	50	ASP	4.8
1	A	327	GLU	4.8
1	I	326	TYR	4.8
1	I	62	GLU	4.7
1	C	398	ASP	4.7
1	A	58	LYS	4.7
1	H	349	ALA	4.6
1	F	395	ASN	4.6
1	A	50	ASP	4.6
1	G	405	LYS	4.6
1	E	386	ILE	4.6
1	L	405	LYS	4.6
1	G	326	TYR	4.6
1	C	401	PRO	4.6
1	F	53	SER	4.6
1	C	53	SER	4.5
1	J	52	SER	4.5
1	A	400	PRO	4.5
1	D	404	ALA	4.5
1	D	402	GLU	4.5
1	D	401	PRO	4.5
1	D	395	ASN	4.5
1	F	396	LEU	4.5
1	J	1	SER	4.4
1	A	351	PRO	4.4
1	J	396	LEU	4.4
1	K	179	TYR	4.4
1	G	394	LYS	4.4
1	G	3	GLU	4.3
1	F	404	ALA	4.3
1	A	347	VAL	4.3
1	F	60	ILE	4.3
1	C	394	LYS	4.3
1	J	404	ALA	4.3
1	L	395	ASN	4.3
1	L	403	GLU	4.2
1	A	278	GLY	4.2
1	A	348	VAL	4.2
1	C	402	GLU	4.2
1	I	403	GLU	4.2
1	D	398	ASP	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	60	ILE	4.1
1	E	52	SER	4.1
1	C	395	ASN	4.1
1	H	400	PRO	4.1
1	A	399	LEU	4.0
1	I	60	ILE	4.0
1	I	3	GLU	4.0
1	A	60	ILE	4.0
1	C	293	GLN	4.0
1	K	406	GLU	4.0
1	A	333	ALA	4.0
1	D	285	ASP	3.9
1	E	396	LEU	3.9
1	A	63	SER	3.9
1	H	61	ASN	3.9
1	B	2	ALA	3.9
1	G	179	TYR	3.9
1	K	405	LYS	3.9
1	B	64	ASP	3.9
1	J	5	VAL	3.8
1	H	12	HIS	3.8
1	F	394	LYS	3.8
1	C	296	TYR	3.8
1	G	53	SER	3.8
1	H	53	SER	3.8
1	K	340	SER	3.8
1	H	8	MET	3.8
1	A	98	GLN	3.8
1	L	63	SER	3.8
1	B	12	HIS	3.8
1	K	327	GLU	3.7
1	C	61	ASN	3.7
1	F	331	MET	3.7
1	H	1	SER	3.7
1	I	327	GLU	3.7
1	C	179	TYR	3.7
1	H	351	PRO	3.7
1	B	46	GLY	3.7
1	E	350	SER	3.7
1	D	397	TYR	3.7
1	E	179	TYR	3.7
1	E	406	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	1	SER	3.7
1	E	12	HIS	3.7
1	C	337	ARG	3.7
1	B	401	PRO	3.7
1	B	58	LYS	3.6
1	E	385	LYS	3.6
1	A	279	THR	3.6
1	H	401	PRO	3.6
1	I	398	ASP	3.6
1	D	179	TYR	3.6
1	F	179	TYR	3.6
1	A	324	PRO	3.6
1	C	62	GLU	3.6
1	B	50	ASP	3.5
1	G	2	ALA	3.5
1	F	407	ILE	3.5
1	B	395	ASN	3.5
1	G	6	LEU	3.5
1	A	335	SER	3.5
1	I	179	TYR	3.5
1	D	50	ASP	3.5
1	H	399	LEU	3.5
1	B	63	SER	3.4
1	J	179	TYR	3.4
1	A	293	GLN	3.4
1	A	62	GLU	3.4
1	E	405	LYS	3.4
1	J	61	ASN	3.4
1	A	402	GLU	3.4
1	E	60	ILE	3.4
1	D	53	SER	3.4
1	D	4	HIS	3.4
1	F	402	GLU	3.4
1	A	179	TYR	3.4
1	H	326	TYR	3.4
1	K	98	GLN	3.4
1	D	400	PRO	3.4
1	B	62	GLU	3.4
1	B	327	GLU	3.4
1	E	403	GLU	3.3
1	L	59	GLY	3.3
1	C	351	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	7	THR	3.3
1	D	117	ALA	3.3
1	C	279	THR	3.3
1	G	339	ARG	3.3
1	H	337	ARG	3.3
1	F	392	MET	3.3
1	F	284	GLY	3.3
1	B	394	LYS	3.3
1	C	327	GLU	3.3
1	G	49	PHE	3.2
1	G	63	SER	3.2
1	A	353	ALA	3.2
1	C	1	SER	3.2
1	B	328	ALA	3.2
1	K	53	SER	3.2
1	F	327	GLU	3.2
1	I	98	GLN	3.2
1	G	62	GLU	3.2
1	E	2	ALA	3.2
1	E	63	SER	3.2
1	C	287	TYR	3.1
1	A	391	PRO	3.1
1	A	276	LYS	3.1
1	J	401	PRO	3.1
1	D	63	SER	3.1
1	I	396	LEU	3.1
1	A	43	PHE	3.1
1	B	8	MET	3.1
1	E	351	PRO	3.1
1	B	179	TYR	3.0
1	A	338	ASN	3.0
1	I	395	ASN	3.0
1	F	40	ALA	3.0
1	A	91	ILE	3.0
1	B	407	ILE	3.0
1	A	339	ARG	3.0
1	B	402	GLU	3.0
1	G	7	THR	3.0
1	A	288	ALA	3.0
1	E	53	SER	3.0
1	E	11	GLU	3.0
1	C	284	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	327	GLU	3.0
1	G	404	ALA	3.0
1	A	5	VAL	2.9
1	A	292	GLU	2.9
1	F	405	LYS	2.9
1	F	98	GLN	2.9
1	J	402	GLU	2.9
1	H	405	LYS	2.9
1	L	61	ASN	2.9
1	C	285	ASP	2.9
1	I	407	ILE	2.9
1	I	59	GLY	2.9
1	B	98	GLN	2.8
1	J	98	GLN	2.8
1	I	54	ILE	2.8
1	L	49	PHE	2.8
1	C	59	GLY	2.8
1	J	4	HIS	2.8
1	A	2	ALA	2.8
1	E	383	LYS	2.8
1	E	404	ALA	2.8
1	H	40	ALA	2.8
1	D	38	VAL	2.8
1	I	401	PRO	2.8
1	F	337	ARG	2.8
1	K	49	PHE	2.8
1	B	39	ASN	2.8
1	B	278	GLY	2.8
1	H	4	HIS	2.8
1	A	6	LEU	2.8
1	F	278	GLY	2.8
1	J	7	THR	2.8
1	A	405	LYS	2.7
1	C	396	LEU	2.7
1	J	6	LEU	2.7
1	C	419	ASN	2.7
1	H	404	ALA	2.7
1	J	8	MET	2.7
1	G	399	LEU	2.7
1	A	387	HIS	2.7
1	C	406	GLU	2.7
1	I	402	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	49	PHE	2.7
1	C	292	GLU	2.7
1	I	331	MET	2.7
1	E	277	ASN	2.7
1	A	352	LYS	2.7
1	C	349	ALA	2.7
1	K	165	GLU	2.7
1	L	58	LYS	2.7
1	E	8	MET	2.6
1	G	403	GLU	2.6
1	E	326	TYR	2.6
1	L	270	CYS	2.6
1	A	3	GLU	2.6
1	I	61	ASN	2.6
1	F	63	SER	2.6
1	E	62	GLU	2.6
1	I	58	LYS	2.6
1	F	340	SER	2.6
1	A	382	ILE	2.6
1	C	286	LYS	2.6
1	I	49	PHE	2.6
1	C	289	GLY	2.6
1	A	275	ALA	2.6
1	B	392	MET	2.6
1	E	3	GLU	2.6
1	E	10	ASN	2.6
1	I	400	PRO	2.6
1	B	393	ASP	2.6
1	D	44	GLU	2.6
1	J	49	PHE	2.6
1	A	346	PRO	2.5
1	G	165	GLU	2.5
1	B	97	LEU	2.5
1	C	282	PHE	2.5
1	I	43	PHE	2.5
1	C	277	ASN	2.5
1	C	399	LEU	2.5
1	E	283	SER	2.5
1	A	401	PRO	2.5
1	K	404	ALA	2.5
1	C	290	LEU	2.5
1	G	396	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	1	SER	2.5
1	L	165	GLU	2.5
1	D	40	ALA	2.5
1	B	11	GLU	2.5
1	C	339	ARG	2.5
1	B	4	HIS	2.5
1	K	2	ALA	2.5
1	E	292	GLU	2.5
1	L	326	TYR	2.5
1	B	122	ASP	2.5
1	B	95	GLY	2.5
1	D	3	GLU	2.5
1	E	401	PRO	2.5
1	C	407	ILE	2.5
1	I	392	MET	2.5
1	L	6	LEU	2.4
1	H	350	SER	2.4
1	F	349	ALA	2.4
1	A	337	ARG	2.4
1	E	337	ARG	2.4
1	A	390	GLU	2.4
1	H	364	ALA	2.4
1	K	331	MET	2.4
1	K	41	GLU	2.4
1	B	290	LEU	2.4
1	A	1	SER	2.4
1	A	340	SER	2.4
1	C	60	ILE	2.4
1	F	324	PRO	2.4
1	K	324	PRO	2.4
1	C	96	THR	2.4
1	F	406	GLU	2.4
1	G	406	GLU	2.4
1	E	387	HIS	2.3
1	L	361	PRO	2.3
1	A	283	SER	2.3
1	A	284	GLY	2.3
1	A	286	LYS	2.3
1	E	278	GLY	2.3
1	H	49	PHE	2.3
1	B	6	LEU	2.3
1	A	299	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	43	PHE	2.3
1	L	98	GLN	2.3
1	A	4	HIS	2.3
1	A	379	LEU	2.3
1	I	64	ASP	2.3
1	F	1	SER	2.3
1	L	328	ALA	2.3
1	K	407	ILE	2.3
1	E	340	SER	2.2
1	I	6	LEU	2.2
1	C	275	ALA	2.2
1	E	423	LEU	2.2
1	H	331	MET	2.2
1	J	339	ARG	2.2
1	B	43	PHE	2.2
1	J	327	GLU	2.2
1	L	327	GLU	2.2
1	A	355	ARG	2.2
1	A	294	ALA	2.2
1	L	404	ALA	2.2
1	K	44	GLU	2.2
1	H	347	VAL	2.2
1	E	392	MET	2.2
1	F	65	MET	2.2
1	I	165	GLU	2.2
1	E	42	PHE	2.2
1	F	338	ASN	2.2
1	D	41	GLU	2.2
1	J	64	ASP	2.2
1	A	287	TYR	2.2
1	G	277	ASN	2.2
1	B	351	PRO	2.2
1	D	396	LEU	2.2
1	F	3	GLU	2.2
1	A	122	ASP	2.2
1	E	64	ASP	2.2
1	E	348	VAL	2.2
1	J	338	ASN	2.2
1	A	336	ALA	2.2
1	F	339	ARG	2.2
1	E	407	ILE	2.1
1	J	41	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	349	ALA	2.1
1	B	42	PHE	2.1
1	K	3	GLU	2.1
1	A	403	GLU	2.1
1	D	165	GLU	2.1
1	B	49	PHE	2.1
1	G	9	LEU	2.1
1	L	40	ALA	2.1
1	J	12	HIS	2.1
1	A	10	ASN	2.1
1	A	42	PHE	2.1
1	J	337	ARG	2.1
1	D	62	GLU	2.1
1	E	341	ALA	2.1
1	A	331	MET	2.1
1	H	338	ASN	2.1
1	H	392	MET	2.1
1	H	277	ASN	2.1
1	A	126	PHE	2.1
1	E	13	GLU	2.1
1	E	402	GLU	2.1
1	D	5	VAL	2.1
1	E	284	GLY	2.1
1	F	352	LYS	2.0
1	D	54	ILE	2.0
1	G	54	ILE	2.0
1	B	117	ALA	2.0
1	E	339	ARG	2.0
1	C	392	MET	2.0
1	L	64	ASP	2.0
1	E	49	PHE	2.0
1	A	38	VAL	2.0
1	F	330	VAL	2.0
1	G	4	HIS	2.0
1	J	165	GLU	2.0
1	C	328	ALA	2.0
1	A	281	LEU	2.0
1	E	4	HIS	2.0
1	B	38	VAL	2.0
1	J	324	PRO	2.0
1	H	407	ILE	2.0
1	J	2	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	293	GLN	2.0
1	C	43	PHE	2.0
1	G	371	PHE	2.0
1	B	339	ARG	2.0
1	D	337	ARG	2.0
1	F	97	LEU	2.0
1	G	97	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	ADP	F	1476	27/27	0.60	0.51	20,78,100,100	27
3	ADP	I	1479	27/27	0.62	0.50	20,78,100,100	27
3	ADP	D	1474	27/27	0.65	0.49	20,78,100,100	27
3	ADP	B	1472	27/27	0.66	0.49	20,78,100,100	27
3	ADP	L	1482	27/27	0.67	0.48	20,78,100,100	27
3	ADP	A	1471	27/27	0.69	0.39	20,78,100,100	27
3	ADP	K	1481	27/27	0.71	0.43	20,78,100,100	27
3	ADP	H	1478	27/27	0.74	0.37	20,78,100,100	27
5	MPD	B	1484	8/8	0.75	0.44	16,43,64,74	8
3	ADP	C	1473	27/27	0.75	0.35	20,78,100,100	27
3	ADP	E	1475	27/27	0.76	0.35	20,78,100,100	27
3	ADP	G	1477	27/27	0.83	0.34	20,78,100,100	27
5	MPD	A	1483	8/8	0.84	0.34	16,43,64,74	8
3	ADP	J	1480	27/27	0.84	0.35	20,78,100,100	27
5	MPD	C	1485	8/8	0.85	0.48	16,43,64,74	8
4	TL	I	473	1/1	0.86	0.22	67,67,67,67	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MPD	D	1486	8/8	0.86	0.39	16,43,64,74	8
5	MPD	F	1488	8/8	0.87	0.43	16,43,64,74	8
4	TL	J	474	1/1	0.89	0.11	75,75,75,75	1
4	TL	A	473	1/1	0.90	0.19	67,67,67,67	1
4	TL	F	473	1/1	0.90	0.11	67,67,67,67	1
4	TL	E	474	1/1	0.91	0.10	75,75,75,75	1
2	MN	A	470	1/1	0.91	0.05	41,41,41,41	0
5	MPD	K	1493	8/8	0.91	0.41	16,43,64,74	8
5	MPD	I	1491	8/8	0.91	0.32	16,43,64,74	8
5	MPD	E	1487	8/8	0.91	0.45	16,43,64,74	8
5	MPD	J	1492	8/8	0.92	0.35	16,43,64,74	8
4	TL	H	474	1/1	0.92	0.05	75,75,75,75	1
5	MPD	L	1494	8/8	0.92	0.45	16,43,64,74	8
5	MPD	H	1490	8/8	0.93	0.41	16,43,64,74	8
4	TL	J	473	1/1	0.93	0.26	67,67,67,67	1
4	TL	B	474	1/1	0.93	0.08	75,75,75,75	1
4	TL	K	473	1/1	0.93	0.12	67,67,67,67	1
4	TL	D	474	1/1	0.93	0.09	75,75,75,75	1
4	TL	L	473	1/1	0.93	0.23	67,67,67,67	1
2	MN	B	470	1/1	0.94	0.04	41,41,41,41	0
4	TL	C	474	1/1	0.94	0.05	75,75,75,75	1
5	MPD	G	1489	8/8	0.94	0.35	16,43,64,74	8
2	MN	H	470	1/1	0.95	0.09	41,41,41,41	0
4	TL	L	474	1/1	0.95	0.12	75,75,75,75	1
2	MN	I	470	1/1	0.95	0.13	41,41,41,41	0
2	MN	A	469	1/1	0.95	0.04	34,34,34,34	0
4	TL	I	474	1/1	0.96	0.13	75,75,75,75	1
4	TL	C	473	1/1	0.96	0.16	67,67,67,67	1
2	MN	F	470	1/1	0.96	0.06	41,41,41,41	0
4	TL	A	474	1/1	0.96	0.08	75,75,75,75	1
4	TL	H	473	1/1	0.96	0.19	67,67,67,67	1
4	TL	G	474	1/1	0.96	0.13	75,75,75,75	1
4	TL	G	473	1/1	0.96	0.17	67,67,67,67	1
2	MN	J	469	1/1	0.96	0.12	34,34,34,34	0
4	TL	E	473	1/1	0.97	0.06	67,67,67,67	1
4	TL	D	473	1/1	0.97	0.05	67,67,67,67	1
2	MN	B	469	1/1	0.97	0.06	34,34,34,34	0
2	MN	C	469	1/1	0.97	0.08	34,34,34,34	0
4	TL	B	473	1/1	0.97	0.05	67,67,67,67	1
4	TL	K	474	1/1	0.97	0.12	75,75,75,75	1
2	MN	D	470	1/1	0.97	0.10	41,41,41,41	0
2	MN	K	469	1/1	0.97	0.13	34,34,34,34	0

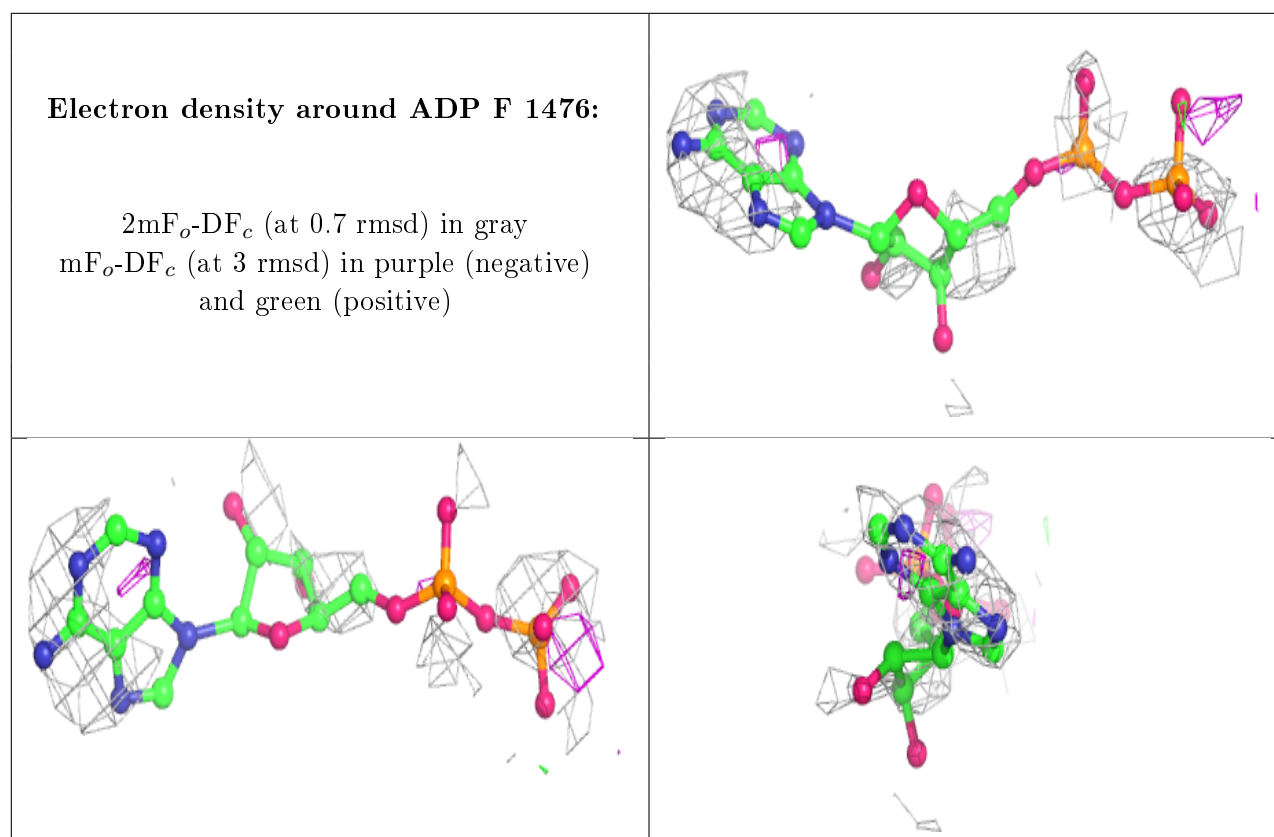
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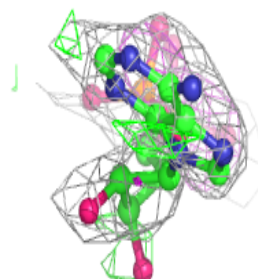
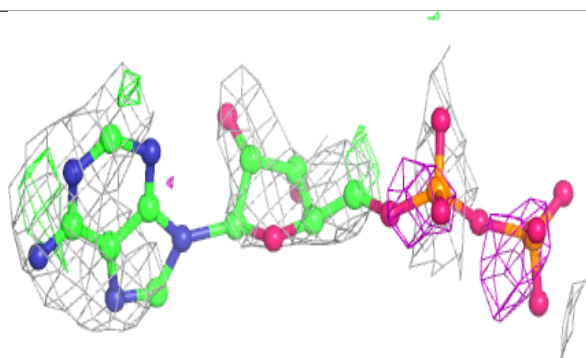
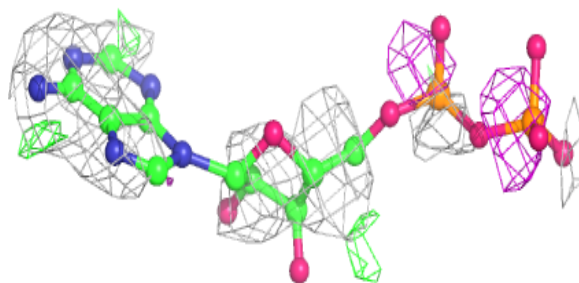
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	L	470	1/1	0.97	0.18	41,41,41,41	0
2	MN	D	469	1/1	0.97	0.10	34,34,34,34	0
4	TL	F	474	1/1	0.97	0.04	75,75,75,75	1
2	MN	G	470	1/1	0.97	0.13	41,41,41,41	0
2	MN	E	470	1/1	0.98	0.09	41,41,41,41	0
2	MN	L	469	1/1	0.98	0.12	34,34,34,34	0
2	MN	E	469	1/1	0.98	0.05	34,34,34,34	0
2	MN	G	469	1/1	0.98	0.07	34,34,34,34	0
2	MN	F	469	1/1	0.99	0.04	34,34,34,34	0
2	MN	C	470	1/1	0.99	0.04	41,41,41,41	0
2	MN	K	470	1/1	0.99	0.16	41,41,41,41	0
2	MN	J	470	1/1	0.99	0.10	41,41,41,41	0
2	MN	I	469	1/1	0.99	0.07	34,34,34,34	0
2	MN	H	469	1/1	0.99	0.08	34,34,34,34	0

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.

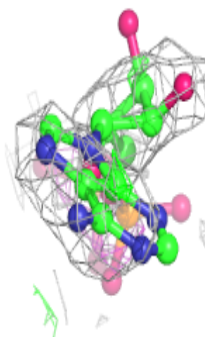
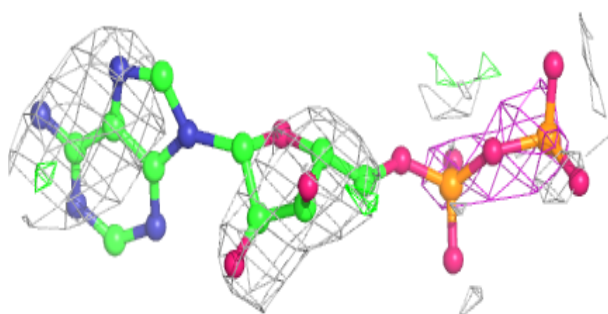
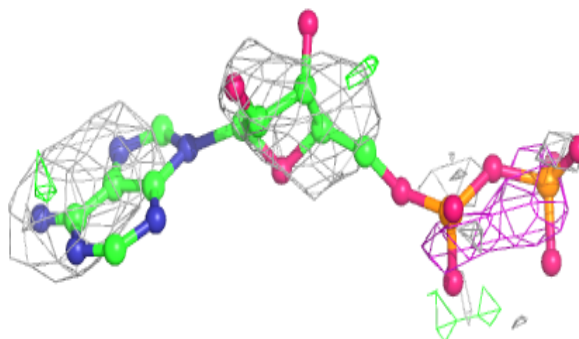


**Electron density around ADP I 1479:**

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

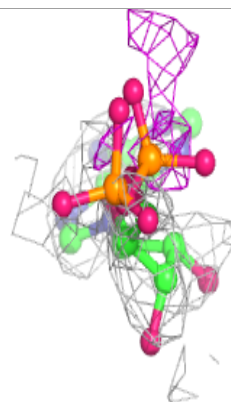
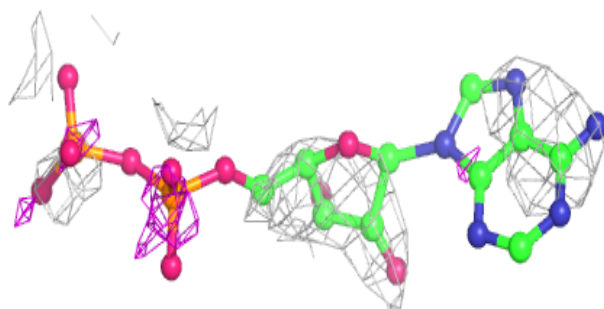
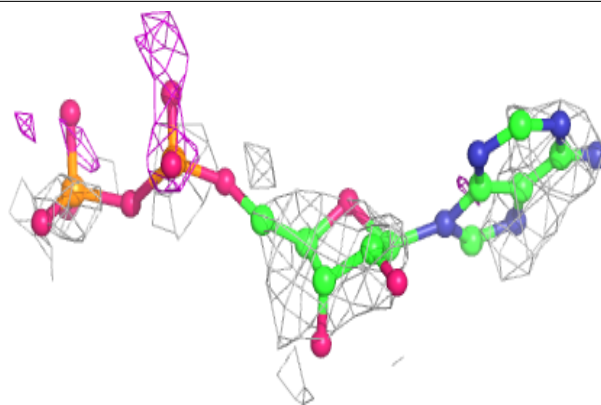
**Electron density around ADP D 1474:**

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

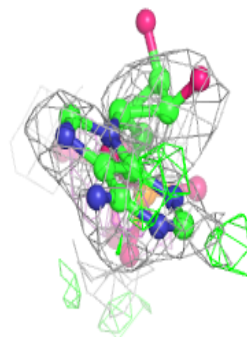
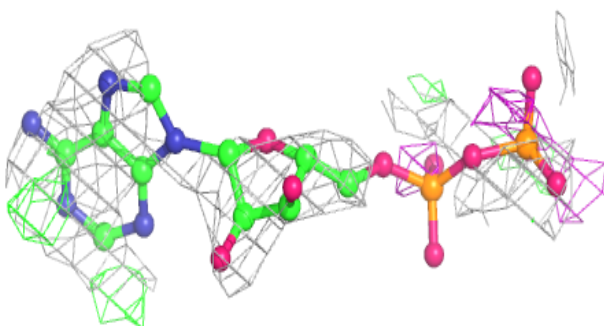
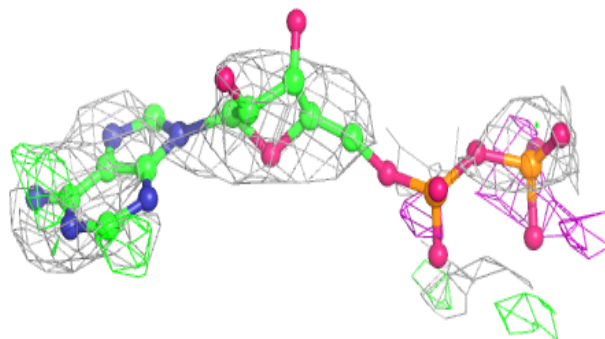


**Electron density around ADP B 1472:**

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

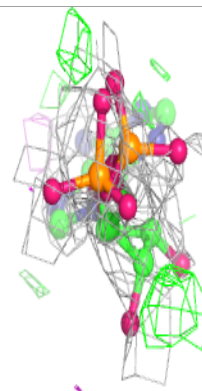
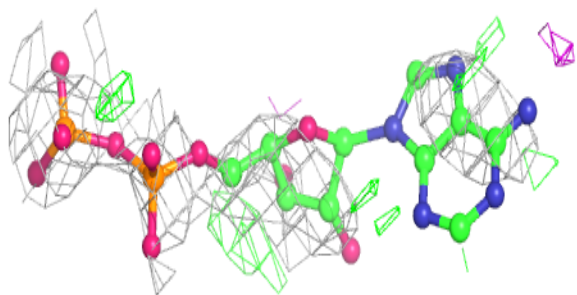
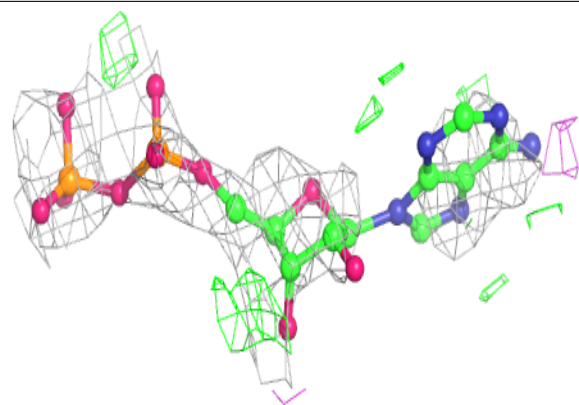
**Electron density around ADP L 1482:**

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

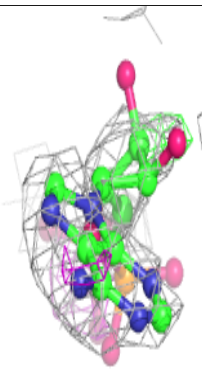
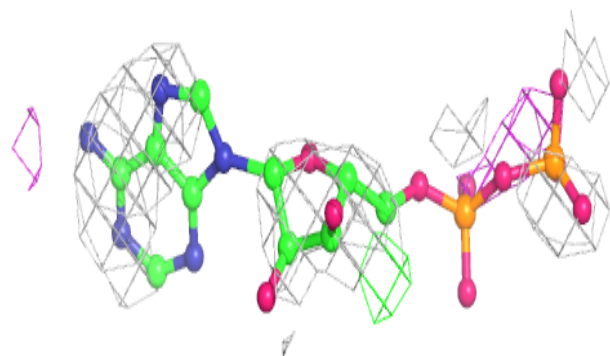
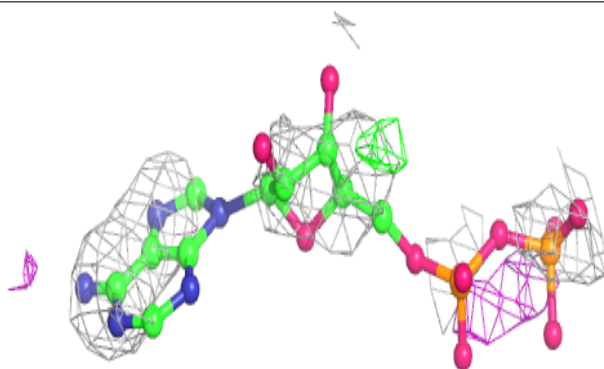


**Electron density around ADP A 1471:**

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

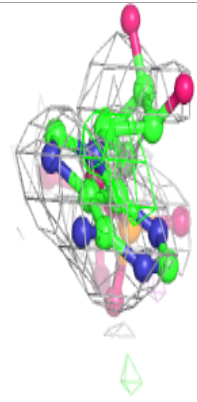
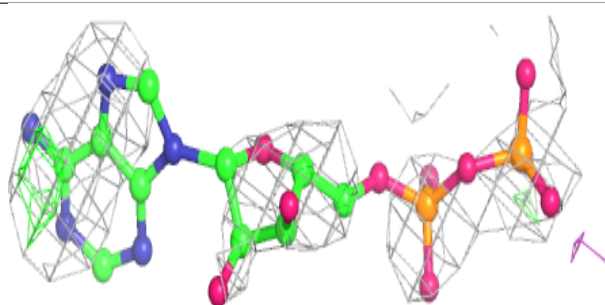
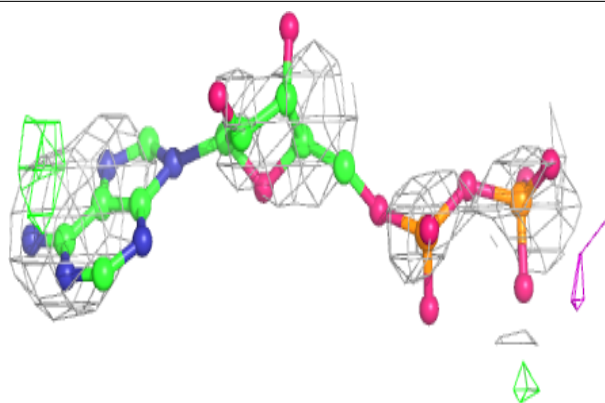
**Electron density around ADP K 1481:**

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

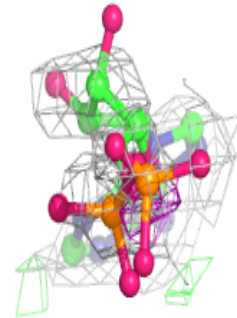
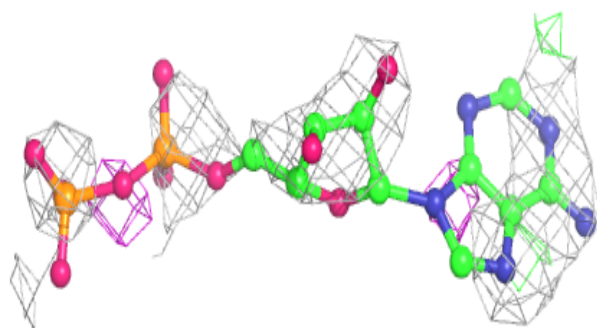
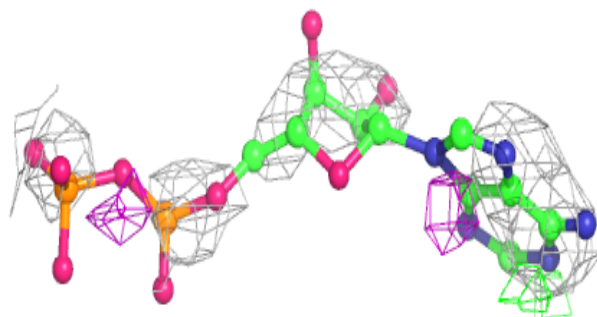


**Electron density around ADP H 1478:**

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

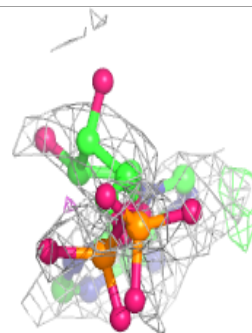
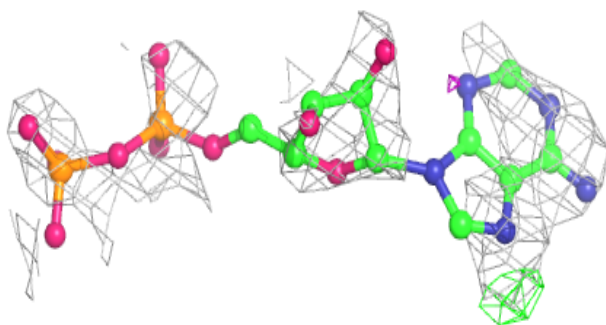
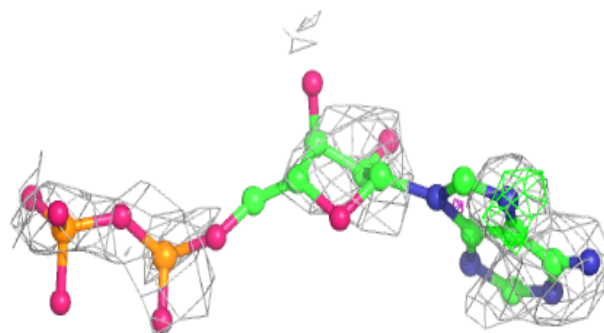
**Electron density around ADP C 1473:**

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

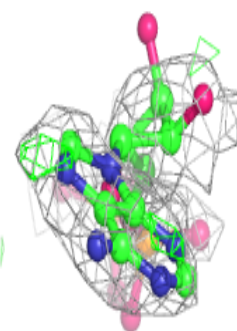
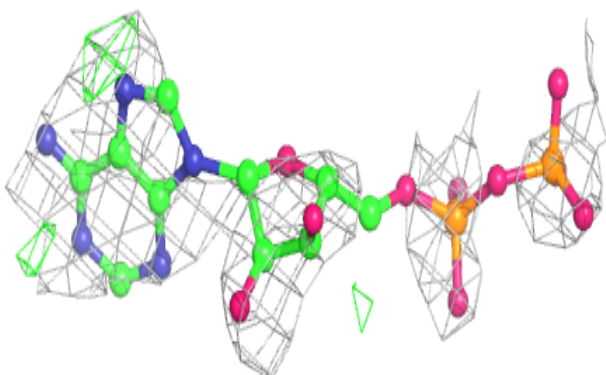
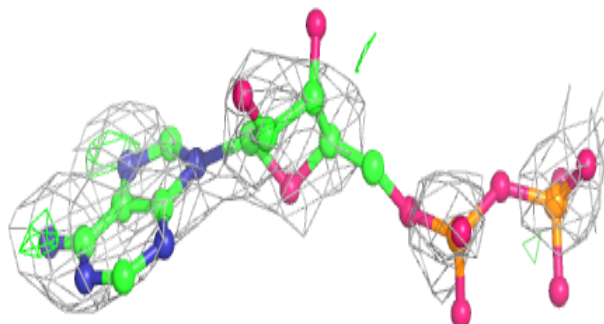


**Electron density around ADP E 1475:**

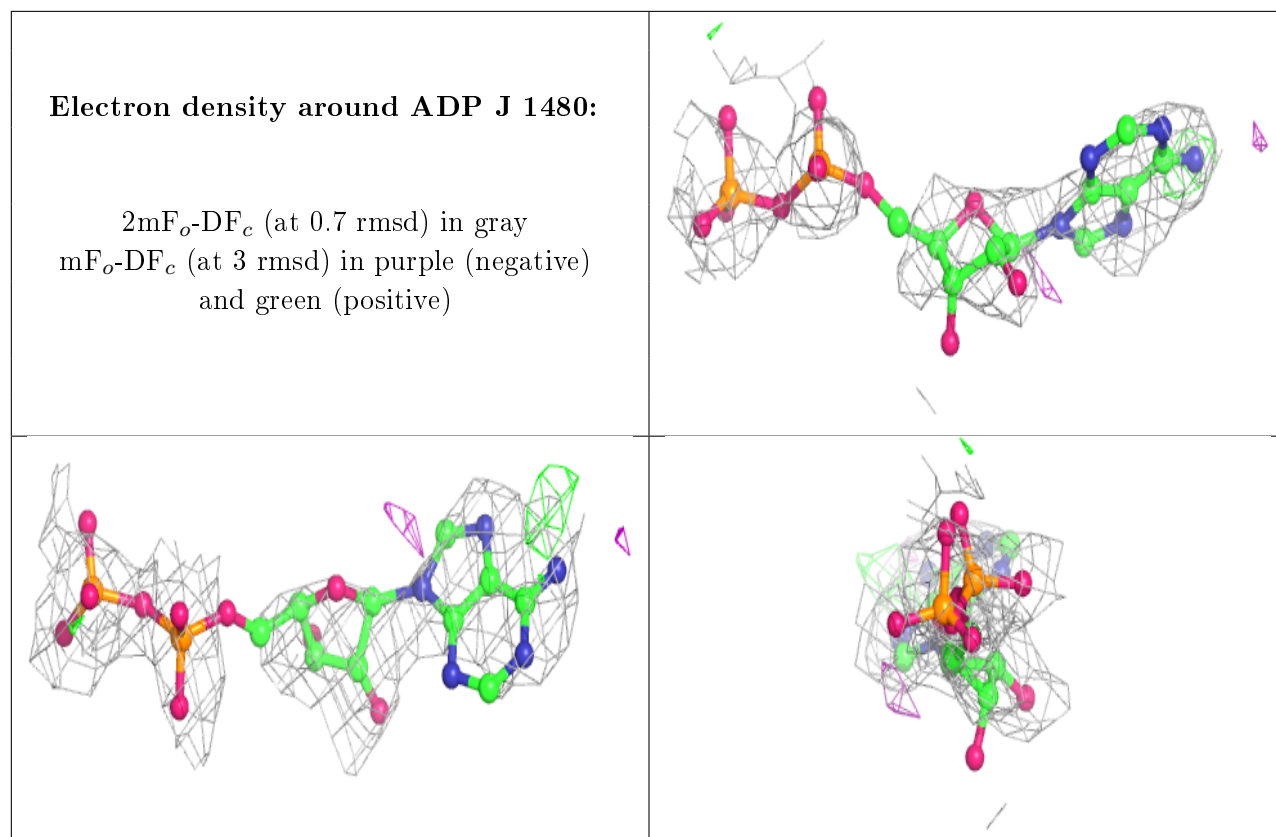
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP G 1477:**

$2mF_o-DF_c$  (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.