



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:30 am BST

PDB ID : 1F52  
Title : CRYSTAL STRUCTURE OF GLUTAMINE SYNTHETASE FROM  
SALMONELLA TYPHIMURIUM CO-CRYSTALLIZED WITH ADP  
Authors : Gill, H.S.; Pfluegl, G.M.U.; Eisenberg, D.  
Deposited on : 2000-06-12  
Resolution : 2.49 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

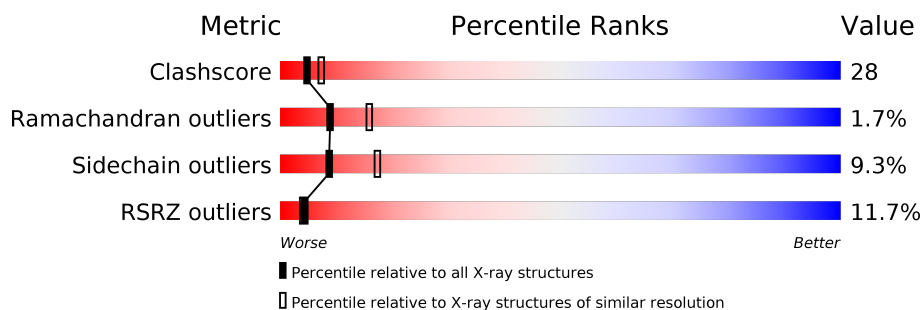
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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.



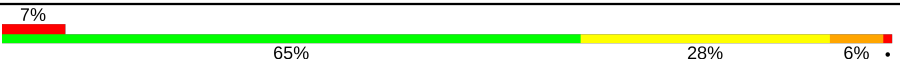


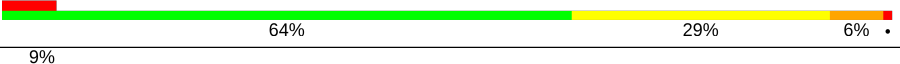

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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>31%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>
1	B	468	<div> <div>15%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>
1	C	468	<div> <div>14%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>
1	D	468	<div> <div>10%</div> <div>66%</div> <div>27%</div> <div>6%</div> </div>
1	E	468	<div> <div>15%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>
1	F	468	<div> <div>10%</div> <div>63%</div> <div>29%</div> <div>6%</div> </div>
1	G	468	<div> <div>9%</div> <div>65%</div> <div>28%</div> <div>6%</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	A	4471	-	-	-	X
3	ADP	B	4472	-	-	-	X
3	ADP	F	4476	-	-	-	X
3	ADP	I	4479	-	-	-	X
3	ADP	K	4481	-	-	-	X
3	ADP	L	4482	-	-	-	X
4	MPD	A	5472	-	-	X	X
4	MPD	A	5481	-	-	X	-
4	MPD	B	5471	-	-	X	X
4	MPD	B	5474	-	-	X	X
4	MPD	C	5473	-	-	X	-
4	MPD	C	5476	-	-	X	X
4	MPD	D	5475	-	-	X	-
4	MPD	D	5478	-	-	X	X
4	MPD	E	5477	-	-	X	-
4	MPD	E	5480	-	-	X	X
4	MPD	F	5479	-	-	X	-
4	MPD	F	5482	-	-	X	-
4	MPD	G	5484	-	-	X	X
4	MPD	G	5485	-	-	X	-
4	MPD	H	5486	-	-	X	X
4	MPD	H	5487	-	-	X	-
4	MPD	I	5488	-	-	X	X
4	MPD	I	5489	-	-	X	-
4	MPD	J	5490	-	-	X	X
4	MPD	J	5491	-	-	X	-
4	MPD	K	5492	-	-	X	X
4	MPD	K	5493	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	L	5483	-	-	X	-
4	MPD	L	5494	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 47688 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called GLUTAMINE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	B	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	C	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	D	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	E	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	F	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	G	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	H	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	I	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	J	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	K	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			
1	L	468	Total	C	N	O	S	8	0	0
			3637	2301	624	692	20			

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

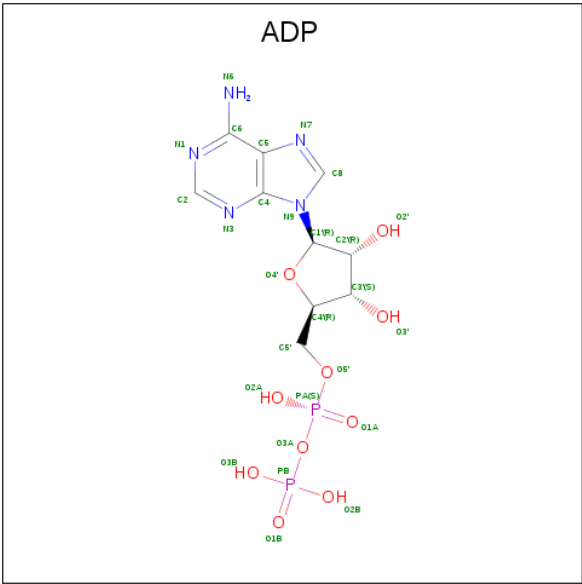
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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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>).



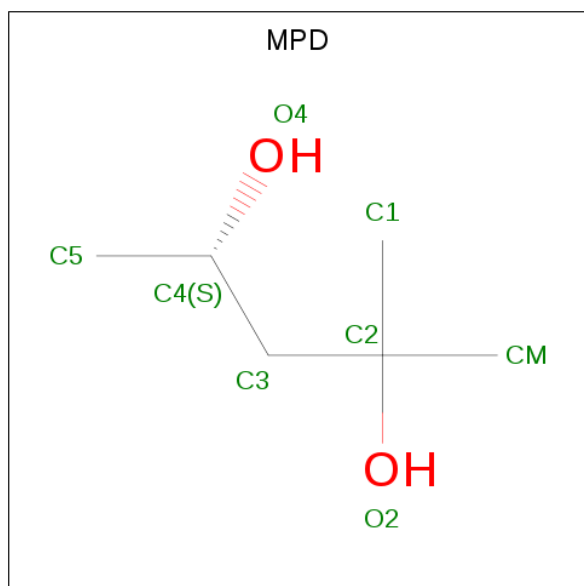
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

- Molecule 4 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
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	G	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	I	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	J	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		
4	K	1	Total	C	O	0	0
			8	6	2		

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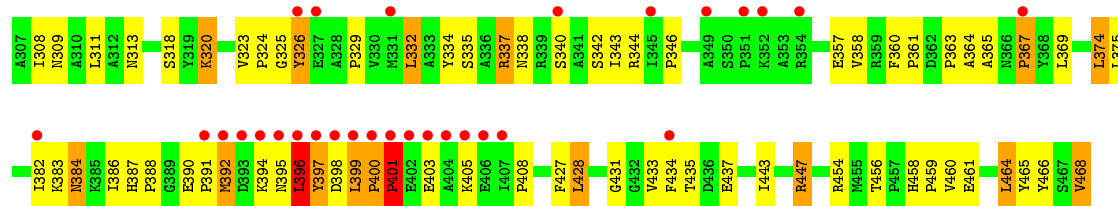
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			8	6	2		
4	L	1	Total	C	O	0	0
			8	6	2		

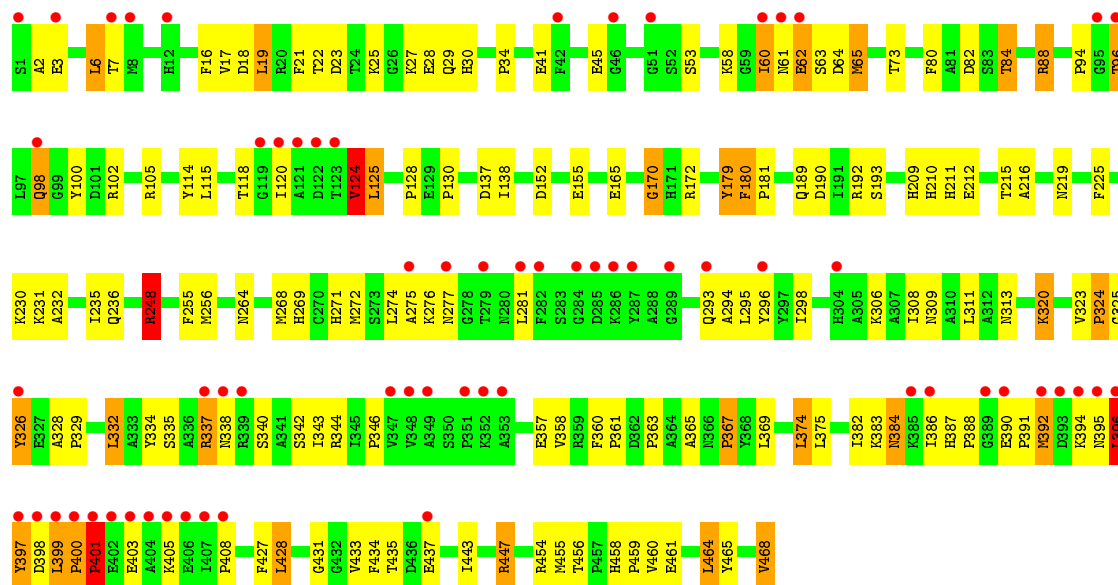
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	294	Total	O	0	0
			294	294		
5	B	297	Total	O	0	0
			297	297		
5	C	293	Total	O	0	0
			293	293		
5	D	295	Total	O	0	0
			295	295		
5	E	294	Total	O	0	0
			294	294		
5	F	293	Total	O	0	0
			293	293		
5	G	288	Total	O	0	0
			288	288		
5	H	288	Total	O	0	0
			288	288		
5	I	295	Total	O	0	0
			295	295		
5	J	287	Total	O	0	0
			287	287		
5	K	288	Total	O	0	0
			288	288		
5	L	292	Total	O	0	0
			292	292		

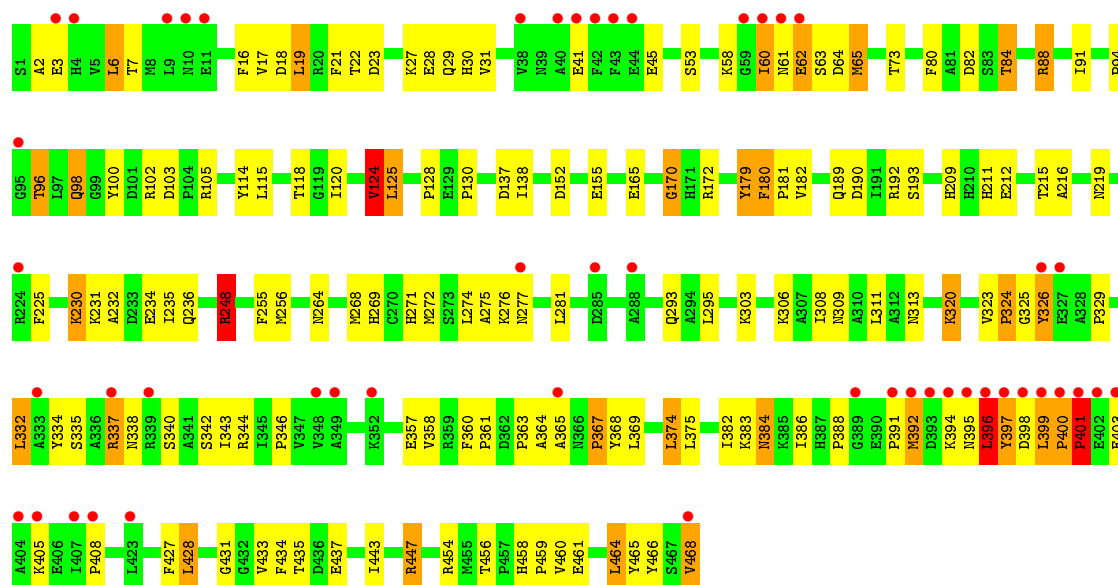




• Molecule 1: GLUTAMINE SYNTHETASE

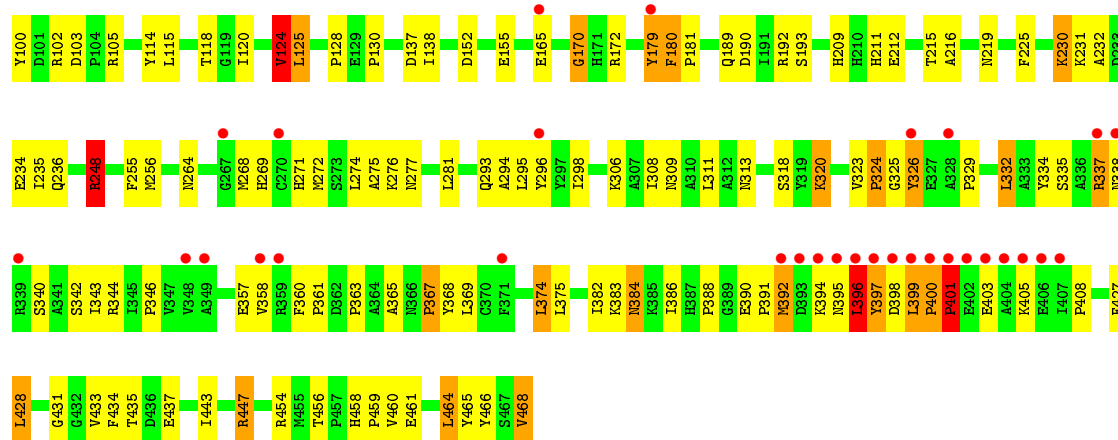


• Molecule 1: GLUTAMINE SYNTHETASE

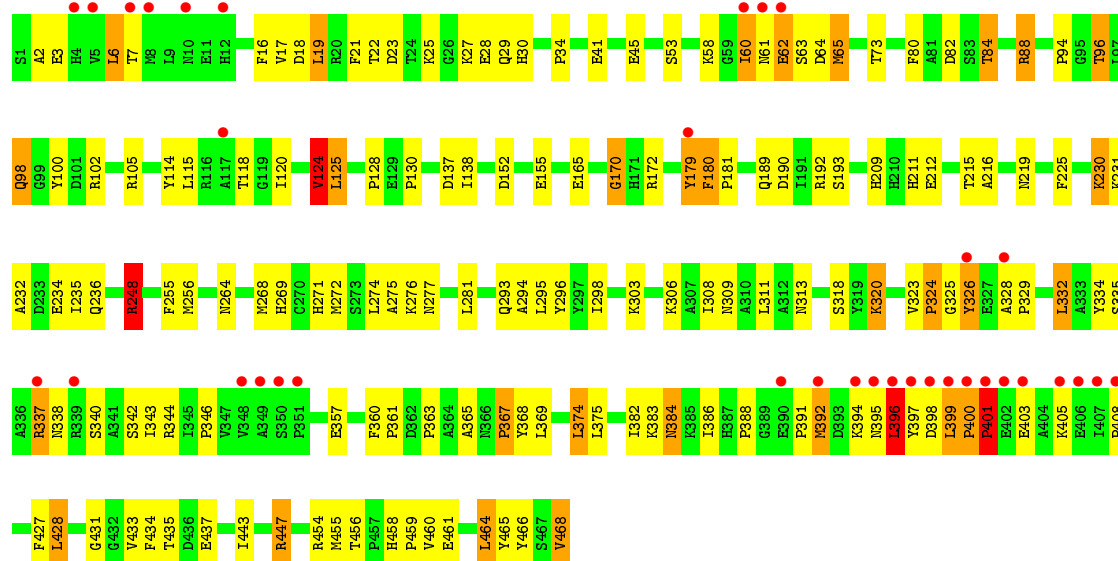


• Molecule 1: GLUTAMINE SYNTHETASE

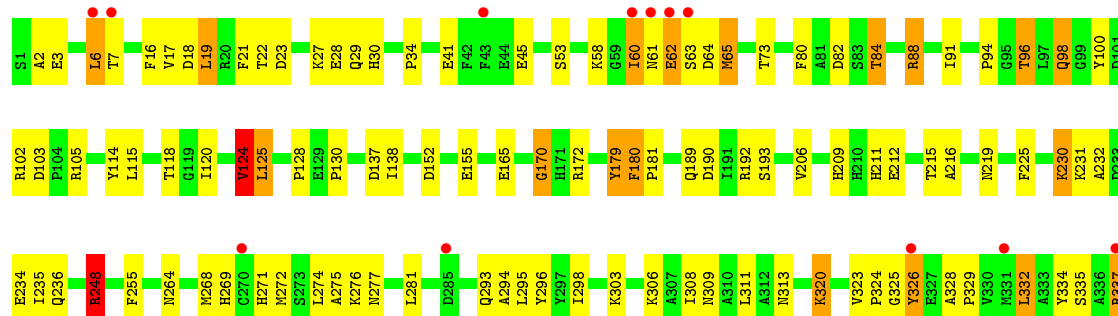




• Molecule 1: GLUTAMINE SYNTHETASE

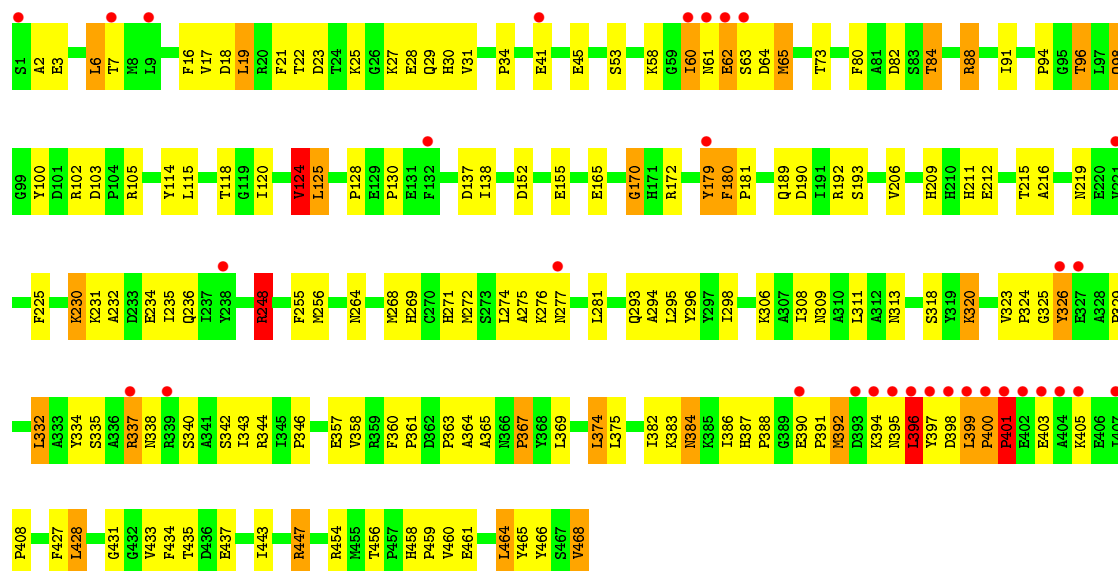


• Molecule 1: GLUTAMINE SYNTHETASE

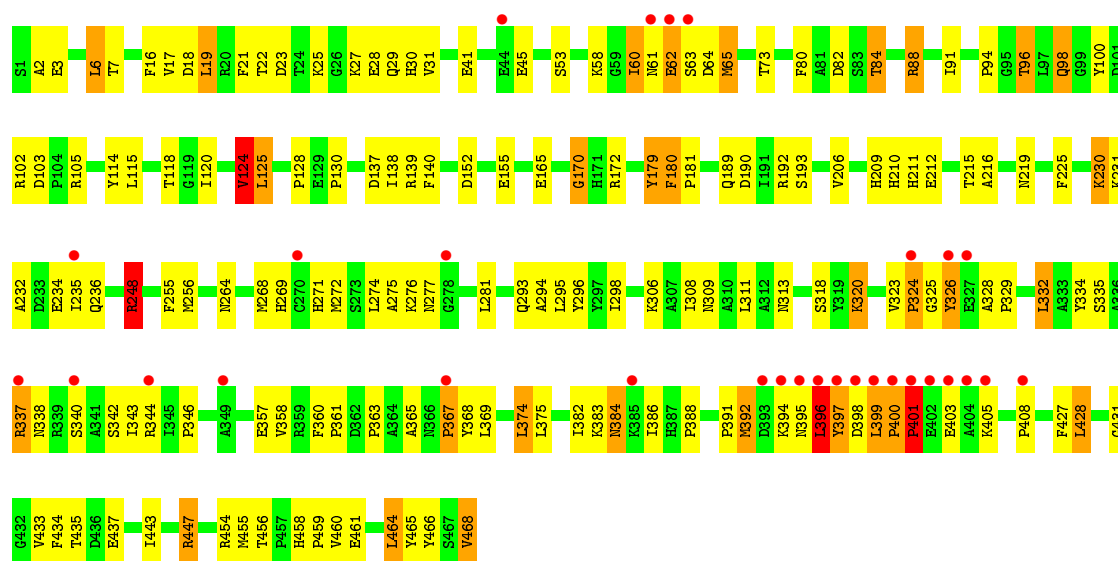




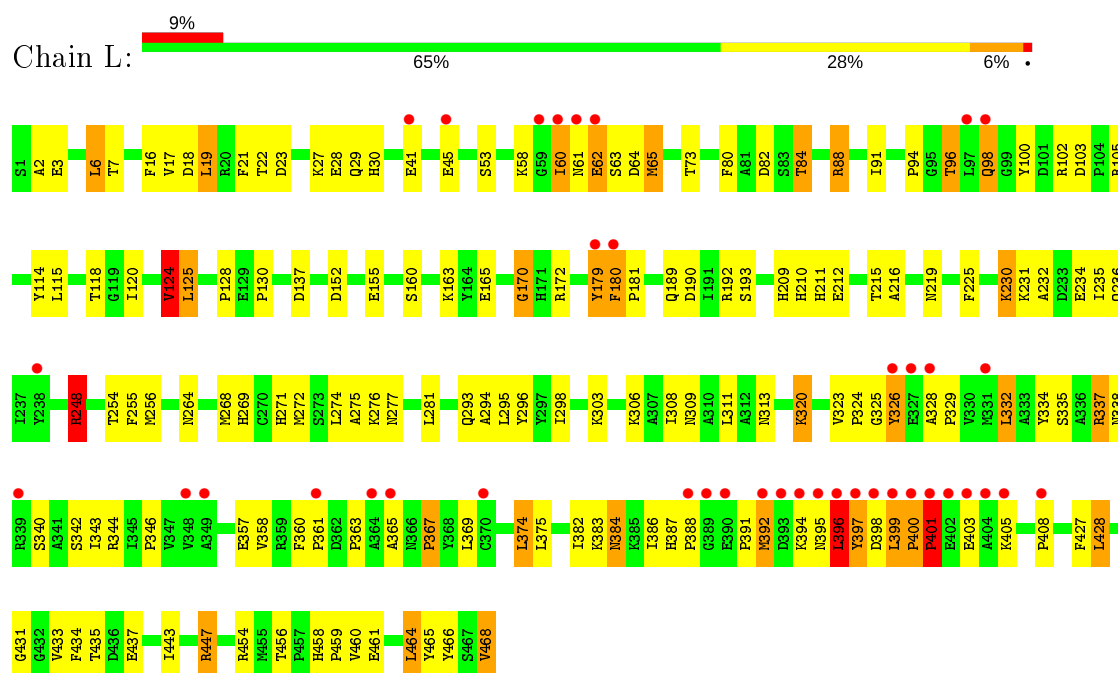
• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	230.60 Å   132.50 Å   195.90 Å 90.00°   102.40°   90.00°	Depositor
Resolution (Å)	34.90 – 2.49 34.90 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (34.90-2.49) 97.9 (34.90-2.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.67 (at 2.48 Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.243   ,   0.257 0.261   ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 57.6	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	47688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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, 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	0.53	0/3724	0.85	4/5043 (0.1%)
1	B	0.53	0/3724	0.85	4/5043 (0.1%)
1	C	0.53	0/3724	0.85	4/5043 (0.1%)
1	D	0.53	0/3724	0.85	4/5043 (0.1%)
1	E	0.53	0/3724	0.85	4/5043 (0.1%)
1	F	0.53	0/3724	0.85	4/5043 (0.1%)
1	G	0.53	0/3724	0.85	4/5043 (0.1%)
1	H	0.53	0/3724	0.85	4/5043 (0.1%)
1	I	0.53	0/3724	0.85	4/5043 (0.1%)
1	J	0.53	0/3724	0.85	4/5043 (0.1%)
1	K	0.53	0/3724	0.85	4/5043 (0.1%)
1	L	0.53	0/3724	0.85	4/5043 (0.1%)
All	All	0.53	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	E	401	PRO	CA-N-CD	-6.91	101.83	111.50
1	J	401	PRO	CA-N-CD	-6.90	101.84	111.50
1	I	401	PRO	CA-N-CD	-6.89	101.86	111.50
1	L	401	PRO	CA-N-CD	-6.89	101.86	111.50
1	F	401	PRO	CA-N-CD	-6.88	101.86	111.50
1	H	401	PRO	CA-N-CD	-6.88	101.87	111.50
1	A	401	PRO	CA-N-CD	-6.88	101.87	111.50
1	G	401	PRO	CA-N-CD	-6.88	101.88	111.50
1	D	401	PRO	CA-N-CD	-6.87	101.89	111.50
1	C	401	PRO	CA-N-CD	-6.87	101.89	111.50
1	B	401	PRO	CA-N-CD	-6.85	101.92	111.50
1	K	401	PRO	CA-N-CD	-6.84	101.92	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	F	248	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	J	248	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	K	248	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	D	248	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	A	248	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	E	248	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	I	248	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	H	248	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	G	248	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	L	248	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	L	367	PRO	O-C-N	5.37	131.29	122.70
1	C	248	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	D	367	PRO	O-C-N	5.36	131.28	122.70
1	K	367	PRO	O-C-N	5.34	131.25	122.70
1	A	367	PRO	O-C-N	5.33	131.23	122.70
1	I	367	PRO	O-C-N	5.33	131.23	122.70
1	C	367	PRO	O-C-N	5.32	131.22	122.70
1	G	367	PRO	O-C-N	5.32	131.21	122.70
1	B	367	PRO	O-C-N	5.32	131.21	122.70
1	H	367	PRO	O-C-N	5.31	131.20	122.70
1	E	367	PRO	O-C-N	5.30	131.18	122.70
1	J	367	PRO	O-C-N	5.30	131.18	122.70
1	F	367	PRO	O-C-N	5.30	131.18	122.70
1	L	124	VAL	CB-CA-C	-5.28	101.37	111.40
1	G	124	VAL	CB-CA-C	-5.28	101.38	111.40
1	C	124	VAL	CB-CA-C	-5.27	101.39	111.40
1	E	124	VAL	CB-CA-C	-5.27	101.39	111.40
1	B	124	VAL	CB-CA-C	-5.27	101.39	111.40
1	H	124	VAL	CB-CA-C	-5.26	101.40	111.40
1	A	124	VAL	CB-CA-C	-5.26	101.40	111.40
1	D	124	VAL	CB-CA-C	-5.25	101.42	111.40
1	I	124	VAL	CB-CA-C	-5.25	101.43	111.40
1	F	124	VAL	CB-CA-C	-5.24	101.44	111.40
1	K	124	VAL	CB-CA-C	-5.24	101.44	111.40
1	J	124	VAL	CB-CA-C	-5.23	101.45	111.40

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	3544	210	0
1	B	3637	0	3544	204	0
1	C	3637	0	3544	207	0
1	D	3637	0	3544	205	0
1	E	3637	0	3544	199	0
1	F	3637	0	3544	218	0
1	G	3637	0	3544	205	0
1	H	3637	0	3544	213	0
1	I	3637	0	3544	211	0
1	J	3637	0	3544	221	0
1	K	3637	0	3544	220	0
1	L	3637	0	3544	216	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	1	0
3	B	27	0	10	1	0
3	C	27	0	10	1	0
3	D	27	0	10	1	0
3	E	27	0	10	1	0
3	F	27	0	10	1	0
3	G	27	0	10	1	0
3	H	27	0	10	1	0
3	I	27	0	10	1	0
3	J	27	0	10	1	0
3	K	27	0	10	1	0
3	L	27	0	10	1	0
4	A	16	0	27	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	16	0	27	60	0
4	C	16	0	27	62	0
4	D	16	0	27	61	0
4	E	16	0	27	54	0
4	F	16	0	27	62	0
4	G	16	0	27	60	0
4	H	16	0	27	65	0
4	I	16	0	27	62	0
4	J	16	0	27	68	0
4	K	16	0	27	66	0
4	L	16	0	27	65	0
5	A	294	0	0	6	0
5	B	297	0	0	7	0
5	C	293	0	0	8	0
5	D	295	0	0	7	0
5	E	294	0	0	8	0
5	F	293	0	0	8	0
5	G	288	0	0	8	0
5	H	288	0	0	7	0
5	I	295	0	0	7	0
5	J	287	0	0	8	0
5	K	288	0	0	7	0
5	L	292	0	0	7	0
All	All	47688	0	42972	2421	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 28.

All (2421) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:84:THR:HG21	4:J:5491:MPD:C5	1.53	1.36
1:F:84:THR:HG21	4:F:5479:MPD:C5	1.57	1.32
1:J:84:THR:CG2	4:J:5491:MPD:H52	1.60	1.32
1:L:84:THR:HG21	4:L:5483:MPD:C5	1.60	1.31
1:I:61:ASN:O	1:J:337:ARG:HB2	1.29	1.29
1:H:80:PHE:CB	4:H:5487:MPD:H12	1.63	1.28
1:F:84:THR:CG2	4:F:5479:MPD:H52	1.63	1.28
1:B:84:THR:HG21	4:B:5471:MPD:C5	1.63	1.27
1:G:84:THR:HG21	4:G:5485:MPD:C5	1.65	1.27
1:I:84:THR:HG21	4:I:5489:MPD:C5	1.64	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:PHE:CB	4:L:5483:MPD:H12	1.65	1.25
1:G:61:ASN:O	1:H:337:ARG:HB2	1.35	1.25
1:K:84:THR:HG21	4:K:5493:MPD:C5	1.65	1.25
1:E:84:THR:HG21	4:E:5477:MPD:C5	1.66	1.24
1:J:80:PHE:CB	4:J:5491:MPD:H12	1.66	1.24
1:D:84:THR:HG21	4:D:5475:MPD:C5	1.66	1.23
1:E:84:THR:CG2	4:E:5477:MPD:H52	1.68	1.23
1:C:337:ARG:HB2	1:D:61:ASN:O	1.37	1.22
1:A:337:ARG:HB2	1:B:61:ASN:O	1.36	1.22
1:L:84:THR:CG2	4:L:5483:MPD:H52	1.66	1.22
1:F:80:PHE:CB	4:F:5479:MPD:H12	1.69	1.22
1:C:84:THR:HG21	4:C:5473:MPD:C5	1.68	1.22
1:B:84:THR:CG2	4:B:5471:MPD:H52	1.68	1.22
1:H:84:THR:HG21	4:H:5487:MPD:C5	1.69	1.21
1:G:84:THR:CG2	4:G:5485:MPD:H52	1.69	1.21
1:D:84:THR:CG2	4:D:5475:MPD:H52	1.70	1.20
1:A:84:THR:HG21	4:A:5481:MPD:C5	1.70	1.20
1:K:84:THR:CG2	4:K:5493:MPD:H52	1.70	1.20
1:I:84:THR:CG2	4:I:5489:MPD:H52	1.70	1.19
1:C:80:PHE:CB	4:C:5473:MPD:H12	1.71	1.19
1:K:80:PHE:CB	4:K:5493:MPD:H12	1.71	1.19
1:C:190:ASP:HA	4:D:5475:MPD:HM3	1.19	1.19
1:A:84:THR:CG2	4:A:5481:MPD:H52	1.72	1.19
4:K:5493:MPD:HM1	1:L:193:SER:HB2	1.25	1.18
1:J:61:ASN:O	1:K:337:ARG:HB2	1.41	1.18
1:A:60:ILE:H	1:A:60:ILE:HD13	1.08	1.18
1:C:84:THR:CG2	4:C:5473:MPD:H52	1.74	1.18
1:L:80:PHE:HB3	4:L:5483:MPD:C1	1.74	1.17
1:J:60:ILE:H	1:J:60:ILE:HD13	1.08	1.17
4:G:5485:MPD:HM1	1:H:193:SER:HB2	1.25	1.16
1:G:360:PHE:CD2	1:G:361:PRO:HD3	1.81	1.16
1:I:80:PHE:CB	4:I:5489:MPD:H12	1.73	1.16
1:B:360:PHE:CD2	1:B:361:PRO:HD3	1.81	1.16
1:E:360:PHE:CD2	1:E:361:PRO:HD3	1.81	1.16
1:K:360:PHE:CD2	1:K:361:PRO:HD3	1.81	1.16
1:J:360:PHE:CD2	1:J:361:PRO:HD3	1.81	1.16
1:E:193:SER:HB2	4:F:5479:MPD:HM1	1.25	1.15
1:H:84:THR:CG2	4:H:5487:MPD:H52	1.76	1.15
1:J:80:PHE:HB3	4:J:5491:MPD:C1	1.73	1.15
1:G:337:ARG:HB2	1:L:61:ASN:O	1.46	1.15
1:A:360:PHE:CD2	1:A:361:PRO:HD3	1.81	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:5481:MPD:HM1	1:F:193:SER:HB2	1.25	1.15
1:B:80:PHE:CB	4:B:5471:MPD:H12	1.77	1.15
1:F:360:PHE:CD2	1:F:361:PRO:HD3	1.81	1.14
1:I:360:PHE:CD2	1:I:361:PRO:HD3	1.81	1.14
1:F:80:PHE:HB3	4:F:5479:MPD:C1	1.77	1.14
1:C:193:SER:HB2	4:D:5475:MPD:HM1	1.25	1.14
1:B:193:SER:HB2	4:C:5473:MPD:HM1	1.25	1.14
1:D:360:PHE:CD2	1:D:361:PRO:HD3	1.81	1.14
1:H:360:PHE:CD2	1:H:361:PRO:HD3	1.81	1.14
4:I:5489:MPD:HM1	1:J:193:SER:HB2	1.25	1.14
1:L:360:PHE:CD2	1:L:361:PRO:HD3	1.81	1.14
1:C:360:PHE:CD2	1:C:361:PRO:HD3	1.81	1.13
4:G:5485:MPD:HM3	1:H:190:ASP:HA	1.19	1.13
1:A:193:SER:HB2	4:B:5471:MPD:HM1	1.25	1.13
1:B:60:ILE:H	1:B:60:ILE:HD13	1.08	1.13
1:H:399:LEU:N	1:H:401:PRO:HG2	1.64	1.13
4:H:5487:MPD:HM3	1:I:190:ASP:HA	1.19	1.13
1:J:399:LEU:N	1:J:401:PRO:HG2	1.64	1.13
1:D:193:SER:HB2	4:E:5477:MPD:HM1	1.25	1.13
1:C:399:LEU:N	1:C:401:PRO:HG2	1.64	1.12
1:E:60:ILE:HD13	1:E:60:ILE:H	1.08	1.12
4:I:5489:MPD:HM3	1:J:190:ASP:HA	1.19	1.12
1:L:399:LEU:N	1:L:401:PRO:HG2	1.64	1.12
1:E:190:ASP:HA	4:F:5479:MPD:HM3	1.19	1.12
1:G:193:SER:HB2	4:L:5483:MPD:HM1	1.25	1.12
1:A:190:ASP:HA	4:B:5471:MPD:HM3	1.19	1.12
1:H:60:ILE:H	1:H:60:ILE:HD13	1.08	1.12
1:K:60:ILE:HD13	1:K:60:ILE:H	1.08	1.12
1:F:60:ILE:HD13	1:F:60:ILE:H	1.08	1.12
4:K:5493:MPD:HM3	1:L:190:ASP:HA	1.19	1.12
1:H:80:PHE:HB3	4:H:5487:MPD:C1	1.77	1.12
4:J:5491:MPD:HM3	1:K:190:ASP:HA	1.19	1.12
1:E:399:LEU:N	1:E:401:PRO:HG2	1.64	1.12
1:G:399:LEU:N	1:G:401:PRO:HG2	1.64	1.12
1:F:399:LEU:H	1:F:401:PRO:HG2	0.95	1.11
1:B:399:LEU:N	1:B:401:PRO:HG2	1.64	1.11
1:F:399:LEU:N	1:F:401:PRO:HG2	1.64	1.11
1:G:60:ILE:H	1:G:60:ILE:HD13	1.08	1.11
1:I:399:LEU:N	1:I:401:PRO:HG2	1.64	1.11
4:A:5481:MPD:HM3	1:F:190:ASP:HA	1.19	1.11
1:A:399:LEU:N	1:A:401:PRO:HG2	1.64	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:PHE:CB	4:D:5475:MPD:H12	1.79	1.11
1:D:399:LEU:N	1:D:401:PRO:HG2	1.64	1.11
1:E:399:LEU:H	1:E:401:PRO:HG2	0.95	1.11
1:K:80:PHE:HB3	4:K:5493:MPD:C1	1.81	1.10
1:A:399:LEU:H	1:A:401:PRO:HG2	0.95	1.10
4:J:5491:MPD:HM1	1:K:193:SER:HB2	1.25	1.10
1:K:399:LEU:N	1:K:401:PRO:HG2	1.64	1.10
1:G:22:THR:N	4:G:5484:MPD:H52	1.67	1.09
1:G:190:ASP:HA	4:L:5483:MPD:HM3	1.19	1.09
1:C:400:PRO:HB3	1:C:405:LYS:HE3	1.34	1.09
1:C:60:ILE:HD13	1:C:60:ILE:H	1.08	1.09
1:B:190:ASP:HA	4:C:5473:MPD:HM3	1.19	1.09
1:L:60:ILE:HD13	1:L:60:ILE:H	1.08	1.09
1:A:400:PRO:HB3	1:A:405:LYS:HE3	1.35	1.09
1:E:22:THR:N	4:E:5480:MPD:H52	1.67	1.09
4:H:5487:MPD:HM1	1:I:193:SER:HB2	1.25	1.09
1:B:22:THR:N	4:B:5474:MPD:H52	1.67	1.09
1:F:22:THR:N	4:F:5482:MPD:H52	1.67	1.09
1:I:22:THR:N	4:I:5488:MPD:H52	1.67	1.09
1:D:190:ASP:HA	4:E:5477:MPD:HM3	1.19	1.09
1:E:400:PRO:HB3	1:E:405:LYS:HE3	1.35	1.09
1:K:400:PRO:HB3	1:K:405:LYS:HE3	1.35	1.09
1:D:22:THR:N	4:D:5478:MPD:H52	1.67	1.09
1:K:22:THR:N	4:K:5492:MPD:H52	1.67	1.09
1:G:400:PRO:HB3	1:G:405:LYS:HE3	1.35	1.08
1:I:60:ILE:H	1:I:60:ILE:HD13	1.08	1.08
1:J:22:THR:N	4:J:5490:MPD:H52	1.67	1.08
1:C:399:LEU:H	1:C:401:PRO:HG2	0.95	1.08
1:C:22:THR:N	4:C:5476:MPD:H52	1.67	1.08
1:H:22:THR:N	4:H:5486:MPD:H52	1.67	1.08
1:J:399:LEU:H	1:J:401:PRO:HG2	0.95	1.08
1:I:400:PRO:HB3	1:I:405:LYS:HE3	1.35	1.08
1:D:60:ILE:H	1:D:60:ILE:HD13	1.08	1.08
1:G:399:LEU:H	1:G:401:PRO:HG2	0.95	1.07
1:L:399:LEU:H	1:L:401:PRO:HG2	0.95	1.07
1:J:400:PRO:HB3	1:J:405:LYS:HE3	1.35	1.07
1:A:22:THR:N	4:A:5472:MPD:H52	1.67	1.07
1:A:61:ASN:O	1:F:337:ARG:HB2	1.54	1.07
1:H:400:PRO:HB3	1:H:405:LYS:HE3	1.35	1.07
1:I:399:LEU:H	1:I:401:PRO:HG2	0.95	1.07
1:L:22:THR:N	4:L:5494:MPD:H52	1.67	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:PHE:HB3	4:I:5489:MPD:C1	1.84	1.06
1:B:400:PRO:HB3	1:B:405:LYS:HE3	1.35	1.06
1:C:80:PHE:HB3	4:C:5473:MPD:C1	1.84	1.06
1:F:400:PRO:HB3	1:F:405:LYS:HE3	1.35	1.06
1:H:399:LEU:H	1:H:401:PRO:HG2	0.95	1.06
1:H:21:PHE:HB2	4:H:5486:MPD:H53	1.38	1.06
1:A:21:PHE:HB2	4:A:5472:MPD:H53	1.38	1.06
1:D:399:LEU:H	1:D:401:PRO:HG2	0.95	1.06
1:D:21:PHE:HB2	4:D:5478:MPD:H53	1.38	1.06
1:K:21:PHE:HB2	4:K:5492:MPD:H53	1.38	1.06
1:H:22:THR:OG1	4:H:5486:MPD:H13	1.56	1.06
1:B:399:LEU:H	1:B:401:PRO:HG2	0.95	1.06
1:K:399:LEU:H	1:K:401:PRO:HG2	0.95	1.05
1:G:80:PHE:CB	4:G:5485:MPD:H12	1.85	1.05
1:B:21:PHE:HB2	4:B:5474:MPD:H53	1.38	1.05
1:E:22:THR:OG1	4:E:5480:MPD:H13	1.56	1.05
1:L:21:PHE:HB2	4:L:5494:MPD:H53	1.38	1.05
1:L:400:PRO:HB3	1:L:405:LYS:HE3	1.35	1.05
1:A:22:THR:OG1	4:A:5472:MPD:H13	1.56	1.05
1:B:80:PHE:HB3	4:B:5471:MPD:C1	1.86	1.05
1:E:21:PHE:HB2	4:E:5480:MPD:H53	1.38	1.05
1:I:21:PHE:HB2	4:I:5488:MPD:H53	1.38	1.05
1:A:80:PHE:CB	4:A:5481:MPD:H12	1.86	1.05
1:C:22:THR:OG1	4:C:5476:MPD:H13	1.56	1.05
1:F:22:THR:OG1	4:F:5482:MPD:H13	1.56	1.04
1:D:80:PHE:HB3	4:D:5475:MPD:C1	1.88	1.04
1:F:21:PHE:HB2	4:F:5482:MPD:H53	1.38	1.04
1:K:22:THR:OG1	4:K:5492:MPD:H13	1.56	1.04
1:A:22:THR:H	4:A:5472:MPD:C5	1.71	1.04
1:D:22:THR:OG1	4:D:5478:MPD:H13	1.56	1.04
1:G:80:PHE:HB3	4:G:5485:MPD:H12	1.05	1.04
1:K:22:THR:H	4:K:5492:MPD:C5	1.71	1.03
1:B:22:THR:H	4:B:5474:MPD:C5	1.71	1.03
1:I:22:THR:H	4:I:5488:MPD:C5	1.71	1.03
1:J:22:THR:OG1	4:J:5490:MPD:H13	1.56	1.03
1:J:21:PHE:HB2	4:J:5490:MPD:H53	1.38	1.03
1:L:22:THR:OG1	4:L:5494:MPD:H13	1.56	1.03
1:G:22:THR:H	4:G:5484:MPD:C5	1.71	1.03
1:E:22:THR:H	4:E:5480:MPD:C5	1.71	1.03
1:C:21:PHE:HB2	4:C:5476:MPD:H53	1.38	1.03
1:D:400:PRO:HB3	1:D:405:LYS:HE3	1.35	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:THR:OG1	4:I:5488:MPD:H13	1.56	1.03
1:L:22:THR:H	4:L:5494:MPD:C5	1.71	1.03
1:C:22:THR:H	4:C:5476:MPD:C5	1.71	1.02
1:D:22:THR:H	4:D:5478:MPD:C5	1.71	1.02
1:B:22:THR:OG1	4:B:5474:MPD:H13	1.56	1.02
1:J:22:THR:H	4:J:5490:MPD:C5	1.71	1.02
1:G:21:PHE:HB2	4:G:5484:MPD:H53	1.38	1.02
1:B:337:ARG:HB2	1:C:61:ASN:O	1.60	1.02
1:H:22:THR:H	4:H:5486:MPD:C5	1.71	1.02
1:G:22:THR:OG1	4:G:5484:MPD:H13	1.56	1.01
1:E:80:PHE:CB	4:E:5477:MPD:H12	1.89	1.01
1:E:80:PHE:HB3	4:E:5477:MPD:H12	1.04	1.01
1:F:22:THR:H	4:F:5482:MPD:C5	1.71	1.01
1:I:22:THR:HG1	4:I:5488:MPD:H13	1.23	1.01
1:K:61:ASN:O	1:L:337:ARG:HB2	1.61	1.01
1:H:61:ASN:O	1:I:337:ARG:HB2	1.61	1.00
1:D:337:ARG:HB2	1:E:61:ASN:O	1.60	1.00
1:A:80:PHE:HB3	4:A:5481:MPD:C1	1.93	0.99
1:A:80:PHE:HB3	4:A:5481:MPD:H12	1.00	0.99
1:G:80:PHE:HB3	4:G:5485:MPD:C1	1.93	0.98
1:C:22:THR:H	4:C:5476:MPD:H52	0.82	0.98
1:L:22:THR:H	4:L:5494:MPD:H52	0.81	0.98
1:E:80:PHE:HB3	4:E:5477:MPD:C1	1.94	0.97
1:E:337:ARG:HB2	1:F:61:ASN:O	1.61	0.97
1:A:22:THR:H	4:A:5472:MPD:H52	0.82	0.97
1:B:80:PHE:HB3	4:B:5471:MPD:H12	0.97	0.97
1:D:22:THR:H	4:D:5478:MPD:H52	0.82	0.97
1:E:22:THR:H	4:E:5480:MPD:H52	0.82	0.97
1:K:22:THR:H	4:K:5492:MPD:H52	0.82	0.97
1:B:22:THR:H	4:B:5474:MPD:H52	0.81	0.96
1:F:22:THR:H	4:F:5482:MPD:H52	0.81	0.96
1:D:80:PHE:HB3	4:D:5475:MPD:H12	0.97	0.96
1:J:22:THR:H	4:J:5490:MPD:H52	0.81	0.96
1:C:80:PHE:HB3	4:C:5473:MPD:H12	0.96	0.95
1:H:22:THR:H	4:H:5486:MPD:H52	0.82	0.95
1:I:22:THR:H	4:I:5488:MPD:H52	0.81	0.95
1:I:80:PHE:HB3	4:I:5489:MPD:H12	0.97	0.95
1:C:235:ILE:HG21	1:C:367:PRO:HG3	1.49	0.95
1:G:22:THR:H	4:G:5484:MPD:H52	0.82	0.95
1:K:235:ILE:HG21	1:K:367:PRO:HG3	1.49	0.94
1:B:235:ILE:HG21	1:B:367:PRO:HG3	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:235:ILE:HG21	1:I:367:PRO:HG3	1.49	0.94
1:J:235:ILE:HG21	1:J:367:PRO:HG3	1.49	0.94
1:H:80:PHE:CD1	4:H:5487:MPD:C5	2.51	0.94
1:G:190:ASP:OD2	4:L:5483:MPD:H13	1.68	0.94
1:C:190:ASP:OD2	4:D:5475:MPD:H13	1.68	0.94
4:A:5481:MPD:H13	1:F:190:ASP:OD2	1.68	0.94
1:F:235:ILE:HG21	1:F:367:PRO:HG3	1.49	0.93
1:G:235:ILE:HG21	1:G:367:PRO:HG3	1.49	0.93
1:L:235:ILE:HG21	1:L:367:PRO:HG3	1.49	0.93
1:H:84:THR:HG21	4:H:5487:MPD:H52	0.93	0.93
1:J:60:ILE:CD1	1:J:60:ILE:H	1.82	0.93
1:E:190:ASP:OD2	4:F:5479:MPD:H13	1.68	0.92
4:I:5489:MPD:H13	1:J:190:ASP:OD2	1.68	0.92
4:K:5493:MPD:H13	1:L:190:ASP:OD2	1.68	0.92
1:A:235:ILE:HG21	1:A:367:PRO:HG3	1.49	0.92
1:G:60:ILE:CD1	1:G:60:ILE:H	1.82	0.92
1:B:190:ASP:OD2	4:C:5473:MPD:H13	1.68	0.92
4:H:5487:MPD:H13	1:I:190:ASP:OD2	1.68	0.92
1:H:80:PHE:CD1	4:H:5487:MPD:H53	2.05	0.92
1:A:190:ASP:OD2	4:B:5471:MPD:H13	1.68	0.92
1:D:235:ILE:HG21	1:D:367:PRO:HG3	1.49	0.92
1:H:235:ILE:HG21	1:H:367:PRO:HG3	1.49	0.92
1:E:235:ILE:HG21	1:E:367:PRO:HG3	1.49	0.91
1:C:60:ILE:CD1	1:C:60:ILE:H	1.82	0.91
4:G:5485:MPD:H13	1:H:190:ASP:OD2	1.68	0.91
1:H:60:ILE:H	1:H:60:ILE:CD1	1.82	0.91
4:J:5491:MPD:H13	1:K:190:ASP:OD2	1.68	0.91
1:K:60:ILE:H	1:K:60:ILE:CD1	1.82	0.91
1:D:190:ASP:OD2	4:E:5477:MPD:H13	1.68	0.91
1:B:395:ASN:HB3	1:B:400:PRO:HD2	1.54	0.90
1:G:60:ILE:N	1:G:60:ILE:HD13	1.87	0.90
1:I:60:ILE:HD13	1:I:60:ILE:N	1.87	0.90
1:K:60:ILE:HD13	1:K:60:ILE:N	1.87	0.90
1:D:60:ILE:N	1:D:60:ILE:HD13	1.87	0.90
1:E:60:ILE:HD13	1:E:60:ILE:N	1.87	0.90
1:H:60:ILE:N	1:H:60:ILE:HD13	1.87	0.90
1:I:395:ASN:HB3	1:I:400:PRO:HD2	1.54	0.90
1:J:395:ASN:HB3	1:J:400:PRO:HD2	1.54	0.90
4:K:5493:MPD:HM1	1:L:193:SER:CB	2.02	0.90
1:K:395:ASN:HB3	1:K:400:PRO:HD2	1.54	0.89
1:D:395:ASN:HB3	1:D:400:PRO:HD2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ILE:N	1:B:60:ILE:HD13	1.87	0.89
1:G:395:ASN:HB3	1:G:400:PRO:HD2	1.54	0.89
1:H:395:ASN:HB3	1:H:400:PRO:HD2	1.54	0.89
1:J:60:ILE:N	1:J:60:ILE:HD13	1.87	0.89
1:L:60:ILE:H	1:L:60:ILE:CD1	1.82	0.89
1:I:60:ILE:CD1	1:I:60:ILE:H	1.82	0.89
1:A:193:SER:CB	4:B:5471:MPD:HM1	2.02	0.89
1:B:60:ILE:H	1:B:60:ILE:CD1	1.82	0.89
1:C:395:ASN:HB3	1:C:400:PRO:HD2	1.54	0.89
4:A:5481:MPD:HM1	1:F:193:SER:CB	2.02	0.89
1:I:80:PHE:CD1	4:I:5489:MPD:C5	2.55	0.89
1:D:193:SER:CB	4:E:5477:MPD:HM1	2.02	0.89
1:L:60:ILE:HD13	1:L:60:ILE:N	1.87	0.89
1:C:80:PHE:CD1	4:C:5473:MPD:C5	2.56	0.89
1:C:60:ILE:HD13	1:C:60:ILE:N	1.87	0.89
4:H:5487:MPD:HM1	1:I:193:SER:CB	2.02	0.89
1:J:80:PHE:CD1	4:J:5491:MPD:C5	2.56	0.89
1:A:60:ILE:CD1	1:A:60:ILE:H	1.82	0.88
1:B:193:SER:CB	4:C:5473:MPD:HM1	2.02	0.88
1:F:60:ILE:HD13	1:F:60:ILE:N	1.87	0.88
1:F:82:ASP:HB2	4:F:5479:MPD:H31	1.55	0.88
1:F:395:ASN:HB3	1:F:400:PRO:HD2	1.54	0.88
1:F:60:ILE:H	1:F:60:ILE:CD1	1.82	0.88
1:A:398:ASP:O	1:A:399:LEU:C	2.11	0.88
1:A:60:ILE:HD13	1:A:60:ILE:N	1.87	0.88
1:L:80:PHE:CD1	4:L:5483:MPD:H53	2.08	0.88
1:E:193:SER:CB	4:F:5479:MPD:HM1	2.02	0.88
4:I:5489:MPD:HM1	1:J:193:SER:CB	2.02	0.88
1:L:80:PHE:CD1	4:L:5483:MPD:C5	2.57	0.88
1:I:398:ASP:O	1:I:399:LEU:C	2.11	0.88
4:J:5491:MPD:HM1	1:K:193:SER:CB	2.02	0.88
1:F:80:PHE:HB3	4:F:5479:MPD:H12	0.89	0.88
1:J:80:PHE:CD1	4:J:5491:MPD:H53	2.09	0.88
1:G:193:SER:CB	4:L:5483:MPD:HM1	2.02	0.88
1:A:395:ASN:HB3	1:A:400:PRO:HD2	1.54	0.88
1:E:398:ASP:O	1:E:399:LEU:C	2.11	0.87
1:L:398:ASP:O	1:L:399:LEU:C	2.11	0.87
1:L:395:ASN:HB3	1:L:400:PRO:HD2	1.54	0.87
1:C:193:SER:CB	4:D:5475:MPD:HM1	2.02	0.87
4:G:5485:MPD:HM1	1:H:193:SER:CB	2.02	0.87
1:J:21:PHE:HA	4:J:5490:MPD:H31	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ASP:O	1:D:399:LEU:C	2.11	0.87
1:F:21:PHE:HA	4:F:5482:MPD:H31	1.56	0.87
1:L:21:PHE:HA	4:L:5494:MPD:H31	1.56	0.87
1:H:398:ASP:O	1:H:399:LEU:C	2.11	0.87
1:H:80:PHE:HB3	4:H:5487:MPD:H12	0.87	0.87
1:J:84:THR:HG21	4:J:5491:MPD:C4	2.05	0.87
1:C:21:PHE:HA	4:C:5476:MPD:H31	1.57	0.87
1:B:398:ASP:O	1:B:399:LEU:C	2.11	0.87
1:E:395:ASN:HB3	1:E:400:PRO:HD2	1.54	0.87
1:J:82:ASP:HB2	4:J:5491:MPD:H31	1.55	0.86
1:K:21:PHE:CA	4:K:5492:MPD:HM2	2.06	0.86
1:K:80:PHE:HB3	4:K:5493:MPD:H12	0.90	0.86
1:B:21:PHE:HA	4:B:5474:MPD:H31	1.56	0.86
1:E:22:THR:OG1	4:E:5480:MPD:C1	2.24	0.86
1:G:21:PHE:CA	4:G:5484:MPD:HM2	2.05	0.86
1:G:22:THR:OG1	4:G:5484:MPD:C1	2.24	0.86
1:L:22:THR:N	4:L:5494:MPD:H11	1.91	0.86
1:A:21:PHE:HA	4:A:5472:MPD:H31	1.56	0.86
1:B:21:PHE:CA	4:B:5474:MPD:HM2	2.05	0.86
1:C:22:THR:OG1	4:C:5476:MPD:C1	2.24	0.86
1:E:22:THR:N	4:E:5480:MPD:H11	1.91	0.86
1:E:21:PHE:CA	4:E:5480:MPD:HM2	2.05	0.86
1:H:21:PHE:CA	4:H:5486:MPD:HM2	2.05	0.86
1:K:22:THR:N	4:K:5492:MPD:H11	1.91	0.86
1:K:22:THR:OG1	4:K:5492:MPD:C1	2.24	0.86
1:D:21:PHE:HA	4:D:5478:MPD:H31	1.56	0.86
1:H:22:THR:N	4:H:5486:MPD:H11	1.91	0.86
1:A:22:THR:N	4:A:5472:MPD:H11	1.91	0.86
1:C:22:THR:N	4:C:5476:MPD:H11	1.91	0.86
1:C:82:ASP:O	1:C:84:THR:HG22	1.76	0.86
1:E:82:ASP:O	1:E:84:THR:HG22	1.76	0.86
1:J:22:THR:OG1	4:J:5490:MPD:C1	2.24	0.86
1:C:21:PHE:CA	4:C:5476:MPD:HM2	2.06	0.85
1:F:22:THR:N	4:F:5482:MPD:H11	1.91	0.85
1:G:82:ASP:O	1:G:84:THR:HG22	1.76	0.85
1:H:22:THR:OG1	4:H:5486:MPD:C1	2.24	0.85
1:I:22:THR:N	4:I:5488:MPD:H11	1.91	0.85
1:I:21:PHE:CA	4:I:5488:MPD:HM2	2.05	0.85
1:B:22:THR:OG1	4:B:5474:MPD:C1	2.24	0.85
1:G:21:PHE:HA	4:G:5484:MPD:H31	1.57	0.85
1:H:82:ASP:O	1:H:84:THR:HG22	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:80:PHE:CD1	4:I:5489:MPD:H53	2.12	0.85
1:B:82:ASP:O	1:B:84:THR:HG22	1.76	0.85
1:F:82:ASP:O	1:F:84:THR:HG22	1.76	0.85
1:C:80:PHE:CD1	4:C:5473:MPD:H53	2.12	0.85
1:D:21:PHE:CA	4:D:5478:MPD:HM2	2.06	0.85
1:J:22:THR:N	4:J:5490:MPD:H11	1.91	0.85
1:J:82:ASP:O	1:J:84:THR:HG22	1.76	0.85
1:K:21:PHE:HA	4:K:5492:MPD:H31	1.57	0.85
1:L:21:PHE:CA	4:L:5494:MPD:HM2	2.05	0.85
1:A:22:THR:OG1	4:A:5472:MPD:C1	2.24	0.85
1:F:22:THR:OG1	4:F:5482:MPD:C1	2.24	0.85
1:K:82:ASP:O	1:K:84:THR:HG22	1.76	0.85
1:A:458:HIS:HD2	1:A:460:VAL:H	1.25	0.85
1:G:22:THR:N	4:G:5484:MPD:H11	1.91	0.85
1:I:21:PHE:HA	4:I:5488:MPD:H31	1.56	0.85
1:I:82:ASP:O	1:I:84:THR:HG22	1.76	0.85
1:D:458:HIS:HD2	1:D:460:VAL:H	1.25	0.85
1:E:21:PHE:HA	4:E:5480:MPD:H31	1.57	0.85
1:A:82:ASP:O	1:A:84:THR:HG22	1.76	0.85
1:D:22:THR:OG1	4:D:5478:MPD:C1	2.24	0.85
1:F:21:PHE:CA	4:F:5482:MPD:HM2	2.05	0.85
1:K:398:ASP:O	1:K:399:LEU:C	2.11	0.85
1:A:21:PHE:CA	4:A:5472:MPD:HM2	2.05	0.84
1:D:82:ASP:O	1:D:84:THR:HG22	1.76	0.84
1:I:22:THR:OG1	4:I:5488:MPD:C1	2.24	0.84
1:B:22:THR:N	4:B:5474:MPD:H11	1.91	0.84
1:D:22:THR:N	4:D:5478:MPD:H11	1.91	0.84
1:J:80:PHE:HB3	4:J:5491:MPD:H12	0.86	0.84
1:L:22:THR:OG1	4:L:5494:MPD:C1	2.24	0.84
1:J:21:PHE:CA	4:J:5490:MPD:HM2	2.05	0.84
1:H:21:PHE:HA	4:H:5486:MPD:H31	1.57	0.84
1:J:398:ASP:O	1:J:399:LEU:C	2.11	0.84
1:C:84:THR:HG21	4:C:5473:MPD:H52	0.87	0.84
1:F:80:PHE:CD1	4:F:5479:MPD:C5	2.61	0.84
1:H:458:HIS:HD2	1:H:460:VAL:H	1.25	0.84
1:I:458:HIS:HD2	1:I:460:VAL:H	1.25	0.84
1:L:458:HIS:HD2	1:L:460:VAL:H	1.25	0.84
1:F:398:ASP:O	1:F:399:LEU:C	2.11	0.83
1:I:22:THR:CB	4:I:5488:MPD:H11	2.09	0.83
1:B:22:THR:CB	4:B:5474:MPD:H11	2.09	0.83
1:K:458:HIS:HD2	1:K:460:VAL:H	1.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:THR:CB	4:C:5476:MPD:H11	2.09	0.83
1:E:22:THR:CB	4:E:5480:MPD:H11	2.09	0.83
1:L:22:THR:CB	4:L:5494:MPD:H11	2.09	0.83
1:L:82:ASP:O	1:L:84:THR:HG22	1.76	0.83
1:E:60:ILE:H	1:E:60:ILE:CD1	1.82	0.83
1:I:61:ASN:O	1:J:337:ARG:CB	2.21	0.83
1:A:22:THR:CB	4:A:5472:MPD:H11	2.09	0.83
1:B:458:HIS:HD2	1:B:460:VAL:H	1.25	0.82
1:D:22:THR:CB	4:D:5478:MPD:H11	2.09	0.82
1:F:22:THR:CB	4:F:5482:MPD:H11	2.09	0.82
1:G:22:THR:CB	4:G:5484:MPD:H11	2.09	0.82
1:H:22:THR:CB	4:H:5486:MPD:H11	2.09	0.82
1:F:80:PHE:CD1	4:F:5479:MPD:H53	2.14	0.82
1:K:22:THR:CB	4:K:5492:MPD:H11	2.09	0.82
1:K:80:PHE:CD1	4:K:5493:MPD:C5	2.63	0.82
1:C:458:HIS:HD2	1:C:460:VAL:H	1.25	0.82
1:E:82:ASP:HB2	4:E:5477:MPD:H31	1.61	0.82
1:J:22:THR:CB	4:J:5490:MPD:H11	2.09	0.82
1:F:105:ARG:HB2	4:F:5482:MPD:H4	1.62	0.82
1:E:458:HIS:HD2	1:E:460:VAL:H	1.25	0.81
1:K:22:THR:CB	4:K:5492:MPD:C1	2.58	0.81
1:K:80:PHE:CD1	4:K:5493:MPD:H53	2.15	0.81
1:D:21:PHE:HA	4:D:5478:MPD:HM2	1.62	0.81
1:J:22:THR:CB	4:J:5490:MPD:C1	2.58	0.81
1:L:84:THR:HG21	4:L:5483:MPD:C4	2.08	0.81
1:C:22:THR:CB	4:C:5476:MPD:C1	2.58	0.81
1:A:22:THR:CB	4:A:5472:MPD:C1	2.58	0.81
1:F:22:THR:CB	4:F:5482:MPD:C1	2.58	0.81
1:G:458:HIS:HD2	1:G:460:VAL:H	1.25	0.81
1:I:105:ARG:HB2	4:I:5488:MPD:H4	1.62	0.81
1:B:21:PHE:HA	4:B:5474:MPD:HM2	1.62	0.81
1:G:21:PHE:HA	4:G:5484:MPD:HM2	1.62	0.81
1:H:84:THR:HG21	4:H:5487:MPD:C4	2.11	0.81
1:I:21:PHE:HA	4:I:5488:MPD:HM2	1.62	0.81
1:B:80:PHE:CD1	4:B:5471:MPD:C5	2.63	0.81
1:J:458:HIS:HD2	1:J:460:VAL:H	1.25	0.81
1:D:105:ARG:HB2	4:D:5478:MPD:H4	1.62	0.81
1:F:458:HIS:HD2	1:F:460:VAL:H	1.25	0.81
1:G:22:THR:CB	4:G:5484:MPD:C1	2.58	0.81
1:J:21:PHE:HA	4:J:5490:MPD:HM2	1.62	0.81
1:G:105:ARG:HB2	4:G:5484:MPD:H4	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:398:ASP:O	1:J:399:LEU:O	1.99	0.81
1:L:22:THR:CB	4:L:5494:MPD:C1	2.58	0.81
1:B:105:ARG:HB2	4:B:5474:MPD:H4	1.62	0.81
1:C:398:ASP:O	1:C:399:LEU:C	2.11	0.81
1:C:21:PHE:HA	4:C:5476:MPD:HM2	1.62	0.81
1:D:22:THR:CB	4:D:5478:MPD:C1	2.58	0.81
1:F:21:PHE:HA	4:F:5482:MPD:HM2	1.62	0.81
1:I:84:THR:HG21	4:I:5489:MPD:H52	0.83	0.81
1:E:398:ASP:O	1:E:399:LEU:O	1.99	0.80
1:K:84:THR:HG21	4:K:5493:MPD:H52	0.85	0.80
1:L:84:THR:HG21	4:L:5483:MPD:H52	0.82	0.80
1:G:82:ASP:HB2	4:G:5485:MPD:H31	1.62	0.80
1:K:105:ARG:HB2	4:K:5492:MPD:H4	1.62	0.80
1:L:82:ASP:HB2	4:L:5483:MPD:H31	1.62	0.80
1:A:84:THR:HG21	4:A:5481:MPD:H52	0.84	0.80
1:B:22:THR:CB	4:B:5474:MPD:C1	2.58	0.80
1:E:22:THR:CB	4:E:5480:MPD:C1	2.58	0.80
1:G:398:ASP:O	1:G:399:LEU:O	1.99	0.80
1:L:105:ARG:HB2	4:L:5494:MPD:H4	1.62	0.80
1:L:398:ASP:O	1:L:399:LEU:O	1.99	0.80
1:L:21:PHE:HA	4:L:5494:MPD:HM2	1.62	0.80
1:C:398:ASP:O	1:C:399:LEU:O	1.99	0.80
1:B:398:ASP:O	1:B:399:LEU:O	1.99	0.80
1:H:398:ASP:O	1:H:399:LEU:O	1.99	0.80
1:I:22:THR:CB	4:I:5488:MPD:C1	2.58	0.80
1:A:398:ASP:O	1:A:399:LEU:O	1.99	0.80
1:I:82:ASP:HB2	4:I:5489:MPD:H31	1.64	0.80
1:B:82:ASP:HB2	4:B:5471:MPD:H31	1.61	0.80
1:E:21:PHE:HA	4:E:5480:MPD:HM2	1.62	0.80
1:H:105:ARG:HB2	4:H:5486:MPD:H4	1.62	0.80
1:H:21:PHE:HA	4:H:5486:MPD:HM2	1.62	0.80
1:H:22:THR:CB	4:H:5486:MPD:C1	2.58	0.80
1:G:398:ASP:O	1:G:399:LEU:C	2.11	0.80
1:K:21:PHE:HA	4:K:5492:MPD:HM2	1.62	0.80
1:K:398:ASP:O	1:K:399:LEU:O	1.99	0.79
1:A:105:ARG:HB2	4:A:5472:MPD:H4	1.62	0.79
1:L:80:PHE:HB3	4:L:5483:MPD:H12	0.84	0.79
1:A:21:PHE:HA	4:A:5472:MPD:HM2	1.62	0.79
1:C:105:ARG:HB2	4:C:5476:MPD:H4	1.62	0.79
1:F:84:THR:HG21	4:F:5479:MPD:C4	2.11	0.79
1:J:105:ARG:HB2	4:J:5490:MPD:H4	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ILE:CD1	1:D:60:ILE:H	1.82	0.79
1:C:337:ARG:CB	1:D:61:ASN:O	2.27	0.79
1:F:398:ASP:O	1:F:399:LEU:O	1.99	0.78
1:E:105:ARG:HB2	4:E:5480:MPD:H4	1.62	0.78
1:I:398:ASP:O	1:I:399:LEU:O	1.99	0.78
1:A:337:ARG:CB	1:B:61:ASN:O	2.26	0.78
1:C:21:PHE:C	4:C:5476:MPD:HM2	2.04	0.78
1:D:84:THR:HG21	4:D:5475:MPD:H52	0.83	0.78
1:L:21:PHE:C	4:L:5494:MPD:HM2	2.04	0.78
1:A:193:SER:HB2	4:B:5471:MPD:CM	2.11	0.78
1:D:193:SER:HB2	4:E:5477:MPD:CM	2.11	0.78
1:D:398:ASP:O	1:D:399:LEU:O	1.99	0.78
1:B:21:PHE:C	4:B:5474:MPD:HM2	2.04	0.78
4:H:5487:MPD:CM	1:I:193:SER:HB2	2.11	0.78
1:J:21:PHE:C	4:J:5490:MPD:HM2	2.04	0.78
1:K:82:ASP:HB2	4:K:5493:MPD:H31	1.66	0.78
1:B:80:PHE:CD1	4:B:5471:MPD:H53	2.18	0.78
1:D:21:PHE:C	4:D:5478:MPD:HM2	2.04	0.78
1:F:21:PHE:C	4:F:5482:MPD:HM2	2.04	0.78
1:H:21:PHE:C	4:H:5486:MPD:HM2	2.04	0.78
1:G:193:SER:HB2	4:L:5483:MPD:CM	2.11	0.77
1:I:21:PHE:C	4:I:5488:MPD:HM2	2.04	0.77
1:C:82:ASP:HB2	4:C:5473:MPD:H31	1.66	0.77
1:K:21:PHE:C	4:K:5492:MPD:HM2	2.04	0.77
1:B:58:LYS:HD2	1:B:62:GLU:HB2	1.67	0.77
1:G:21:PHE:C	4:G:5484:MPD:HM2	2.04	0.77
1:A:21:PHE:C	4:A:5472:MPD:HM2	2.04	0.77
1:E:21:PHE:C	4:E:5480:MPD:HM2	2.04	0.77
1:D:58:LYS:HD2	1:D:62:GLU:HB2	1.67	0.77
1:F:58:LYS:HD2	1:F:62:GLU:HB2	1.67	0.77
1:G:399:LEU:HA	1:G:400:PRO:C	2.06	0.77
1:G:61:ASN:O	1:H:337:ARG:CB	2.28	0.77
1:I:84:THR:HG21	4:I:5489:MPD:C4	2.15	0.77
1:J:58:LYS:HD2	1:J:62:GLU:HB2	1.67	0.77
1:L:58:LYS:HD2	1:L:62:GLU:HB2	1.67	0.77
1:I:58:LYS:HD2	1:I:62:GLU:HB2	1.67	0.76
4:G:5485:MPD:CM	1:H:193:SER:HB2	2.11	0.76
1:A:399:LEU:HA	1:A:400:PRO:C	2.06	0.76
1:C:193:SER:HB2	4:D:5475:MPD:CM	2.11	0.76
1:C:58:LYS:HD2	1:C:62:GLU:HB2	1.67	0.76
1:I:399:LEU:HA	1:I:400:PRO:C	2.06	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:58:LYS:HD2	1:H:62:GLU:HB2	1.67	0.76
1:D:399:LEU:HA	1:D:400:PRO:C	2.06	0.76
1:F:399:LEU:HA	1:F:400:PRO:C	2.06	0.76
1:G:58:LYS:HD2	1:G:62:GLU:HB2	1.67	0.76
1:I:395:ASN:HB3	1:I:400:PRO:CD	2.16	0.76
1:D:82:ASP:HB2	4:D:5475:MPD:H31	1.68	0.76
1:E:395:ASN:HB3	1:E:400:PRO:CD	2.16	0.76
1:G:395:ASN:HB3	1:G:400:PRO:CD	2.16	0.76
1:D:80:PHE:CD1	4:D:5475:MPD:C5	2.68	0.76
1:D:80:PHE:CD1	4:D:5475:MPD:H53	2.21	0.76
1:G:80:PHE:CD1	4:G:5485:MPD:C5	2.68	0.76
1:H:399:LEU:HA	1:H:400:PRO:C	2.06	0.76
1:K:395:ASN:HB3	1:K:400:PRO:CD	2.16	0.76
4:I:5489:MPD:CM	1:J:193:SER:HB2	2.11	0.76
1:C:399:LEU:HA	1:C:400:PRO:C	2.06	0.76
1:K:399:LEU:HA	1:K:400:PRO:C	2.06	0.76
1:L:395:ASN:HB3	1:L:400:PRO:CD	2.16	0.76
1:A:395:ASN:HB3	1:A:400:PRO:CD	2.16	0.76
1:B:395:ASN:HB3	1:B:400:PRO:CD	2.16	0.75
1:D:395:ASN:HB3	1:D:400:PRO:CD	2.16	0.75
1:J:399:LEU:HA	1:J:400:PRO:C	2.06	0.75
1:L:399:LEU:HA	1:L:400:PRO:C	2.06	0.75
1:A:58:LYS:HD2	1:A:62:GLU:HB2	1.67	0.75
1:C:84:THR:HG21	4:C:5473:MPD:C4	2.16	0.75
1:K:58:LYS:HD2	1:K:62:GLU:HB2	1.67	0.75
4:K:5493:MPD:CM	1:L:193:SER:HB2	2.11	0.75
1:C:395:ASN:HB3	1:C:400:PRO:CD	2.16	0.75
1:J:395:ASN:HB3	1:J:400:PRO:CD	2.16	0.75
1:A:27:LYS:HA	5:A:5743:HOH:O	1.87	0.75
1:K:84:THR:HG21	4:K:5493:MPD:C4	2.16	0.75
1:G:190:ASP:CA	4:L:5483:MPD:HM3	2.11	0.75
1:B:399:LEU:HA	1:B:400:PRO:C	2.06	0.75
1:E:193:SER:HB2	4:F:5479:MPD:CM	2.11	0.75
1:G:27:LYS:HA	5:G:5754:HOH:O	1.87	0.75
1:I:27:LYS:HA	5:I:5769:HOH:O	1.87	0.75
1:J:248:ARG:HH21	1:J:248:ARG:CG	2.00	0.75
1:E:399:LEU:HA	1:E:400:PRO:C	2.06	0.75
1:I:248:ARG:CG	1:I:248:ARG:HH21	2.00	0.75
1:B:248:ARG:CG	1:B:248:ARG:HH21	2.00	0.74
1:E:27:LYS:HA	5:E:1454:HOH:O	1.87	0.74
1:E:58:LYS:HD2	1:E:62:GLU:HB2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:5489:MPD:HM3	1:J:190:ASP:CA	2.11	0.74
1:C:248:ARG:CG	1:C:248:ARG:HH21	2.00	0.74
1:D:27:LYS:HA	5:D:1162:HOH:O	1.87	0.74
1:F:248:ARG:CG	1:F:248:ARG:HH21	2.00	0.74
1:J:27:LYS:HA	5:J:2914:HOH:O	1.87	0.74
1:B:193:SER:HB2	4:C:5473:MPD:CM	2.11	0.74
1:H:395:ASN:HB3	1:H:400:PRO:CD	2.16	0.74
1:B:192:ARG:HH21	1:B:219:ASN:ND2	1.86	0.74
1:B:84:THR:HG21	4:B:5471:MPD:H52	0.80	0.74
1:L:248:ARG:HH21	1:L:248:ARG:CG	2.00	0.74
1:B:27:LYS:HA	5:B:5744:HOH:O	1.87	0.74
1:F:395:ASN:HB3	1:F:400:PRO:CD	2.16	0.74
1:G:192:ARG:HH21	1:G:219:ASN:ND2	1.86	0.74
1:B:84:THR:HG21	4:B:5471:MPD:C4	2.18	0.74
1:D:248:ARG:HH21	1:D:248:ARG:CG	2.00	0.74
4:A:5481:MPD:CM	1:F:193:SER:HB2	2.11	0.74
1:H:27:LYS:HA	5:H:5762:HOH:O	1.87	0.74
1:K:248:ARG:HH21	1:K:248:ARG:CG	2.00	0.74
1:K:27:LYS:HA	5:K:3206:HOH:O	1.87	0.74
1:F:27:LYS:HA	5:F:5756:HOH:O	1.87	0.74
1:L:27:LYS:HA	5:L:3498:HOH:O	1.87	0.74
1:E:248:ARG:CG	1:E:248:ARG:HH21	2.00	0.74
1:H:248:ARG:HH21	1:H:248:ARG:CG	2.00	0.74
1:I:192:ARG:HH21	1:I:219:ASN:ND2	1.86	0.74
1:D:192:ARG:HH21	1:D:219:ASN:ND2	1.86	0.73
1:J:192:ARG:HH21	1:J:219:ASN:ND2	1.86	0.73
1:K:192:ARG:HH21	1:K:219:ASN:ND2	1.86	0.73
1:A:248:ARG:CG	1:A:248:ARG:HH21	2.00	0.73
1:E:192:ARG:HH21	1:E:219:ASN:ND2	1.86	0.73
4:K:5493:MPD:HM3	1:L:190:ASP:CA	2.11	0.73
1:G:248:ARG:CG	1:G:248:ARG:HH21	2.00	0.73
1:C:192:ARG:HH21	1:C:219:ASN:ND2	1.86	0.73
1:C:27:LYS:HA	5:C:5744:HOH:O	1.87	0.73
4:A:5481:MPD:HM3	1:F:190:ASP:CA	2.11	0.73
1:C:88:ARG:HE	4:C:5476:MPD:CM	2.02	0.73
1:E:82:ASP:HB2	4:E:5477:MPD:C3	2.18	0.73
1:F:88:ARG:HE	4:F:5482:MPD:CM	2.02	0.73
1:J:88:ARG:HE	4:J:5490:MPD:CM	2.02	0.73
1:L:88:ARG:HE	4:L:5494:MPD:CM	2.02	0.73
1:A:192:ARG:HH21	1:A:219:ASN:ND2	1.86	0.72
1:D:88:ARG:HE	4:D:5478:MPD:CM	2.02	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:ARG:HH21	1:F:219:ASN:ND2	1.86	0.72
1:H:88:ARG:HE	4:H:5486:MPD:CM	2.02	0.72
1:C:190:ASP:CA	4:D:5475:MPD:HM3	2.11	0.72
1:H:192:ARG:HH21	1:H:219:ASN:ND2	1.86	0.72
1:L:192:ARG:HH21	1:L:219:ASN:ND2	1.86	0.72
1:A:82:ASP:HB2	4:A:5481:MPD:H31	1.70	0.72
1:H:82:ASP:HB2	4:H:5487:MPD:H31	1.71	0.72
4:J:5491:MPD:CM	1:K:193:SER:HB2	2.11	0.72
1:I:88:ARG:HE	4:I:5488:MPD:CM	2.02	0.72
1:A:88:ARG:HE	4:A:5472:MPD:CM	2.02	0.72
1:B:88:ARG:HE	4:B:5474:MPD:CM	2.02	0.72
4:I:5489:MPD:O4	4:I:5489:MPD:HM2	1.90	0.72
1:E:88:ARG:HE	4:E:5480:MPD:CM	2.02	0.72
1:A:96:THR:OG1	1:A:98:GLN:HB2	1.90	0.72
1:E:96:THR:OG1	1:E:98:GLN:HB2	1.90	0.72
1:G:88:ARG:HE	4:G:5484:MPD:CM	2.02	0.72
4:C:5473:MPD:HM2	4:C:5473:MPD:O4	1.90	0.71
4:D:5475:MPD:HM2	4:D:5475:MPD:O4	1.90	0.71
1:J:96:THR:OG1	1:J:98:GLN:HB2	1.90	0.71
1:K:88:ARG:HE	4:K:5492:MPD:CM	2.02	0.71
4:L:5483:MPD:O4	4:L:5483:MPD:HM2	1.90	0.71
1:C:96:THR:OG1	1:C:98:GLN:HB2	1.90	0.71
1:G:96:THR:OG1	1:G:98:GLN:HB2	1.90	0.71
1:L:96:THR:OG1	1:L:98:GLN:HB2	1.90	0.71
1:F:96:THR:OG1	1:F:98:GLN:HB2	1.90	0.71
1:G:80:PHE:CD1	4:G:5485:MPD:H53	2.24	0.71
1:K:96:THR:OG1	1:K:98:GLN:HB2	1.90	0.71
1:D:96:THR:OG1	1:D:98:GLN:HB2	1.90	0.71
1:F:22:THR:HB	4:F:5482:MPD:C1	2.21	0.71
1:F:84:THR:HG21	4:F:5479:MPD:H52	0.76	0.71
1:H:22:THR:HB	4:H:5486:MPD:C1	2.21	0.71
4:H:5487:MPD:HM2	4:H:5487:MPD:O4	1.90	0.71
4:J:5491:MPD:HM2	4:J:5491:MPD:O4	1.90	0.71
4:E:5477:MPD:O4	4:E:5477:MPD:HM2	1.90	0.71
4:G:5485:MPD:HM2	4:G:5485:MPD:O4	1.90	0.71
4:B:5471:MPD:O4	4:B:5471:MPD:HM2	1.90	0.71
1:I:96:THR:OG1	1:I:98:GLN:HB2	1.90	0.71
1:B:22:THR:HB	4:B:5474:MPD:C1	2.21	0.70
1:E:190:ASP:CA	4:F:5479:MPD:HM3	2.11	0.70
1:J:84:THR:HG21	4:J:5491:MPD:H52	0.75	0.70
1:K:384:ASN:HD22	1:K:384:ASN:N	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:22:THR:HB	4:L:5494:MPD:C1	2.21	0.70
1:A:22:THR:HB	4:A:5472:MPD:C1	2.21	0.70
4:A:5481:MPD:HM2	4:A:5481:MPD:O4	1.90	0.70
4:F:5479:MPD:O4	4:F:5479:MPD:HM2	1.90	0.70
1:D:22:THR:HB	4:D:5478:MPD:C1	2.21	0.70
1:L:399:LEU:H	1:L:401:PRO:CG	1.90	0.70
1:F:82:ASP:HB2	4:F:5479:MPD:C3	2.21	0.70
4:K:5493:MPD:HM2	4:K:5493:MPD:O4	1.90	0.70
1:H:384:ASN:HD22	1:H:384:ASN:N	1.89	0.70
1:I:22:THR:HB	4:I:5488:MPD:C1	2.21	0.70
1:A:384:ASN:HD22	1:A:384:ASN:N	1.89	0.70
1:E:384:ASN:HD22	1:E:384:ASN:N	1.89	0.70
1:E:22:THR:HB	4:E:5480:MPD:C1	2.21	0.70
1:J:22:THR:HB	4:J:5490:MPD:C1	2.21	0.70
1:H:96:THR:OG1	1:H:98:GLN:HB2	1.90	0.70
1:L:384:ASN:N	1:L:384:ASN:HD22	1.89	0.70
1:C:384:ASN:N	1:C:384:ASN:HD22	1.89	0.70
1:E:21:PHE:HA	4:E:5480:MPD:CM	2.22	0.70
1:K:22:THR:HB	4:K:5492:MPD:C1	2.21	0.70
4:G:5485:MPD:HM3	1:H:190:ASP:CA	2.11	0.69
1:G:22:THR:HB	4:G:5484:MPD:C1	2.21	0.69
1:G:82:ASP:HB2	4:G:5485:MPD:C3	2.22	0.69
1:H:21:PHE:HA	4:H:5486:MPD:CM	2.22	0.69
1:B:96:THR:OG1	1:B:98:GLN:HB2	1.90	0.69
1:G:21:PHE:HA	4:G:5484:MPD:CM	2.22	0.69
1:K:21:PHE:HA	4:K:5492:MPD:CM	2.22	0.69
1:I:384:ASN:HD22	1:I:384:ASN:N	1.89	0.69
1:G:384:ASN:N	1:G:384:ASN:HD22	1.89	0.69
1:G:84:THR:HG21	4:G:5485:MPD:H52	0.78	0.69
1:G:337:ARG:CB	1:L:61:ASN:O	2.34	0.69
1:A:190:ASP:CA	4:B:5471:MPD:HM3	2.11	0.69
1:C:22:THR:HB	4:C:5476:MPD:C1	2.21	0.69
1:J:384:ASN:N	1:J:384:ASN:HD22	1.89	0.69
1:L:21:PHE:HA	4:L:5494:MPD:CM	2.22	0.69
1:L:22:THR:HB	4:L:5494:MPD:H11	1.75	0.69
1:C:21:PHE:HA	4:C:5476:MPD:CM	2.22	0.69
1:C:22:THR:HB	4:C:5476:MPD:H11	1.75	0.69
1:E:399:LEU:H	1:E:401:PRO:CG	1.90	0.69
1:A:21:PHE:HA	4:A:5472:MPD:CM	2.22	0.69
1:I:22:THR:HB	4:I:5488:MPD:H11	1.75	0.69
1:D:22:THR:HB	4:D:5478:MPD:H11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:82:ASP:HB2	4:J:5491:MPD:C3	2.22	0.69
1:I:21:PHE:HA	4:I:5488:MPD:CM	2.22	0.68
1:E:22:THR:HB	4:E:5480:MPD:H11	1.75	0.68
1:F:21:PHE:HA	4:F:5482:MPD:CM	2.22	0.68
1:H:22:THR:HB	4:H:5486:MPD:H11	1.75	0.68
1:D:399:LEU:HA	1:D:400:PRO:O	1.94	0.68
1:B:21:PHE:HA	4:B:5474:MPD:CM	2.22	0.68
1:D:21:PHE:HA	4:D:5478:MPD:CM	2.22	0.68
1:H:399:LEU:HA	1:H:400:PRO:O	1.94	0.68
4:H:5487:MPD:HM3	1:I:190:ASP:CA	2.11	0.68
1:A:399:LEU:HA	1:A:400:PRO:O	1.94	0.68
1:B:190:ASP:CA	4:C:5473:MPD:HM3	2.10	0.68
1:D:84:THR:HG21	4:D:5475:MPD:C4	2.22	0.68
1:E:399:LEU:HA	1:E:400:PRO:O	1.94	0.68
1:K:399:LEU:HA	1:K:400:PRO:O	1.94	0.68
1:B:399:LEU:HA	1:B:400:PRO:O	1.94	0.68
1:E:461:GLU:OE1	1:K:320:LYS:NZ	2.27	0.68
4:J:5491:MPD:HM3	1:K:190:ASP:CA	2.11	0.68
1:B:384:ASN:N	1:B:384:ASN:HD22	1.89	0.68
1:D:384:ASN:HD22	1:D:384:ASN:N	1.89	0.68
1:F:384:ASN:N	1:F:384:ASN:HD22	1.89	0.68
1:I:88:ARG:HE	4:I:5488:MPD:HM1	1.60	0.68
1:L:88:ARG:HE	4:L:5494:MPD:HM1	1.59	0.68
1:A:22:THR:HB	4:A:5472:MPD:H11	1.75	0.67
4:C:5473:MPD:H11	4:C:5473:MPD:H53	1.77	0.67
1:G:84:THR:HG21	4:G:5485:MPD:C4	2.24	0.67
1:I:399:LEU:HA	1:I:400:PRO:O	1.94	0.67
1:C:399:LEU:HA	1:C:400:PRO:O	1.94	0.67
4:L:5483:MPD:H53	4:L:5483:MPD:H11	1.76	0.67
1:A:399:LEU:N	1:A:401:PRO:CG	2.52	0.67
1:A:88:ARG:HE	4:A:5472:MPD:HM1	1.60	0.67
1:E:458:HIS:CD2	1:E:460:VAL:H	2.11	0.67
1:J:399:LEU:HA	1:J:400:PRO:O	1.94	0.67
1:J:21:PHE:HA	4:J:5490:MPD:CM	2.22	0.67
1:L:399:LEU:HA	1:L:400:PRO:O	1.94	0.67
1:C:399:LEU:N	1:C:401:PRO:CG	2.52	0.67
1:G:295:LEU:O	1:G:388:PRO:CG	2.43	0.67
1:G:399:LEU:HA	1:G:400:PRO:O	1.94	0.67
4:I:5489:MPD:H53	4:I:5489:MPD:H11	1.76	0.67
1:K:22:THR:HB	4:K:5492:MPD:H11	1.75	0.67
1:D:295:LEU:O	1:D:388:PRO:CG	2.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:399:LEU:N	1:L:401:PRO:CG	2.52	0.67
4:A:5481:MPD:H11	4:A:5481:MPD:H53	1.77	0.67
4:D:5478:MPD:H11	4:D:5478:MPD:H52	1.77	0.67
1:K:295:LEU:O	1:K:388:PRO:CG	2.43	0.67
4:K:5492:MPD:H52	4:K:5492:MPD:H11	1.77	0.67
1:C:295:LEU:O	1:C:388:PRO:CG	2.43	0.67
4:E:5477:MPD:H53	4:E:5477:MPD:H11	1.77	0.67
1:F:88:ARG:HE	4:F:5482:MPD:HM1	1.60	0.67
4:H:5486:MPD:H11	4:H:5486:MPD:H52	1.77	0.67
1:H:295:LEU:O	1:H:388:PRO:CG	2.43	0.67
1:H:399:LEU:N	1:H:401:PRO:CG	2.52	0.67
1:H:88:ARG:HE	4:H:5486:MPD:HM1	1.60	0.67
1:I:458:HIS:CD2	1:I:460:VAL:H	2.12	0.67
1:J:88:ARG:HE	4:J:5490:MPD:HM1	1.60	0.67
1:L:80:PHE:CB	4:L:5483:MPD:C1	2.53	0.67
1:B:295:LEU:O	1:B:388:PRO:CG	2.43	0.67
1:B:399:LEU:N	1:B:401:PRO:CG	2.52	0.67
4:B:5474:MPD:H11	4:B:5474:MPD:H52	1.77	0.67
1:F:295:LEU:O	1:F:388:PRO:CG	2.43	0.67
1:A:295:LEU:O	1:A:388:PRO:CG	2.43	0.67
1:D:461:GLU:OE1	1:J:320:LYS:NZ	2.26	0.67
1:D:190:ASP:CA	4:E:5477:MPD:HM3	2.11	0.67
4:J:5491:MPD:H53	4:J:5491:MPD:H11	1.76	0.67
1:J:30:HIS:H	1:K:180:PHE:HB3	1.58	0.67
1:E:295:LEU:O	1:E:388:PRO:CG	2.43	0.66
1:G:458:HIS:CD2	1:G:460:VAL:H	2.11	0.66
1:G:88:ARG:HE	4:G:5484:MPD:HM1	1.59	0.66
1:H:80:PHE:CB	4:H:5487:MPD:C1	2.53	0.66
1:J:80:PHE:HD1	4:J:5491:MPD:C5	2.09	0.66
1:D:88:ARG:HE	4:D:5478:MPD:HM1	1.59	0.66
1:I:295:LEU:O	1:I:388:PRO:CG	2.43	0.66
1:L:295:LEU:O	1:L:388:PRO:CG	2.43	0.66
4:A:5472:MPD:H11	4:A:5472:MPD:H52	1.77	0.66
1:A:80:PHE:CD1	4:A:5481:MPD:H53	2.30	0.66
1:C:105:ARG:HB2	4:C:5476:MPD:C4	2.26	0.66
1:D:399:LEU:H	1:D:401:PRO:CG	1.90	0.66
1:A:53:SER:HB2	1:F:179:TYR:CD2	2.30	0.66
4:F:5482:MPD:H52	4:F:5482:MPD:H11	1.77	0.66
1:F:399:LEU:HA	1:F:400:PRO:O	1.94	0.66
1:J:295:LEU:O	1:J:388:PRO:CG	2.43	0.66
4:K:5493:MPD:H11	4:K:5493:MPD:H53	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:5471:MPD:H53	4:B:5471:MPD:H11	1.76	0.66
1:B:82:ASP:HB2	4:B:5471:MPD:C3	2.24	0.66
1:C:88:ARG:HE	4:C:5476:MPD:HM1	1.59	0.66
1:J:80:PHE:CB	4:J:5491:MPD:C1	2.53	0.66
1:A:29:GLN:OE1	1:F:181:PRO:HD3	1.96	0.66
1:G:22:THR:HB	4:G:5484:MPD:H11	1.75	0.66
4:G:5485:MPD:H11	4:G:5485:MPD:H53	1.77	0.66
4:H:5487:MPD:H53	4:H:5487:MPD:H11	1.77	0.66
1:I:399:LEU:N	1:I:401:PRO:CG	2.52	0.66
1:A:82:ASP:HB2	4:A:5481:MPD:C3	2.25	0.66
1:G:105:ARG:HB2	4:G:5484:MPD:C4	2.26	0.66
1:J:22:THR:HB	4:J:5490:MPD:H11	1.75	0.66
4:J:5490:MPD:H52	4:J:5490:MPD:H11	1.77	0.66
1:A:365:ALA:O	1:A:367:PRO:HD3	1.96	0.66
4:F:5479:MPD:H11	4:F:5479:MPD:H53	1.77	0.66
1:J:105:ARG:HB2	4:J:5490:MPD:C4	2.26	0.66
1:L:365:ALA:O	1:L:367:PRO:HD3	1.96	0.66
1:B:105:ARG:HB2	4:B:5474:MPD:C4	2.26	0.66
4:G:5484:MPD:H52	4:G:5484:MPD:H11	1.77	0.66
1:J:458:HIS:CD2	1:J:460:VAL:H	2.11	0.66
1:D:105:ARG:HB2	4:D:5478:MPD:C4	2.26	0.65
1:E:88:ARG:HE	4:E:5480:MPD:HM1	1.60	0.65
1:G:30:HIS:H	1:H:180:PHE:HB3	1.61	0.65
1:H:105:ARG:HB2	4:H:5486:MPD:C4	2.26	0.65
1:F:320:LYS:NZ	1:L:461:GLU:OE1	2.27	0.65
4:D:5475:MPD:H53	4:D:5475:MPD:H11	1.76	0.65
4:E:5480:MPD:H52	4:E:5480:MPD:H11	1.77	0.65
1:I:365:ALA:O	1:I:367:PRO:HD3	1.96	0.65
4:I:5488:MPD:H11	4:I:5488:MPD:H52	1.77	0.65
1:I:30:HIS:H	1:J:180:PHE:HB3	1.62	0.65
4:L:5494:MPD:H11	4:L:5494:MPD:H52	1.77	0.65
1:B:88:ARG:HE	4:B:5474:MPD:HM1	1.59	0.65
1:D:365:ALA:O	1:D:367:PRO:HD3	1.96	0.65
1:I:105:ARG:HB2	4:I:5488:MPD:C4	2.26	0.65
4:C:5476:MPD:H52	4:C:5476:MPD:H11	1.77	0.65
1:K:88:ARG:HE	4:K:5492:MPD:HM1	1.59	0.65
1:L:458:HIS:CD2	1:L:460:VAL:H	2.11	0.65
1:C:365:ALA:O	1:C:367:PRO:HD3	1.96	0.65
1:F:105:ARG:HB2	4:F:5482:MPD:C4	2.26	0.65
1:A:320:LYS:NZ	1:G:461:GLU:OE1	2.24	0.65
1:H:365:ALA:O	1:H:367:PRO:HD3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:80:PHE:HD1	4:H:5487:MPD:H52	1.61	0.65
1:D:320:LYS:NZ	1:J:461:GLU:OE1	2.28	0.65
1:F:22:THR:HB	4:F:5482:MPD:H11	1.75	0.65
1:H:53:SER:HB2	1:I:179:TYR:CD2	2.32	0.65
1:A:80:PHE:CD1	4:A:5481:MPD:C5	2.80	0.65
1:C:399:LEU:H	1:C:401:PRO:CG	1.90	0.65
1:K:105:ARG:HB2	4:K:5492:MPD:C4	2.26	0.65
1:L:105:ARG:HB2	4:L:5494:MPD:C4	2.26	0.65
1:A:105:ARG:HB2	4:A:5472:MPD:C4	2.26	0.65
1:B:22:THR:HB	4:B:5474:MPD:H11	1.75	0.65
1:E:105:ARG:HB2	4:E:5480:MPD:C4	2.26	0.65
1:C:179:TYR:CD2	1:D:53:SER:HB2	2.32	0.64
1:G:399:LEU:N	1:G:401:PRO:CG	2.52	0.64
1:F:365:ALA:O	1:F:367:PRO:HD3	1.96	0.64
1:K:458:HIS:CD2	1:K:460:VAL:H	2.11	0.64
1:I:170:GLY:HA2	1:I:172:ARG:NH2	2.13	0.64
1:J:80:PHE:CA	4:J:5491:MPD:H12	2.28	0.64
1:D:458:HIS:CD2	1:D:460:VAL:H	2.11	0.64
1:E:399:LEU:N	1:E:401:PRO:CG	2.52	0.64
1:D:82:ASP:HB2	4:D:5475:MPD:C3	2.28	0.64
1:K:365:ALA:O	1:K:367:PRO:HD3	1.96	0.64
1:G:211:HIS:HD2	1:G:212:GLU:O	1.81	0.64
1:I:211:HIS:HD2	1:I:212:GLU:O	1.81	0.64
1:J:170:GLY:HA2	1:J:172:ARG:NH2	2.13	0.64
1:F:170:GLY:HA2	1:F:172:ARG:NH2	2.13	0.64
1:F:399:LEU:N	1:F:401:PRO:CG	2.52	0.64
1:J:399:LEU:N	1:J:401:PRO:CG	2.52	0.64
1:K:170:GLY:HA2	1:K:172:ARG:NH2	2.13	0.64
1:L:211:HIS:HD2	1:L:212:GLU:O	1.81	0.64
1:A:170:GLY:HA2	1:A:172:ARG:NH2	2.13	0.64
1:D:170:GLY:HA2	1:D:172:ARG:NH2	2.13	0.64
1:G:399:LEU:H	1:G:401:PRO:CG	1.90	0.64
1:J:211:HIS:HD2	1:J:212:GLU:O	1.81	0.64
1:B:365:ALA:O	1:B:367:PRO:HD3	1.96	0.64
1:E:80:PHE:CD1	4:E:5477:MPD:C5	2.81	0.64
1:G:365:ALA:O	1:G:367:PRO:HD3	1.96	0.64
1:J:365:ALA:O	1:J:367:PRO:HD3	1.96	0.64
1:E:365:ALA:O	1:E:367:PRO:HD3	1.96	0.63
1:E:80:PHE:CD1	4:E:5477:MPD:H53	2.34	0.63
1:F:211:HIS:HD2	1:F:212:GLU:O	1.81	0.63
1:B:170:GLY:HA2	1:B:172:ARG:NH2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:HIS:CD2	1:C:460:VAL:H	2.11	0.63
1:H:170:GLY:HA2	1:H:172:ARG:NH2	2.13	0.63
1:H:211:HIS:HD2	1:H:212:GLU:O	1.81	0.63
1:K:399:LEU:N	1:K:401:PRO:CG	2.52	0.63
1:C:211:HIS:HD2	1:C:212:GLU:O	1.81	0.63
1:H:458:HIS:CD2	1:H:460:VAL:H	2.11	0.63
1:H:80:PHE:CA	4:H:5487:MPD:H12	2.29	0.63
1:K:211:HIS:HD2	1:K:212:GLU:O	1.81	0.63
1:L:386:ILE:O	1:L:388:PRO:HD3	1.99	0.63
1:B:386:ILE:O	1:B:388:PRO:HD3	1.99	0.63
1:G:170:GLY:HA2	1:G:172:ARG:NH2	2.13	0.63
1:E:386:ILE:O	1:E:388:PRO:HD3	1.99	0.63
1:C:170:GLY:HA2	1:C:172:ARG:NH2	2.13	0.63
1:A:211:HIS:HD2	1:A:212:GLU:O	1.81	0.63
1:A:461:GLU:OE1	1:G:320:LYS:NZ	2.25	0.63
1:E:211:HIS:HD2	1:E:212:GLU:O	1.81	0.63
1:L:170:GLY:HA2	1:L:172:ARG:NH2	2.13	0.63
1:B:399:LEU:H	1:B:401:PRO:CG	1.90	0.63
1:F:396:LEU:HD12	1:F:398:ASP:H	1.64	0.63
1:G:386:ILE:O	1:G:388:PRO:HD3	1.99	0.63
1:D:211:HIS:HD2	1:D:212:GLU:O	1.81	0.62
1:E:170:GLY:HA2	1:E:172:ARG:NH2	2.13	0.62
1:F:386:ILE:O	1:F:388:PRO:HD3	1.99	0.62
1:F:437:GLU:HG3	5:F:5724:HOH:O	1.99	0.62
1:H:386:ILE:O	1:H:388:PRO:HD3	1.99	0.62
1:I:386:ILE:O	1:I:388:PRO:HD3	1.99	0.62
1:I:82:ASP:HB2	4:I:5489:MPD:C3	2.29	0.62
1:L:82:ASP:HB2	4:L:5483:MPD:C3	2.28	0.62
1:A:396:LEU:HD12	1:A:398:ASP:H	1.64	0.62
1:B:211:HIS:HD2	1:B:212:GLU:O	1.81	0.62
1:C:386:ILE:O	1:C:388:PRO:HD3	1.99	0.62
1:D:386:ILE:O	1:D:388:PRO:HD3	1.99	0.62
1:J:386:ILE:O	1:J:388:PRO:HD3	1.99	0.62
1:A:458:HIS:CD2	1:A:460:VAL:H	2.11	0.62
1:D:399:LEU:N	1:D:401:PRO:CG	2.52	0.62
1:I:396:LEU:HD12	1:I:398:ASP:H	1.64	0.62
1:J:437:GLU:HG3	5:J:2881:HOH:O	1.99	0.62
1:L:396:LEU:HD12	1:L:398:ASP:H	1.64	0.62
1:A:386:ILE:O	1:A:388:PRO:HD3	1.99	0.62
1:C:396:LEU:HD12	1:C:398:ASP:H	1.64	0.62
1:F:80:PHE:CA	4:F:5479:MPD:H12	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:235:ILE:CG2	1:H:367:PRO:HG3	2.28	0.62
1:I:80:PHE:HD1	4:I:5489:MPD:C5	2.12	0.62
1:E:84:THR:HG21	4:E:5477:MPD:H52	0.77	0.62
1:F:458:HIS:CD2	1:F:460:VAL:H	2.11	0.62
1:J:396:LEU:HD12	1:J:398:ASP:H	1.64	0.62
1:L:437:GLU:HG3	5:L:3465:HOH:O	1.99	0.62
1:C:437:GLU:HG3	5:C:5712:HOH:O	1.99	0.62
1:J:235:ILE:CG2	1:J:367:PRO:HG3	2.28	0.62
1:K:386:ILE:O	1:K:388:PRO:HD3	1.99	0.62
1:K:396:LEU:HD12	1:K:398:ASP:H	1.64	0.62
1:A:155:GLU:OE1	1:A:211:HIS:HE1	1.83	0.62
1:E:396:LEU:HD12	1:E:398:ASP:H	1.64	0.62
1:H:396:LEU:HD12	1:H:398:ASP:H	1.64	0.62
1:G:437:GLU:HG3	5:G:5723:HOH:O	1.99	0.62
1:K:82:ASP:HB2	4:K:5493:MPD:C3	2.30	0.62
1:B:437:GLU:HG3	5:B:5712:HOH:O	1.99	0.62
1:D:235:ILE:CG2	1:D:367:PRO:HG3	2.28	0.62
1:H:399:LEU:H	1:H:401:PRO:CG	1.90	0.62
1:D:155:GLU:OE1	1:D:211:HIS:HE1	1.83	0.62
1:G:396:LEU:HD12	1:G:398:ASP:H	1.64	0.62
1:I:437:GLU:HG3	5:I:5738:HOH:O	1.99	0.62
1:B:360:PHE:CG	1:B:361:PRO:HD3	2.35	0.61
1:I:235:ILE:CG2	1:I:367:PRO:HG3	2.27	0.61
1:B:155:GLU:OE1	1:B:211:HIS:HE1	1.83	0.61
1:A:180:PHE:HB3	1:B:30:HIS:H	1.65	0.61
1:A:437:GLU:HG3	5:A:5711:HOH:O	1.99	0.61
1:A:84:THR:HG21	4:A:5481:MPD:C4	2.30	0.61
1:B:248:ARG:HG2	1:B:248:ARG:HH21	1.66	0.61
1:B:427:PHE:CE1	1:B:428:LEU:HD13	2.36	0.61
1:C:427:PHE:CE1	1:C:428:LEU:HD13	2.36	0.61
1:D:360:PHE:CG	1:D:361:PRO:HD3	2.35	0.61
1:D:437:GLU:HG3	5:D:1129:HOH:O	1.99	0.61
1:H:437:GLU:HG3	5:H:5731:HOH:O	1.99	0.61
1:L:155:GLU:OE1	1:L:211:HIS:HE1	1.83	0.61
1:E:155:GLU:OE1	1:E:211:HIS:HE1	1.83	0.61
1:J:248:ARG:HH21	1:J:248:ARG:HG2	1.65	0.61
1:J:427:PHE:CE1	1:J:428:LEU:HD13	2.36	0.61
1:K:155:GLU:OE1	1:K:211:HIS:HE1	1.83	0.61
1:K:437:GLU:HG3	5:K:3173:HOH:O	1.99	0.61
1:K:53:SER:HB2	1:L:179:TYR:CD2	2.35	0.61
1:C:248:ARG:HH21	1:C:248:ARG:HG2	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:LEU:HD12	1:D:398:ASP:H	1.64	0.61
1:I:427:PHE:CE1	1:I:428:LEU:HD13	2.35	0.61
1:A:427:PHE:CE1	1:A:428:LEU:HD13	2.36	0.61
1:B:396:LEU:HD12	1:B:398:ASP:H	1.64	0.61
1:E:437:GLU:HG3	5:E:1421:HOH:O	1.99	0.61
1:H:155:GLU:OE1	1:H:211:HIS:HE1	1.83	0.61
1:J:155:GLU:OE1	1:J:211:HIS:HE1	1.83	0.61
1:F:155:GLU:OE1	1:F:211:HIS:HE1	1.83	0.61
1:H:248:ARG:HG2	1:H:248:ARG:HH21	1.66	0.61
1:D:427:PHE:CE1	1:D:428:LEU:HD13	2.36	0.61
1:E:22:THR:H	4:E:5480:MPD:H11	1.66	0.61
1:E:427:PHE:CE1	1:E:428:LEU:HD13	2.36	0.61
1:G:155:GLU:OE1	1:G:211:HIS:HE1	1.83	0.61
1:G:248:ARG:HG2	1:G:248:ARG:HH21	1.66	0.61
1:I:155:GLU:OE1	1:I:211:HIS:HE1	1.83	0.61
1:I:248:ARG:HH21	1:I:248:ARG:HG2	1.66	0.61
1:C:80:PHE:CA	4:C:5473:MPD:H12	2.30	0.61
1:G:427:PHE:CE1	1:G:428:LEU:HD13	2.36	0.61
1:I:80:PHE:CA	4:I:5489:MPD:H12	2.30	0.61
1:K:427:PHE:CE1	1:K:428:LEU:HD13	2.35	0.61
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.36	0.60
1:B:458:HIS:CD2	1:B:460:VAL:H	2.11	0.60
1:C:235:ILE:CG2	1:C:367:PRO:HG3	2.28	0.60
1:F:235:ILE:CG2	1:F:367:PRO:HG3	2.28	0.60
1:G:22:THR:H	4:G:5484:MPD:H11	1.66	0.60
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.36	0.60
1:L:427:PHE:CE1	1:L:428:LEU:HD13	2.36	0.60
1:F:248:ARG:HG2	1:F:248:ARG:HH21	1.66	0.60
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.36	0.60
1:C:155:GLU:OE1	1:C:211:HIS:HE1	1.83	0.60
1:F:427:PHE:CE1	1:F:428:LEU:HD13	2.35	0.60
1:G:21:PHE:HB2	4:G:5484:MPD:C5	2.25	0.60
1:H:427:PHE:CE1	1:H:428:LEU:HD13	2.36	0.60
1:J:360:PHE:CG	1:J:361:PRO:HD3	2.35	0.60
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.36	0.60
1:A:235:ILE:CG2	1:A:367:PRO:HG3	2.28	0.60
1:B:323:VAL:O	1:B:325:GLY:N	2.35	0.60
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.36	0.60
1:E:248:ARG:HG2	1:E:248:ARG:HH21	1.65	0.60
1:K:22:THR:H	4:K:5492:MPD:H11	1.66	0.60
1:C:360:PHE:CG	1:C:361:PRO:HD3	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:323:VAL:O	1:E:325:GLY:N	2.35	0.60
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.36	0.60
1:I:399:LEU:H	1:I:401:PRO:CG	1.90	0.60
1:E:320:LYS:NZ	1:K:461:GLU:OE1	2.27	0.60
1:F:323:VAL:O	1:F:325:GLY:N	2.35	0.60
1:K:248:ARG:HH21	1:K:248:ARG:HG2	1.65	0.60
1:K:29:GLN:OE1	1:L:181:PRO:HD3	2.01	0.60
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.36	0.60
1:K:360:PHE:CE2	1:K:361:PRO:HD3	2.36	0.60
1:L:80:PHE:CA	4:L:5483:MPD:H12	2.30	0.60
1:A:248:ARG:HH21	1:A:248:ARG:HG2	1.66	0.60
1:A:360:PHE:CG	1:A:361:PRO:HD3	2.35	0.60
1:D:323:VAL:O	1:D:325:GLY:N	2.35	0.60
1:G:360:PHE:CG	1:G:361:PRO:HD3	2.35	0.60
1:H:323:VAL:O	1:H:325:GLY:N	2.35	0.60
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.36	0.60
1:K:323:VAL:O	1:K:325:GLY:N	2.35	0.60
1:C:80:PHE:HD1	4:C:5473:MPD:H52	1.67	0.59
1:J:323:VAL:O	1:J:325:GLY:N	2.35	0.59
1:L:323:VAL:O	1:L:325:GLY:N	2.35	0.59
1:A:399:LEU:H	1:A:401:PRO:CG	1.90	0.59
1:A:22:THR:H	4:A:5472:MPD:H11	1.66	0.59
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.36	0.59
1:A:323:VAL:O	1:A:325:GLY:N	2.35	0.59
1:E:84:THR:HG21	4:E:5477:MPD:C4	2.30	0.59
1:F:80:PHE:HD1	4:F:5479:MPD:C5	2.14	0.59
1:I:323:VAL:O	1:I:325:GLY:N	2.35	0.59
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.36	0.59
1:K:332:LEU:HB2	1:K:408:PRO:HB2	1.85	0.59
1:L:80:PHE:HD1	4:L:5483:MPD:C5	2.10	0.59
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.36	0.59
1:C:320:LYS:NZ	1:I:461:GLU:OE1	2.30	0.59
1:A:332:LEU:HB2	1:A:408:PRO:HB2	1.85	0.59
1:B:332:LEU:HB2	1:B:408:PRO:HB2	1.85	0.59
1:C:80:PHE:CB	4:C:5473:MPD:C1	2.60	0.59
1:D:181:PRO:HD3	1:E:29:GLN:OE1	2.03	0.59
1:F:22:THR:H	4:F:5482:MPD:H11	1.66	0.59
1:C:181:PRO:HD3	1:D:29:GLN:OE1	2.01	0.59
1:D:248:ARG:HH21	1:D:248:ARG:HG2	1.65	0.59
1:G:323:VAL:O	1:G:325:GLY:N	2.35	0.59
1:I:332:LEU:HB2	1:I:408:PRO:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:PHE:HD1	4:L:5483:MPD:H52	1.68	0.59
1:C:360:PHE:CE2	1:C:361:PRO:HD3	2.36	0.59
1:E:360:PHE:CG	1:E:361:PRO:HD3	2.35	0.59
1:E:180:PHE:HB3	1:F:30:HIS:H	1.66	0.59
5:H:5633:HOH:O	1:I:181:PRO:HG3	2.01	0.59
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.36	0.59
1:J:399:LEU:H	1:J:401:PRO:CG	1.90	0.59
1:K:235:ILE:CG2	1:K:367:PRO:HG3	2.28	0.59
1:C:21:PHE:HB2	4:C:5476:MPD:C5	2.25	0.59
1:C:332:LEU:HB2	1:C:408:PRO:HB2	1.85	0.59
1:E:235:ILE:CG2	1:E:367:PRO:HG3	2.28	0.59
1:H:18:ASP:OD2	1:H:30:HIS:HD2	1.86	0.59
1:I:21:PHE:HB2	4:I:5488:MPD:C5	2.25	0.59
1:I:80:PHE:HD1	4:I:5489:MPD:H52	1.68	0.59
1:K:18:ASP:OD2	1:K:30:HIS:HD2	1.86	0.59
1:L:248:ARG:HG2	1:L:248:ARG:HH21	1.66	0.59
1:C:180:PHE:HB3	1:D:30:HIS:H	1.66	0.58
1:D:332:LEU:HB2	1:D:408:PRO:HB2	1.85	0.58
1:G:235:ILE:CG2	1:G:367:PRO:HG3	2.28	0.58
1:L:22:THR:H	4:L:5494:MPD:H11	1.66	0.58
1:B:18:ASP:OD2	1:B:30:HIS:HD2	1.86	0.58
1:B:22:THR:H	4:B:5474:MPD:H11	1.66	0.58
1:C:80:PHE:CD1	4:C:5473:MPD:H52	2.38	0.58
1:E:18:ASP:OD2	1:E:30:HIS:HD2	1.86	0.58
1:H:118:THR:OG1	1:H:120:ILE:HG13	2.04	0.58
1:I:22:THR:H	4:I:5488:MPD:H11	1.66	0.58
1:A:18:ASP:OD2	1:A:30:HIS:HD2	1.86	0.58
1:A:360:PHE:CE2	1:A:361:PRO:HD3	2.36	0.58
1:C:82:ASP:HB2	4:C:5473:MPD:C3	2.33	0.58
1:L:18:ASP:OD2	1:L:30:HIS:HD2	1.86	0.58
1:L:332:LEU:HB2	1:L:408:PRO:HB2	1.85	0.58
1:C:323:VAL:O	1:C:325:GLY:N	2.35	0.58
1:B:179:TYR:CD2	1:C:53:SER:HB2	2.38	0.58
1:F:80:PHE:CB	4:F:5479:MPD:C1	2.56	0.58
1:G:332:LEU:HB2	1:G:408:PRO:HB2	1.85	0.58
1:H:360:PHE:CG	1:H:361:PRO:HD3	2.35	0.58
1:I:360:PHE:CE2	1:I:361:PRO:HD3	2.36	0.58
1:D:22:THR:H	4:D:5478:MPD:H11	1.66	0.58
1:E:118:THR:OG1	1:E:120:ILE:HG13	2.04	0.58
1:G:360:PHE:CE2	1:G:361:PRO:HD3	2.36	0.58
1:I:53:SER:HB2	1:J:179:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:21:PHE:HB2	4:J:5490:MPD:C5	2.25	0.58
1:C:18:ASP:OD2	1:C:30:HIS:HD2	1.86	0.58
1:D:118:THR:OG1	1:D:120:ILE:HG13	2.04	0.58
1:H:332:LEU:HB2	1:H:408:PRO:HB2	1.85	0.58
1:I:118:THR:OG1	1:I:120:ILE:HG13	2.03	0.58
1:J:118:THR:OG1	1:J:120:ILE:HG13	2.03	0.58
1:L:360:PHE:CG	1:L:361:PRO:HD3	2.35	0.58
1:L:235:ILE:CG2	1:L:367:PRO:HG3	2.28	0.58
1:B:21:PHE:HB2	4:B:5474:MPD:C5	2.25	0.58
1:E:360:PHE:CE2	1:E:361:PRO:HD3	2.36	0.58
1:C:22:THR:H	4:C:5476:MPD:H11	1.66	0.58
1:E:308:ILE:HG21	1:E:374:LEU:HD13	1.86	0.58
1:G:443:ILE:O	1:G:447:ARG:HG3	2.04	0.58
1:I:18:ASP:OD2	1:I:30:HIS:HD2	1.86	0.58
1:J:332:LEU:HB2	1:J:408:PRO:HB2	1.85	0.58
1:J:443:ILE:O	1:J:447:ARG:HG3	2.04	0.58
1:K:308:ILE:HG21	1:K:374:LEU:HD13	1.86	0.58
1:A:118:THR:OG1	1:A:120:ILE:HG13	2.03	0.58
1:A:21:PHE:HB2	4:A:5472:MPD:C5	2.25	0.58
1:F:443:ILE:O	1:F:447:ARG:HG3	2.04	0.58
1:J:22:THR:H	4:J:5490:MPD:H11	1.66	0.58
1:J:82:ASP:O	1:J:84:THR:CG2	2.51	0.58
1:B:308:ILE:HG21	1:B:374:LEU:HD13	1.86	0.58
1:D:18:ASP:OD2	1:D:30:HIS:HD2	1.86	0.58
1:D:443:ILE:O	1:D:447:ARG:HG3	2.04	0.58
1:L:118:THR:OG1	1:L:120:ILE:HG13	2.03	0.58
1:B:118:THR:OG1	1:B:120:ILE:HG13	2.04	0.57
1:C:118:THR:OG1	1:C:120:ILE:HG13	2.04	0.57
1:E:82:ASP:O	1:E:84:THR:CG2	2.51	0.57
1:F:332:LEU:HB2	1:F:408:PRO:HB2	1.85	0.57
1:J:18:ASP:OD2	1:J:30:HIS:HD2	1.86	0.57
1:F:360:PHE:CG	1:F:361:PRO:HD3	2.35	0.57
1:G:118:THR:OG1	1:G:120:ILE:HG13	2.04	0.57
1:H:308:ILE:HG21	1:H:374:LEU:HD13	1.86	0.57
1:K:360:PHE:CG	1:K:361:PRO:HD3	2.35	0.57
1:B:443:ILE:O	1:B:447:ARG:HG3	2.04	0.57
1:K:443:ILE:O	1:K:447:ARG:HG3	2.04	0.57
1:C:443:ILE:O	1:C:447:ARG:HG3	2.04	0.57
1:E:332:LEU:HB2	1:E:408:PRO:HB2	1.85	0.57
1:L:360:PHE:CE2	1:L:361:PRO:HD3	2.36	0.57
1:A:332:LEU:CB	1:A:408:PRO:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LYS:C	1:B:384:ASN:HD22	2.08	0.57
1:F:435:THR:HG23	5:F:5531:HOH:O	2.05	0.57
1:H:443:ILE:O	1:H:447:ARG:HG3	2.04	0.57
1:J:360:PHE:CE2	1:J:361:PRO:HD3	2.36	0.57
1:K:21:PHE:HB2	4:K:5492:MPD:C5	2.25	0.57
1:G:435:THR:HG23	5:G:5529:HOH:O	2.05	0.57
1:J:383:LYS:C	1:J:384:ASN:HD22	2.08	0.57
1:K:118:THR:OG1	1:K:120:ILE:HG13	2.04	0.57
1:C:435:THR:HG23	5:C:5518:HOH:O	2.05	0.57
1:E:435:THR:HG23	5:E:1210:HOH:O	2.05	0.57
1:F:120:ILE:HD13	1:F:382:ILE:HG21	1.87	0.57
1:F:118:THR:OG1	1:F:120:ILE:HG13	2.04	0.57
1:G:332:LEU:CB	1:G:408:PRO:HB2	2.35	0.57
1:G:383:LYS:C	1:G:384:ASN:HD22	2.08	0.57
1:I:120:ILE:HD13	1:I:382:ILE:HG21	1.87	0.57
1:I:82:ASP:O	1:I:84:THR:CG2	2.51	0.57
1:K:332:LEU:CB	1:K:408:PRO:HB2	2.35	0.57
1:G:180:PHE:HB3	1:L:30:HIS:H	1.68	0.57
1:L:435:THR:HG23	5:L:3254:HOH:O	2.05	0.57
1:B:332:LEU:CB	1:B:408:PRO:HB2	2.35	0.57
1:G:120:ILE:HD13	1:G:382:ILE:HG21	1.87	0.57
1:G:53:SER:HB2	1:H:179:TYR:CD2	2.40	0.57
1:G:82:ASP:O	1:G:84:THR:CG2	2.51	0.57
1:H:192:ARG:HH21	1:H:219:ASN:HD22	1.52	0.57
1:I:80:PHE:CD1	4:I:5489:MPD:H52	2.39	0.57
1:A:308:ILE:HG21	1:A:374:LEU:HD13	1.86	0.57
1:A:443:ILE:O	1:A:447:ARG:HG3	2.04	0.57
1:B:235:ILE:CG2	1:B:367:PRO:HG3	2.28	0.57
1:F:192:ARG:HH21	1:F:219:ASN:HD22	1.52	0.57
1:G:308:ILE:HG21	1:G:374:LEU:HD13	1.86	0.57
1:H:383:LYS:C	1:H:384:ASN:HD22	2.08	0.57
1:I:360:PHE:CG	1:I:361:PRO:HD3	2.35	0.57
1:K:399:LEU:H	1:K:401:PRO:CG	1.90	0.57
4:K:5493:MPD:H11	1:L:189:GLN:HG3	1.87	0.57
1:A:179:TYR:CD2	1:B:53:SER:HB2	2.40	0.57
1:C:180:PHE:O	1:D:29:GLN:HA	2.04	0.57
1:C:192:ARG:HH21	1:C:219:ASN:HD22	1.52	0.57
1:D:120:ILE:HD13	1:D:382:ILE:HG21	1.87	0.57
1:D:192:ARG:HH21	1:D:219:ASN:HD22	1.52	0.57
1:D:180:PHE:HB3	1:E:30:HIS:H	1.70	0.57
1:E:383:LYS:C	1:E:384:ASN:HD22	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:443:ILE:O	1:E:447:ARG:HG3	2.04	0.57
1:F:21:PHE:HB2	4:F:5482:MPD:C5	2.25	0.57
1:H:22:THR:H	4:H:5486:MPD:H11	1.66	0.57
1:L:332:LEU:CB	1:L:408:PRO:HB2	2.35	0.57
1:C:189:GLN:HG3	4:D:5475:MPD:H11	1.87	0.56
1:C:120:ILE:HD13	1:C:382:ILE:HG21	1.87	0.56
1:D:383:LYS:C	1:D:384:ASN:HD22	2.08	0.56
1:J:326:TYR:HA	1:J:396:LEU:HD13	1.87	0.56
1:K:120:ILE:HD13	1:K:382:ILE:HG21	1.87	0.56
1:A:189:GLN:HG3	4:B:5471:MPD:H11	1.87	0.56
1:G:460:VAL:HG12	1:G:464:LEU:HD22	1.88	0.56
1:H:435:THR:HG23	5:H:5540:HOH:O	2.05	0.56
1:I:435:THR:HG23	5:I:5542:HOH:O	2.05	0.56
1:K:80:PHE:CB	4:K:5493:MPD:C1	2.60	0.56
1:L:443:ILE:O	1:L:447:ARG:HG3	2.04	0.56
1:B:120:ILE:HD13	1:B:382:ILE:HG21	1.87	0.56
1:D:360:PHE:CE2	1:D:361:PRO:HD3	2.36	0.56
1:F:18:ASP:OD2	1:F:30:HIS:HD2	1.86	0.56
1:F:326:TYR:HA	1:F:396:LEU:HD13	1.87	0.56
1:G:18:ASP:OD2	1:G:30:HIS:HD2	1.86	0.56
4:H:5487:MPD:H11	1:I:189:GLN:HG3	1.87	0.56
1:L:120:ILE:HD13	1:L:382:ILE:HG21	1.87	0.56
1:L:308:ILE:HG21	1:L:374:LEU:HD13	1.86	0.56
1:B:80:PHE:HD1	4:B:5471:MPD:C5	2.18	0.56
1:C:340:SER:HB3	1:C:396:LEU:HA	1.88	0.56
1:D:332:LEU:CB	1:D:408:PRO:HB2	2.35	0.56
1:F:308:ILE:HG21	1:F:374:LEU:HD13	1.86	0.56
1:A:383:LYS:C	1:A:384:ASN:HD22	2.08	0.56
1:B:435:THR:HG23	5:B:5518:HOH:O	2.05	0.56
1:C:460:VAL:HG12	1:C:464:LEU:HD22	1.88	0.56
1:F:383:LYS:C	1:F:384:ASN:HD22	2.08	0.56
1:F:460:VAL:HG12	1:F:464:LEU:HD22	1.88	0.56
1:L:383:LYS:C	1:L:384:ASN:HD22	2.08	0.56
1:E:332:LEU:CB	1:E:408:PRO:HB2	2.35	0.56
1:D:179:TYR:CD2	1:E:53:SER:HB2	2.41	0.56
1:G:340:SER:HB3	1:G:396:LEU:HA	1.88	0.56
1:H:332:LEU:CB	1:H:408:PRO:HB2	2.35	0.56
4:I:5489:MPD:H11	1:J:189:GLN:HG3	1.87	0.56
1:J:340:SER:HB3	1:J:396:LEU:HA	1.87	0.56
1:K:192:ARG:HH21	1:K:219:ASN:HD22	1.52	0.56
1:K:435:THR:HG23	5:K:2962:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:80:PHE:HD1	4:K:5493:MPD:C5	2.17	0.56
1:L:326:TYR:HA	1:L:396:LEU:HD13	1.87	0.56
1:A:120:ILE:HD13	1:A:382:ILE:HG21	1.87	0.56
1:D:130:PRO:HB3	1:D:268:MET:HE3	1.88	0.56
1:E:192:ARG:HH21	1:E:219:ASN:HD22	1.52	0.56
1:L:82:ASP:O	1:L:84:THR:CG2	2.51	0.56
1:B:326:TYR:HA	1:B:396:LEU:HD13	1.88	0.56
1:B:82:ASP:O	1:B:84:THR:CG2	2.51	0.56
1:F:248:ARG:CG	1:F:248:ARG:NH2	2.67	0.56
1:F:332:LEU:CB	1:F:408:PRO:HB2	2.35	0.56
1:E:189:GLN:HG3	4:F:5479:MPD:H11	1.87	0.56
1:G:326:TYR:HA	1:G:396:LEU:HD13	1.87	0.56
1:I:443:ILE:O	1:I:447:ARG:HG3	2.04	0.56
1:I:460:VAL:HG12	1:I:464:LEU:HD22	1.88	0.56
1:J:120:ILE:HD13	1:J:382:ILE:HG21	1.87	0.56
1:J:435:THR:HG23	5:J:2670:HOH:O	2.05	0.56
1:L:192:ARG:HH21	1:L:219:ASN:HD22	1.52	0.56
1:A:435:THR:HG23	5:A:5515:HOH:O	2.05	0.56
1:C:326:TYR:HA	1:C:396:LEU:HD13	1.87	0.56
1:D:308:ILE:HG21	1:D:374:LEU:HD13	1.86	0.56
1:D:398:ASP:O	1:D:399:LEU:HG	2.06	0.56
1:E:340:SER:HB3	1:E:396:LEU:HA	1.88	0.56
1:H:398:ASP:O	1:H:399:LEU:HG	2.06	0.56
1:I:332:LEU:CB	1:I:408:PRO:HB2	2.35	0.56
1:K:82:ASP:O	1:K:84:THR:CG2	2.51	0.56
1:A:326:TYR:HA	1:A:396:LEU:HD13	1.87	0.56
1:C:332:LEU:CB	1:C:408:PRO:HB2	2.35	0.56
1:D:21:PHE:HB2	4:D:5478:MPD:C5	2.25	0.56
1:J:308:ILE:HG21	1:J:374:LEU:HD13	1.86	0.56
1:J:61:ASN:O	1:K:337:ARG:CB	2.34	0.56
1:K:383:LYS:C	1:K:384:ASN:HD22	2.08	0.56
1:G:192:ARG:HH21	1:G:219:ASN:HD22	1.52	0.56
4:J:5491:MPD:H11	1:K:189:GLN:HG3	1.87	0.56
1:K:398:ASP:O	1:K:399:LEU:HG	2.06	0.56
1:G:179:TYR:CD2	1:L:53:SER:HB2	2.40	0.56
1:A:114:TYR:CD2	1:A:431:GLY:HA3	2.41	0.55
1:B:398:ASP:O	1:B:399:LEU:HG	2.06	0.55
1:B:189:GLN:HG3	4:C:5473:MPD:H11	1.87	0.55
1:E:120:ILE:HD13	1:E:382:ILE:HG21	1.87	0.55
1:F:114:TYR:CD2	1:F:431:GLY:HA3	2.41	0.55
1:H:340:SER:HB3	1:H:396:LEU:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:383:LYS:C	1:I:384:ASN:HD22	2.08	0.55
1:I:340:SER:HB3	1:I:396:LEU:HA	1.87	0.55
1:K:326:TYR:HA	1:K:396:LEU:HD13	1.87	0.55
1:C:114:TYR:CD2	1:C:431:GLY:HA3	2.41	0.55
1:E:360:PHE:CD2	1:E:361:PRO:CD	2.74	0.55
1:E:460:VAL:HG12	1:E:464:LEU:HD22	1.88	0.55
1:F:340:SER:HB3	1:F:396:LEU:HA	1.88	0.55
1:H:114:TYR:CD2	1:H:431:GLY:HA3	2.41	0.55
1:J:332:LEU:CB	1:J:408:PRO:HB2	2.35	0.55
1:J:460:VAL:HG12	1:J:464:LEU:HD22	1.88	0.55
1:B:181:PRO:HG3	5:C:5611:HOH:O	2.07	0.55
1:B:360:PHE:CD2	1:B:361:PRO:CD	2.74	0.55
1:E:326:TYR:HA	1:E:396:LEU:HD13	1.87	0.55
4:A:5481:MPD:H11	1:F:189:GLN:HG3	1.87	0.55
1:H:326:TYR:HA	1:H:396:LEU:HD13	1.87	0.55
1:J:192:ARG:HH21	1:J:219:ASN:HD22	1.52	0.55
1:A:340:SER:HB3	1:A:396:LEU:HA	1.88	0.55
1:A:460:VAL:HG12	1:A:464:LEU:HD22	1.88	0.55
1:C:308:ILE:HG21	1:C:374:LEU:HD13	1.86	0.55
1:C:82:ASP:O	1:C:84:THR:CG2	2.51	0.55
1:J:398:ASP:O	1:J:399:LEU:HG	2.06	0.55
1:L:114:TYR:CD2	1:L:431:GLY:HA3	2.41	0.55
1:L:340:SER:HB3	1:L:396:LEU:HA	1.88	0.55
1:D:435:THR:HG23	5:D:918:HOH:O	2.05	0.55
1:F:461:GLU:OE1	1:L:320:LYS:NZ	2.30	0.55
1:G:189:GLN:HG3	4:L:5483:MPD:H11	1.87	0.55
1:H:120:ILE:HD13	1:H:382:ILE:HG21	1.87	0.55
1:J:80:PHE:HD1	4:J:5491:MPD:H52	1.69	0.55
1:C:383:LYS:C	1:C:384:ASN:HD22	2.08	0.55
1:D:340:SER:HB3	1:D:396:LEU:HA	1.88	0.55
1:D:189:GLN:HG3	4:E:5477:MPD:H11	1.87	0.55
1:I:308:ILE:HG21	1:I:374:LEU:HD13	1.86	0.55
1:L:398:ASP:O	1:L:399:LEU:HG	2.06	0.55
1:A:398:ASP:O	1:A:399:LEU:HG	2.06	0.55
1:B:114:TYR:CD2	1:B:431:GLY:HA3	2.41	0.55
1:D:114:TYR:CD2	1:D:431:GLY:HA3	2.41	0.55
1:D:82:ASP:O	1:D:84:THR:CG2	2.51	0.55
1:G:360:PHE:CD2	1:G:361:PRO:CD	2.74	0.55
1:I:398:ASP:O	1:I:399:LEU:HG	2.06	0.55
1:B:80:PHE:CA	4:B:5471:MPD:H12	2.36	0.55
1:E:21:PHE:HB2	4:E:5480:MPD:C5	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:5485:MPD:H11	1:H:189:GLN:HG3	1.87	0.55
1:H:460:VAL:HG12	1:H:464:LEU:HD22	1.88	0.55
1:H:84:THR:CG2	4:H:5487:MPD:H32	2.37	0.55
1:I:29:GLN:HA	1:J:180:PHE:O	2.06	0.55
1:B:340:SER:HB3	1:B:396:LEU:HA	1.88	0.55
1:B:460:VAL:HG12	1:B:464:LEU:HD22	1.88	0.55
1:D:326:TYR:HA	1:D:396:LEU:HD13	1.87	0.55
1:J:114:TYR:CD2	1:J:431:GLY:HA3	2.41	0.55
1:K:460:VAL:HG12	1:K:464:LEU:HD22	1.87	0.55
1:A:82:ASP:O	1:A:84:THR:CG2	2.51	0.55
1:D:460:VAL:HG12	1:D:464:LEU:HD22	1.88	0.55
1:L:128:PRO:HD2	1:L:231:LYS:HE2	1.89	0.55
1:C:398:ASP:O	1:C:399:LEU:HG	2.06	0.54
1:G:29:GLN:OE1	1:H:181:PRO:HD3	2.07	0.54
1:G:398:ASP:O	1:G:399:LEU:HG	2.06	0.54
1:H:248:ARG:NH2	1:H:248:ARG:CG	2.67	0.54
1:I:114:TYR:CD2	1:I:431:GLY:HA3	2.41	0.54
1:K:340:SER:HB3	1:K:396:LEU:HA	1.88	0.54
1:B:192:ARG:HH21	1:B:219:ASN:HD22	1.52	0.54
1:C:181:PRO:HG3	5:D:1020:HOH:O	2.07	0.54
1:E:398:ASP:O	1:E:399:LEU:HG	2.06	0.54
1:F:360:PHE:CE2	1:F:361:PRO:HD3	2.37	0.54
1:I:192:ARG:HH21	1:I:219:ASN:HD22	1.52	0.54
1:I:22:THR:HG1	4:I:5488:MPD:C1	2.08	0.54
1:J:128:PRO:HD2	1:J:231:LYS:HE2	1.89	0.54
1:J:248:ARG:NH2	1:J:248:ARG:HG2	2.23	0.54
1:J:360:PHE:CD2	1:J:361:PRO:CD	2.74	0.54
1:J:105:ARG:HD2	4:J:5490:MPD:H32	1.90	0.54
1:J:29:GLN:HA	1:K:180:PHE:O	2.07	0.54
1:L:460:VAL:HG12	1:L:464:LEU:HD22	1.88	0.54
1:B:128:PRO:HD2	1:B:231:LYS:HE2	1.89	0.54
1:E:114:TYR:CD2	1:E:431:GLY:HA3	2.41	0.54
1:E:248:ARG:HG2	1:E:248:ARG:NH2	2.23	0.54
1:G:114:TYR:CD2	1:G:431:GLY:HA3	2.41	0.54
1:K:114:TYR:CD2	1:K:431:GLY:HA3	2.41	0.54
1:L:21:PHE:HB2	4:L:5494:MPD:C5	2.25	0.54
1:B:360:PHE:CE2	1:B:361:PRO:HD3	2.36	0.54
1:F:128:PRO:HD2	1:F:231:LYS:HE2	1.89	0.54
1:F:398:ASP:O	1:F:399:LEU:HG	2.06	0.54
1:H:128:PRO:HD2	1:H:231:LYS:HE2	1.89	0.54
1:K:30:HIS:H	1:L:180:PHE:HB3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:29:GLN:HA	1:L:180:PHE:O	2.08	0.54
1:B:456:THR:O	1:H:458:HIS:HE1	1.91	0.54
1:D:128:PRO:HD2	1:D:231:LYS:HE2	1.89	0.54
1:G:248:ARG:NH2	1:G:248:ARG:HG2	2.23	0.54
1:H:248:ARG:HG2	1:H:248:ARG:NH2	2.23	0.54
1:L:84:THR:CG2	4:L:5483:MPD:H32	2.37	0.54
1:C:248:ARG:NH2	1:C:248:ARG:HG2	2.23	0.54
1:B:320:LYS:NZ	1:H:461:GLU:OE1	2.35	0.54
1:H:82:ASP:O	1:H:84:THR:CG2	2.51	0.54
1:A:61:ASN:O	1:F:337:ARG:CB	2.44	0.54
1:H:21:PHE:HB2	4:H:5486:MPD:C5	2.25	0.54
1:H:360:PHE:CE2	1:H:361:PRO:HD3	2.36	0.54
1:C:105:ARG:HD2	4:C:5476:MPD:H32	1.90	0.54
1:J:29:GLN:OE1	1:K:181:PRO:HD3	2.08	0.54
1:L:248:ARG:HG2	1:L:248:ARG:NH2	2.23	0.54
1:B:180:PHE:HB3	1:C:30:HIS:H	1.73	0.54
1:B:105:ARG:HD2	4:B:5474:MPD:H32	1.90	0.54
1:I:326:TYR:HA	1:I:396:LEU:HD13	1.88	0.54
1:K:80:PHE:HD1	4:K:5493:MPD:H52	1.73	0.54
1:E:128:PRO:HD2	1:E:231:LYS:HE2	1.89	0.54
5:K:3064:HOH:O	1:L:181:PRO:HG3	2.07	0.54
1:H:105:ARG:HD2	4:H:5486:MPD:H32	1.90	0.53
1:L:105:ARG:HD2	4:L:5494:MPD:H32	1.90	0.53
1:A:192:ARG:HH21	1:A:219:ASN:HD22	1.52	0.53
1:A:128:PRO:HD2	1:A:231:LYS:HE2	1.89	0.53
1:C:461:GLU:OE1	1:I:320:LYS:NZ	2.33	0.53
1:D:105:ARG:HD2	4:D:5478:MPD:H32	1.90	0.53
1:H:80:PHE:CG	4:H:5487:MPD:H12	2.37	0.53
1:B:248:ARG:NH2	1:B:248:ARG:HG2	2.23	0.53
1:H:80:PHE:CG	4:H:5487:MPD:C1	2.92	0.53
5:I:5635:HOH:O	1:J:181:PRO:HG3	2.07	0.53
1:D:248:ARG:HG2	1:D:248:ARG:NH2	2.23	0.53
1:H:80:PHE:CD1	4:H:5487:MPD:H52	2.33	0.53
1:K:105:ARG:HD2	4:K:5492:MPD:H32	1.90	0.53
1:A:105:ARG:HD2	4:A:5472:MPD:H32	1.90	0.53
1:E:105:ARG:HD2	4:E:5480:MPD:H32	1.90	0.53
1:I:128:PRO:HD2	1:I:231:LYS:HE2	1.89	0.53
1:I:80:PHE:CB	4:I:5489:MPD:C1	2.61	0.53
1:C:128:PRO:HD2	1:C:231:LYS:HE2	1.89	0.53
1:C:360:PHE:CD2	1:C:361:PRO:CD	2.74	0.53
1:A:29:GLN:HA	1:F:180:PHE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:360:PHE:CD2	1:L:361:PRO:CD	2.74	0.53
1:B:461:GLU:OE1	1:H:320:LYS:NZ	2.33	0.53
1:F:105:ARG:HD2	4:F:5482:MPD:H32	1.90	0.53
1:F:399:LEU:H	1:F:401:PRO:CG	1.90	0.53
1:I:360:PHE:CD2	1:I:361:PRO:CD	2.74	0.53
1:K:128:PRO:HD2	1:K:231:LYS:HE2	1.89	0.53
1:B:295:LEU:O	1:B:388:PRO:HG3	2.09	0.53
1:F:82:ASP:O	1:F:84:THR:CG2	2.51	0.53
1:G:105:ARG:HD2	4:G:5484:MPD:H32	1.90	0.53
1:H:29:GLN:HA	1:I:180:PHE:O	2.09	0.53
1:D:295:LEU:O	1:D:388:PRO:HG3	2.09	0.52
1:F:256:MET:HG3	1:L:466:TYR:HA	1.91	0.52
1:F:80:PHE:HD1	4:F:5479:MPD:H52	1.74	0.52
1:A:248:ARG:HG3	1:A:248:ARG:HH21	1.75	0.52
1:G:128:PRO:HD2	1:G:231:LYS:HE2	1.89	0.52
1:G:21:PHE:HA	4:G:5484:MPD:C3	2.36	0.52
1:H:360:PHE:CD2	1:H:361:PRO:CD	2.74	0.52
1:K:248:ARG:NH2	1:K:248:ARG:HG2	2.23	0.52
1:K:295:LEU:O	1:K:388:PRO:HG3	2.09	0.52
1:B:80:PHE:HD1	4:B:5471:MPD:H52	1.75	0.52
1:I:105:ARG:HD2	4:I:5488:MPD:H32	1.90	0.52
1:I:29:GLN:HB3	1:J:180:PHE:HB2	1.91	0.52
1:J:16:PHE:HB2	1:J:84:THR:HB	1.92	0.52
1:K:360:PHE:CD2	1:K:361:PRO:CD	2.74	0.52
1:A:88:ARG:HH11	4:A:5472:MPD:HM3	1.75	0.52
1:B:16:PHE:HB2	1:B:84:THR:HB	1.92	0.52
1:H:295:LEU:O	1:H:388:PRO:HG3	2.09	0.52
1:H:16:PHE:HB2	1:H:84:THR:HB	1.92	0.52
1:J:295:LEU:O	1:J:388:PRO:HG3	2.09	0.52
1:L:295:LEU:O	1:L:388:PRO:HG3	2.09	0.52
1:A:248:ARG:NH2	1:A:248:ARG:HG2	2.23	0.52
1:C:88:ARG:HH11	4:C:5476:MPD:HM3	1.75	0.52
1:A:30:HIS:H	1:F:180:PHE:HB3	1.73	0.52
1:I:29:GLN:HB3	1:J:180:PHE:CB	2.40	0.52
1:J:88:ARG:HH11	4:J:5490:MPD:HM3	1.75	0.52
1:K:80:PHE:CA	4:K:5493:MPD:H12	2.38	0.52
1:A:256:MET:HG3	1:G:466:TYR:HA	1.91	0.52
1:D:80:PHE:HD1	4:D:5475:MPD:C5	2.23	0.52
1:F:88:ARG:HH11	4:F:5482:MPD:HM3	1.75	0.52
1:I:295:LEU:O	1:I:388:PRO:HG3	2.09	0.52
1:B:248:ARG:HH21	1:B:248:ARG:HG3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:THR:O	1:J:458:HIS:HE1	1.93	0.52
1:E:16:PHE:HB2	1:E:84:THR:HB	1.92	0.52
1:J:29:GLN:HB3	1:K:180:PHE:HB2	1.92	0.52
1:B:181:PRO:HD3	1:C:29:GLN:OE1	2.10	0.52
1:B:88:ARG:HH11	4:B:5474:MPD:HM3	1.75	0.52
1:D:16:PHE:HB2	1:D:84:THR:HB	1.92	0.52
1:H:88:ARG:HH11	4:H:5486:MPD:HM3	1.75	0.52
1:I:248:ARG:HG3	1:I:248:ARG:HH21	1.75	0.52
1:C:16:PHE:HB2	1:C:84:THR:HB	1.92	0.51
1:I:311:LEU:HD22	1:I:369:LEU:HB3	1.93	0.51
1:F:248:ARG:HG2	1:F:248:ARG:NH2	2.23	0.51
1:I:88:ARG:HH11	4:I:5488:MPD:HM3	1.75	0.51
1:L:311:LEU:HD22	1:L:369:LEU:HB3	1.93	0.51
1:L:399:LEU:CA	1:L:400:PRO:C	2.78	0.51
1:A:295:LEU:O	1:A:388:PRO:HG3	2.09	0.51
1:B:399:LEU:CA	1:B:400:PRO:C	2.78	0.51
1:E:295:LEU:O	1:E:388:PRO:HG3	2.09	0.51
5:A:5609:HOH:O	1:F:181:PRO:HG3	2.10	0.51
1:I:21:PHE:HA	4:I:5488:MPD:C3	2.36	0.51
1:I:29:GLN:OE1	1:J:181:PRO:HD3	2.10	0.51
1:A:311:LEU:HD22	1:A:369:LEU:HB3	1.93	0.51
1:B:311:LEU:HD22	1:B:369:LEU:HB3	1.93	0.51
1:D:88:ARG:HH11	4:D:5478:MPD:HM3	1.75	0.51
1:E:311:LEU:HD22	1:E:369:LEU:HB3	1.93	0.51
1:H:84:THR:HG21	4:H:5487:MPD:H32	1.92	0.51
1:I:248:ARG:NH2	1:I:248:ARG:HG2	2.23	0.51
1:C:295:LEU:O	1:C:388:PRO:HG3	2.09	0.51
1:F:399:LEU:CA	1:F:400:PRO:C	2.78	0.51
1:I:399:LEU:CA	1:I:400:PRO:C	2.78	0.51
1:C:180:PHE:CB	1:D:29:GLN:HB3	2.41	0.51
1:D:458:HIS:HE1	1:J:456:THR:O	1.94	0.51
1:I:16:PHE:HB2	1:I:84:THR:HB	1.92	0.51
1:K:399:LEU:CA	1:K:400:PRO:C	2.78	0.51
1:F:16:PHE:HB2	1:F:84:THR:HB	1.92	0.51
1:G:29:GLN:HA	1:H:180:PHE:O	2.11	0.51
1:J:84:THR:CG2	4:J:5491:MPD:H32	2.40	0.51
1:K:311:LEU:HD22	1:K:369:LEU:HB3	1.93	0.51
1:B:458:HIS:HE1	1:H:456:THR:O	1.93	0.51
1:F:295:LEU:O	1:F:388:PRO:HG3	2.09	0.51
1:G:295:LEU:O	1:G:388:PRO:HG3	2.09	0.51
1:K:403:GLU:C	1:K:405:LYS:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:CG	1:A:248:ARG:NH2	2.67	0.51
1:C:311:LEU:HD22	1:C:369:LEU:HB3	1.93	0.51
1:F:311:LEU:HD22	1:F:369:LEU:HB3	1.93	0.51
1:G:396:LEU:O	1:G:400:PRO:HG2	2.11	0.51
1:G:403:GLU:C	1:G:405:LYS:H	2.14	0.51
1:H:29:GLN:OE1	1:I:181:PRO:HD3	2.10	0.51
1:K:88:ARG:HH11	4:K:5492:MPD:HM3	1.75	0.51
1:G:248:ARG:HG3	1:G:248:ARG:HH21	1.75	0.51
1:J:248:ARG:HH21	1:J:248:ARG:HG3	1.75	0.51
1:K:16:PHE:HB2	1:K:84:THR:HB	1.92	0.51
1:L:88:ARG:HH11	4:L:5494:MPD:HM3	1.75	0.51
1:C:248:ARG:HG3	1:C:248:ARG:HH21	1.75	0.50
1:D:130:PRO:HB3	1:D:268:MET:CE	2.41	0.50
1:D:360:PHE:CD2	1:D:361:PRO:CD	2.74	0.50
1:G:16:PHE:HB2	1:G:84:THR:HB	1.92	0.50
1:J:53:SER:HB2	1:K:179:TYR:CD2	2.46	0.50
1:L:130:PRO:HB3	1:L:268:MET:CE	2.41	0.50
1:G:180:PHE:O	1:L:29:GLN:HA	2.10	0.50
1:F:403:GLU:C	1:F:405:LYS:H	2.14	0.50
1:B:403:GLU:C	1:B:405:LYS:H	2.14	0.50
1:C:21:PHE:CB	4:C:5476:MPD:H53	2.27	0.50
1:G:88:ARG:HH11	4:G:5484:MPD:HM3	1.75	0.50
1:J:130:PRO:HB3	1:J:268:MET:CE	2.41	0.50
1:J:403:GLU:C	1:J:405:LYS:H	2.14	0.50
1:J:82:ASP:N	4:J:5491:MPD:O2	2.39	0.50
1:A:399:LEU:CA	1:A:400:PRO:C	2.78	0.50
1:B:124:VAL:HG13	1:B:274:LEU:HD21	1.94	0.50
1:E:124:VAL:HG13	1:E:274:LEU:HD21	1.94	0.50
1:F:335:SER:HB2	1:F:392:MET:O	2.12	0.50
1:C:396:LEU:O	1:C:400:PRO:HG2	2.11	0.50
1:D:124:VAL:HG13	1:D:274:LEU:HD21	1.94	0.50
1:D:335:SER:HB2	1:D:392:MET:O	2.12	0.50
1:E:396:LEU:O	1:E:400:PRO:HG2	2.11	0.50
1:E:88:ARG:HH11	4:E:5480:MPD:HM3	1.75	0.50
1:H:192:ARG:HD3	1:H:219:ASN:HD22	1.77	0.50
1:I:124:VAL:HG13	1:I:274:LEU:HD21	1.94	0.50
1:I:28:GLU:OE1	1:I:88:ARG:NH1	2.45	0.50
1:I:403:GLU:C	1:I:405:LYS:H	2.14	0.50
1:L:16:PHE:HB2	1:L:84:THR:HB	1.92	0.50
1:L:124:VAL:HG13	1:L:274:LEU:HD21	1.94	0.50
1:A:124:VAL:HG13	1:A:274:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PRO:HB3	1:A:268:MET:CE	2.41	0.50
1:A:16:PHE:HB2	1:A:84:THR:HB	1.92	0.50
1:B:396:LEU:O	1:B:400:PRO:HG2	2.12	0.50
1:C:192:ARG:HD3	1:C:219:ASN:HD22	1.77	0.50
1:C:180:PHE:HB2	1:D:29:GLN:HB3	1.92	0.50
1:D:255:PHE:HB3	1:D:363:PRO:HB2	1.94	0.50
1:D:311:LEU:HD22	1:D:369:LEU:HB3	1.93	0.50
1:H:124:VAL:HG13	1:H:274:LEU:HD21	1.94	0.50
1:C:458:HIS:HE1	1:I:456:THR:O	1.95	0.50
1:J:335:SER:HB2	1:J:392:MET:O	2.12	0.50
1:K:192:ARG:HD3	1:K:219:ASN:HD22	1.77	0.50
1:K:124:VAL:HG13	1:K:274:LEU:HD21	1.94	0.50
1:L:335:SER:HB2	1:L:392:MET:O	2.12	0.50
1:A:255:PHE:HB3	1:A:363:PRO:HB2	1.94	0.50
1:C:403:GLU:C	1:C:405:LYS:H	2.14	0.50
1:D:399:LEU:CA	1:D:400:PRO:C	2.78	0.50
1:E:399:LEU:CA	1:E:400:PRO:C	2.78	0.50
1:F:82:ASP:N	4:F:5479:MPD:O2	2.40	0.50
1:F:22:THR:CA	4:F:5482:MPD:H11	2.42	0.50
1:G:29:GLN:HB3	1:H:180:PHE:HB2	1.94	0.50
1:H:255:PHE:HB3	1:H:363:PRO:HB2	1.94	0.50
1:B:22:THR:CA	4:B:5474:MPD:H11	2.42	0.50
1:D:396:LEU:O	1:D:400:PRO:HG2	2.12	0.50
1:G:335:SER:HB2	1:G:392:MET:O	2.12	0.50
1:H:248:ARG:HG3	1:H:248:ARG:HH21	1.75	0.50
1:H:311:LEU:HD22	1:H:369:LEU:HB3	1.93	0.50
1:J:396:LEU:O	1:J:400:PRO:HG2	2.12	0.50
1:K:255:PHE:HB3	1:K:363:PRO:HB2	1.94	0.50
1:E:256:MET:HG3	1:K:466:TYR:HA	1.94	0.50
1:K:84:THR:CG2	4:K:5493:MPD:H32	2.42	0.50
1:L:22:THR:CA	4:L:5494:MPD:H11	2.42	0.50
1:B:255:PHE:HB3	1:B:363:PRO:HB2	1.94	0.50
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.77	0.50
4:F:5479:MPD:O4	4:F:5479:MPD:CM	2.60	0.50
1:H:130:PRO:HB3	1:H:268:MET:CE	2.41	0.50
1:H:335:SER:HB2	1:H:392:MET:O	2.12	0.50
1:J:311:LEU:HD22	1:J:369:LEU:HB3	1.93	0.50
4:K:5493:MPD:CM	4:K:5493:MPD:O4	2.60	0.50
1:B:335:SER:HB2	1:B:392:MET:O	2.12	0.49
1:D:248:ARG:HH21	1:D:248:ARG:HG3	1.75	0.49
1:F:21:PHE:HA	4:F:5482:MPD:C3	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:PHE:HB3	1:F:363:PRO:HB2	1.94	0.49
1:G:399:LEU:CA	1:G:400:PRO:C	2.78	0.49
1:I:396:LEU:O	1:I:400:PRO:HG2	2.11	0.49
1:L:255:PHE:HB3	1:L:363:PRO:HB2	1.94	0.49
1:A:360:PHE:CD2	1:A:361:PRO:CD	2.74	0.49
1:A:335:SER:HB2	1:A:392:MET:O	2.12	0.49
1:C:21:PHE:HA	4:C:5476:MPD:C3	2.36	0.49
1:C:80:PHE:HD1	4:C:5473:MPD:C5	2.13	0.49
1:D:28:GLU:OE1	1:D:88:ARG:NH1	2.45	0.49
1:E:22:THR:CA	4:E:5480:MPD:H11	2.42	0.49
1:F:192:ARG:HD3	1:F:219:ASN:HD22	1.77	0.49
1:F:80:PHE:CD1	4:F:5479:MPD:H52	2.46	0.49
1:G:130:PRO:HB3	1:G:268:MET:CE	2.42	0.49
1:G:80:PHE:HD1	4:G:5485:MPD:C5	2.25	0.49
1:H:396:LEU:O	1:H:400:PRO:HG2	2.11	0.49
1:I:22:THR:CA	4:I:5488:MPD:H11	2.42	0.49
1:J:124:VAL:HG13	1:J:274:LEU:HD21	1.94	0.49
1:L:192:ARG:HD3	1:L:219:ASN:HD22	1.77	0.49
1:B:80:PHE:CD1	4:B:5471:MPD:H52	2.46	0.49
1:C:130:PRO:HB3	1:C:268:MET:CE	2.41	0.49
1:C:399:LEU:CA	1:C:400:PRO:C	2.78	0.49
4:D:5475:MPD:CM	4:D:5475:MPD:O4	2.60	0.49
1:E:255:PHE:HB3	1:E:363:PRO:HB2	1.94	0.49
1:F:396:LEU:O	1:F:400:PRO:HG2	2.11	0.49
1:G:124:VAL:HG13	1:G:274:LEU:HD21	1.94	0.49
1:G:311:LEU:HD22	1:G:369:LEU:HB3	1.93	0.49
1:H:84:THR:HG21	4:H:5487:MPD:C3	2.41	0.49
1:I:255:PHE:HB3	1:I:363:PRO:HB2	1.94	0.49
1:J:255:PHE:HB3	1:J:363:PRO:HB2	1.94	0.49
1:K:28:GLU:OE1	1:K:88:ARG:NH1	2.45	0.49
1:L:84:THR:CB	4:L:5483:MPD:H52	2.38	0.49
1:A:403:GLU:C	1:A:405:LYS:H	2.14	0.49
1:A:84:THR:CB	4:A:5481:MPD:H52	2.38	0.49
1:B:180:PHE:O	1:C:29:GLN:HA	2.13	0.49
1:B:130:PRO:HB3	1:B:268:MET:CE	2.41	0.49
4:B:5471:MPD:CM	4:B:5471:MPD:O4	2.60	0.49
1:D:403:GLU:C	1:D:405:LYS:H	2.14	0.49
1:E:88:ARG:HD2	5:E:1252:HOH:O	2.13	0.49
1:F:130:PRO:HB3	1:F:268:MET:CE	2.41	0.49
1:G:384:ASN:N	1:G:384:ASN:ND2	2.60	0.49
1:I:130:PRO:HB3	1:I:268:MET:CE	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:335:SER:HB2	1:I:392:MET:O	2.12	0.49
1:J:21:PHE:HA	4:J:5490:MPD:C3	2.36	0.49
1:K:130:PRO:HB3	1:K:268:MET:CE	2.42	0.49
1:K:396:LEU:O	1:K:400:PRO:HG2	2.11	0.49
1:A:88:ARG:HD2	5:A:5553:HOH:O	2.13	0.49
1:B:192:ARG:HD3	1:B:219:ASN:HD22	1.77	0.49
1:C:335:SER:HB2	1:C:392:MET:O	2.12	0.49
1:E:130:PRO:HB3	1:E:268:MET:CE	2.42	0.49
1:E:403:GLU:C	1:E:405:LYS:H	2.14	0.49
1:G:192:ARG:HD3	1:G:219:ASN:HD22	1.77	0.49
1:I:248:ARG:CG	1:I:248:ARG:NH2	2.67	0.49
1:C:454:ARG:O	1:I:320:LYS:HG3	2.11	0.49
1:K:335:SER:HB2	1:K:392:MET:O	2.12	0.49
1:K:84:THR:CB	4:K:5493:MPD:H52	2.40	0.49
1:L:403:GLU:C	1:L:405:LYS:H	2.14	0.49
1:A:396:LEU:O	1:A:400:PRO:HG2	2.11	0.49
1:A:22:THR:CA	4:A:5472:MPD:H11	2.42	0.49
1:H:403:GLU:C	1:H:405:LYS:H	2.14	0.49
1:L:28:GLU:OE1	1:L:88:ARG:NH1	2.45	0.49
1:F:456:THR:O	1:L:458:HIS:HE1	1.96	0.49
1:G:88:ARG:HD2	5:G:5566:HOH:O	2.13	0.49
1:H:399:LEU:CA	1:H:400:PRO:C	2.78	0.49
1:H:22:THR:CA	4:H:5486:MPD:H11	2.42	0.49
1:K:22:THR:CA	4:K:5492:MPD:H11	2.42	0.49
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.77	0.49
1:C:22:THR:CA	4:C:5476:MPD:H11	2.42	0.49
1:E:181:PRO:HD3	1:F:29:GLN:OE1	2.12	0.49
1:E:335:SER:HB2	1:E:392:MET:O	2.12	0.49
1:F:124:VAL:HG13	1:F:274:LEU:HD21	1.94	0.49
1:F:364:ALA:HA	1:L:468:VAL:HG13	1.95	0.49
1:H:21:PHE:HA	4:H:5486:MPD:C3	2.36	0.49
1:H:82:ASP:HB2	4:H:5487:MPD:C3	2.39	0.49
1:G:181:PRO:HD3	1:L:29:GLN:OE1	2.13	0.49
1:L:396:LEU:O	1:L:400:PRO:HG2	2.11	0.49
1:L:88:ARG:HD2	5:L:3296:HOH:O	2.13	0.49
1:D:22:THR:CA	4:D:5478:MPD:H11	2.42	0.49
1:G:181:PRO:HG3	5:L:3356:HOH:O	2.11	0.49
1:C:124:VAL:HG13	1:C:274:LEU:HD21	1.94	0.49
1:E:248:ARG:HH21	1:E:248:ARG:HG3	1.75	0.49
1:F:88:ARG:HD2	5:F:5568:HOH:O	2.13	0.49
1:A:454:ARG:O	1:G:320:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:384:ASN:N	1:I:384:ASN:ND2	2.60	0.49
1:I:88:ARG:HD2	5:I:5579:HOH:O	2.13	0.49
1:E:466:TYR:HA	1:K:256:MET:HG3	1.94	0.49
1:A:384:ASN:N	1:A:384:ASN:ND2	2.60	0.48
1:C:387:HIS:HA	1:C:388:PRO:HD2	1.73	0.48
1:G:22:THR:CA	4:G:5484:MPD:H11	2.42	0.48
1:I:192:ARG:HD3	1:I:219:ASN:HD22	1.77	0.48
1:K:88:ARG:HD2	5:K:3004:HOH:O	2.13	0.48
1:L:248:ARG:HH21	1:L:248:ARG:HG3	1.75	0.48
1:B:306:LYS:HE2	5:B:5572:HOH:O	2.13	0.48
1:B:396:LEU:HB2	1:B:397:TYR:H	1.36	0.48
1:C:384:ASN:ND2	1:C:384:ASN:N	2.60	0.48
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.77	0.48
1:J:306:LYS:HE2	5:J:2729:HOH:O	2.13	0.48
1:K:21:PHE:CB	4:K:5492:MPD:H53	2.27	0.48
1:C:255:PHE:HB3	1:C:363:PRO:HB2	1.94	0.48
1:D:21:PHE:HA	4:D:5478:MPD:C3	2.36	0.48
1:D:22:THR:HG22	1:D:23:ASP:O	2.14	0.48
1:D:396:LEU:HB2	1:D:397:TYR:H	1.36	0.48
1:G:306:LYS:HE2	5:G:5583:HOH:O	2.13	0.48
1:H:88:ARG:HD2	5:H:5577:HOH:O	2.13	0.48
1:J:384:ASN:ND2	1:J:384:ASN:N	2.60	0.48
1:J:22:THR:CA	4:J:5490:MPD:H11	2.42	0.48
1:J:88:ARG:HD2	5:J:2712:HOH:O	2.13	0.48
1:D:84:THR:CB	4:D:5475:MPD:H52	2.41	0.48
1:E:22:THR:HG22	1:E:23:ASP:O	2.14	0.48
1:G:22:THR:HG22	1:G:23:ASP:O	2.14	0.48
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.77	0.48
1:J:399:LEU:CA	1:J:400:PRO:C	2.78	0.48
4:K:5493:MPD:CM	1:L:193:SER:CB	2.84	0.48
1:L:84:THR:HG21	4:L:5483:MPD:H32	1.96	0.48
1:E:179:TYR:CD2	1:F:53:SER:HB2	2.49	0.48
1:G:21:PHE:CB	4:G:5484:MPD:H53	2.27	0.48
1:I:96:THR:HG1	1:I:98:GLN:HB2	1.76	0.48
1:J:398:ASP:OD1	1:J:399:LEU:HD23	2.14	0.48
1:K:329:PRO:O	1:K:342:SER:HB3	2.14	0.48
1:G:255:PHE:HB3	1:G:363:PRO:HB2	1.94	0.48
1:I:22:THR:HG22	1:I:23:ASP:O	2.14	0.48
4:I:5489:MPD:O4	4:I:5489:MPD:CM	2.60	0.48
1:B:329:PRO:O	1:B:342:SER:HB3	2.14	0.48
1:C:22:THR:HG22	1:C:23:ASP:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:PRO:O	1:C:342:SER:HB3	2.14	0.48
1:E:306:LYS:HE2	5:E:1269:HOH:O	2.13	0.48
1:E:398:ASP:OD1	1:E:399:LEU:HD23	2.14	0.48
1:F:458:HIS:HE1	1:L:456:THR:O	1.96	0.48
4:G:5485:MPD:CM	1:H:193:SER:CB	2.84	0.48
1:J:329:PRO:O	1:J:342:SER:HB3	2.14	0.48
1:K:22:THR:HG22	1:K:23:ASP:O	2.14	0.48
1:L:398:ASP:OD1	1:L:399:LEU:HD23	2.14	0.48
1:A:28:GLU:OE1	1:A:88:ARG:NH1	2.45	0.48
1:A:329:PRO:O	1:A:342:SER:HB3	2.14	0.48
1:B:22:THR:HG22	1:B:23:ASP:O	2.14	0.48
1:H:22:THR:HG22	1:H:23:ASP:O	2.14	0.48
1:J:29:GLN:HB3	1:K:180:PHE:CB	2.44	0.48
1:A:398:ASP:OD1	1:A:399:LEU:HD23	2.14	0.48
1:A:180:PHE:O	1:B:29:GLN:HA	2.13	0.48
1:D:329:PRO:O	1:D:342:SER:HB3	2.14	0.48
1:F:329:PRO:O	1:F:342:SER:HB3	2.14	0.48
1:F:364:ALA:HA	1:L:468:VAL:CG1	2.44	0.48
1:H:329:PRO:O	1:H:342:SER:HB3	2.14	0.48
1:H:30:HIS:H	1:I:180:PHE:HB3	1.78	0.48
1:L:329:PRO:O	1:L:342:SER:HB3	2.14	0.48
1:A:22:THR:HG22	1:A:23:ASP:O	2.14	0.48
1:C:398:ASP:OD1	1:C:399:LEU:HD23	2.14	0.48
1:F:360:PHE:CD2	1:F:361:PRO:CD	2.74	0.48
1:J:84:THR:CB	4:J:5491:MPD:H52	2.37	0.48
4:L:5483:MPD:CM	4:L:5483:MPD:O4	2.60	0.48
1:L:84:THR:HG21	4:L:5483:MPD:C3	2.43	0.48
1:A:181:PRO:HD3	1:B:29:GLN:OE1	2.14	0.47
1:B:396:LEU:H	1:B:396:LEU:HG	1.46	0.47
1:C:88:ARG:HD2	5:C:5555:HOH:O	2.13	0.47
1:F:22:THR:HG22	1:F:23:ASP:O	2.14	0.47
1:K:130:PRO:HB3	1:K:268:MET:HE3	1.96	0.47
1:K:328:ALA:HA	1:K:329:PRO:HD3	1.73	0.47
4:K:5493:MPD:O4	1:L:193:SER:OG	2.28	0.47
1:L:306:LYS:HE2	5:L:3313:HOH:O	2.13	0.47
1:D:88:ARG:HD2	5:D:960:HOH:O	2.13	0.47
1:E:384:ASN:N	1:E:384:ASN:ND2	2.60	0.47
1:F:306:LYS:HE2	5:F:5585:HOH:O	2.13	0.47
1:G:398:ASP:OD1	1:G:399:LEU:HD23	2.14	0.47
1:J:124:VAL:HG13	1:J:274:LEU:CD2	2.45	0.47
1:B:398:ASP:OD1	1:B:399:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:VAL:HG13	1:D:274:LEU:CD2	2.45	0.47
1:D:384:ASN:ND2	1:D:384:ASN:N	2.60	0.47
1:E:329:PRO:O	1:E:342:SER:HB3	2.14	0.47
1:E:232:ALA:HB1	1:E:367:PRO:HB2	1.97	0.47
1:G:124:VAL:HG13	1:G:274:LEU:CD2	2.45	0.47
1:J:82:ASP:O	4:J:5491:MPD:H32	2.14	0.47
1:K:306:LYS:HE2	5:K:3021:HOH:O	2.14	0.47
1:K:271:HIS:CD2	1:K:357:GLU:HG3	2.50	0.47
1:B:21:PHE:HA	4:B:5474:MPD:C3	2.36	0.47
1:D:100:TYR:CE2	1:D:102:ARG:HB2	2.50	0.47
1:F:124:VAL:HG13	1:F:274:LEU:CD2	2.45	0.47
1:G:271:HIS:CD2	1:G:357:GLU:HG3	2.50	0.47
1:G:329:PRO:O	1:G:342:SER:HB3	2.14	0.47
1:I:271:HIS:CD2	1:I:357:GLU:HG3	2.50	0.47
1:I:124:VAL:HG13	1:I:274:LEU:CD2	2.45	0.47
1:J:22:THR:HG22	1:J:23:ASP:O	2.13	0.47
1:C:320:LYS:HG3	1:I:454:ARG:O	2.15	0.47
1:C:396:LEU:HB2	1:C:397:TYR:H	1.36	0.47
1:C:465:TYR:O	1:C:468:VAL:HB	2.15	0.47
1:E:193:SER:CB	4:F:5479:MPD:CM	2.84	0.47
1:E:271:HIS:CD2	1:E:357:GLU:HG3	2.50	0.47
1:E:320:LYS:HG3	1:K:454:ARG:O	2.13	0.47
1:G:232:ALA:HB1	1:G:367:PRO:HB2	1.97	0.47
1:K:465:TYR:O	1:K:468:VAL:HB	2.15	0.47
1:L:21:PHE:CB	4:L:5494:MPD:H53	2.27	0.47
1:A:271:HIS:CD2	1:A:357:GLU:HG3	2.50	0.47
1:A:124:VAL:HG13	1:A:274:LEU:CD2	2.45	0.47
1:B:271:HIS:CD2	1:B:357:GLU:HG3	2.50	0.47
1:F:21:PHE:CB	4:F:5482:MPD:H53	2.27	0.47
1:H:28:GLU:OE1	1:H:88:ARG:NH1	2.45	0.47
1:H:306:LYS:HE2	5:H:5594:HOH:O	2.13	0.47
1:J:232:ALA:HB1	1:J:367:PRO:HB2	1.97	0.47
1:K:124:VAL:HG13	1:K:274:LEU:CD2	2.45	0.47
1:A:21:PHE:CB	4:A:5472:MPD:H53	2.27	0.47
1:B:232:ALA:HB1	1:B:367:PRO:HB2	1.97	0.47
1:C:124:VAL:HG13	1:C:274:LEU:CD2	2.45	0.47
1:D:306:LYS:HE2	5:D:977:HOH:O	2.14	0.47
1:D:465:TYR:O	1:D:468:VAL:HB	2.15	0.47
1:F:248:ARG:HG3	1:F:248:ARG:HH21	1.75	0.47
1:J:248:ARG:NH2	1:J:248:ARG:CG	2.66	0.47
1:J:272:MET:HE1	1:J:358:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:22:THR:HG22	1:L:23:ASP:O	2.14	0.47
1:L:80:PHE:CG	4:L:5483:MPD:C1	2.97	0.47
1:A:100:TYR:CE2	1:A:102:ARG:HB2	2.50	0.47
1:C:100:TYR:CE2	1:C:102:ARG:HB2	2.50	0.47
1:C:456:THR:O	1:I:458:HIS:HE1	1.98	0.47
1:D:232:ALA:HB1	1:D:367:PRO:HB2	1.97	0.47
1:E:454:ARG:O	1:K:320:LYS:HG3	2.13	0.47
1:H:232:ALA:HB1	1:H:367:PRO:HB2	1.97	0.47
1:A:193:SER:CB	4:B:5471:MPD:CM	2.84	0.47
1:A:306:LYS:HE2	5:A:5570:HOH:O	2.13	0.47
1:B:28:GLU:OE1	1:B:88:ARG:NH1	2.45	0.47
1:C:232:ALA:HB1	1:C:367:PRO:HB2	1.97	0.47
1:C:455:MET:HG2	1:I:323:VAL:HG11	1.97	0.47
1:F:232:ALA:HB1	1:F:367:PRO:HB2	1.97	0.47
1:G:80:PHE:CA	4:G:5485:MPD:H12	2.42	0.47
1:H:398:ASP:OD1	1:H:399:LEU:HD23	2.14	0.47
1:H:465:TYR:O	1:H:468:VAL:HB	2.15	0.47
1:L:100:TYR:CE2	1:L:102:ARG:HB2	2.50	0.47
1:L:21:PHE:HA	4:L:5494:MPD:C3	2.36	0.47
1:L:272:MET:HE1	1:L:358:VAL:HG21	1.97	0.47
1:B:88:ARG:HD2	5:B:5555:HOH:O	2.13	0.47
1:E:124:VAL:HG13	1:E:274:LEU:CD2	2.45	0.47
1:E:21:PHE:CB	4:E:5480:MPD:H53	2.27	0.47
1:F:100:TYR:CE2	1:F:102:ARG:HB2	2.50	0.47
1:F:398:ASP:OD1	1:F:399:LEU:HD23	2.14	0.47
1:G:100:TYR:CE2	1:G:102:ARG:HB2	2.50	0.47
1:G:28:GLU:OE1	1:G:88:ARG:NH1	2.45	0.47
1:G:465:TYR:O	1:G:468:VAL:HB	2.15	0.47
1:H:328:ALA:HA	1:H:329:PRO:HD3	1.73	0.47
1:I:306:LYS:HE2	5:I:5596:HOH:O	2.13	0.47
1:I:329:PRO:O	1:I:342:SER:HB3	2.14	0.47
1:K:295:LEU:O	1:K:388:PRO:HG2	2.15	0.47
1:L:271:HIS:CD2	1:L:357:GLU:HG3	2.50	0.47
1:A:320:LYS:HG3	1:G:454:ARG:O	2.15	0.47
1:B:100:TYR:CE2	1:B:102:ARG:HB2	2.50	0.47
1:C:256:MET:HG3	1:I:466:TYR:HA	1.97	0.47
1:C:193:SER:OG	4:D:5475:MPD:O4	2.28	0.47
1:E:28:GLU:OE1	1:E:88:ARG:NH1	2.45	0.47
1:A:31:VAL:HG23	1:F:210:HIS:HB3	1.97	0.47
1:I:398:ASP:OD1	1:I:399:LEU:HD23	2.14	0.47
1:J:84:THR:HG21	4:J:5491:MPD:C3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:GLU:OE1	1:J:88:ARG:NH1	2.45	0.47
1:K:368:TYR:OH	4:K:5492:MPD:O2	2.27	0.47
1:L:465:TYR:O	1:L:468:VAL:HB	2.15	0.47
1:A:41:GLU:OE2	1:A:45:GLU:OE2	2.34	0.46
1:A:465:TYR:O	1:A:468:VAL:HB	2.15	0.46
1:C:306:LYS:HE2	5:C:5572:HOH:O	2.13	0.46
1:D:398:ASP:OD1	1:D:399:LEU:HD23	2.14	0.46
1:D:466:TYR:HA	1:J:256:MET:HG3	1.97	0.46
1:D:80:PHE:HD1	4:D:5475:MPD:H52	1.80	0.46
1:F:271:HIS:CD2	1:F:357:GLU:HG3	2.50	0.46
1:K:398:ASP:OD1	1:K:399:LEU:HD23	2.14	0.46
1:K:41:GLU:OE2	1:K:45:GLU:OE2	2.34	0.46
1:L:384:ASN:ND2	1:L:384:ASN:N	2.60	0.46
1:A:181:PRO:HG3	5:B:5611:HOH:O	2.14	0.46
1:E:100:TYR:CE2	1:E:102:ARG:HB2	2.50	0.46
1:H:130:PRO:HB3	1:H:268:MET:HE3	1.96	0.46
5:G:5622:HOH:O	1:H:181:PRO:HG3	2.13	0.46
1:J:100:TYR:CE2	1:J:102:ARG:HB2	2.50	0.46
1:J:80:PHE:CG	4:J:5491:MPD:H53	2.50	0.46
1:K:232:ALA:HB1	1:K:367:PRO:HB2	1.97	0.46
1:L:41:GLU:OE2	1:L:45:GLU:OE2	2.34	0.46
1:A:272:MET:HE1	1:A:358:VAL:HG21	1.98	0.46
1:F:465:TYR:O	1:F:468:VAL:HB	2.15	0.46
1:G:368:TYR:OH	4:G:5484:MPD:O2	2.26	0.46
1:I:465:TYR:O	1:I:468:VAL:HB	2.15	0.46
1:K:248:ARG:HG3	1:K:248:ARG:HH21	1.75	0.46
1:K:80:PHE:CD1	4:K:5493:MPD:H52	2.46	0.46
1:B:295:LEU:O	1:B:388:PRO:HG2	2.15	0.46
1:B:41:GLU:OE2	1:B:45:GLU:OE2	2.34	0.46
1:B:465:TYR:O	1:B:468:VAL:HB	2.15	0.46
1:C:271:HIS:CD2	1:C:357:GLU:HG3	2.50	0.46
1:D:41:GLU:OE2	1:D:45:GLU:OE2	2.34	0.46
1:E:396:LEU:H	1:E:396:LEU:HG	1.46	0.46
1:E:41:GLU:OE2	1:E:45:GLU:OE2	2.34	0.46
1:H:295:LEU:O	1:H:388:PRO:HG2	2.15	0.46
1:H:271:HIS:CD2	1:H:357:GLU:HG3	2.50	0.46
1:H:41:GLU:OE2	1:H:45:GLU:OE2	2.34	0.46
1:I:41:GLU:OE2	1:I:45:GLU:OE2	2.34	0.46
4:I:5489:MPD:CM	1:J:193:SER:CB	2.84	0.46
1:J:271:HIS:CD2	1:J:357:GLU:HG3	2.50	0.46
1:J:465:TYR:O	1:J:468:VAL:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:328:ALA:HA	1:L:329:PRO:HD3	1.73	0.46
1:A:21:PHE:HA	4:A:5472:MPD:C3	2.36	0.46
1:B:130:PRO:HB3	1:B:268:MET:HE3	1.98	0.46
1:I:3:GLU:O	1:I:7:THR:HG23	2.16	0.46
1:L:232:ALA:HB1	1:L:367:PRO:HB2	1.97	0.46
1:B:124:VAL:HG13	1:B:274:LEU:CD2	2.44	0.46
1:D:272:MET:HE1	1:D:358:VAL:HG21	1.97	0.46
1:E:128:PRO:HA	1:E:269:HIS:O	2.16	0.46
1:E:465:TYR:O	1:E:468:VAL:HB	2.15	0.46
1:G:41:GLU:OE2	1:G:45:GLU:OE2	2.34	0.46
1:H:100:TYR:CE2	1:H:102:ARG:HB2	2.50	0.46
1:A:128:PRO:HA	1:A:269:HIS:O	2.16	0.46
1:A:387:HIS:HA	1:A:388:PRO:HD2	1.73	0.46
1:C:88:ARG:NE	4:C:5476:MPD:HM1	2.30	0.46
1:D:271:HIS:CD2	1:D:357:GLU:HG3	2.50	0.46
1:G:3:GLU:O	1:G:7:THR:HG23	2.16	0.46
1:I:100:TYR:CE2	1:I:102:ARG:HB2	2.50	0.46
1:J:41:GLU:OE2	1:J:45:GLU:OE2	2.34	0.46
1:F:454:ARG:O	1:L:320:LYS:HG3	2.16	0.46
1:A:232:ALA:HB1	1:A:367:PRO:HB2	1.97	0.46
1:B:320:LYS:HG3	1:H:454:ARG:O	2.16	0.46
1:F:328:ALA:HA	1:F:329:PRO:HD3	1.73	0.46
1:F:272:MET:HE1	1:F:358:VAL:HG21	1.98	0.46
1:H:128:PRO:HA	1:H:269:HIS:O	2.16	0.46
1:H:124:VAL:HG13	1:H:274:LEU:CD2	2.45	0.46
1:I:21:PHE:CB	4:I:5488:MPD:H53	2.27	0.46
1:J:295:LEU:O	1:J:388:PRO:HG2	2.15	0.46
1:B:88:ARG:NE	4:B:5474:MPD:HM1	2.30	0.46
1:D:3:GLU:O	1:D:7:THR:HG23	2.16	0.46
1:E:295:LEU:O	1:E:388:PRO:HG2	2.15	0.46
1:F:254:THR:HB	1:L:466:TYR:CE1	2.51	0.46
1:F:384:ASN:N	1:F:384:ASN:ND2	2.60	0.46
1:J:84:THR:CG2	4:J:5491:MPD:C5	2.48	0.46
1:K:100:TYR:CE2	1:K:102:ARG:HB2	2.50	0.46
1:B:80:PHE:CB	4:B:5471:MPD:C1	2.65	0.46
1:C:128:PRO:HA	1:C:269:HIS:O	2.16	0.46
1:F:3:GLU:O	1:F:7:THR:HG23	2.16	0.46
1:G:128:PRO:HA	1:G:269:HIS:O	2.16	0.46
1:G:396:LEU:HB2	1:G:397:TYR:H	1.36	0.46
1:I:232:ALA:HB1	1:I:367:PRO:HB2	1.97	0.46
1:J:128:PRO:HA	1:J:269:HIS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3:GLU:O	1:L:7:THR:HG23	2.16	0.46
4:A:5481:MPD:CM	4:A:5481:MPD:O4	2.60	0.45
1:A:3:GLU:O	1:A:7:THR:HG23	2.16	0.45
1:B:313:ASN:HD21	1:B:360:PHE:HD2	1.65	0.45
1:G:80:PHE:HD1	4:G:5485:MPD:H52	1.81	0.45
1:J:3:GLU:O	1:J:7:THR:HG23	2.16	0.45
5:J:2772:HOH:O	1:K:181:PRO:HG3	2.15	0.45
1:L:124:VAL:HG13	1:L:274:LEU:CD2	2.45	0.45
1:A:396:LEU:HG	1:A:396:LEU:H	1.46	0.45
1:A:466:TYR:HA	1:G:256:MET:HG3	1.97	0.45
1:C:41:GLU:OE2	1:C:45:GLU:OE2	2.34	0.45
1:D:80:PHE:CA	4:D:5475:MPD:H12	2.45	0.45
1:E:3:GLU:O	1:E:7:THR:HG23	2.16	0.45
1:F:313:ASN:HD21	1:F:360:PHE:HD2	1.65	0.45
1:F:84:THR:CG2	4:F:5479:MPD:H32	2.46	0.45
1:G:313:ASN:HD21	1:G:360:PHE:HD2	1.65	0.45
1:B:128:PRO:HA	1:B:269:HIS:O	2.16	0.45
1:C:210:HIS:HB3	1:D:31:VAL:HG23	1.99	0.45
1:D:180:PHE:O	1:E:29:GLN:HA	2.16	0.45
1:F:41:GLU:OE2	1:F:45:GLU:OE2	2.34	0.45
1:G:29:GLN:HB3	1:H:180:PHE:CB	2.46	0.45
1:J:21:PHE:CB	4:J:5490:MPD:H53	2.27	0.45
1:J:84:THR:CG2	4:J:5491:MPD:C4	2.88	0.45
1:K:128:PRO:HA	1:K:269:HIS:O	2.16	0.45
1:K:231:LYS:HD2	1:K:231:LYS:HA	1.74	0.45
1:C:28:GLU:OE1	1:C:88:ARG:NH1	2.45	0.45
1:C:3:GLU:O	1:C:7:THR:HG23	2.16	0.45
1:E:180:PHE:O	1:F:29:GLN:HA	2.16	0.45
1:G:80:PHE:CD1	4:G:5485:MPD:H52	2.51	0.45
1:J:313:ASN:HD21	1:J:360:PHE:HD2	1.65	0.45
1:D:128:PRO:HA	1:D:269:HIS:O	2.16	0.45
1:I:128:PRO:HA	1:I:269:HIS:O	2.16	0.45
1:I:328:ALA:HA	1:I:329:PRO:HD3	1.73	0.45
1:K:248:ARG:NH2	1:K:248:ARG:CG	2.66	0.45
1:K:313:ASN:HD21	1:K:360:PHE:HD2	1.65	0.45
1:H:170:GLY:HA2	1:H:172:ARG:HH22	1.81	0.45
1:B:323:VAL:HG11	1:H:455:MET:HG2	1.98	0.45
1:H:3:GLU:O	1:H:7:THR:HG23	2.16	0.45
1:L:295:LEU:O	1:L:388:PRO:HG2	2.15	0.45
1:I:80:PHE:CG	4:I:5489:MPD:H53	2.50	0.45
1:K:3:GLU:O	1:K:7:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:180:PHE:O	1:L:181:PRO:C	2.54	0.45
1:C:80:PHE:CG	4:C:5473:MPD:H12	2.48	0.45
1:H:21:PHE:CB	4:H:5486:MPD:H53	2.27	0.45
1:J:31:VAL:HG23	1:K:210:HIS:HB3	1.98	0.45
1:J:34:PRO:HG2	1:K:206:VAL:O	2.17	0.45
1:A:235:ILE:HA	1:A:235:ILE:HD13	1.82	0.45
1:A:458:HIS:CD2	1:A:459:PRO:HD2	2.52	0.45
1:A:180:PHE:HB2	1:B:29:GLN:HB3	1.99	0.45
1:B:387:HIS:HA	1:B:388:PRO:HD2	1.73	0.45
1:B:454:ARG:O	1:H:320:LYS:HG3	2.17	0.45
1:C:340:SER:HB3	1:C:396:LEU:HB3	1.99	0.45
1:E:84:THR:CB	4:E:5477:MPD:H52	2.41	0.45
1:F:128:PRO:HA	1:F:269:HIS:O	2.16	0.45
1:F:28:GLU:OE1	1:F:88:ARG:NH1	2.45	0.45
1:H:84:THR:CB	4:H:5487:MPD:H52	2.45	0.45
1:I:170:GLY:HA2	1:I:172:ARG:HH22	1.81	0.45
1:K:21:PHE:HA	4:K:5492:MPD:C3	2.36	0.45
1:K:340:SER:HB3	1:K:396:LEU:HB3	1.99	0.45
1:B:340:SER:HB3	1:B:396:LEU:HB3	1.99	0.45
1:D:65:MET:HA	1:D:94:PRO:HG3	1.99	0.45
1:E:340:SER:HB3	1:E:396:LEU:HB3	1.99	0.45
1:G:340:SER:HB3	1:G:396:LEU:HB3	1.99	0.45
1:I:276:LYS:HG2	1:I:277:ASN:ND2	2.33	0.45
1:I:340:SER:HB3	1:I:396:LEU:HB3	1.99	0.45
1:K:458:HIS:CD2	1:K:459:PRO:HD2	2.52	0.45
1:K:84:THR:HG21	4:K:5493:MPD:H32	1.99	0.45
1:L:128:PRO:HA	1:L:269:HIS:O	2.16	0.45
1:A:276:LYS:HG2	1:A:277:ASN:ND2	2.33	0.44
1:A:295:LEU:O	1:A:388:PRO:HG2	2.15	0.44
1:A:340:SER:HB3	1:A:396:LEU:HB3	1.99	0.44
1:D:276:LYS:HG2	1:D:277:ASN:ND2	2.33	0.44
1:D:88:ARG:NE	4:D:5478:MPD:HM1	2.30	0.44
1:E:180:PHE:O	1:E:181:PRO:C	2.54	0.44
1:E:181:PRO:HG3	5:F:5624:HOH:O	2.18	0.44
1:F:25:LYS:NZ	5:F:5746:HOH:O	2.44	0.44
1:L:276:LYS:HG2	1:L:277:ASN:ND2	2.32	0.44
1:B:3:GLU:O	1:B:7:THR:HG23	2.16	0.44
1:C:328:ALA:HA	1:C:329:PRO:HD3	1.73	0.44
1:D:180:PHE:O	1:D:181:PRO:C	2.54	0.44
1:E:458:HIS:CD2	1:E:459:PRO:HD2	2.52	0.44
1:G:276:LYS:HG2	1:G:277:ASN:ND2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:313:ASN:HD21	1:L:360:PHE:HD2	1.65	0.44
1:A:65:MET:HA	1:A:94:PRO:HG3	2.00	0.44
1:D:295:LEU:O	1:D:388:PRO:HG2	2.15	0.44
1:D:320:LYS:HG3	1:J:454:ARG:O	2.18	0.44
1:D:458:HIS:CD2	1:D:459:PRO:HD2	2.52	0.44
1:E:313:ASN:HD21	1:E:360:PHE:HD2	1.65	0.44
1:J:340:SER:HB3	1:J:396:LEU:HB3	1.99	0.44
1:J:88:ARG:NE	4:J:5490:MPD:HM1	2.30	0.44
1:A:328:ALA:HA	1:A:329:PRO:HD3	1.73	0.44
1:C:80:PHE:CG	4:C:5473:MPD:H53	2.51	0.44
1:E:215:THR:O	1:E:216:ALA:HB3	2.18	0.44
1:G:180:PHE:O	1:G:181:PRO:C	2.54	0.44
1:I:295:LEU:O	1:I:388:PRO:HG2	2.15	0.44
1:K:65:MET:HA	1:K:94:PRO:HG3	2.00	0.44
1:A:215:THR:O	1:A:216:ALA:HB3	2.18	0.44
1:A:313:ASN:HD21	1:A:360:PHE:HD2	1.65	0.44
1:B:170:GLY:HA2	1:B:172:ARG:HH22	1.81	0.44
1:B:276:LYS:HG2	1:B:277:ASN:ND2	2.33	0.44
1:B:458:HIS:CD2	1:B:459:PRO:HD2	2.52	0.44
1:C:17:VAL:HG12	1:C:19:LEU:HD13	2.00	0.44
1:F:88:ARG:NE	4:F:5482:MPD:HM1	2.30	0.44
1:H:458:HIS:CD2	1:H:459:PRO:HD2	2.52	0.44
1:L:215:THR:O	1:L:216:ALA:HB3	2.18	0.44
1:A:17:VAL:HG12	1:A:19:LEU:HD13	2.00	0.44
1:A:396:LEU:HB2	1:A:397:TYR:H	1.36	0.44
1:C:313:ASN:HD21	1:C:360:PHE:HD2	1.64	0.44
1:E:21:PHE:HA	4:E:5480:MPD:C3	2.36	0.44
1:E:130:PRO:HB3	1:E:268:MET:HE3	1.98	0.44
1:E:272:MET:HE1	1:E:358:VAL:HG21	1.99	0.44
1:F:295:LEU:O	1:F:388:PRO:HG2	2.15	0.44
1:G:130:PRO:HB3	1:G:268:MET:HE3	1.99	0.44
1:H:88:ARG:NE	4:H:5486:MPD:HM1	2.30	0.44
1:H:61:ASN:O	1:I:337:ARG:CB	2.50	0.44
1:I:309:ASN:HD22	1:I:313:ASN:HD22	1.66	0.44
1:J:80:PHE:CG	4:J:5491:MPD:C1	3.00	0.44
1:J:73:THR:HG21	1:J:88:ARG:HB3	2.00	0.44
1:C:180:PHE:O	1:C:181:PRO:C	2.54	0.44
1:C:275:ALA:HA	1:C:281:LEU:HD13	2.00	0.44
1:D:193:SER:CB	4:E:5477:MPD:CM	2.84	0.44
1:D:84:THR:CG2	4:D:5475:MPD:H32	2.48	0.44
1:F:180:PHE:O	1:F:181:PRO:C	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:275:ALA:HA	1:F:281:LEU:HD13	2.00	0.44
1:F:340:SER:HB3	1:F:396:LEU:HB3	1.99	0.44
1:G:275:ALA:HA	1:G:281:LEU:HD13	2.00	0.44
1:G:458:HIS:CD2	1:G:459:PRO:HD2	2.52	0.44
4:G:5485:MPD:O4	1:H:193:SER:OG	2.28	0.44
1:H:215:THR:O	1:H:216:ALA:HB3	2.18	0.44
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.74	0.44
1:I:231:LYS:HD2	1:I:231:LYS:HA	1.74	0.44
1:I:275:ALA:HA	1:I:281:LEU:HD13	2.00	0.44
1:I:65:MET:HA	1:I:94:PRO:HG3	2.00	0.44
1:K:17:VAL:HG12	1:K:19:LEU:HD13	2.00	0.44
1:K:276:LYS:HG2	1:K:277:ASN:ND2	2.32	0.44
1:L:458:HIS:CD2	1:L:459:PRO:HD2	2.53	0.44
1:A:130:PRO:HB3	1:A:268:MET:HE3	1.99	0.44
1:B:73:THR:HG21	1:B:88:ARG:HB3	2.00	0.44
1:C:272:MET:HE1	1:C:358:VAL:HG21	2.00	0.44
1:C:458:HIS:CD2	1:C:459:PRO:HD2	2.53	0.44
1:E:276:LYS:HG2	1:E:277:ASN:ND2	2.33	0.44
1:F:231:LYS:HA	1:F:231:LYS:HD2	1.74	0.44
1:G:17:VAL:HG12	1:G:19:LEU:HD13	2.00	0.44
1:G:309:ASN:HD22	1:G:313:ASN:HD22	1.66	0.44
1:K:215:THR:O	1:K:216:ALA:HB3	2.18	0.44
1:G:180:PHE:CB	1:L:29:GLN:HB3	2.48	0.44
1:B:231:LYS:HA	1:B:231:LYS:HD2	1.74	0.44
1:C:295:LEU:O	1:C:388:PRO:HG2	2.15	0.44
1:D:309:ASN:HD22	1:D:313:ASN:HD22	1.66	0.44
1:E:17:VAL:HG12	1:E:19:LEU:HD13	2.00	0.44
1:E:309:ASN:HD22	1:E:313:ASN:HD22	1.66	0.44
1:A:139:ARG:HD3	1:F:163:LYS:HG2	1.99	0.44
1:H:340:SER:HB3	1:H:396:LEU:HB3	1.99	0.44
1:I:215:THR:O	1:I:216:ALA:HB3	2.18	0.44
1:I:313:ASN:HD21	1:I:360:PHE:HD2	1.64	0.44
1:C:276:LYS:HG2	1:C:277:ASN:ND2	2.32	0.43
1:D:215:THR:O	1:D:216:ALA:HB3	2.18	0.43
1:F:125:LEU:O	1:F:272:MET:HA	2.18	0.43
1:F:458:HIS:CD2	1:F:459:PRO:HD2	2.52	0.43
1:F:82:ASP:O	4:F:5479:MPD:H32	2.18	0.43
1:G:65:MET:HA	1:G:94:PRO:HG3	2.00	0.43
1:H:313:ASN:HD21	1:H:360:PHE:HD2	1.65	0.43
1:H:65:MET:HA	1:H:94:PRO:HG3	2.00	0.43
1:I:458:HIS:CD2	1:I:459:PRO:HD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:VAL:HG13	1:J:364:ALA:HA	1.99	0.43
1:B:125:LEU:O	1:B:272:MET:HA	2.19	0.43
1:B:344:ARG:NH1	1:B:346:PRO:HA	2.34	0.43
1:C:215:THR:O	1:C:216:ALA:HB3	2.18	0.43
1:E:344:ARG:NH1	1:E:346:PRO:HA	2.34	0.43
4:E:5477:MPD:O4	4:E:5477:MPD:CM	2.60	0.43
1:F:396:LEU:HB2	1:F:397:TYR:H	1.36	0.43
1:F:73:THR:HG21	1:F:88:ARG:HB3	2.00	0.43
4:G:5485:MPD:H11	1:H:189:GLN:CG	2.48	0.43
1:H:137:ASP:HB3	1:H:152:ASP:HB3	2.01	0.43
1:H:17:VAL:HG12	1:H:19:LEU:HD13	2.00	0.43
1:J:170:GLY:HA2	1:J:172:ARG:HH22	1.81	0.43
1:J:215:THR:O	1:J:216:ALA:HB3	2.18	0.43
1:J:458:HIS:CD2	1:J:459:PRO:HD2	2.52	0.43
1:K:235:ILE:HA	1:K:235:ILE:HD13	1.82	0.43
1:L:236:GLN:HA	1:L:236:GLN:OE1	2.19	0.43
1:A:189:GLN:CG	4:B:5471:MPD:H11	2.48	0.43
1:A:125:LEU:O	1:A:272:MET:HA	2.19	0.43
1:A:344:ARG:NH1	1:A:346:PRO:HA	2.34	0.43
1:B:272:MET:HE1	1:B:358:VAL:HG21	2.00	0.43
1:B:21:PHE:CB	4:B:5474:MPD:H53	2.27	0.43
1:C:235:ILE:HA	1:C:235:ILE:HD13	1.82	0.43
1:D:468:VAL:CG1	1:J:364:ALA:HA	2.49	0.43
1:D:189:GLN:CG	4:E:5477:MPD:H11	2.48	0.43
1:F:17:VAL:HG12	1:F:19:LEU:HD13	2.00	0.43
1:F:215:THR:O	1:F:216:ALA:HB3	2.18	0.43
1:F:236:GLN:OE1	1:F:236:GLN:HA	2.19	0.43
1:F:256:MET:CG	1:L:466:TYR:HA	2.49	0.43
1:G:236:GLN:OE1	1:G:236:GLN:HA	2.19	0.43
1:G:272:MET:HE1	1:G:358:VAL:HG21	2.00	0.43
1:H:344:ARG:NH1	1:H:346:PRO:HA	2.34	0.43
1:I:88:ARG:NE	4:I:5488:MPD:HM1	2.30	0.43
1:J:17:VAL:HG12	1:J:19:LEU:HD13	2.00	0.43
1:J:125:LEU:O	1:J:272:MET:HA	2.19	0.43
1:J:276:LYS:HG2	1:J:277:ASN:ND2	2.33	0.43
1:K:236:GLN:OE1	1:K:236:GLN:HA	2.19	0.43
1:B:65:MET:HA	1:B:94:PRO:HG3	2.00	0.43
1:C:125:LEU:O	1:C:272:MET:HA	2.19	0.43
1:C:65:MET:HA	1:C:94:PRO:HG3	2.00	0.43
1:D:344:ARG:NH1	1:D:346:PRO:HA	2.34	0.43
1:D:313:ASN:HD21	1:D:360:PHE:HD2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:276:LYS:HG2	1:F:277:ASN:ND2	2.33	0.43
1:H:236:GLN:OE1	1:H:236:GLN:HA	2.19	0.43
1:H:276:LYS:HG2	1:H:277:ASN:ND2	2.33	0.43
1:H:309:ASN:HD22	1:H:313:ASN:HD22	1.66	0.43
1:I:344:ARG:NH1	1:I:346:PRO:HA	2.34	0.43
1:J:236:GLN:OE1	1:J:236:GLN:HA	2.19	0.43
4:J:5491:MPD:H11	1:K:189:GLN:CG	2.48	0.43
1:K:275:ALA:HA	1:K:281:LEU:HD13	2.00	0.43
1:L:344:ARG:NH1	1:L:346:PRO:HA	2.34	0.43
1:L:396:LEU:HB2	1:L:397:TYR:H	1.36	0.43
4:L:5483:MPD:C1	4:L:5483:MPD:H53	2.48	0.43
1:L:65:MET:HA	1:L:94:PRO:HG3	2.00	0.43
1:A:309:ASN:HD22	1:A:313:ASN:HD22	1.66	0.43
1:B:215:THR:O	1:B:216:ALA:HB3	2.18	0.43
1:A:180:PHE:CB	1:B:29:GLN:HB3	2.49	0.43
1:B:309:ASN:HD22	1:B:313:ASN:HD22	1.66	0.43
1:C:236:GLN:HA	1:C:236:GLN:OE1	2.19	0.43
1:D:170:GLY:HA2	1:D:172:ARG:HH22	1.81	0.43
1:D:275:ALA:HA	1:D:281:LEU:HD13	2.00	0.43
1:D:73:THR:HG21	1:D:88:ARG:HB3	2.00	0.43
1:J:387:HIS:HA	1:J:388:PRO:HD2	1.73	0.43
1:K:309:ASN:HD22	1:K:313:ASN:HD22	1.66	0.43
4:K:5493:MPD:H11	1:L:189:GLN:CG	2.48	0.43
1:D:137:ASP:HB3	1:D:152:ASP:HB3	2.01	0.43
1:D:125:LEU:O	1:D:272:MET:HA	2.19	0.43
1:E:125:LEU:O	1:E:272:MET:HA	2.19	0.43
1:G:231:LYS:HA	1:G:231:LYS:HD2	1.74	0.43
1:I:73:THR:HG21	1:I:88:ARG:HB3	2.00	0.43
1:L:125:LEU:O	1:L:272:MET:HA	2.19	0.43
1:A:236:GLN:HA	1:A:236:GLN:OE1	2.19	0.43
1:A:29:GLN:HB3	1:F:180:PHE:HB2	2.00	0.43
1:A:80:PHE:CB	4:A:5481:MPD:C1	2.75	0.43
1:B:320:LYS:HG2	1:H:455:MET:O	2.19	0.43
1:D:368:TYR:OH	4:D:5478:MPD:O2	2.27	0.43
1:E:231:LYS:HD2	1:E:231:LYS:HA	1.74	0.43
1:E:275:ALA:HA	1:E:281:LEU:HD13	2.00	0.43
1:F:309:ASN:HD22	1:F:313:ASN:HD22	1.66	0.43
1:F:65:MET:HA	1:F:94:PRO:HG3	2.00	0.43
1:H:396:LEU:H	1:H:396:LEU:HG	1.46	0.43
4:H:5487:MPD:O4	4:H:5487:MPD:CM	2.60	0.43
4:I:5489:MPD:H11	1:J:189:GLN:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:80:PHE:CD1	4:J:5491:MPD:H52	2.44	0.43
1:J:65:MET:HA	1:J:94:PRO:HG3	1.99	0.43
1:K:25:LYS:NZ	5:K:3196:HOH:O	2.44	0.43
1:B:236:GLN:HA	1:B:236:GLN:OE1	2.19	0.43
1:D:340:SER:HB3	1:D:396:LEU:HB3	1.99	0.43
1:E:137:ASP:HB3	1:E:152:ASP:HB3	2.01	0.43
1:F:137:ASP:HB3	1:F:152:ASP:HB3	2.01	0.43
4:A:5481:MPD:CM	1:F:193:SER:CB	2.84	0.43
1:G:344:ARG:NH1	1:G:346:PRO:HA	2.34	0.43
1:G:73:THR:HG21	1:G:88:ARG:HB3	2.00	0.43
1:H:180:PHE:O	1:H:181:PRO:C	2.54	0.43
1:I:130:PRO:HB3	1:I:268:MET:HE3	2.01	0.43
1:H:29:GLN:HB3	1:I:180:PHE:CB	2.49	0.43
4:H:5487:MPD:CM	1:I:193:SER:CB	2.84	0.43
1:I:17:VAL:HG12	1:I:19:LEU:HD13	2.00	0.43
1:J:25:LYS:NZ	5:J:2904:HOH:O	2.44	0.43
1:J:275:ALA:HA	1:J:281:LEU:HD13	2.00	0.43
1:L:137:ASP:HB3	1:L:152:ASP:HB3	2.01	0.43
1:L:275:ALA:HA	1:L:281:LEU:HD13	2.00	0.43
1:L:334:TYR:HA	1:L:343:ILE:O	2.19	0.43
1:L:88:ARG:NE	4:L:5494:MPD:HM1	2.30	0.43
1:L:2:ALA:O	1:L:6:LEU:HD12	2.19	0.43
1:A:275:ALA:HA	1:A:281:LEU:HD13	2.00	0.43
1:B:275:ALA:HA	1:B:281:LEU:HD13	2.00	0.43
1:C:231:LYS:HA	1:C:231:LYS:HD2	1.74	0.43
4:C:5473:MPD:CM	4:C:5473:MPD:O4	2.60	0.43
1:C:189:GLN:CG	4:D:5475:MPD:H11	2.48	0.43
1:D:21:PHE:CB	4:D:5478:MPD:H53	2.27	0.43
1:D:2:ALA:O	1:D:6:LEU:HD12	2.19	0.43
1:I:236:GLN:HA	1:I:236:GLN:OE1	2.19	0.43
1:K:396:LEU:HG	1:K:396:LEU:H	1.46	0.43
1:L:340:SER:HB3	1:L:396:LEU:HB3	1.99	0.43
1:L:73:THR:HG21	1:L:88:ARG:HB3	2.00	0.43
1:C:2:ALA:O	1:C:6:LEU:HD12	2.19	0.43
1:C:309:ASN:HD22	1:C:313:ASN:HD22	1.66	0.43
1:C:73:THR:HG21	1:C:88:ARG:HB3	2.00	0.43
1:F:130:PRO:HB3	1:F:268:MET:HE3	2.01	0.43
1:F:466:TYR:HA	1:L:256:MET:HG3	2.01	0.43
1:F:2:ALA:O	1:F:6:LEU:HD12	2.19	0.43
1:G:125:LEU:O	1:G:272:MET:HA	2.19	0.43
1:G:88:ARG:NE	4:G:5484:MPD:HM1	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:ALA:O	1:H:6:LEU:HD12	2.19	0.43
1:H:334:TYR:HA	1:H:343:ILE:O	2.19	0.43
1:I:2:ALA:O	1:I:6:LEU:HD12	2.19	0.43
1:K:125:LEU:O	1:K:272:MET:HA	2.19	0.43
1:K:80:PHE:CG	4:K:5493:MPD:H12	2.48	0.43
1:K:139:ARG:HD3	1:L:163:LYS:HG2	2.01	0.43
1:G:189:GLN:CG	4:L:5483:MPD:H11	2.48	0.43
1:A:2:ALA:O	1:A:6:LEU:HD12	2.19	0.42
1:B:466:TYR:HA	1:H:256:MET:HG3	2.02	0.42
1:C:334:TYR:HA	1:C:343:ILE:O	2.19	0.42
1:C:80:PHE:CG	4:C:5473:MPD:C1	3.01	0.42
1:D:80:PHE:CB	4:D:5475:MPD:C1	2.68	0.42
1:D:80:PHE:CD1	4:D:5475:MPD:H52	2.51	0.42
1:E:2:ALA:O	1:E:6:LEU:HD12	2.19	0.42
1:E:334:TYR:HA	1:E:343:ILE:O	2.19	0.42
1:F:170:GLY:HA2	1:F:172:ARG:HH22	1.81	0.42
1:G:215:THR:O	1:G:216:ALA:HB3	2.18	0.42
1:I:272:MET:HE1	1:I:358:VAL:HG21	2.01	0.42
1:I:387:HIS:HA	1:I:388:PRO:HD2	1.73	0.42
1:J:390:GLU:HA	1:J:391:PRO:HD3	1.89	0.42
1:J:84:THR:HG21	4:J:5491:MPD:H32	2.01	0.42
1:K:344:ARG:NH1	1:K:346:PRO:HA	2.34	0.42
1:K:29:GLN:HB3	1:L:180:PHE:CB	2.49	0.42
1:K:31:VAL:HG23	1:L:210:HIS:HB3	2.01	0.42
1:A:73:THR:HG21	1:A:88:ARG:HB3	2.00	0.42
1:B:390:GLU:HA	1:B:391:PRO:HD3	1.89	0.42
1:C:170:GLY:HA2	1:C:172:ARG:HH22	1.81	0.42
1:E:65:MET:HA	1:E:94:PRO:HG3	2.00	0.42
1:A:29:GLN:HB3	1:F:180:PHE:CB	2.49	0.42
1:A:30:HIS:HB3	1:F:182:VAL:HG12	2.01	0.42
1:H:125:LEU:O	1:H:272:MET:HA	2.19	0.42
1:J:334:TYR:HA	1:J:343:ILE:O	2.19	0.42
1:J:344:ARG:NH1	1:J:346:PRO:HA	2.33	0.42
1:K:396:LEU:HB2	1:K:397:TYR:H	1.36	0.42
1:K:73:THR:HG21	1:K:88:ARG:HB3	2.00	0.42
1:A:88:ARG:NE	4:A:5472:MPD:HM1	2.30	0.42
1:D:334:TYR:HA	1:D:343:ILE:O	2.19	0.42
1:E:25:LYS:NZ	5:E:1444:HOH:O	2.44	0.42
1:E:458:HIS:HE1	1:K:456:THR:O	2.03	0.42
4:A:5481:MPD:H11	1:F:189:GLN:CG	2.49	0.42
1:H:275:ALA:HA	1:H:281:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:THR:HG21	1:H:88:ARG:HB3	2.00	0.42
1:I:137:ASP:HB3	1:I:152:ASP:HB3	2.01	0.42
1:I:332:LEU:HB2	1:I:408:PRO:CB	2.50	0.42
1:J:137:ASP:HB3	1:J:152:ASP:HB3	2.01	0.42
1:J:2:ALA:O	1:J:6:LEU:HD12	2.19	0.42
1:K:2:ALA:O	1:K:6:LEU:HD12	2.19	0.42
1:A:138:ILE:HG23	1:A:138:ILE:O	2.20	0.42
4:A:5481:MPD:H53	4:A:5481:MPD:C1	2.48	0.42
4:C:5473:MPD:H53	4:C:5473:MPD:C1	2.48	0.42
1:E:88:ARG:NE	4:E:5480:MPD:HM1	2.30	0.42
1:F:334:TYR:HA	1:F:343:ILE:O	2.19	0.42
1:G:138:ILE:O	1:G:138:ILE:HG23	2.20	0.42
1:G:193:SER:CB	4:L:5483:MPD:CM	2.84	0.42
1:G:334:TYR:HA	1:G:343:ILE:O	2.19	0.42
1:I:180:PHE:O	1:I:181:PRO:C	2.54	0.42
1:I:125:LEU:O	1:I:272:MET:HA	2.19	0.42
1:J:130:PRO:HB3	1:J:268:MET:HE2	2.02	0.42
1:J:180:PHE:O	1:J:181:PRO:C	2.54	0.42
1:K:80:PHE:CG	4:K:5493:MPD:C1	3.01	0.42
1:L:17:VAL:HG12	1:L:19:LEU:HD13	2.00	0.42
1:A:364:ALA:HA	1:G:468:VAL:HG13	2.01	0.42
1:B:332:LEU:HB2	1:B:408:PRO:CB	2.50	0.42
1:B:384:ASN:ND2	1:B:384:ASN:N	2.60	0.42
1:C:344:ARG:NH1	1:C:346:PRO:HA	2.34	0.42
1:F:332:LEU:HB2	1:F:408:PRO:CB	2.50	0.42
1:F:396:LEU:H	1:F:396:LEU:HG	1.46	0.42
1:K:138:ILE:O	1:K:138:ILE:HG23	2.20	0.42
1:K:170:GLY:HA2	1:K:172:ARG:HH22	1.81	0.42
1:K:29:GLN:HB3	1:L:180:PHE:HB2	2.01	0.42
1:L:309:ASN:HD22	1:L:313:ASN:HD22	1.66	0.42
1:B:17:VAL:HG12	1:B:19:LEU:HD13	2.00	0.42
1:B:25:LYS:NZ	5:B:5734:HOH:O	2.44	0.42
1:B:334:TYR:HA	1:B:343:ILE:O	2.19	0.42
1:C:137:ASP:HB3	1:C:152:ASP:HB3	2.01	0.42
1:C:281:LEU:HB3	1:C:293:GLN:OE1	2.20	0.42
1:E:138:ILE:HG23	1:E:138:ILE:O	2.20	0.42
1:E:236:GLN:OE1	1:E:236:GLN:HA	2.19	0.42
1:F:344:ARG:NH1	1:F:346:PRO:HA	2.34	0.42
1:I:138:ILE:HG23	1:I:138:ILE:O	2.20	0.42
1:I:334:TYR:HA	1:I:343:ILE:O	2.19	0.42
1:K:137:ASP:HB3	1:K:152:ASP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASP:HB3	1:A:152:ASP:HB3	2.01	0.42
1:B:281:LEU:HB3	1:B:293:GLN:OE1	2.20	0.42
1:D:192:ARG:NH2	1:D:219:ASN:ND2	2.63	0.42
1:D:454:ARG:O	1:J:320:LYS:HG3	2.20	0.42
1:G:170:GLY:HA2	1:G:172:ARG:HH22	1.81	0.42
1:A:256:MET:CG	1:G:466:TYR:HA	2.49	0.42
1:J:309:ASN:HD22	1:J:313:ASN:HD22	1.66	0.42
1:K:84:THR:HG21	4:K:5493:MPD:C3	2.48	0.42
1:L:130:PRO:HB3	1:L:268:MET:HE3	2.01	0.42
1:L:80:PHE:CG	4:L:5483:MPD:H53	2.53	0.42
1:A:170:GLY:HA2	1:A:172:ARG:HH22	1.81	0.42
1:A:281:LEU:HB3	1:A:293:GLN:OE1	2.20	0.42
1:B:137:ASP:HB3	1:B:152:ASP:HB3	2.01	0.42
1:B:189:GLN:CG	4:C:5473:MPD:H11	2.49	0.42
1:D:17:VAL:HG12	1:D:19:LEU:HD13	2.00	0.42
1:D:332:LEU:HB2	1:D:408:PRO:CB	2.50	0.42
1:E:281:LEU:HB3	1:E:293:GLN:OE1	2.20	0.42
1:E:456:THR:O	1:K:458:HIS:HE1	2.02	0.42
1:A:53:SER:CB	1:F:179:TYR:CD2	3.01	0.42
1:G:137:ASP:HB3	1:G:152:ASP:HB3	2.01	0.42
1:H:281:LEU:HB3	1:H:293:GLN:OE1	2.20	0.42
1:I:281:LEU:HB3	1:I:293:GLN:OE1	2.20	0.42
1:L:170:GLY:HA2	1:L:172:ARG:HH22	1.81	0.42
1:G:180:PHE:HB2	1:L:29:GLN:HB3	2.00	0.42
1:D:181:PRO:HG3	5:E:1312:HOH:O	2.19	0.42
1:D:256:MET:HG3	1:J:466:TYR:HA	2.02	0.42
1:G:295:LEU:O	1:G:388:PRO:HG2	2.15	0.42
1:J:138:ILE:O	1:J:138:ILE:HG23	2.20	0.42
1:L:231:LYS:HA	1:L:231:LYS:HD2	1.74	0.42
1:L:281:LEU:HB3	1:L:293:GLN:OE1	2.20	0.42
1:L:332:LEU:HD12	1:L:332:LEU:HA	1.90	0.42
1:L:387:HIS:HA	1:L:388:PRO:HD2	1.73	0.42
1:A:84:THR:CG2	4:A:5481:MPD:H32	2.50	0.42
1:B:138:ILE:HG23	1:B:138:ILE:O	2.20	0.42
4:B:5474:MPD:H4	4:B:5474:MPD:H12	1.82	0.42
1:C:396:LEU:HG	1:C:396:LEU:H	1.46	0.42
1:C:84:THR:CG2	4:C:5473:MPD:H32	2.49	0.42
1:E:272:MET:HE1	1:E:358:VAL:CG2	2.50	0.42
1:E:73:THR:HG21	1:E:88:ARG:HB3	2.00	0.42
1:F:192:ARG:NH2	1:F:219:ASN:ND2	2.63	0.42
1:H:332:LEU:HB2	1:H:408:PRO:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:PHE:HD1	3:C:4473:ADP:O2'	2.03	0.41
1:C:332:LEU:HB2	1:C:408:PRO:CB	2.50	0.41
1:D:281:LEU:HB3	1:D:293:GLN:OE1	2.20	0.41
1:E:170:GLY:HA2	1:E:172:ARG:HH22	1.81	0.41
1:G:68:MET:HA	1:G:69:PRO:HD2	1.95	0.41
1:J:332:LEU:HA	1:J:332:LEU:HD12	1.90	0.41
1:K:281:LEU:HB3	1:K:293:GLN:OE1	2.20	0.41
1:K:334:TYR:HA	1:K:343:ILE:O	2.19	0.41
1:A:334:TYR:HA	1:A:343:ILE:O	2.19	0.41
1:A:296:TYR:HB3	1:A:382:ILE:HA	2.03	0.41
1:A:456:THR:O	1:G:458:HIS:HE1	2.02	0.41
1:B:91:ILE:HB	1:B:103:ASP:HB2	2.02	0.41
1:C:433:VAL:HG12	1:C:434:PHE:CD2	2.55	0.41
1:D:138:ILE:O	1:D:138:ILE:HG23	2.20	0.41
1:A:364:ALA:HA	1:G:468:VAL:CG1	2.50	0.41
1:G:91:ILE:HB	1:G:103:ASP:HB2	2.02	0.41
1:I:84:THR:CG2	4:I:5489:MPD:H32	2.50	0.41
1:K:180:PHE:O	1:K:181:PRO:C	2.54	0.41
4:J:5491:MPD:CM	1:K:193:SER:CB	2.84	0.41
1:K:192:ARG:NH2	1:K:219:ASN:ND2	2.63	0.41
1:L:230:LYS:O	1:L:234:GLU:HG3	2.20	0.41
1:L:433:VAL:HG12	1:L:434:PHE:CD2	2.55	0.41
1:A:180:PHE:O	1:A:181:PRO:C	2.54	0.41
1:E:296:TYR:HB3	1:E:382:ILE:HA	2.03	0.41
1:F:138:ILE:O	1:F:138:ILE:HG23	2.20	0.41
1:F:433:VAL:HG12	1:F:434:PHE:CD2	2.55	0.41
1:G:281:LEU:HB3	1:G:293:GLN:OE1	2.20	0.41
1:G:433:VAL:HG12	1:G:434:PHE:CD2	2.56	0.41
1:H:138:ILE:O	1:H:138:ILE:HG23	2.20	0.41
4:H:5487:MPD:H11	1:I:189:GLN:CG	2.48	0.41
1:K:88:ARG:NE	4:K:5492:MPD:HM1	2.30	0.41
1:L:225:PHE:HD1	3:L:4482:ADP:O2'	2.03	0.41
1:C:296:TYR:HB3	1:C:382:ILE:HA	2.03	0.41
1:G:2:ALA:O	1:G:6:LEU:HD12	2.19	0.41
1:H:25:LYS:NZ	5:H:5752:HOH:O	2.44	0.41
1:H:80:PHE:CG	4:H:5487:MPD:H53	2.50	0.41
1:F:230:LYS:O	1:F:234:GLU:HG3	2.21	0.41
1:F:91:ILE:HB	1:F:103:ASP:HB2	2.03	0.41
1:H:433:VAL:HG12	1:H:434:PHE:CD2	2.55	0.41
1:K:225:PHE:HD1	3:K:4481:ADP:O2'	2.03	0.41
1:K:332:LEU:HB2	1:K:408:PRO:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PHE:HD1	3:A:4471:ADP:O2'	2.03	0.41
1:A:403:GLU:C	1:A:405:LYS:N	2.74	0.41
1:B:254:THR:HB	1:H:466:TYR:CE1	2.56	0.41
1:C:138:ILE:O	1:C:138:ILE:HG23	2.20	0.41
1:C:390:GLU:HA	1:C:391:PRO:HD3	1.89	0.41
1:C:403:GLU:C	1:C:405:LYS:N	2.74	0.41
1:D:236:GLN:OE1	1:D:236:GLN:HA	2.19	0.41
1:F:281:LEU:HB3	1:F:293:GLN:OE1	2.20	0.41
1:F:318:SER:OG	1:F:362:ASP:OD2	2.27	0.41
1:G:231:LYS:HE2	5:G:5504:HOH:O	2.21	0.41
1:I:231:LYS:HE2	5:I:5517:HOH:O	2.21	0.41
1:I:396:LEU:H	1:I:396:LEU:HG	1.46	0.41
1:I:433:VAL:HG12	1:I:434:PHE:CD2	2.55	0.41
1:K:91:ILE:HB	1:K:103:ASP:HB2	2.03	0.41
1:L:332:LEU:HB2	1:L:408:PRO:CB	2.50	0.41
1:E:225:PHE:HD1	3:E:4475:ADP:O2'	2.03	0.41
1:E:80:PHE:CB	4:E:5477:MPD:C1	2.76	0.41
1:F:296:TYR:HB3	1:F:382:ILE:HA	2.03	0.41
1:A:458:HIS:HE1	1:G:456:THR:O	2.03	0.41
1:H:230:LYS:O	1:H:234:GLU:HG3	2.20	0.41
1:H:384:ASN:N	1:H:384:ASN:ND2	2.60	0.41
1:I:296:TYR:HB3	1:I:382:ILE:HA	2.03	0.41
1:J:230:LYS:O	1:J:234:GLU:HG3	2.21	0.41
1:J:281:LEU:HB3	1:J:293:GLN:OE1	2.20	0.41
1:J:396:LEU:HG	1:J:396:LEU:H	1.46	0.41
1:J:433:VAL:HG12	1:J:434:PHE:CD2	2.55	0.41
1:J:91:ILE:HB	1:J:103:ASP:HB2	2.03	0.41
1:K:272:MET:HE1	1:K:358:VAL:HG21	2.01	0.41
1:F:320:LYS:HG3	1:L:454:ARG:O	2.21	0.41
1:L:91:ILE:HB	1:L:103:ASP:HB2	2.02	0.41
1:B:230:LYS:O	1:B:234:GLU:HG3	2.20	0.41
1:C:130:PRO:HB3	1:C:268:MET:HE3	2.02	0.41
1:C:231:LYS:HE2	5:C:5493:HOH:O	2.21	0.41
1:B:206:VAL:O	1:C:34:PRO:HG2	2.20	0.41
1:D:225:PHE:HD1	3:D:4474:ADP:O2'	2.03	0.41
1:G:296:TYR:HB3	1:G:382:ILE:HA	2.03	0.41
1:H:114:TYR:O	1:H:118:THR:HG23	2.21	0.41
1:H:296:TYR:HB3	1:H:382:ILE:HA	2.03	0.41
1:I:225:PHE:HD1	3:I:4479:ADP:O2'	2.03	0.41
1:J:231:LYS:HE2	5:J:2640:HOH:O	2.21	0.41
1:J:296:TYR:HB3	1:J:382:ILE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:5491:MPD:C1	4:J:5491:MPD:H53	2.48	0.41
1:K:403:GLU:C	1:K:405:LYS:N	2.74	0.41
1:K:433:VAL:HG12	1:K:434:PHE:CD2	2.55	0.41
1:A:230:LYS:O	1:A:234:GLU:HG3	2.21	0.41
1:A:272:MET:HE1	1:A:358:VAL:CG2	2.51	0.41
1:C:193:SER:CB	4:D:5475:MPD:CM	2.84	0.41
1:D:114:TYR:O	1:D:118:THR:HG23	2.21	0.41
1:D:332:LEU:HA	1:D:332:LEU:HD12	1.90	0.41
1:D:364:ALA:HA	1:J:468:VAL:HG13	2.03	0.41
1:E:231:LYS:HE2	5:E:1180:HOH:O	2.21	0.41
1:G:114:TYR:O	1:G:118:THR:HG23	2.21	0.41
1:G:230:LYS:O	1:G:234:GLU:HG3	2.21	0.41
1:G:25:LYS:NZ	5:G:5744:HOH:O	2.44	0.41
1:I:403:GLU:C	1:I:405:LYS:N	2.74	0.41
1:I:34:PRO:HG2	1:J:206:VAL:O	2.20	0.41
1:L:296:TYR:HB3	1:L:382:ILE:HA	2.03	0.41
1:A:433:VAL:HG12	1:A:434:PHE:CD2	2.55	0.41
1:B:2:ALA:O	1:B:6:LEU:HD12	2.19	0.41
1:B:313:ASN:HB3	1:B:318:SER:HB3	2.03	0.41
1:B:320:LYS:HG2	1:H:455:MET:C	2.42	0.41
1:C:294:ALA:O	1:C:298:ILE:HG13	2.21	0.41
1:D:91:ILE:HB	1:D:103:ASP:HB2	2.03	0.41
1:E:206:VAL:O	1:F:34:PRO:HG2	2.20	0.41
1:E:230:LYS:O	1:E:234:GLU:HG3	2.21	0.41
1:E:323:VAL:HG11	1:K:455:MET:HG2	2.03	0.41
1:E:390:GLU:HA	1:E:391:PRO:HD3	1.89	0.41
1:E:433:VAL:HG12	1:E:434:PHE:CD2	2.56	0.41
4:G:5484:MPD:C5	4:G:5484:MPD:H11	2.45	0.41
1:H:368:TYR:OH	4:H:5486:MPD:O2	2.27	0.41
4:J:5491:MPD:CM	4:J:5491:MPD:O4	2.60	0.41
1:L:114:TYR:O	1:L:118:THR:HG23	2.21	0.41
1:A:91:ILE:HB	1:A:103:ASP:HB2	2.03	0.41
1:B:114:TYR:O	1:B:118:THR:HG23	2.21	0.41
1:B:225:PHE:HD1	3:B:4472:ADP:O2'	2.03	0.41
1:D:231:LYS:HE2	5:D:888:HOH:O	2.21	0.41
1:D:303:LYS:HD2	1:D:386:ILE:HD13	2.04	0.41
1:F:294:ALA:O	1:F:298:ILE:HG13	2.21	0.41
1:H:294:ALA:O	1:H:298:ILE:HG13	2.21	0.41
1:I:114:TYR:O	1:I:118:THR:HG23	2.21	0.41
1:K:114:TYR:O	1:K:118:THR:HG23	2.21	0.41
1:K:140:PHE:CE1	1:L:160:SER:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:THR:HB	1:K:466:TYR:CE1	2.56	0.41
4:K:5493:MPD:H53	4:K:5493:MPD:C1	2.48	0.41
1:L:231:LYS:HE2	5:L:3224:HOH:O	2.21	0.41
1:A:114:TYR:O	1:A:118:THR:HG23	2.21	0.40
1:B:84:THR:CG2	4:B:5471:MPD:H32	2.51	0.40
1:D:433:VAL:HG12	1:D:434:PHE:CD2	2.55	0.40
1:E:294:ALA:O	1:E:298:ILE:HG13	2.21	0.40
1:E:313:ASN:HB3	1:E:318:SER:HB3	2.03	0.40
1:F:225:PHE:HD1	3:F:4476:ADP:O2'	2.03	0.40
1:F:80:PHE:CG	4:F:5479:MPD:C1	3.04	0.40
1:G:294:ALA:O	1:G:298:ILE:HG13	2.21	0.40
1:G:313:ASN:HB3	1:G:318:SER:HB3	2.03	0.40
1:G:332:LEU:HA	1:G:332:LEU:HD12	1.90	0.40
1:H:303:LYS:HD2	1:H:386:ILE:HD13	2.03	0.40
1:I:80:PHE:CG	4:I:5489:MPD:C1	3.04	0.40
1:J:114:TYR:O	1:J:118:THR:HG23	2.21	0.40
1:J:313:ASN:HB3	1:J:318:SER:HB3	2.03	0.40
1:K:294:ALA:O	1:K:298:ILE:HG13	2.22	0.40
1:K:296:TYR:HB3	1:K:382:ILE:HA	2.03	0.40
1:L:248:ARG:NH2	1:L:248:ARG:CG	2.67	0.40
1:F:466:TYR:CE1	1:L:254:THR:HB	2.56	0.40
1:L:294:ALA:O	1:L:298:ILE:HG13	2.21	0.40
1:L:82:ASP:O	4:L:5483:MPD:H32	2.20	0.40
1:A:294:ALA:O	1:A:298:ILE:HG13	2.21	0.40
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.82	0.40
1:B:294:ALA:O	1:B:298:ILE:HG13	2.21	0.40
1:C:25:LYS:NZ	5:C:5734:HOH:O	2.44	0.40
1:D:230:LYS:O	1:D:234:GLU:HG3	2.21	0.40
1:F:231:LYS:HE2	5:F:5506:HOH:O	2.21	0.40
1:F:332:LEU:HA	1:F:332:LEU:HD12	1.90	0.40
1:E:189:GLN:CG	4:F:5479:MPD:H11	2.48	0.40
1:G:390:GLU:HA	1:G:391:PRO:HD3	1.89	0.40
4:H:5487:MPD:H53	4:H:5487:MPD:C1	2.48	0.40
1:H:34:PRO:HG2	1:I:206:VAL:O	2.21	0.40
1:I:230:LYS:O	1:I:234:GLU:HG3	2.21	0.40
1:J:225:PHE:HD1	3:J:4480:ADP:O2'	2.03	0.40
1:J:235:ILE:HA	1:J:235:ILE:HD13	1.82	0.40
1:K:105:ARG:HD3	1:K:105:ARG:HH21	1.76	0.40
1:A:140:PHE:CE1	1:F:160:SER:HB2	2.56	0.40
1:B:180:PHE:O	1:B:181:PRO:C	2.54	0.40
1:B:433:VAL:HG12	1:B:434:PHE:CD2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:5471:MPD:C1	4:B:5471:MPD:H53	2.48	0.40
1:C:22:THR:HG1	4:C:5476:MPD:C1	2.33	0.40
1:D:182:VAL:HG12	1:E:30:HIS:HB3	2.03	0.40
1:D:235:ILE:HD13	1:D:235:ILE:HA	1.82	0.40
1:D:403:GLU:C	1:D:405:LYS:N	2.74	0.40
1:E:114:TYR:O	1:E:118:THR:HG23	2.21	0.40
1:E:328:ALA:HA	1:E:329:PRO:HD3	1.73	0.40
1:G:225:PHE:HD1	3:G:4477:ADP:O2'	2.03	0.40
1:B:364:ALA:HA	1:H:468:VAL:CG1	2.51	0.40
1:I:91:ILE:HB	1:I:103:ASP:HB2	2.02	0.40
1:K:230:LYS:O	1:K:234:GLU:HG3	2.21	0.40
1:K:313:ASN:HB3	1:K:318:SER:HB3	2.03	0.40
1:E:364:ALA:HA	1:K:468:VAL:HG13	2.03	0.40
1:L:303:LYS:HD2	1:L:386:ILE:HD13	2.04	0.40
1:A:332:LEU:HA	1:A:332:LEU:HD12	1.90	0.40
1:E:303:LYS:HD2	1:E:386:ILE:HD13	2.03	0.40
1:F:403:GLU:C	1:F:405:LYS:N	2.74	0.40
1:H:403:GLU:C	1:H:405:LYS:N	2.74	0.40
1:I:294:ALA:O	1:I:298:ILE:HG13	2.22	0.40
1:I:332:LEU:HD12	1:I:332:LEU:HA	1.90	0.40
1:I:303:LYS:HD2	1:I:386:ILE:HD13	2.04	0.40
1:J:332:LEU:HB2	1:J:408:PRO:CB	2.50	0.40
1:A:332:LEU:HB3	1:A:408:PRO:HB2	2.04	0.40
1:F:303:LYS:HD2	1:F:386:ILE:HD13	2.04	0.40
1:E:193:SER:OG	4:F:5479:MPD:O4	2.28	0.40
4:G:5484:MPD:H12	4:G:5484:MPD:H4	1.82	0.40
4:G:5485:MPD:CM	4:G:5485:MPD:O4	2.60	0.40
1:H:225:PHE:HD1	3:H:4478:ADP:O2'	2.03	0.40
1:H:313:ASN:HB3	1:H:318:SER:HB3	2.03	0.40
1:J:125:LEU:HD12	1:J:125:LEU:HA	1.91	0.40
1:J:294:ALA:O	1:J:298:ILE:HG13	2.21	0.40
1:K:384:ASN:N	1:K:384:ASN:ND2	2.60	0.40
4:L:5494:MPD:C5	4:L:5494:MPD:H11	2.45	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%)	426 (91%)	32 (7%)	8 (2%)	9	16
1	B	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	9	16
1	C	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	9	16
1	D	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	9	16
1	E	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	9	16
1	F	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	9	16
1	G	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	9	16
1	H	466/468 (100%)	427 (92%)	31 (7%)	8 (2%)	9	16
1	I	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	9	16
1	J	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	9	16
1	K	466/468 (100%)	427 (92%)	31 (7%)	8 (2%)	9	16
1	L	466/468 (100%)	426 (91%)	32 (7%)	8 (2%)	9	16
All	All	5592/5616 (100%)	5114 (92%)	382 (7%)	96 (2%)	9	16

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	A	400	PRO
1	A	401	PRO
1	B	180	PHE
1	B	400	PRO
1	B	401	PRO
1	C	180	PHE
1	C	400	PRO
1	C	401	PRO
1	D	180	PHE
1	D	400	PRO
1	D	401	PRO

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Mol	Chain	Res	Type
1	E	180	PHE
1	E	400	PRO
1	E	401	PRO
1	F	180	PHE
1	F	400	PRO
1	F	401	PRO
1	G	180	PHE
1	G	400	PRO
1	G	401	PRO
1	H	180	PHE
1	H	400	PRO
1	H	401	PRO
1	I	180	PHE
1	I	400	PRO
1	I	401	PRO
1	J	180	PHE
1	J	400	PRO
1	J	401	PRO
1	K	180	PHE
1	K	400	PRO
1	K	401	PRO
1	L	180	PHE
1	L	400	PRO
1	L	401	PRO
1	A	170	GLY
1	B	170	GLY
1	C	170	GLY
1	D	170	GLY
1	E	170	GLY
1	F	170	GLY
1	G	170	GLY
1	H	170	GLY
1	I	170	GLY
1	J	170	GLY
1	K	170	GLY
1	L	170	GLY
1	A	324	PRO
1	A	338	ASN
1	A	394	LYS
1	B	324	PRO
1	B	338	ASN
1	B	394	LYS

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Mol	Chain	Res	Type
1	C	324	PRO
1	C	338	ASN
1	C	394	LYS
1	D	324	PRO
1	D	338	ASN
1	D	394	LYS
1	E	324	PRO
1	E	338	ASN
1	E	394	LYS
1	F	324	PRO
1	F	338	ASN
1	F	394	LYS
1	G	324	PRO
1	G	338	ASN
1	G	394	LYS
1	H	324	PRO
1	H	338	ASN
1	H	394	LYS
1	I	324	PRO
1	I	338	ASN
1	I	394	LYS
1	J	324	PRO
1	J	338	ASN
1	J	394	LYS
1	K	324	PRO
1	K	338	ASN
1	K	394	LYS
1	L	324	PRO
1	L	338	ASN
1	L	394	LYS
1	A	396	LEU
1	B	396	LEU
1	C	396	LEU
1	D	396	LEU
1	E	396	LEU
1	F	396	LEU
1	G	396	LEU
1	H	396	LEU
1	I	396	LEU
1	J	396	LEU
1	K	396	LEU
1	L	396	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/384 (100%)	348 (91%)	36 (9%)	8	17
1	B	384/384 (100%)	349 (91%)	35 (9%)	9	18
1	C	384/384 (100%)	348 (91%)	36 (9%)	8	17
1	D	384/384 (100%)	348 (91%)	36 (9%)	8	17
1	E	384/384 (100%)	348 (91%)	36 (9%)	8	17
1	F	384/384 (100%)	349 (91%)	35 (9%)	9	18
1	G	384/384 (100%)	348 (91%)	36 (9%)	8	17
1	H	384/384 (100%)	348 (91%)	36 (9%)	8	17
1	I	384/384 (100%)	349 (91%)	35 (9%)	9	18
1	J	384/384 (100%)	349 (91%)	35 (9%)	9	18
1	K	384/384 (100%)	348 (91%)	36 (9%)	8	17
1	L	384/384 (100%)	349 (91%)	35 (9%)	9	18
All	All	4608/4608 (100%)	4181 (91%)	427 (9%)	9	17

All (427) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	19	LEU
1	A	60	ILE
1	A	62	GLU
1	A	63	SER
1	A	64	ASP
1	A	65	MET
1	A	84	THR
1	A	88	ARG
1	A	96	THR
1	A	98	GLN
1	A	115	LEU
1	A	124	VAL
1	A	125	LEU

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Mol	Chain	Res	Type
1	A	165	GLU
1	A	179	TYR
1	A	209	HIS
1	A	230	LYS
1	A	248	ARG
1	A	264	ASN
1	A	320	LYS
1	A	324	PRO
1	A	326	TYR
1	A	332	LEU
1	A	337	ARG
1	A	374	LEU
1	A	375	LEU
1	A	384	ASN
1	A	392	MET
1	A	396	LEU
1	A	397	TYR
1	A	399	LEU
1	A	428	LEU
1	A	447	ARG
1	A	464	LEU
1	A	468	VAL
1	B	6	LEU
1	B	19	LEU
1	B	60	ILE
1	B	62	GLU
1	B	63	SER
1	B	64	ASP
1	B	65	MET
1	B	84	THR
1	B	88	ARG
1	B	96	THR
1	B	98	GLN
1	B	115	LEU
1	B	124	VAL
1	B	125	LEU
1	B	165	GLU
1	B	179	TYR
1	B	209	HIS
1	B	230	LYS
1	B	248	ARG
1	B	264	ASN

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Mol	Chain	Res	Type
1	B	320	LYS
1	B	326	TYR
1	B	332	LEU
1	B	337	ARG
1	B	374	LEU
1	B	375	LEU
1	B	384	ASN
1	B	392	MET
1	B	396	LEU
1	B	397	TYR
1	B	399	LEU
1	B	428	LEU
1	B	447	ARG
1	B	464	LEU
1	B	468	VAL
1	C	6	LEU
1	C	19	LEU
1	C	60	ILE
1	C	62	GLU
1	C	63	SER
1	C	64	ASP
1	C	65	MET
1	C	84	THR
1	C	88	ARG
1	C	96	THR
1	C	98	GLN
1	C	115	LEU
1	C	124	VAL
1	C	125	LEU
1	C	165	GLU
1	C	179	TYR
1	C	209	HIS
1	C	230	LYS
1	C	248	ARG
1	C	264	ASN
1	C	320	LYS
1	C	324	PRO
1	C	326	TYR
1	C	332	LEU
1	C	337	ARG
1	C	374	LEU
1	C	375	LEU

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Mol	Chain	Res	Type
1	C	384	ASN
1	C	392	MET
1	C	396	LEU
1	C	397	TYR
1	C	399	LEU
1	C	428	LEU
1	C	447	ARG
1	C	464	LEU
1	C	468	VAL
1	D	6	LEU
1	D	19	LEU
1	D	60	ILE
1	D	62	GLU
1	D	63	SER
1	D	64	ASP
1	D	65	MET
1	D	84	THR
1	D	88	ARG
1	D	96	THR
1	D	98	GLN
1	D	115	LEU
1	D	124	VAL
1	D	125	LEU
1	D	165	GLU
1	D	179	TYR
1	D	209	HIS
1	D	230	LYS
1	D	248	ARG
1	D	264	ASN
1	D	320	LYS
1	D	324	PRO
1	D	326	TYR
1	D	332	LEU
1	D	337	ARG
1	D	374	LEU
1	D	375	LEU
1	D	384	ASN
1	D	392	MET
1	D	396	LEU
1	D	397	TYR
1	D	399	LEU
1	D	428	LEU

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Mol	Chain	Res	Type
1	D	447	ARG
1	D	464	LEU
1	D	468	VAL
1	E	6	LEU
1	E	19	LEU
1	E	60	ILE
1	E	62	GLU
1	E	63	SER
1	E	64	ASP
1	E	65	MET
1	E	84	THR
1	E	88	ARG
1	E	96	THR
1	E	98	GLN
1	E	115	LEU
1	E	124	VAL
1	E	125	LEU
1	E	165	GLU
1	E	179	TYR
1	E	209	HIS
1	E	230	LYS
1	E	248	ARG
1	E	264	ASN
1	E	320	LYS
1	E	324	PRO
1	E	326	TYR
1	E	332	LEU
1	E	337	ARG
1	E	374	LEU
1	E	375	LEU
1	E	384	ASN
1	E	392	MET
1	E	396	LEU
1	E	397	TYR
1	E	399	LEU
1	E	428	LEU
1	E	447	ARG
1	E	464	LEU
1	E	468	VAL
1	F	6	LEU
1	F	19	LEU
1	F	60	ILE

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Mol	Chain	Res	Type
1	F	62	GLU
1	F	63	SER
1	F	64	ASP
1	F	65	MET
1	F	84	THR
1	F	88	ARG
1	F	96	THR
1	F	98	GLN
1	F	115	LEU
1	F	124	VAL
1	F	125	LEU
1	F	165	GLU
1	F	179	TYR
1	F	209	HIS
1	F	230	LYS
1	F	248	ARG
1	F	264	ASN
1	F	320	LYS
1	F	326	TYR
1	F	332	LEU
1	F	337	ARG
1	F	374	LEU
1	F	375	LEU
1	F	384	ASN
1	F	392	MET
1	F	396	LEU
1	F	397	TYR
1	F	399	LEU
1	F	428	LEU
1	F	447	ARG
1	F	464	LEU
1	F	468	VAL
1	G	6	LEU
1	G	19	LEU
1	G	60	ILE
1	G	62	GLU
1	G	63	SER
1	G	64	ASP
1	G	65	MET
1	G	84	THR
1	G	88	ARG
1	G	96	THR

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Mol	Chain	Res	Type
1	G	98	GLN
1	G	115	LEU
1	G	124	VAL
1	G	125	LEU
1	G	165	GLU
1	G	179	TYR
1	G	209	HIS
1	G	230	LYS
1	G	248	ARG
1	G	264	ASN
1	G	320	LYS
1	G	324	PRO
1	G	326	TYR
1	G	332	LEU
1	G	337	ARG
1	G	374	LEU
1	G	375	LEU
1	G	384	ASN
1	G	392	MET
1	G	396	LEU
1	G	397	TYR
1	G	399	LEU
1	G	428	LEU
1	G	447	ARG
1	G	464	LEU
1	G	468	VAL
1	H	6	LEU
1	H	19	LEU
1	H	60	ILE
1	H	62	GLU
1	H	63	SER
1	H	64	ASP
1	H	65	MET
1	H	84	THR
1	H	88	ARG
1	H	96	THR
1	H	98	GLN
1	H	115	LEU
1	H	124	VAL
1	H	125	LEU
1	H	165	GLU
1	H	179	TYR

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Mol	Chain	Res	Type
1	H	209	HIS
1	H	230	LYS
1	H	248	ARG
1	H	264	ASN
1	H	320	LYS
1	H	324	PRO
1	H	326	TYR
1	H	332	LEU
1	H	337	ARG
1	H	374	LEU
1	H	375	LEU
1	H	384	ASN
1	H	392	MET
1	H	396	LEU
1	H	397	TYR
1	H	399	LEU
1	H	428	LEU
1	H	447	ARG
1	H	464	LEU
1	H	468	VAL
1	I	6	LEU
1	I	19	LEU
1	I	60	ILE
1	I	62	GLU
1	I	63	SER
1	I	64	ASP
1	I	65	MET
1	I	84	THR
1	I	88	ARG
1	I	96	THR
1	I	98	GLN
1	I	115	LEU
1	I	124	VAL
1	I	125	LEU
1	I	165	GLU
1	I	179	TYR
1	I	209	HIS
1	I	230	LYS
1	I	248	ARG
1	I	264	ASN
1	I	320	LYS
1	I	326	TYR

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Mol	Chain	Res	Type
1	I	332	LEU
1	I	337	ARG
1	I	374	LEU
1	I	375	LEU
1	I	384	ASN
1	I	392	MET
1	I	396	LEU
1	I	397	TYR
1	I	399	LEU
1	I	428	LEU
1	I	447	ARG
1	I	464	LEU
1	I	468	VAL
1	J	6	LEU
1	J	19	LEU
1	J	60	ILE
1	J	62	GLU
1	J	63	SER
1	J	64	ASP
1	J	65	MET
1	J	84	THR
1	J	88	ARG
1	J	96	THR
1	J	98	GLN
1	J	115	LEU
1	J	124	VAL
1	J	125	LEU
1	J	165	GLU
1	J	179	TYR
1	J	209	HIS
1	J	230	LYS
1	J	248	ARG
1	J	264	ASN
1	J	320	LYS
1	J	326	TYR
1	J	332	LEU
1	J	337	ARG
1	J	374	LEU
1	J	375	LEU
1	J	384	ASN
1	J	392	MET
1	J	396	LEU

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Mol	Chain	Res	Type
1	J	397	TYR
1	J	399	LEU
1	J	428	LEU
1	J	447	ARG
1	J	464	LEU
1	J	468	VAL
1	K	6	LEU
1	K	19	LEU
1	K	60	ILE
1	K	62	GLU
1	K	63	SER
1	K	64	ASP
1	K	65	MET
1	K	84	THR
1	K	88	ARG
1	K	96	THR
1	K	98	GLN
1	K	115	LEU
1	K	124	VAL
1	K	125	LEU
1	K	165	GLU
1	K	179	TYR
1	K	209	HIS
1	K	230	LYS
1	K	248	ARG
1	K	264	ASN
1	K	320	LYS
1	K	324	PRO
1	K	326	TYR
1	K	332	LEU
1	K	337	ARG
1	K	374	LEU
1	K	375	LEU
1	K	384	ASN
1	K	392	MET
1	K	396	LEU
1	K	397	TYR
1	K	399	LEU
1	K	428	LEU
1	K	447	ARG
1	K	464	LEU
1	K	468	VAL

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Mol	Chain	Res	Type
1	L	6	LEU
1	L	19	LEU
1	L	60	ILE
1	L	62	GLU
1	L	63	SER
1	L	64	ASP
1	L	65	MET
1	L	84	THR
1	L	88	ARG
1	L	96	THR
1	L	98	GLN
1	L	115	LEU
1	L	124	VAL
1	L	125	LEU
1	L	165	GLU
1	L	179	TYR
1	L	209	HIS
1	L	230	LYS
1	L	248	ARG
1	L	264	ASN
1	L	320	LYS
1	L	326	TYR
1	L	332	LEU
1	L	337	ARG
1	L	374	LEU
1	L	375	LEU
1	L	384	ASN
1	L	392	MET
1	L	396	LEU
1	L	397	TYR
1	L	399	LEU
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 (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	211	HIS
1	A	218	GLN

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Mol	Chain	Res	Type
1	A	219	ASN
1	A	244	ASN
1	A	264	ASN
1	A	277	ASN
1	A	313	ASN
1	A	384	ASN
1	A	458	HIS
1	B	30	HIS
1	B	211	HIS
1	B	218	GLN
1	B	219	ASN
1	B	244	ASN
1	B	264	ASN
1	B	277	ASN
1	B	313	ASN
1	B	384	ASN
1	B	458	HIS
1	C	30	HIS
1	C	211	HIS
1	C	218	GLN
1	C	219	ASN
1	C	244	ASN
1	C	264	ASN
1	C	277	ASN
1	C	313	ASN
1	C	384	ASN
1	C	458	HIS
1	D	30	HIS
1	D	211	HIS
1	D	218	GLN
1	D	219	ASN
1	D	244	ASN
1	D	264	ASN
1	D	277	ASN
1	D	313	ASN
1	D	384	ASN
1	D	458	HIS
1	E	30	HIS
1	E	211	HIS
1	E	218	GLN
1	E	219	ASN
1	E	244	ASN

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Mol	Chain	Res	Type
1	E	264	ASN
1	E	277	ASN
1	E	313	ASN
1	E	384	ASN
1	E	458	HIS
1	F	30	HIS
1	F	211	HIS
1	F	218	GLN
1	F	219	ASN
1	F	244	ASN
1	F	264	ASN
1	F	277	ASN
1	F	313	ASN
1	F	384	ASN
1	F	458	HIS
1	G	30	HIS
1	G	211	HIS
1	G	218	GLN
1	G	219	ASN
1	G	244	ASN
1	G	264	ASN
1	G	277	ASN
1	G	313	ASN
1	G	384	ASN
1	G	458	HIS
1	H	30	HIS
1	H	211	HIS
1	H	218	GLN
1	H	219	ASN
1	H	244	ASN
1	H	264	ASN
1	H	277	ASN
1	H	313	ASN
1	H	384	ASN
1	H	458	HIS
1	I	30	HIS
1	I	211	HIS
1	I	218	GLN
1	I	219	ASN
1	I	244	ASN
1	I	264	ASN
1	I	277	ASN

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Mol	Chain	Res	Type
1	I	313	ASN
1	I	384	ASN
1	I	458	HIS
1	J	30	HIS
1	J	211	HIS
1	J	218	GLN
1	J	219	ASN
1	J	244	ASN
1	J	264	ASN
1	J	277	ASN
1	J	313	ASN
1	J	384	ASN
1	J	458	HIS
1	K	30	HIS
1	K	211	HIS
1	K	218	GLN
1	K	219	ASN
1	K	244	ASN
1	K	264	ASN
1	K	277	ASN
1	K	313	ASN
1	K	384	ASN
1	K	458	HIS
1	L	30	HIS
1	L	211	HIS
1	L	218	GLN
1	L	219	ASN
1	L	244	ASN
1	L	264	ASN
1	L	277	ASN
1	L	313	ASN
1	L	384	ASN
1	L	458	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 60 ligands modelled in this entry, 24 are monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	MPD	K	5492	-	7,7,7	3.31	4 (57%)	9,10,10	1.56	1 (11%)
4	MPD	B	5471	-	7,7,7	1.55	2 (28%)	9,10,10	1.00	0
3	ADP	F	4476	2	24,29,29	2.92	8 (33%)	29,45,45	3.33	11 (37%)
4	MPD	E	5480	-	7,7,7	3.32	4 (57%)	9,10,10	1.57	1 (11%)
4	MPD	I	5489	-	7,7,7	1.55	2 (28%)	9,10,10	1.00	0
3	ADP	A	4471	2	24,29,29	2.91	8 (33%)	29,45,45	3.34	11 (37%)
3	ADP	H	4478	2	24,29,29	2.91	8 (33%)	29,45,45	3.34	11 (37%)
4	MPD	D	5478	-	7,7,7	3.31	4 (57%)	9,10,10	1.56	1 (11%)
3	ADP	C	4473	2	24,29,29	2.91	8 (33%)	29,45,45	3.33	11 (37%)
4	MPD	K	5493	-	7,7,7	1.54	2 (28%)	9,10,10	1.00	0
4	MPD	J	5491	-	7,7,7	1.54	2 (28%)	9,10,10	1.00	0
4	MPD	I	5488	-	7,7,7	3.31	4 (57%)	9,10,10	1.57	1 (11%)
4	MPD	C	5476	-	7,7,7	3.31	4 (57%)	9,10,10	1.57	1 (11%)
4	MPD	G	5484	-	7,7,7	3.31	4 (57%)	9,10,10	1.57	1 (11%)
4	MPD	A	5472	-	7,7,7	3.31	4 (57%)	9,10,10	1.56	1 (11%)
3	ADP	E	4475	2	24,29,29	2.91	8 (33%)	29,45,45	3.34	12 (41%)
4	MPD	C	5473	-	7,7,7	1.54	2 (28%)	9,10,10	1.00	0
4	MPD	E	5477	-	7,7,7	1.55	2 (28%)	9,10,10	1.00	0
3	ADP	K	4481	2	24,29,29	2.92	8 (33%)	29,45,45	3.33	11 (37%)
4	MPD	H	5486	-	7,7,7	3.31	4 (57%)	9,10,10	1.56	1 (11%)
3	ADP	G	4477	2	24,29,29	2.91	8 (33%)	29,45,45	3.34	11 (37%)
4	MPD	A	5481	-	7,7,7	1.55	2 (28%)	9,10,10	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MPD	L	5483	-	7,7,7	1.54	2 (28%)	9,10,10	1.00	0
4	MPD	J	5490	-	7,7,7	3.31	4 (57%)	9,10,10	1.57	1 (11%)
4	MPD	F	5482	-	7,7,7	3.31	4 (57%)	9,10,10	1.57	1 (11%)
3	ADP	I	4479	2	24,29,29	2.91	8 (33%)	29,45,45	3.34	12 (41%)
3	ADP	L	4482	2	24,29,29	2.92	8 (33%)	29,45,45	3.34	11 (37%)
4	MPD	L	5494	-	7,7,7	3.32	4 (57%)	9,10,10	1.56	1 (11%)
3	ADP	B	4472	2	24,29,29	2.90	8 (33%)	29,45,45	3.34	11 (37%)
3	ADP	J	4480	2	24,29,29	2.91	8 (33%)	29,45,45	3.34	11 (37%)
4	MPD	D	5475	-	7,7,7	1.54	2 (28%)	9,10,10	1.00	0
4	MPD	B	5474	-	7,7,7	3.32	4 (57%)	9,10,10	1.56	1 (11%)
3	ADP	D	4474	2	24,29,29	2.92	8 (33%)	29,45,45	3.33	11 (37%)
4	MPD	H	5487	-	7,7,7	1.55	2 (28%)	9,10,10	1.00	0
4	MPD	G	5485	-	7,7,7	1.55	2 (28%)	9,10,10	1.00	0
4	MPD	F	5479	-	7,7,7	1.55	2 (28%)	9,10,10	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	K	5492	-	-	3/5/5/5	-
4	MPD	B	5471	-	-	0/5/5/5	-
3	ADP	F	4476	2	-	3/12/32/32	0/3/3/3
4	MPD	E	5480	-	-	3/5/5/5	-
4	MPD	I	5489	-	-	0/5/5/5	-
3	ADP	A	4471	2	-	3/12/32/32	0/3/3/3
3	ADP	H	4478	2	-	3/12/32/32	0/3/3/3
4	MPD	D	5478	-	-	3/5/5/5	-
3	ADP	C	4473	2	-	3/12/32/32	0/3/3/3
4	MPD	K	5493	-	-	0/5/5/5	-
4	MPD	J	5491	-	-	0/5/5/5	-
4	MPD	I	5488	-	-	3/5/5/5	-
4	MPD	C	5476	-	-	3/5/5/5	-
4	MPD	G	5484	-	-	3/5/5/5	-
4	MPD	A	5472	-	-	3/5/5/5	-
3	ADP	E	4475	2	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	C	5473	-	-	0/5/5/5	-
4	MPD	E	5477	-	-	0/5/5/5	-
3	ADP	K	4481	2	-	3/12/32/32	0/3/3/3
4	MPD	H	5486	-	-	3/5/5/5	-
3	ADP	G	4477	2	-	3/12/32/32	0/3/3/3
4	MPD	A	5481	-	-	0/5/5/5	-
4	MPD	L	5483	-	-	0/5/5/5	-
4	MPD	J	5490	-	-	3/5/5/5	-
4	MPD	F	5482	-	-	3/5/5/5	-
3	ADP	I	4479	2	-	3/12/32/32	0/3/3/3
3	ADP	L	4482	2	-	3/12/32/32	0/3/3/3
4	MPD	L	5494	-	-	3/5/5/5	-
3	ADP	B	4472	2	-	3/12/32/32	0/3/3/3
3	ADP	J	4480	2	-	3/12/32/32	0/3/3/3
4	MPD	D	5475	-	-	0/5/5/5	-
4	MPD	B	5474	-	-	3/5/5/5	-
3	ADP	D	4474	2	-	3/12/32/32	0/3/3/3
4	MPD	H	5487	-	-	0/5/5/5	-
4	MPD	G	5485	-	-	0/5/5/5	-
4	MPD	F	5479	-	-	0/5/5/5	-

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	4481	ADP	O4'-C1'	8.85	1.53	1.41
3	L	4482	ADP	O4'-C1'	8.83	1.53	1.41
3	F	4476	ADP	O4'-C1'	8.82	1.53	1.41
3	C	4473	ADP	O4'-C1'	8.81	1.53	1.41
3	D	4474	ADP	O4'-C1'	8.80	1.53	1.41
3	H	4478	ADP	O4'-C1'	8.80	1.53	1.41
3	A	4471	ADP	O4'-C1'	8.79	1.53	1.41
3	J	4480	ADP	O4'-C1'	8.79	1.53	1.41
3	G	4477	ADP	O4'-C1'	8.78	1.53	1.41
3	E	4475	ADP	O4'-C1'	8.78	1.53	1.41
3	I	4479	ADP	O4'-C1'	8.77	1.53	1.41
3	B	4472	ADP	O4'-C1'	8.75	1.53	1.41
4	L	5494	MPD	C1-C2	-6.74	1.31	1.52
4	E	5480	MPD	C1-C2	-6.73	1.31	1.52
4	C	5476	MPD	C1-C2	-6.73	1.31	1.52
4	B	5474	MPD	C1-C2	-6.72	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5472	MPD	C1-C2	-6.71	1.31	1.52
4	K	5492	MPD	C1-C2	-6.71	1.31	1.52
4	D	5478	MPD	C1-C2	-6.71	1.31	1.52
4	I	5488	MPD	C1-C2	-6.70	1.31	1.52
4	G	5484	MPD	C1-C2	-6.70	1.31	1.52
4	H	5486	MPD	C1-C2	-6.70	1.31	1.52
4	J	5490	MPD	C1-C2	-6.70	1.31	1.52
4	F	5482	MPD	C1-C2	-6.69	1.31	1.52
3	E	4475	ADP	O4'-C4'	5.77	1.57	1.45
3	I	4479	ADP	O4'-C4'	5.74	1.57	1.45
3	D	4474	ADP	O4'-C4'	5.74	1.57	1.45
3	F	4476	ADP	O4'-C4'	5.74	1.57	1.45
3	J	4480	ADP	O4'-C4'	5.74	1.57	1.45
3	A	4471	ADP	O4'-C4'	5.73	1.57	1.45
3	G	4477	ADP	O4'-C4'	5.73	1.57	1.45
3	L	4482	ADP	O4'-C4'	5.72	1.57	1.45
3	K	4481	ADP	O4'-C4'	5.71	1.57	1.45
3	B	4472	ADP	O4'-C4'	5.71	1.57	1.45
3	C	4473	ADP	O4'-C4'	5.70	1.57	1.45
3	H	4478	ADP	O4'-C4'	5.70	1.57	1.45
3	L	4482	ADP	C4-N3	5.03	1.42	1.35
3	H	4478	ADP	C4-N3	5.01	1.42	1.35
3	F	4476	ADP	C4-N3	5.01	1.42	1.35
3	D	4474	ADP	C4-N3	4.98	1.42	1.35
3	G	4477	ADP	C4-N3	4.98	1.42	1.35
3	A	4471	ADP	C4-N3	4.97	1.42	1.35
3	J	4480	ADP	C4-N3	4.97	1.42	1.35
3	C	4473	ADP	C4-N3	4.97	1.42	1.35
3	K	4481	ADP	C4-N3	4.96	1.42	1.35
3	E	4475	ADP	C4-N3	4.96	1.42	1.35
3	I	4479	ADP	C4-N3	4.95	1.42	1.35
3	B	4472	ADP	C4-N3	4.95	1.42	1.35
4	B	5474	MPD	O2-C2	-4.41	1.33	1.44
4	F	5482	MPD	O2-C2	-4.41	1.33	1.44
4	A	5472	MPD	O2-C2	-4.40	1.33	1.44
4	J	5490	MPD	O2-C2	-4.40	1.33	1.44
4	L	5494	MPD	O2-C2	-4.40	1.33	1.44
4	K	5492	MPD	O2-C2	-4.40	1.33	1.44
4	I	5488	MPD	O2-C2	-4.39	1.33	1.44
4	H	5486	MPD	O2-C2	-4.39	1.33	1.44
4	E	5480	MPD	O2-C2	-4.39	1.33	1.44
4	G	5484	MPD	O2-C2	-4.39	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5476	MPD	O2-C2	-4.38	1.33	1.44
4	D	5478	MPD	O2-C2	-4.38	1.33	1.44
3	K	4481	ADP	C2-N3	3.91	1.38	1.32
3	J	4480	ADP	C2-N3	3.90	1.38	1.32
3	I	4479	ADP	C2-N3	3.90	1.38	1.32
3	G	4477	ADP	C2-N3	3.90	1.38	1.32
3	C	4473	ADP	C2-N3	3.89	1.38	1.32
3	A	4471	ADP	C2-N3	3.89	1.38	1.32
3	H	4478	ADP	C2-N3	3.88	1.38	1.32
3	D	4474	ADP	C2-N3	3.88	1.38	1.32
3	B	4472	ADP	C2-N3	3.87	1.38	1.32
3	E	4475	ADP	C2-N3	3.86	1.38	1.32
3	F	4476	ADP	C2-N3	3.85	1.38	1.32
3	L	4482	ADP	C2-N3	3.83	1.38	1.32
3	D	4474	ADP	PB-O3B	3.33	1.67	1.54
3	H	4478	ADP	PB-O3B	3.33	1.67	1.54
3	I	4479	ADP	PB-O3B	3.33	1.67	1.54
3	A	4471	ADP	PB-O3B	3.33	1.67	1.54
3	G	4477	ADP	PB-O3B	3.32	1.67	1.54
3	L	4482	ADP	PB-O3B	3.32	1.67	1.54
3	E	4475	ADP	PB-O3B	3.32	1.67	1.54
3	C	4473	ADP	PB-O3B	3.32	1.67	1.54
3	B	4472	ADP	PB-O3B	3.32	1.67	1.54
3	J	4480	ADP	PB-O3B	3.31	1.67	1.54
3	K	4481	ADP	PB-O3B	3.31	1.67	1.54
3	F	4476	ADP	PB-O3B	3.30	1.67	1.54
3	B	4472	ADP	C6-N6	-3.18	1.22	1.34
3	D	4474	ADP	C6-N6	-3.18	1.22	1.34
3	I	4479	ADP	C6-N6	-3.17	1.22	1.34
3	J	4480	ADP	C6-N6	-3.17	1.22	1.34
3	A	4471	ADP	C6-N6	-3.17	1.22	1.34
3	F	4476	ADP	C6-N6	-3.16	1.22	1.34
3	H	4478	ADP	C6-N6	-3.16	1.22	1.34
3	K	4481	ADP	C6-N6	-3.16	1.22	1.34
3	L	4482	ADP	C6-N6	-3.16	1.22	1.34
3	C	4473	ADP	C6-N6	-3.16	1.22	1.34
3	E	4475	ADP	C6-N6	-3.16	1.22	1.34
3	G	4477	ADP	C6-N6	-3.15	1.22	1.34
3	E	4475	ADP	C2'-C1'	-3.12	1.49	1.53
3	K	4481	ADP	C2'-C1'	-3.11	1.49	1.53
3	D	4474	ADP	C2'-C1'	-3.09	1.49	1.53
3	F	4476	ADP	C2'-C1'	-3.09	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4471	ADP	C2'-C1'	-3.08	1.49	1.53
3	G	4477	ADP	C2'-C1'	-3.08	1.49	1.53
3	B	4472	ADP	C2'-C1'	-3.07	1.49	1.53
3	C	4473	ADP	C2'-C1'	-3.07	1.49	1.53
3	H	4478	ADP	C2'-C1'	-3.07	1.49	1.53
3	I	4479	ADP	C2'-C1'	-3.05	1.49	1.53
3	J	4480	ADP	C2'-C1'	-3.04	1.49	1.53
3	L	4482	ADP	C2'-C1'	-3.04	1.49	1.53
4	H	5487	MPD	CM-C2	-3.01	1.43	1.52
4	E	5477	MPD	CM-C2	-3.01	1.43	1.52
4	F	5479	MPD	CM-C2	-3.01	1.43	1.52
4	L	5483	MPD	CM-C2	-3.00	1.43	1.52
4	I	5489	MPD	CM-C2	-2.99	1.43	1.52
4	G	5485	MPD	CM-C2	-2.99	1.43	1.52
4	B	5471	MPD	CM-C2	-2.99	1.43	1.52
4	K	5493	MPD	CM-C2	-2.98	1.43	1.52
4	A	5481	MPD	CM-C2	-2.98	1.43	1.52
4	C	5473	MPD	CM-C2	-2.98	1.43	1.52
4	J	5491	MPD	CM-C2	-2.97	1.43	1.52
4	D	5475	MPD	CM-C2	-2.96	1.43	1.52
4	F	5482	MPD	C3-C2	-2.65	1.46	1.53
4	I	5488	MPD	C3-C2	-2.65	1.46	1.53
4	H	5486	MPD	C3-C2	-2.65	1.46	1.53
4	K	5492	MPD	C3-C2	-2.64	1.46	1.53
4	E	5480	MPD	C3-C2	-2.64	1.46	1.53
4	J	5490	MPD	C3-C2	-2.64	1.46	1.53
4	C	5476	MPD	C3-C2	-2.64	1.46	1.53
4	A	5472	MPD	C3-C2	-2.63	1.46	1.53
4	L	5494	MPD	C3-C2	-2.63	1.46	1.53
4	D	5478	MPD	C3-C2	-2.63	1.46	1.53
4	B	5474	MPD	C3-C2	-2.62	1.46	1.53
4	G	5484	MPD	C3-C2	-2.61	1.46	1.53
3	F	4476	ADP	C3'-C4'	-2.49	1.46	1.53
3	J	4480	ADP	C3'-C4'	-2.49	1.46	1.53
3	I	4479	ADP	C3'-C4'	-2.48	1.46	1.53
3	D	4474	ADP	C3'-C4'	-2.47	1.46	1.53
3	L	4482	ADP	C3'-C4'	-2.47	1.46	1.53
3	C	4473	ADP	C3'-C4'	-2.47	1.46	1.53
3	A	4471	ADP	C3'-C4'	-2.47	1.46	1.53
3	E	4475	ADP	C3'-C4'	-2.47	1.46	1.53
3	H	4478	ADP	C3'-C4'	-2.46	1.46	1.53
3	B	4472	ADP	C3'-C4'	-2.46	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	4481	ADP	C3'-C4'	-2.45	1.46	1.53
3	G	4477	ADP	C3'-C4'	-2.45	1.46	1.53
4	D	5478	MPD	CM-C2	-2.14	1.45	1.52
4	H	5486	MPD	CM-C2	-2.13	1.45	1.52
4	G	5484	MPD	CM-C2	-2.12	1.45	1.52
4	E	5480	MPD	CM-C2	-2.12	1.45	1.52
4	J	5490	MPD	CM-C2	-2.11	1.45	1.52
4	I	5488	MPD	CM-C2	-2.11	1.45	1.52
4	A	5472	MPD	CM-C2	-2.11	1.45	1.52
4	B	5474	MPD	CM-C2	-2.10	1.45	1.52
4	L	5494	MPD	CM-C2	-2.09	1.45	1.52
4	F	5482	MPD	CM-C2	-2.09	1.45	1.52
4	K	5492	MPD	CM-C2	-2.09	1.45	1.52
4	C	5476	MPD	CM-C2	-2.08	1.46	1.52
4	C	5473	MPD	C1-C2	-2.04	1.46	1.52
4	I	5489	MPD	C1-C2	-2.03	1.46	1.52
4	J	5491	MPD	C1-C2	-2.03	1.46	1.52
4	B	5471	MPD	C1-C2	-2.03	1.46	1.52
4	D	5475	MPD	C1-C2	-2.03	1.46	1.52
4	H	5487	MPD	C1-C2	-2.03	1.46	1.52
4	A	5481	MPD	C1-C2	-2.03	1.46	1.52
4	F	5479	MPD	C1-C2	-2.02	1.46	1.52
4	G	5485	MPD	C1-C2	-2.02	1.46	1.52
4	E	5477	MPD	C1-C2	-2.01	1.46	1.52
4	L	5483	MPD	C1-C2	-2.01	1.46	1.52
4	K	5493	MPD	C1-C2	-2.01	1.46	1.52

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4477	ADP	O4'-C1'-C2'	-10.30	91.87	106.93
3	H	4478	ADP	O4'-C1'-C2'	-10.30	91.87	106.93
3	K	4481	ADP	O4'-C1'-C2'	-10.29	91.89	106.93
3	J	4480	ADP	O4'-C1'-C2'	-10.29	91.89	106.93
3	A	4471	ADP	O4'-C1'-C2'	-10.29	91.89	106.93
3	I	4479	ADP	O4'-C1'-C2'	-10.28	91.90	106.93
3	L	4482	ADP	O4'-C1'-C2'	-10.28	91.90	106.93
3	B	4472	ADP	O4'-C1'-C2'	-10.28	91.90	106.93
3	D	4474	ADP	O4'-C1'-C2'	-10.28	91.91	106.93
3	C	4473	ADP	O4'-C1'-C2'	-10.27	91.92	106.93
3	F	4476	ADP	O4'-C1'-C2'	-10.27	91.92	106.93
3	E	4475	ADP	O4'-C1'-C2'	-10.26	91.93	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	4482	ADP	O5'-C5'-C4'	8.35	137.73	108.99
3	J	4480	ADP	O5'-C5'-C4'	8.35	137.73	108.99
3	I	4479	ADP	O5'-C5'-C4'	8.34	137.71	108.99
3	F	4476	ADP	O5'-C5'-C4'	8.34	137.70	108.99
3	D	4474	ADP	O5'-C5'-C4'	8.34	137.69	108.99
3	C	4473	ADP	O5'-C5'-C4'	8.34	137.69	108.99
3	H	4478	ADP	O5'-C5'-C4'	8.34	137.69	108.99
3	E	4475	ADP	O5'-C5'-C4'	8.34	137.69	108.99
3	A	4471	ADP	O5'-C5'-C4'	8.34	137.68	108.99
3	K	4481	ADP	O5'-C5'-C4'	8.33	137.66	108.99
3	G	4477	ADP	O5'-C5'-C4'	8.33	137.66	108.99
3	B	4472	ADP	O5'-C5'-C4'	8.32	137.64	108.99
3	H	4478	ADP	C1'-N9-C4	5.10	135.61	126.64
3	L	4482	ADP	C1'-N9-C4	5.10	135.60	126.64
3	J	4480	ADP	C1'-N9-C4	5.09	135.59	126.64
3	C	4473	ADP	C1'-N9-C4	5.09	135.59	126.64
3	I	4479	ADP	C1'-N9-C4	5.09	135.59	126.64
3	A	4471	ADP	C1'-N9-C4	5.09	135.58	126.64
3	K	4481	ADP	C1'-N9-C4	5.08	135.57	126.64
3	E	4475	ADP	C1'-N9-C4	5.08	135.56	126.64
3	D	4474	ADP	C1'-N9-C4	5.07	135.55	126.64
3	F	4476	ADP	C1'-N9-C4	5.07	135.55	126.64
3	G	4477	ADP	C1'-N9-C4	5.07	135.54	126.64
3	B	4472	ADP	C1'-N9-C4	5.07	135.54	126.64
3	B	4472	ADP	C4-C5-N7	4.86	114.46	109.40
3	E	4475	ADP	C4-C5-N7	4.83	114.43	109.40
3	I	4479	ADP	C4-C5-N7	4.81	114.42	109.40
3	H	4478	ADP	C4-C5-N7	4.81	114.41	109.40
3	L	4482	ADP	C4-C5-N7	4.81	114.41	109.40
3	A	4471	ADP	C4-C5-N7	4.80	114.40	109.40
3	C	4473	ADP	C4-C5-N7	4.80	114.40	109.40
3	J	4480	ADP	C4-C5-N7	4.79	114.39	109.40
3	F	4476	ADP	C4-C5-N7	4.79	114.39	109.40
3	K	4481	ADP	C4-C5-N7	4.78	114.38	109.40
3	G	4477	ADP	C4-C5-N7	4.78	114.38	109.40
3	D	4474	ADP	C4-C5-N7	4.76	114.36	109.40
3	J	4480	ADP	C3'-C2'-C1'	-4.59	94.07	100.98
3	E	4475	ADP	C3'-C2'-C1'	-4.58	94.08	100.98
3	I	4479	ADP	C3'-C2'-C1'	-4.57	94.09	100.98
3	C	4473	ADP	C3'-C2'-C1'	-4.57	94.09	100.98
3	L	4482	ADP	C3'-C2'-C1'	-4.56	94.11	100.98
3	A	4471	ADP	C3'-C2'-C1'	-4.56	94.11	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	4478	ADP	C3'-C2'-C1'	-4.56	94.11	100.98
3	F	4476	ADP	C3'-C2'-C1'	-4.55	94.12	100.98
3	K	4481	ADP	C3'-C2'-C1'	-4.55	94.12	100.98
3	B	4472	ADP	C3'-C2'-C1'	-4.55	94.13	100.98
3	G	4477	ADP	C3'-C2'-C1'	-4.55	94.13	100.98
3	D	4474	ADP	C3'-C2'-C1'	-4.53	94.15	100.98
3	G	4477	ADP	C5'-C4'-C3'	-4.13	99.71	115.18
3	D	4474	ADP	C5'-C4'-C3'	-4.13	99.71	115.18
3	B	4472	ADP	C5'-C4'-C3'	-4.13	99.72	115.18
3	C	4473	ADP	C5'-C4'-C3'	-4.12	99.74	115.18
3	L	4482	ADP	C5'-C4'-C3'	-4.12	99.74	115.18
3	K	4481	ADP	C5'-C4'-C3'	-4.12	99.74	115.18
3	A	4471	ADP	C5'-C4'-C3'	-4.12	99.75	115.18
3	H	4478	ADP	C5'-C4'-C3'	-4.12	99.76	115.18
3	F	4476	ADP	C5'-C4'-C3'	-4.11	99.77	115.18
3	J	4480	ADP	C5'-C4'-C3'	-4.11	99.77	115.18
3	E	4475	ADP	C5'-C4'-C3'	-4.11	99.78	115.18
3	I	4479	ADP	C5'-C4'-C3'	-4.11	99.78	115.18
4	J	5490	MPD	O2-C2-C1	-3.47	96.93	108.08
4	I	5488	MPD	O2-C2-C1	-3.47	96.93	108.08
4	E	5480	MPD	O2-C2-C1	-3.47	96.94	108.08
4	F	5482	MPD	O2-C2-C1	-3.47	96.96	108.08
4	C	5476	MPD	O2-C2-C1	-3.46	96.96	108.08
4	A	5472	MPD	O2-C2-C1	-3.46	96.97	108.08
4	G	5484	MPD	O2-C2-C1	-3.46	96.97	108.08
4	H	5486	MPD	O2-C2-C1	-3.46	96.97	108.08
4	D	5478	MPD	O2-C2-C1	-3.46	96.98	108.08
4	B	5474	MPD	O2-C2-C1	-3.46	96.99	108.08
4	L	5494	MPD	O2-C2-C1	-3.46	96.99	108.08
4	K	5492	MPD	O2-C2-C1	-3.45	97.00	108.08
3	B	4472	ADP	O4'-C4'-C5'	3.45	120.71	109.37
3	J	4480	ADP	O4'-C4'-C5'	3.44	120.68	109.37
3	K	4481	ADP	O4'-C4'-C5'	3.44	120.68	109.37
3	L	4482	ADP	O4'-C4'-C5'	3.44	120.68	109.37
3	H	4478	ADP	O4'-C4'-C5'	3.44	120.68	109.37
3	A	4471	ADP	O4'-C4'-C5'	3.43	120.67	109.37
3	D	4474	ADP	O4'-C4'-C5'	3.43	120.66	109.37
3	G	4477	ADP	O4'-C4'-C5'	3.43	120.66	109.37
3	E	4475	ADP	O4'-C4'-C5'	3.43	120.66	109.37
3	F	4476	ADP	O4'-C4'-C5'	3.43	120.65	109.37
3	C	4473	ADP	O4'-C4'-C5'	3.43	120.64	109.37
3	I	4479	ADP	O4'-C4'-C5'	3.43	120.64	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4472	ADP	PA-O5'-C5'	2.85	138.37	121.68
3	E	4475	ADP	PA-O5'-C5'	2.85	138.37	121.68
3	C	4473	ADP	PA-O5'-C5'	2.84	138.36	121.68
3	H	4478	ADP	PA-O5'-C5'	2.84	138.36	121.68
3	J	4480	ADP	PA-O5'-C5'	2.84	138.34	121.68
3	G	4477	ADP	PA-O5'-C5'	2.84	138.32	121.68
3	A	4471	ADP	PA-O5'-C5'	2.84	138.32	121.68
3	I	4479	ADP	PA-O5'-C5'	2.84	138.32	121.68
3	D	4474	ADP	PA-O5'-C5'	2.84	138.32	121.68
3	K	4481	ADP	PA-O5'-C5'	2.84	138.32	121.68
3	F	4476	ADP	PA-O5'-C5'	2.84	138.31	121.68
3	L	4482	ADP	PA-O5'-C5'	2.83	138.30	121.68
3	E	4475	ADP	O2'-C2'-C1'	2.68	120.75	110.85
3	C	4473	ADP	O2'-C2'-C1'	2.67	120.71	110.85
3	K	4481	ADP	O2'-C2'-C1'	2.67	120.70	110.85
3	D	4474	ADP	O2'-C2'-C1'	2.67	120.70	110.85
3	F	4476	ADP	O2'-C2'-C1'	2.67	120.70	110.85
3	L	4482	ADP	O2'-C2'-C1'	2.67	120.70	110.85
3	G	4477	ADP	O2'-C2'-C1'	2.66	120.69	110.85
3	A	4471	ADP	O2'-C2'-C1'	2.66	120.69	110.85
3	H	4478	ADP	O2'-C2'-C1'	2.66	120.68	110.85
3	I	4479	ADP	O2'-C2'-C1'	2.66	120.68	110.85
3	B	4472	ADP	O2'-C2'-C1'	2.66	120.66	110.85
3	J	4480	ADP	O2'-C2'-C1'	2.65	120.66	110.85
3	E	4475	ADP	O2B-PB-O3A	2.31	112.38	104.64
3	G	4477	ADP	O2B-PB-O3A	2.30	112.36	104.64
3	D	4474	ADP	O2B-PB-O3A	2.30	112.36	104.64
3	L	4482	ADP	O2B-PB-O3A	2.30	112.36	104.64
3	K	4481	ADP	O2B-PB-O3A	2.30	112.36	104.64
3	H	4478	ADP	O2B-PB-O3A	2.30	112.36	104.64
3	A	4471	ADP	O2B-PB-O3A	2.30	112.35	104.64
3	B	4472	ADP	O2B-PB-O3A	2.30	112.35	104.64
3	I	4479	ADP	O2B-PB-O3A	2.30	112.35	104.64
3	C	4473	ADP	O2B-PB-O3A	2.30	112.34	104.64
3	F	4476	ADP	O2B-PB-O3A	2.29	112.32	104.64
3	H	4478	ADP	O3'-C3'-C2'	2.29	119.22	111.82
3	I	4479	ADP	O3'-C3'-C2'	2.29	119.22	111.82
3	J	4480	ADP	O2B-PB-O3A	2.29	112.31	104.64
3	B	4472	ADP	O3'-C3'-C2'	2.28	119.21	111.82
3	E	4475	ADP	O3'-C3'-C2'	2.28	119.20	111.82
3	J	4480	ADP	O3'-C3'-C2'	2.28	119.19	111.82
3	A	4471	ADP	O3'-C3'-C2'	2.28	119.19	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	K	4481	ADP	O3'-C3'-C2'	2.28	119.18	111.82
3	G	4477	ADP	O3'-C3'-C2'	2.28	119.18	111.82
3	C	4473	ADP	O3'-C3'-C2'	2.27	119.17	111.82
3	F	4476	ADP	O3'-C3'-C2'	2.27	119.16	111.82
3	D	4474	ADP	O3'-C3'-C2'	2.27	119.16	111.82
3	L	4482	ADP	O3'-C3'-C2'	2.26	119.13	111.82
3	E	4475	ADP	C5-C6-N6	-2.01	117.29	120.35
3	I	4479	ADP	C5-C6-N6	-2.01	117.30	120.35

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	4476	ADP	C4'-C5'-O5'-PA
4	E	5480	MPD	C1-C2-C3-C4
4	E	5480	MPD	O2-C2-C3-C4
4	E	5480	MPD	C2-C3-C4-O4
3	A	4471	ADP	C4'-C5'-O5'-PA
3	H	4478	ADP	C4'-C5'-O5'-PA
3	L	4482	ADP	C4'-C5'-O5'-PA
4	D	5478	MPD	C1-C2-C3-C4
4	D	5478	MPD	O2-C2-C3-C4
4	D	5478	MPD	C2-C3-C4-O4
3	C	4473	ADP	C4'-C5'-O5'-PA
4	A	5472	MPD	C1-C2-C3-C4
4	A	5472	MPD	O2-C2-C3-C4
4	A	5472	MPD	C2-C3-C4-O4
4	C	5476	MPD	C1-C2-C3-C4
4	C	5476	MPD	O2-C2-C3-C4
4	C	5476	MPD	C2-C3-C4-O4
4	G	5484	MPD	C1-C2-C3-C4
4	G	5484	MPD	O2-C2-C3-C4
4	G	5484	MPD	C2-C3-C4-O4
3	E	4475	ADP	C4'-C5'-O5'-PA
3	K	4481	ADP	C4'-C5'-O5'-PA
4	H	5486	MPD	C1-C2-C3-C4
4	H	5486	MPD	O2-C2-C3-C4
4	H	5486	MPD	C2-C3-C4-O4
3	G	4477	ADP	C4'-C5'-O5'-PA
4	I	5488	MPD	C1-C2-C3-C4
4	I	5488	MPD	O2-C2-C3-C4
4	I	5488	MPD	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
4	J	5490	MPD	C1-C2-C3-C4
4	J	5490	MPD	O2-C2-C3-C4
4	J	5490	MPD	C2-C3-C4-O4
4	F	5482	MPD	C1-C2-C3-C4
4	F	5482	MPD	O2-C2-C3-C4
4	F	5482	MPD	C2-C3-C4-O4
3	I	4479	ADP	C4'-C5'-O5'-PA
4	L	5494	MPD	C1-C2-C3-C4
4	L	5494	MPD	O2-C2-C3-C4
4	L	5494	MPD	C2-C3-C4-O4
3	B	4472	ADP	C4'-C5'-O5'-PA
4	K	5492	MPD	C1-C2-C3-C4
4	K	5492	MPD	O2-C2-C3-C4
4	K	5492	MPD	C2-C3-C4-O4
3	J	4480	ADP	C4'-C5'-O5'-PA
4	B	5474	MPD	C1-C2-C3-C4
4	B	5474	MPD	O2-C2-C3-C4
4	B	5474	MPD	C2-C3-C4-O4
3	D	4474	ADP	C4'-C5'-O5'-PA
3	F	4476	ADP	C5'-O5'-PA-O1A
3	A	4471	ADP	C5'-O5'-PA-O1A
3	H	4478	ADP	C5'-O5'-PA-O1A
3	L	4482	ADP	C5'-O5'-PA-O1A
3	C	4473	ADP	C5'-O5'-PA-O1A
3	E	4475	ADP	C5'-O5'-PA-O1A
3	K	4481	ADP	C5'-O5'-PA-O1A
3	G	4477	ADP	C5'-O5'-PA-O1A
3	I	4479	ADP	C5'-O5'-PA-O1A
3	B	4472	ADP	C5'-O5'-PA-O1A
3	J	4480	ADP	C5'-O5'-PA-O1A
3	D	4474	ADP	C5'-O5'-PA-O1A
3	F	4476	ADP	C5'-O5'-PA-O3A
3	A	4471	ADP	C5'-O5'-PA-O3A
3	H	4478	ADP	C5'-O5'-PA-O3A
3	L	4482	ADP	C5'-O5'-PA-O3A
3	C	4473	ADP	C5'-O5'-PA-O3A
3	E	4475	ADP	C5'-O5'-PA-O3A
3	K	4481	ADP	C5'-O5'-PA-O3A
3	G	4477	ADP	C5'-O5'-PA-O3A
3	I	4479	ADP	C5'-O5'-PA-O3A
3	B	4472	ADP	C5'-O5'-PA-O3A
3	J	4480	ADP	C5'-O5'-PA-O3A

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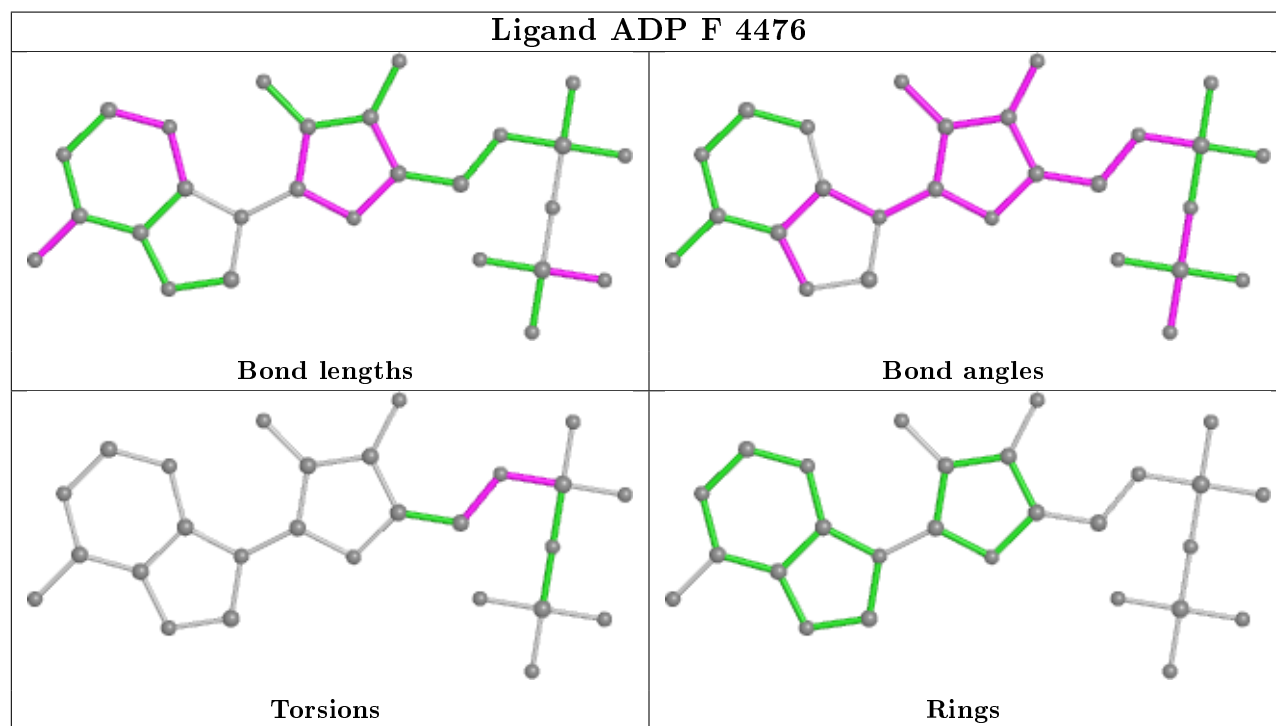
Mol	Chain	Res	Type	Atoms
3	D	4474	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

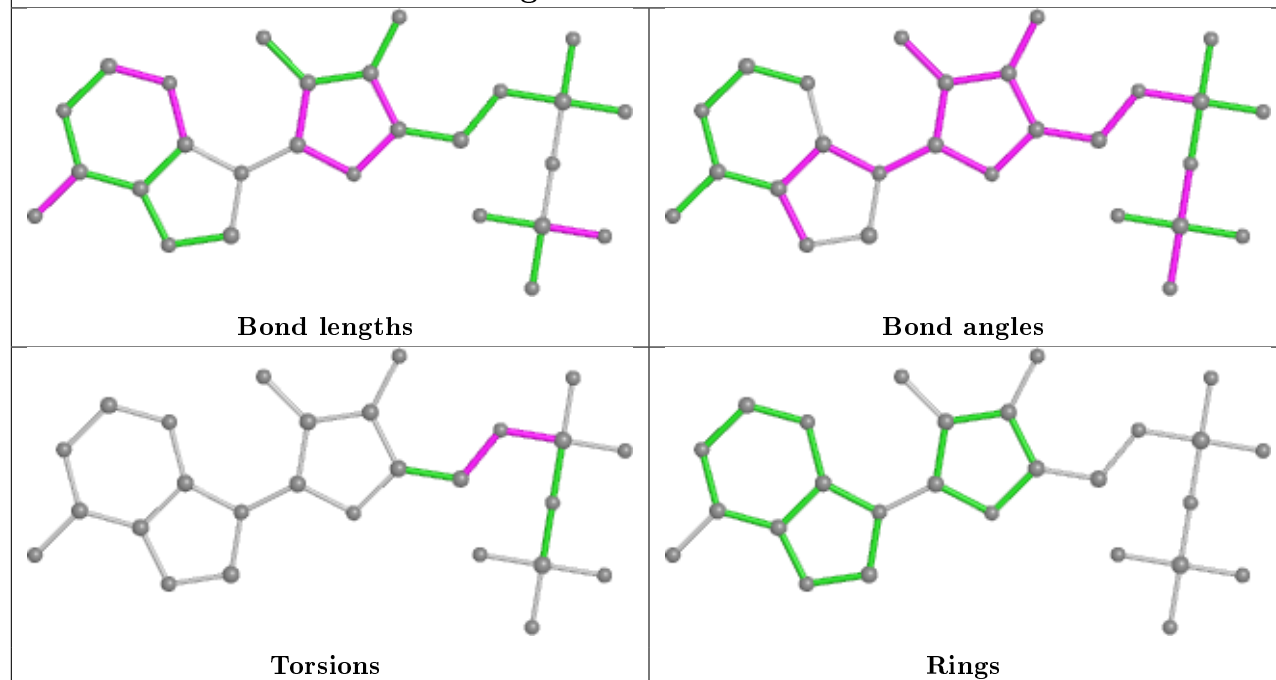
36 monomers are involved in 753 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	5492	MPD	30	0
4	B	5471	MPD	30	0
3	F	4476	ADP	1	0
4	E	5480	MPD	29	0
4	I	5489	MPD	31	0
3	A	4471	ADP	1	0
3	H	4478	ADP	1	0
4	D	5478	MPD	30	0
3	C	4473	ADP	1	0
4	K	5493	MPD	36	0
4	J	5491	MPD	39	0
4	I	5488	MPD	31	0
4	C	5476	MPD	30	0
4	G	5484	MPD	32	0
4	A	5472	MPD	29	0
3	E	4475	ADP	1	0
4	C	5473	MPD	32	0
4	E	5477	MPD	25	0
3	K	4481	ADP	1	0
4	H	5486	MPD	30	0
3	G	4477	ADP	1	0
4	A	5481	MPD	27	0
4	L	5483	MPD	35	0
4	J	5490	MPD	29	0
4	F	5482	MPD	29	0
3	I	4479	ADP	1	0
3	L	4482	ADP	1	0
4	L	5494	MPD	30	0
3	B	4472	ADP	1	0
3	J	4480	ADP	1	0
4	D	5475	MPD	31	0
4	B	5474	MPD	30	0
3	D	4474	ADP	1	0
4	H	5487	MPD	35	0
4	G	5485	MPD	28	0
4	F	5479	MPD	33	0

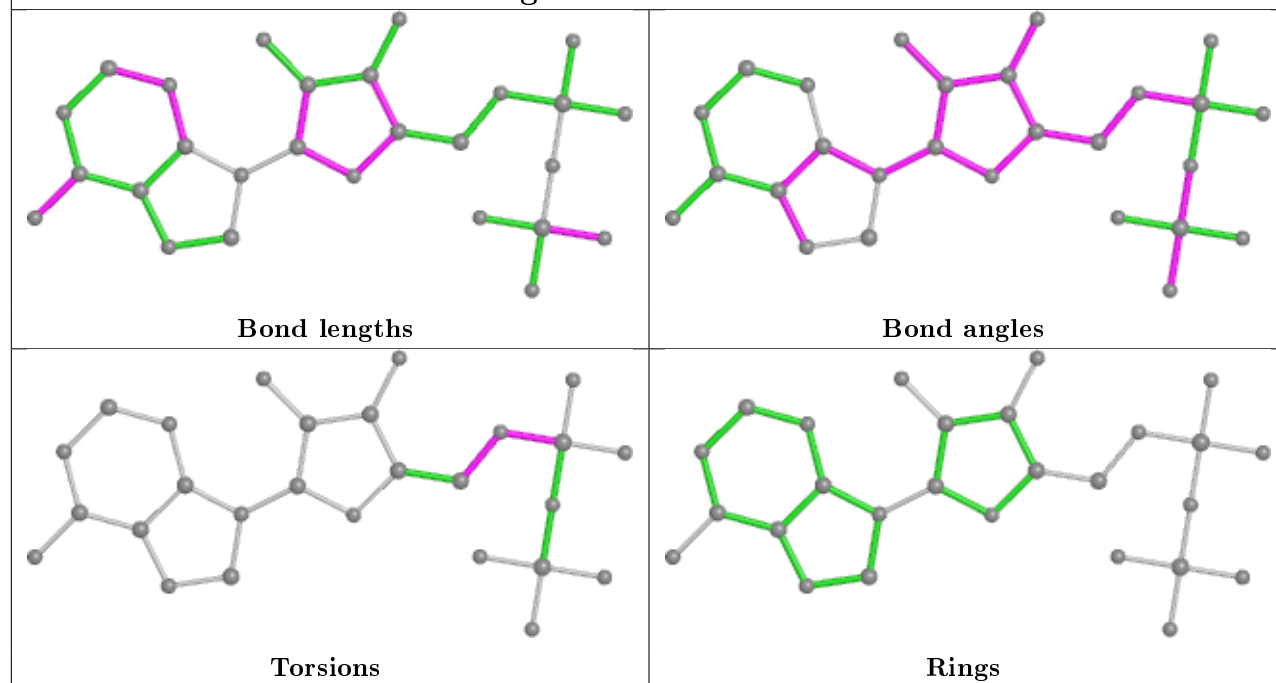
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



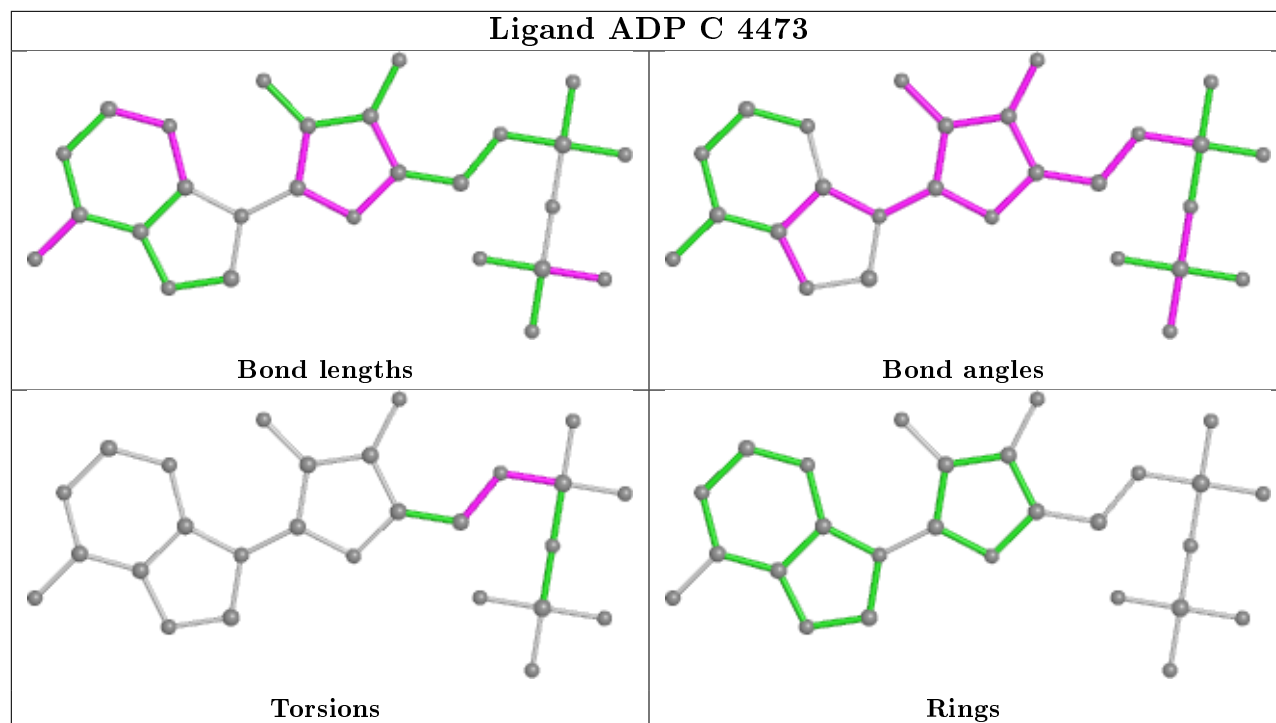
## Ligand ADP A 4471



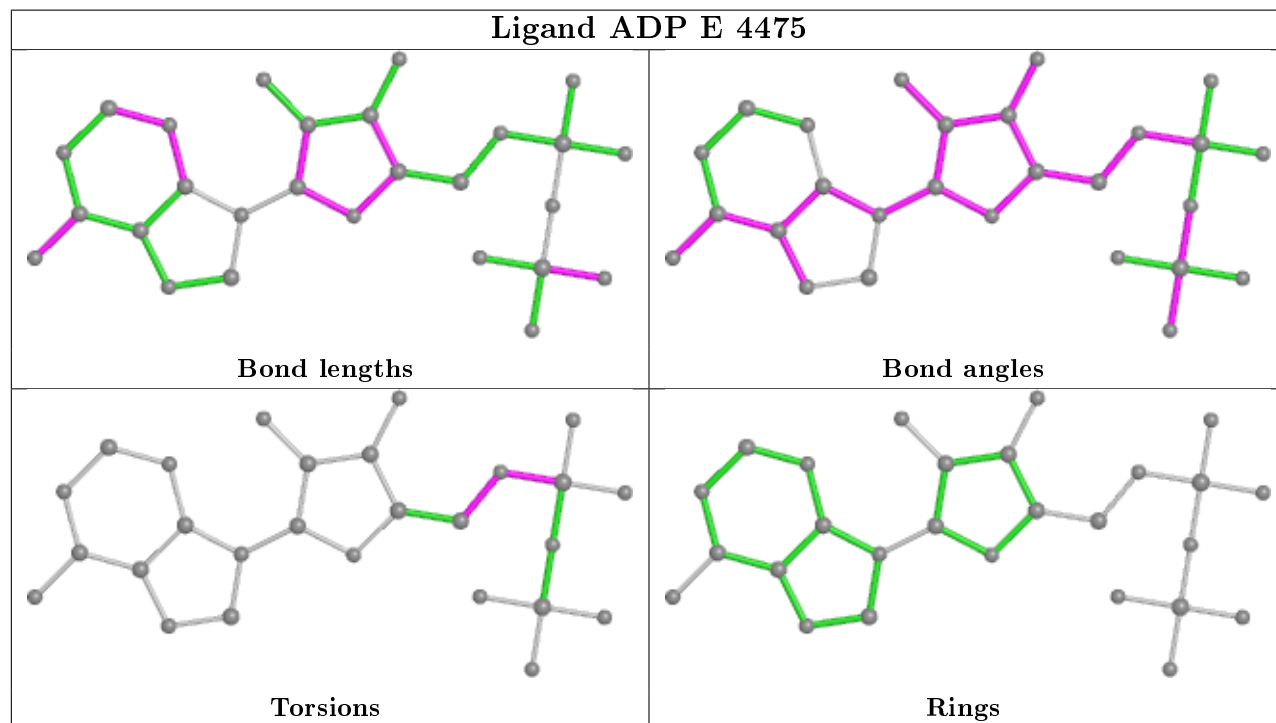
## Ligand ADP H 4478



## Ligand ADP C 4473

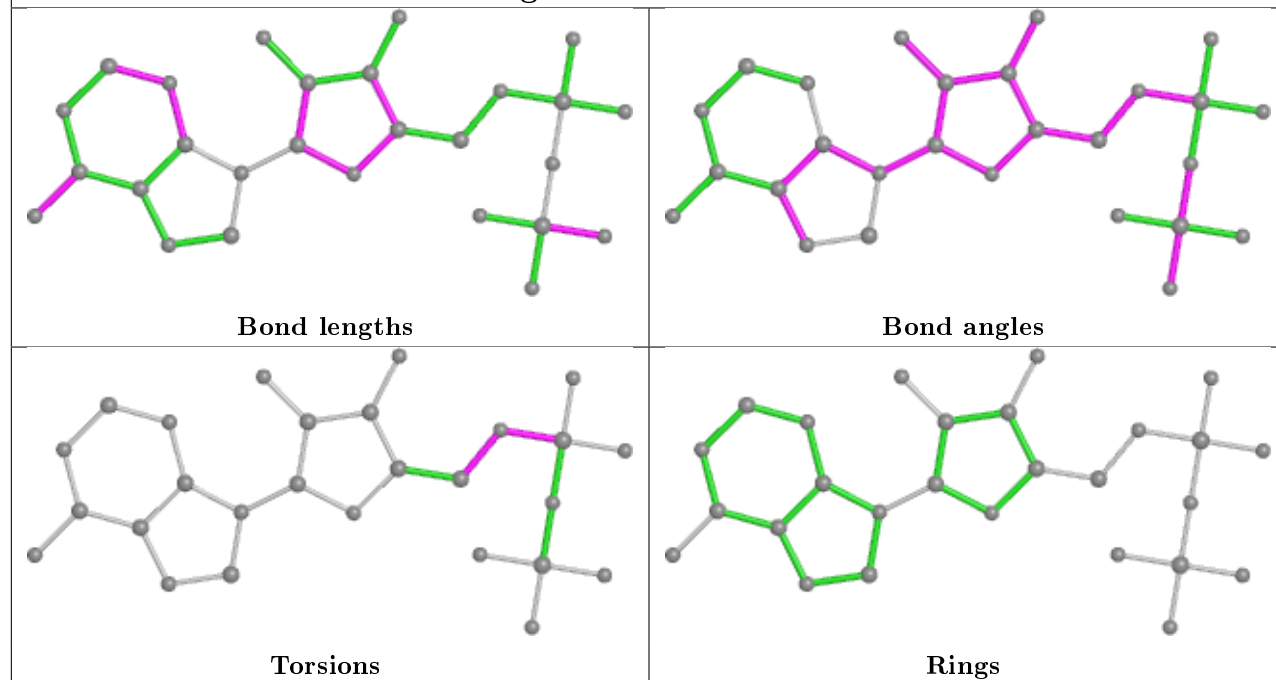


## Ligand ADP E 4475

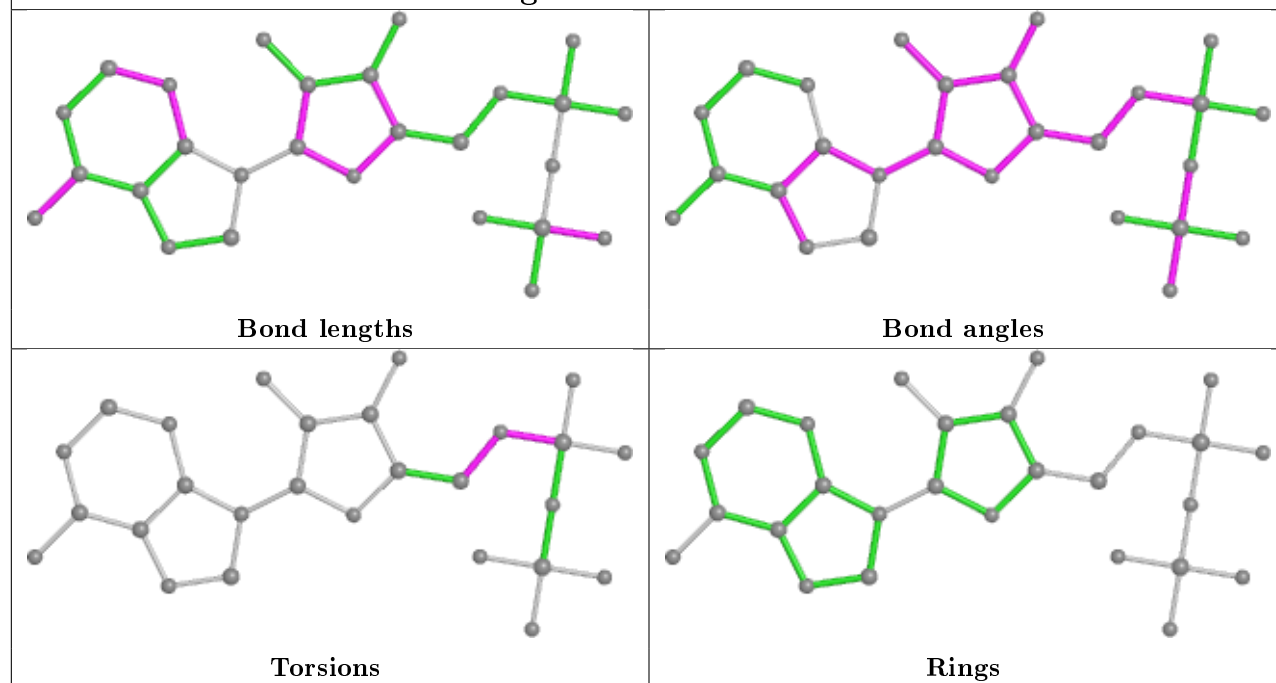


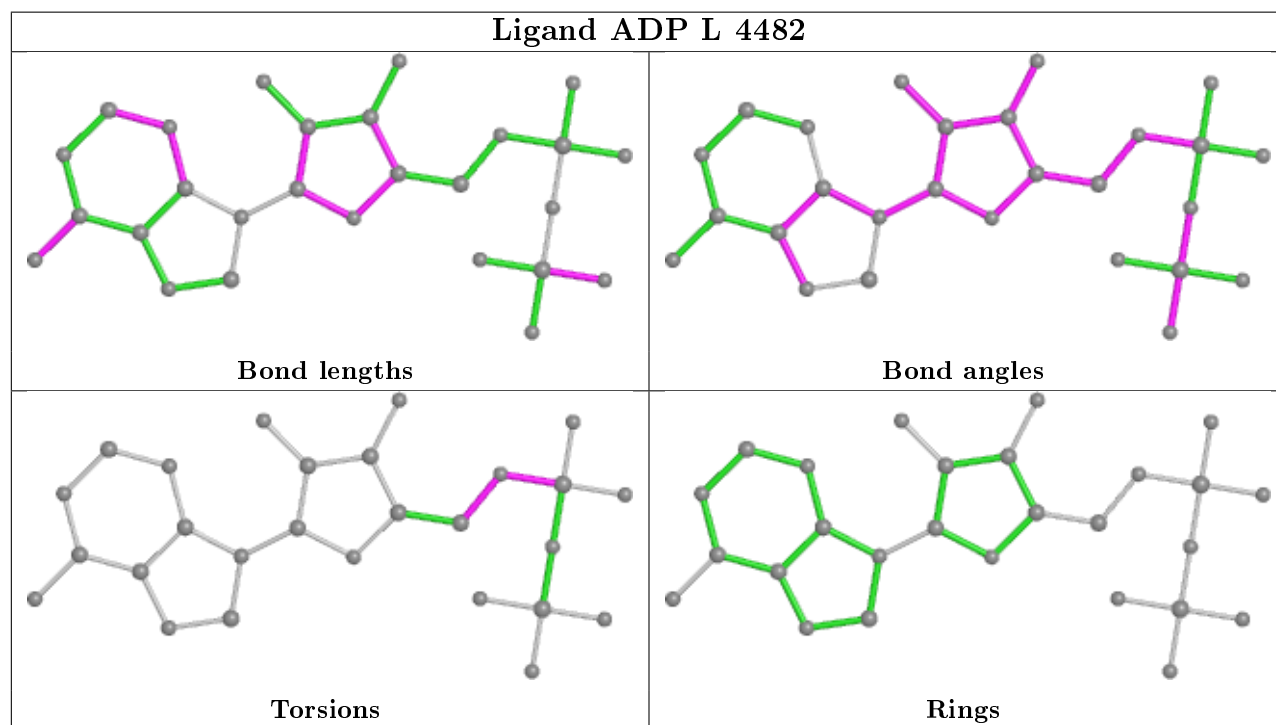
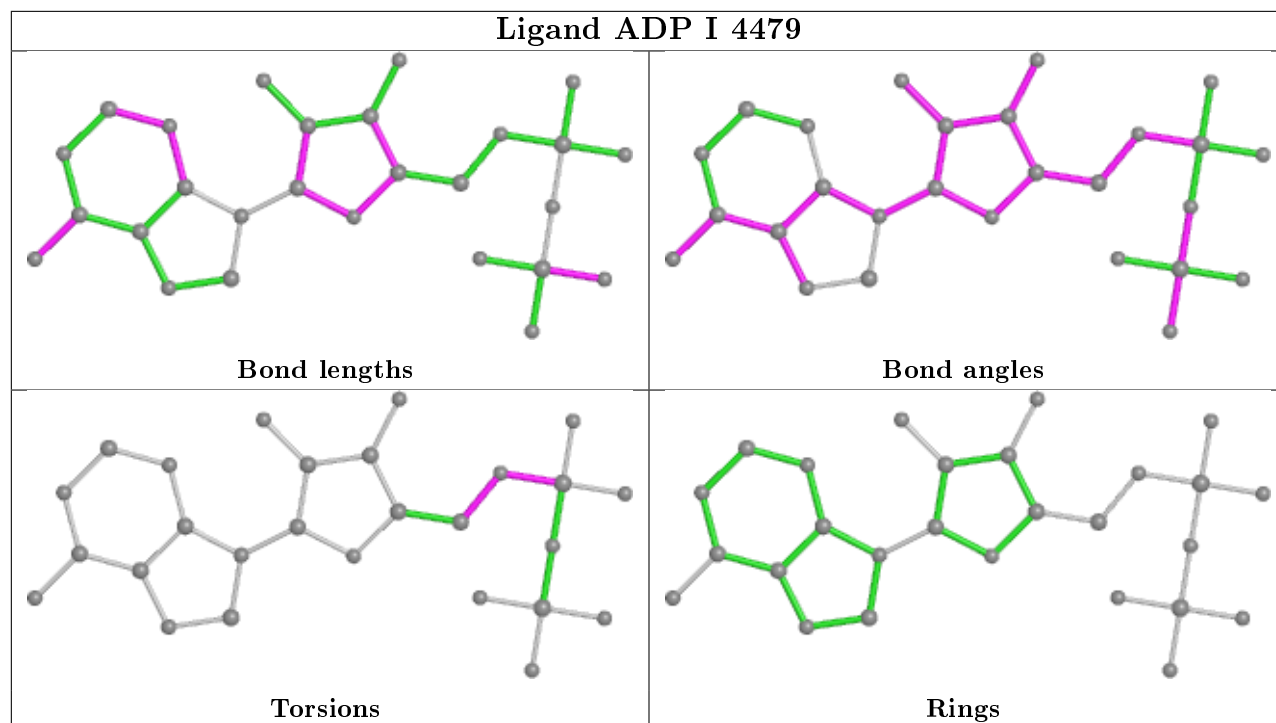


## Ligand ADP K 4481

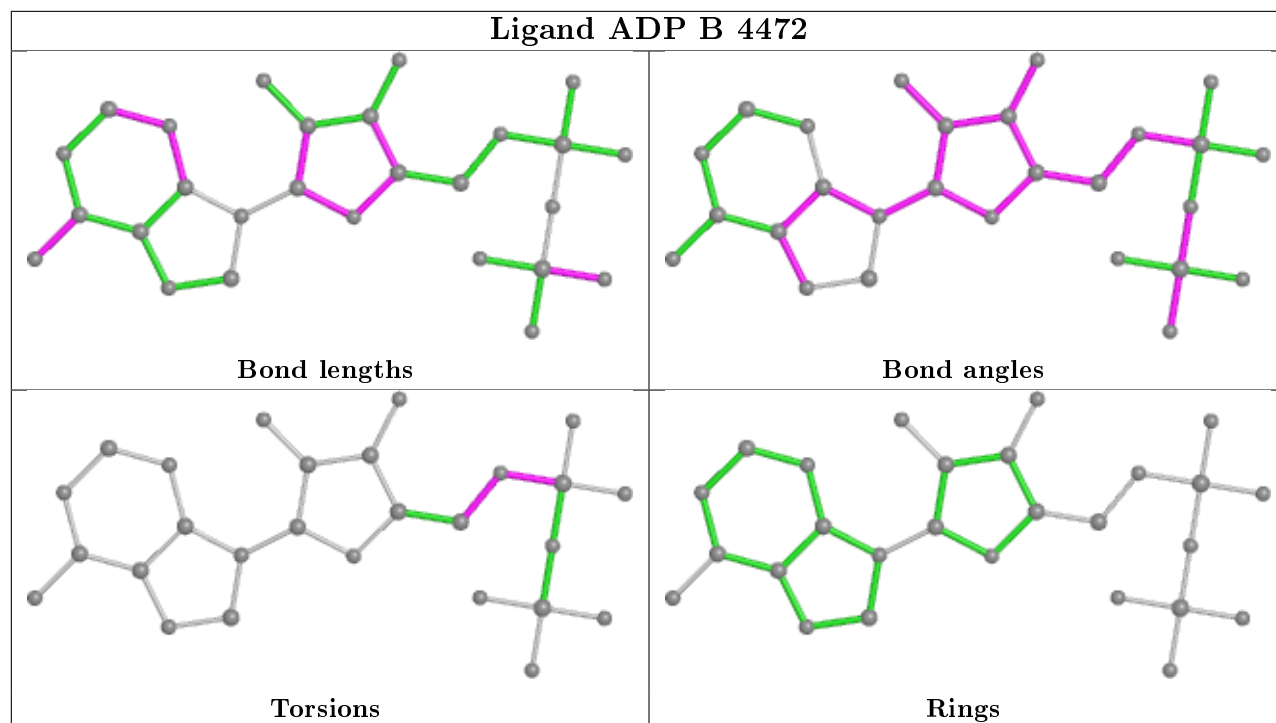


## Ligand ADP G 4477

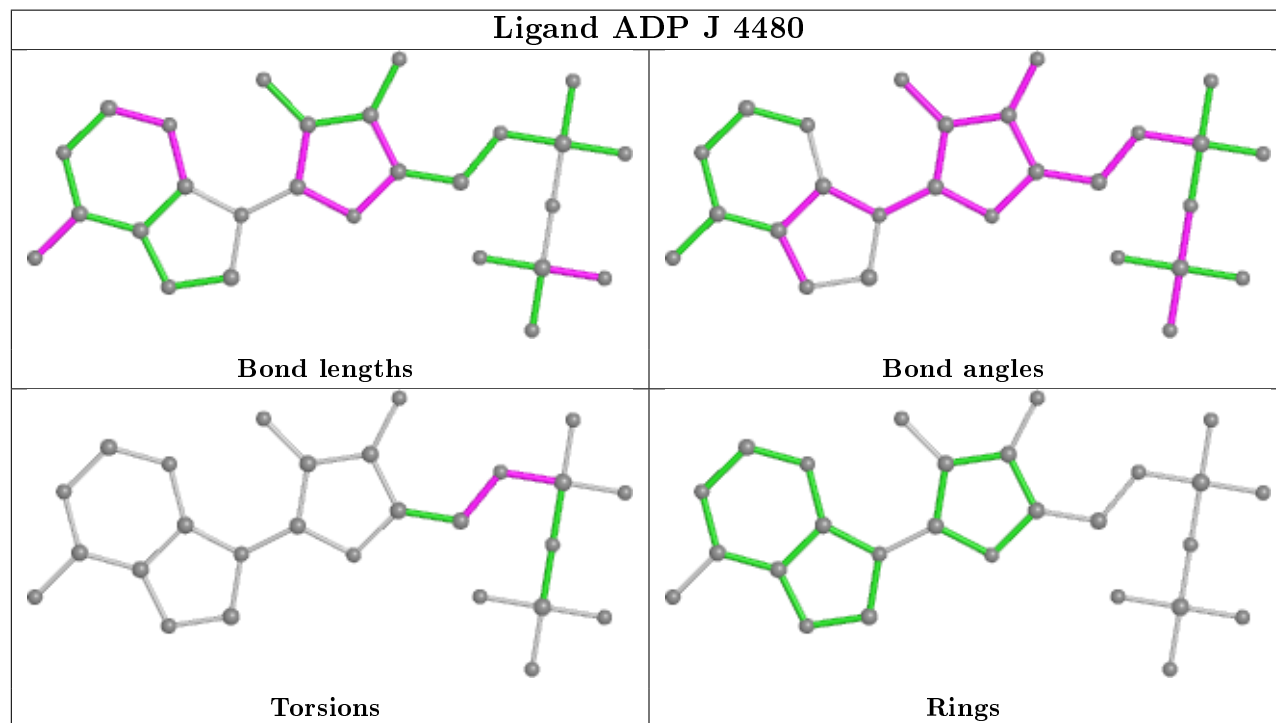


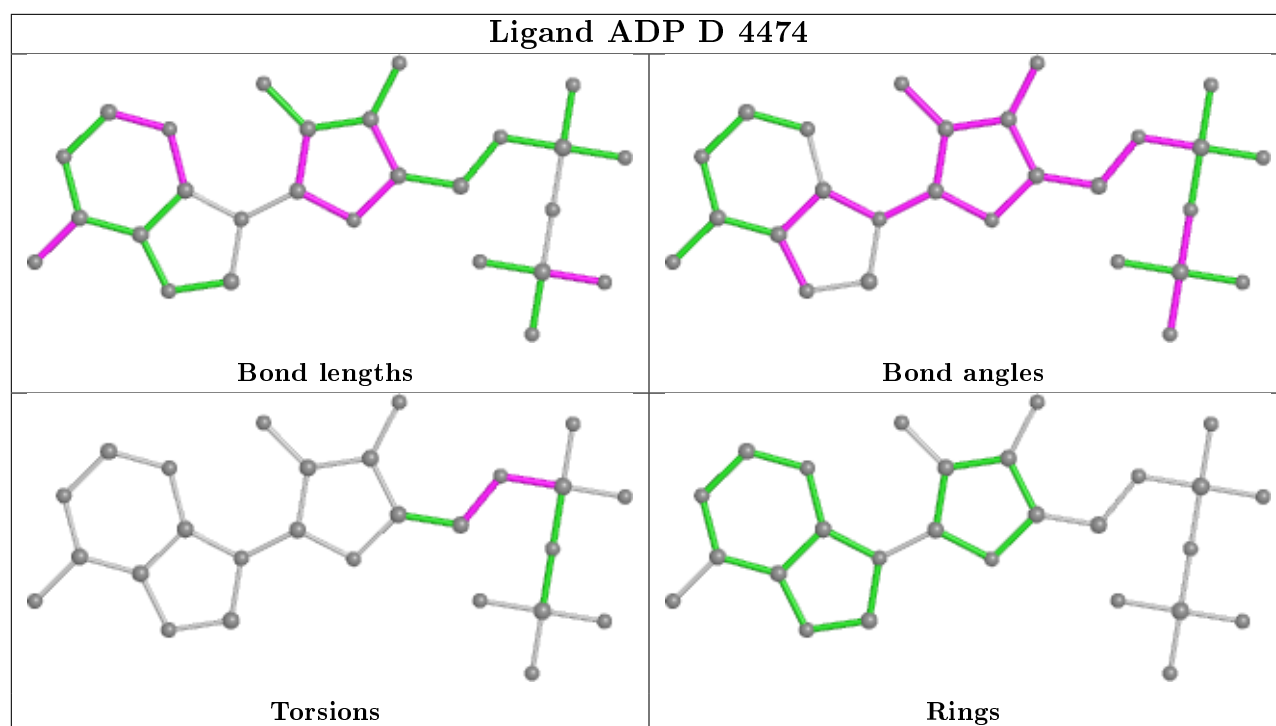


## Ligand ADP B 4472



## Ligand ADP J 4480





## 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%)	1.47	145 (30%)	0 0	28, 48, 96, 100	19 (4%)
1	B	468/468 (100%)	0.84	69 (14%)	2 2	28, 48, 96, 100	19 (4%)
1	C	468/468 (100%)	0.76	64 (13%)	3 2	28, 48, 96, 100	19 (4%)
1	D	468/468 (100%)	0.44	49 (10%)	6 6	28, 48, 96, 100	19 (4%)
1	E	468/468 (100%)	0.77	71 (15%)	2 1	28, 48, 96, 100	19 (4%)
1	F	468/468 (100%)	0.78	48 (10%)	6 6	28, 48, 96, 100	19 (4%)
1	G	468/468 (100%)	0.52	42 (8%)	9 9	28, 48, 96, 100	19 (4%)
1	H	468/468 (100%)	0.51	35 (7%)	14 14	28, 48, 96, 100	19 (4%)
1	I	468/468 (100%)	0.46	33 (7%)	16 16	28, 48, 96, 100	19 (4%)
1	J	468/468 (100%)	0.48	32 (6%)	17 17	28, 48, 96, 100	19 (4%)
1	K	468/468 (100%)	0.40	30 (6%)	19 20	28, 48, 96, 100	19 (4%)
1	L	468/468 (100%)	0.63	40 (8%)	10 10	28, 48, 96, 100	19 (4%)
All	All	5616/5616 (100%)	0.67	658 (11%)	4 4	28, 48, 96, 100	228 (4%)

All (658) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	397	TYR	13.5
1	A	397	TYR	12.8
1	J	397	TYR	12.7
1	B	397	TYR	12.5
1	A	398	ASP	12.5
1	C	398	ASP	12.4
1	I	397	TYR	12.2
1	F	398	ASP	12.2
1	F	397	TYR	11.9
1	G	397	TYR	11.2
1	E	397	TYR	10.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	399	LEU	10.9
1	L	397	TYR	10.5
1	F	404	ALA	10.4
1	E	395	ASN	10.3
1	G	399	LEU	10.2
1	D	326	TYR	10.2
1	E	399	LEU	10.1
1	A	277	ASN	10.1
1	C	404	ALA	9.8
1	A	351	PRO	9.5
1	D	399	LEU	9.5
1	L	399	LEU	9.4
1	B	399	LEU	9.3
1	A	326	TYR	9.2
1	A	395	ASN	9.2
1	K	397	TYR	9.0
1	I	398	ASP	9.0
1	A	334	TYR	8.9
1	E	404	ALA	8.9
1	F	399	LEU	8.8
1	K	399	LEU	8.6
1	B	398	ASP	8.5
1	H	395	ASN	8.4
1	A	285	ASP	8.4
1	I	399	LEU	8.3
1	E	400	PRO	8.2
1	B	394	LYS	8.2
1	D	400	PRO	8.2
1	H	399	LEU	8.1
1	B	326	TYR	8.0
1	F	326	TYR	8.0
1	D	397	TYR	8.0
1	H	402	GLU	7.8
1	H	398	ASP	7.8
1	B	61	ASN	7.8
1	B	401	PRO	7.8
1	C	396	LEU	7.7
1	F	395	ASN	7.6
1	B	404	ALA	7.5
1	F	401	PRO	7.5
1	E	396	LEU	7.4
1	A	337	ARG	7.3

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Mol	Chain	Res	Type	RSRZ
1	B	395	ASN	7.2
1	G	398	ASP	7.2
1	A	296	TYR	7.2
1	D	394	LYS	7.2
1	H	403	GLU	7.0
1	A	404	ALA	7.0
1	K	398	ASP	7.0
1	A	116	ARG	6.9
1	F	394	LYS	6.9
1	I	404	ALA	6.8
1	K	326	TYR	6.8
1	B	396	LEU	6.8
1	J	398	ASP	6.8
1	L	61	ASN	6.8
1	C	400	PRO	6.7
1	C	394	LYS	6.7
1	E	394	LYS	6.7
1	F	396	LEU	6.7
1	F	400	PRO	6.6
1	L	326	TYR	6.6
1	D	395	ASN	6.5
1	A	347	VAL	6.5
1	A	345	ILE	6.5
1	I	405	LYS	6.4
1	A	396	LEU	6.4
1	A	399	LEU	6.4
1	J	326	TYR	6.4
1	H	397	TYR	6.4
1	L	405	LYS	6.3
1	E	349	ALA	6.3
1	F	60	ILE	6.3
1	E	326	TYR	6.2
1	E	398	ASP	6.1
1	F	337	ARG	6.0
1	F	402	GLU	6.0
1	C	401	PRO	6.0
1	I	326	TYR	5.9
1	G	403	GLU	5.9
1	F	62	GLU	5.9
1	A	348	VAL	5.9
1	H	61	ASN	5.8
1	A	333	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	354	ARG	5.8
1	A	278	GLY	5.8
1	E	402	GLU	5.7
1	C	395	ASN	5.7
1	B	392	MET	5.6
1	A	286	LYS	5.6
1	D	60	ILE	5.6
1	I	61	ASN	5.6
1	D	403	GLU	5.5
1	H	326	TYR	5.5
1	E	12	HIS	5.4
1	C	326	TYR	5.4
1	G	404	ALA	5.4
1	A	288	ALA	5.4
1	A	287	TYR	5.4
1	C	1	SER	5.3
1	A	123	THR	5.3
1	L	398	ASP	5.3
1	A	292	GLU	5.3
1	F	405	LYS	5.3
1	B	60	ILE	5.3
1	G	61	ASN	5.2
1	C	402	GLU	5.2
1	A	61	ASN	5.2
1	A	401	PRO	5.1
1	A	91	ILE	5.1
1	I	402	GLU	5.1
1	B	95	GLY	5.1
1	H	405	LYS	5.0
1	A	338	ASN	5.0
1	G	400	PRO	5.0
1	L	62	GLU	5.0
1	C	287	TYR	5.0
1	K	395	ASN	4.9
1	I	337	ARG	4.9
1	C	61	ASN	4.9
1	A	274	LEU	4.9
1	C	403	GLU	4.9
1	A	392	MET	4.8
1	G	62	GLU	4.8
1	E	61	ASN	4.8
1	L	60	ILE	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	326	TYR	4.8
1	C	337	ARG	4.8
1	A	60	ILE	4.8
1	A	391	PRO	4.8
1	G	405	LYS	4.8
1	F	403	GLU	4.7
1	K	402	GLU	4.7
1	F	98	GLN	4.7
1	A	275	ALA	4.7
1	C	405	LYS	4.7
1	D	401	PRO	4.7
1	D	398	ASP	4.7
1	F	406	GLU	4.7
1	L	400	PRO	4.6
1	B	393	ASP	4.6
1	K	403	GLU	4.6
1	A	382	ILE	4.6
1	A	344	ARG	4.6
1	F	349	ALA	4.6
1	J	399	LEU	4.6
1	B	402	GLU	4.6
1	A	402	GLU	4.6
1	B	406	GLU	4.6
1	A	299	GLY	4.5
1	G	402	GLU	4.5
1	L	395	ASN	4.5
1	G	406	GLU	4.5
1	E	348	VAL	4.5
1	L	401	PRO	4.5
1	E	7	THR	4.5
1	H	12	HIS	4.5
1	B	400	PRO	4.5
1	A	352	LYS	4.5
1	F	61	ASN	4.5
1	L	396	LEU	4.5
1	I	401	PRO	4.4
1	I	403	GLU	4.4
1	A	3	GLU	4.4
1	J	60	ILE	4.4
1	A	294	ALA	4.4
1	E	4	HIS	4.4
1	E	337	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	402	GLU	4.4
1	A	280	ASN	4.3
1	E	401	PRO	4.3
1	B	351	PRO	4.3
1	G	63	SER	4.3
1	F	353	ALA	4.2
1	G	395	ASN	4.2
1	H	337	ARG	4.2
1	E	283	SER	4.2
1	C	62	GLU	4.2
1	I	62	GLU	4.2
1	L	394	LYS	4.1
1	H	400	PRO	4.1
1	I	400	PRO	4.1
1	H	60	ILE	4.1
1	E	405	LYS	4.1
1	B	407	ILE	4.1
1	E	62	GLU	4.0
1	A	405	LYS	4.0
1	C	406	GLU	4.0
1	A	380	ASP	4.0
1	D	405	LYS	4.0
1	A	117	ALA	4.0
1	B	327	GLU	4.0
1	C	282	PHE	4.0
1	K	396	LEU	4.0
1	A	2	ALA	4.0
1	F	351	PRO	4.0
1	A	293	GLN	3.9
1	G	1	SER	3.9
1	G	394	LYS	3.9
1	E	60	ILE	3.9
1	A	390	GLU	3.9
1	H	62	GLU	3.9
1	G	396	LEU	3.9
1	A	121	ALA	3.9
1	A	276	LYS	3.9
1	E	277	ASN	3.9
1	A	122	ASP	3.8
1	H	7	THR	3.8
1	E	279	THR	3.8
1	A	118	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	124	VAL	3.8
1	J	337	ARG	3.7
1	E	285	ASP	3.7
1	J	400	PRO	3.7
1	B	117	ALA	3.7
1	E	392	MET	3.7
1	G	339	ARG	3.7
1	L	404	ALA	3.7
1	E	282	PHE	3.7
1	A	335	SER	3.7
1	B	403	GLU	3.7
1	E	339	ARG	3.7
1	C	285	ASP	3.7
1	G	401	PRO	3.7
1	C	296	TYR	3.6
1	D	396	LEU	3.6
1	A	328	ALA	3.6
1	B	405	LYS	3.6
1	F	296	TYR	3.6
1	K	394	LYS	3.6
1	A	179	TYR	3.6
1	L	339	ARG	3.6
1	B	62	GLU	3.6
1	E	42	PHE	3.6
1	J	405	LYS	3.6
1	A	340	SER	3.5
1	D	348	VAL	3.5
1	F	348	VAL	3.5
1	H	8	MET	3.5
1	A	273	SER	3.5
1	J	401	PRO	3.5
1	C	60	ILE	3.5
1	A	327	GLU	3.5
1	B	42	PHE	3.5
1	C	386	ILE	3.5
1	F	333	ALA	3.5
1	C	293	GLN	3.5
1	A	379	LEU	3.5
1	A	290	LEU	3.4
1	A	387	HIS	3.4
1	A	126	PHE	3.4
1	A	330	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	337	ARG	3.4
1	L	402	GLU	3.4
1	B	12	HIS	3.3
1	C	348	VAL	3.3
1	J	403	GLU	3.3
1	E	353	ALA	3.3
1	A	355	ARG	3.3
1	B	331	MET	3.3
1	E	278	GLY	3.3
1	J	395	ASN	3.3
1	D	393	ASP	3.3
1	F	327	GLU	3.3
1	I	285	ASP	3.3
1	I	393	ASP	3.3
1	E	354	ARG	3.3
1	A	356	ILE	3.3
1	G	349	ALA	3.3
1	K	385	LYS	3.3
1	A	403	GLU	3.3
1	K	327	GLU	3.3
1	D	40	ALA	3.3
1	A	62	GLU	3.3
1	L	403	GLU	3.3
1	K	405	LYS	3.3
1	A	353	ALA	3.2
1	H	394	LYS	3.2
1	G	44	GLU	3.2
1	D	391	PRO	3.2
1	K	401	PRO	3.2
1	A	284	GLY	3.2
1	F	390	GLU	3.2
1	A	375	LEU	3.2
1	A	108	ALA	3.2
1	J	7	THR	3.2
1	K	404	ALA	3.2
1	G	60	ILE	3.2
1	L	59	GLY	3.2
1	A	38	VAL	3.2
1	C	392	MET	3.1
1	B	11	GLU	3.1
1	A	7	THR	3.1
1	A	349	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	389	GLY	3.1
1	D	352	LYS	3.1
1	J	394	LYS	3.1
1	A	224	ARG	3.1
1	H	401	PRO	3.1
1	K	337	ARG	3.1
1	L	349	ALA	3.1
1	A	339	ARG	3.1
1	A	343	ILE	3.1
1	H	407	ILE	3.1
1	A	431	GLY	3.1
1	A	279	THR	3.1
1	A	63	SER	3.1
1	I	60	ILE	3.1
1	J	393	ASP	3.1
1	A	51	GLY	3.1
1	C	281	LEU	3.1
1	D	9	LEU	3.1
1	D	404	ALA	3.1
1	J	61	ASN	3.1
1	K	62	GLU	3.1
1	B	354	ARG	3.0
1	G	393	ASP	3.0
1	F	324	PRO	3.0
1	D	61	ASN	3.0
1	J	404	ALA	3.0
1	K	349	ALA	3.0
1	F	352	LYS	3.0
1	A	324	PRO	3.0
1	B	391	PRO	3.0
1	K	400	PRO	3.0
1	J	339	ARG	3.0
1	B	65	MET	3.0
1	G	179	TYR	3.0
1	H	339	ARG	3.0
1	B	123	THR	3.0
1	H	4	HIS	3.0
1	C	407	ILE	3.0
1	A	383	LYS	3.0
1	A	120	ILE	2.9
1	A	406	GLU	2.9
1	A	381	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	51	GLY	2.9
1	C	437	GLU	2.9
1	H	5	VAL	2.9
1	J	402	GLU	2.9
1	A	282	PHE	2.9
1	H	351	PRO	2.9
1	C	279	THR	2.9
1	G	348	VAL	2.9
1	A	11	GLU	2.9
1	A	423	LEU	2.9
1	D	423	LEU	2.9
1	A	291	SER	2.9
1	E	351	PRO	2.9
1	B	6	LEU	2.9
1	A	323	VAL	2.8
1	E	393	ASP	2.8
1	A	408	PRO	2.8
1	J	407	ILE	2.8
1	C	275	ALA	2.8
1	D	4	HIS	2.8
1	F	277	ASN	2.8
1	H	350	SER	2.8
1	A	400	PRO	2.8
1	B	35	ALA	2.8
1	A	332	LEU	2.8
1	C	277	ASN	2.8
1	A	52	SER	2.8
1	A	289	GLY	2.8
1	L	388	PRO	2.8
1	B	58	LYS	2.8
1	A	10	ASN	2.8
1	C	284	GLY	2.8
1	L	408	PRO	2.8
1	C	393	ASP	2.8
1	G	2	ALA	2.8
1	G	96	THR	2.8
1	E	423	LEU	2.8
1	A	389	GLY	2.8
1	A	272	MET	2.8
1	A	5	VAL	2.8
1	E	347	VAL	2.8
1	A	100	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	179	TYR	2.8
1	I	395	ASN	2.8
1	E	403	GLU	2.8
1	A	94	PRO	2.8
1	F	116	ARG	2.8
1	E	293	GLN	2.8
1	C	120	ILE	2.8
1	H	10	ASN	2.8
1	H	179	TYR	2.7
1	C	349	ALA	2.7
1	D	42	PHE	2.7
1	F	2	ALA	2.7
1	I	6	LEU	2.7
1	L	393	ASP	2.7
1	C	339	ARG	2.7
1	J	62	GLU	2.7
1	I	407	ILE	2.7
1	B	8	MET	2.7
1	C	408	PRO	2.7
1	A	46	GLY	2.7
1	D	288	ALA	2.7
1	F	407	ILE	2.7
1	H	408	PRO	2.7
1	D	285	ASP	2.7
1	A	40	ALA	2.7
1	E	323	VAL	2.7
1	A	281	LEU	2.7
1	F	282	PHE	2.6
1	A	45	GLU	2.6
1	F	392	MET	2.6
1	J	390	GLU	2.6
1	C	338	ASN	2.6
1	E	434	PHE	2.6
1	C	122	ASP	2.6
1	G	165	GLU	2.6
1	H	406	GLU	2.6
1	I	406	GLU	2.6
1	A	342	SER	2.6
1	E	340	SER	2.6
1	C	7	THR	2.6
1	C	51	GLY	2.6
1	J	327	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	327	GLU	2.6
1	A	203	GLY	2.6
1	B	98	GLN	2.6
1	C	96	THR	2.6
1	A	125	LEU	2.6
1	D	339	ARG	2.6
1	E	350	SER	2.6
1	F	59	GLY	2.6
1	A	346	PRO	2.6
1	L	331	MET	2.6
1	A	336	ALA	2.6
1	B	275	ALA	2.6
1	C	347	VAL	2.6
1	E	292	GLU	2.6
1	L	390	GLU	2.6
1	B	48	MET	2.6
1	D	95	GLY	2.6
1	D	224	ARG	2.6
1	A	331	MET	2.5
1	D	392	MET	2.5
1	F	331	MET	2.5
1	A	303	LYS	2.5
1	C	46	GLY	2.5
1	D	10	ASN	2.5
1	I	63	SER	2.5
1	C	121	ALA	2.5
1	D	333	ALA	2.5
1	L	179	TYR	2.5
1	E	428	LEU	2.5
1	C	286	LYS	2.5
1	E	386	ILE	2.5
1	C	98	GLN	2.5
1	E	44	GLU	2.5
1	B	85	LEU	2.5
1	B	282	PHE	2.5
1	A	48	MET	2.5
1	D	44	GLU	2.5
1	K	367	PRO	2.5
1	K	61	ASN	2.5
1	C	351	PRO	2.5
1	C	119	GLY	2.5
1	B	4	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	304	HIS	2.5
1	A	371	PHE	2.5
1	A	394	LYS	2.5
1	C	123	THR	2.5
1	L	98	GLN	2.4
1	A	434	PHE	2.4
1	J	63	SER	2.4
1	E	41	GLU	2.4
1	G	407	ILE	2.4
1	I	390	GLU	2.4
1	E	123	THR	2.4
1	I	349	ALA	2.4
1	A	6	LEU	2.4
1	E	290	LEU	2.4
1	A	283	SER	2.4
1	A	86	ILE	2.4
1	C	385	LYS	2.4
1	J	277	ASN	2.4
1	C	353	ALA	2.4
1	K	393	ASP	2.4
1	A	432	GLY	2.4
1	D	43	PHE	2.4
1	F	44	GLU	2.4
1	F	165	GLU	2.4
1	E	430	ALA	2.4
1	J	238	TYR	2.4
1	I	361	PRO	2.4
1	D	349	ALA	2.4
1	A	112	GLU	2.4
1	B	41	GLU	2.4
1	B	352	LYS	2.4
1	C	42	PHE	2.4
1	A	1	SER	2.4
1	A	115	LEU	2.4
1	D	41	GLU	2.4
1	E	286	LYS	2.3
1	F	325	GLY	2.3
1	B	39	ASN	2.3
1	J	396	LEU	2.3
1	C	304	HIS	2.3
1	D	38	VAL	2.3
1	B	285	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	235	ILE	2.3
1	A	230	LYS	2.3
1	B	349	ALA	2.3
1	H	117	ALA	2.3
1	E	284	GLY	2.3
1	E	9	LEU	2.3
1	B	64	ASP	2.3
1	A	407	ILE	2.3
1	B	273	SER	2.3
1	D	365	ALA	2.3
1	C	289	GLY	2.3
1	D	59	GLY	2.3
1	E	295	LEU	2.3
1	E	280	ASN	2.3
1	A	426	GLU	2.3
1	F	1	SER	2.3
1	K	278	GLY	2.3
1	F	334	TYR	2.3
1	J	221	VAL	2.3
1	C	3	GLU	2.3
1	C	390	GLU	2.3
1	H	392	MET	2.3
1	B	52	SER	2.3
1	G	267	GLY	2.3
1	G	328	ALA	2.3
1	B	96	THR	2.3
1	E	11	GLU	2.3
1	A	376	MET	2.3
1	D	389	GLY	2.3
1	K	63	SER	2.3
1	A	180	PHE	2.3
1	A	44	GLU	2.3
1	E	13	GLU	2.3
1	D	408	PRO	2.2
1	H	348	VAL	2.2
1	E	1	SER	2.2
1	J	1	SER	2.2
1	E	341	ALA	2.2
1	L	327	GLU	2.2
1	G	97	LEU	2.2
1	E	388	PRO	2.2
1	E	276	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	336	ALA	2.2
1	B	274	LEU	2.2
1	H	396	LEU	2.2
1	K	324	PRO	2.2
1	K	408	PRO	2.2
1	A	99	GLY	2.2
1	F	66	VAL	2.2
1	I	331	MET	2.2
1	F	393	ASP	2.2
1	B	179	TYR	2.2
1	E	3	GLU	2.2
1	L	41	GLU	2.2
1	B	367	PRO	2.2
1	G	338	ASN	2.2
1	I	339	ARG	2.2
1	C	12	HIS	2.2
1	D	62	GLU	2.2
1	L	364	ALA	2.2
1	A	386	ILE	2.2
1	B	345	ILE	2.2
1	B	290	LEU	2.2
1	G	270	CYS	2.2
1	H	349	ALA	2.2
1	F	123	THR	2.2
1	E	43	PHE	2.2
1	B	9	LEU	2.2
1	A	53	SER	2.2
1	K	340	SER	2.2
1	G	358	VAL	2.1
1	H	328	ALA	2.1
1	B	118	THR	2.1
1	E	289	GLY	2.1
1	I	371	PHE	2.1
1	J	41	GLU	2.1
1	G	6	LEU	2.1
1	L	328	ALA	2.1
1	L	348	VAL	2.1
1	K	44	GLU	2.1
1	E	346	PRO	2.1
1	G	371	PHE	2.1
1	I	43	PHE	2.1
1	G	392	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	288	ALA	2.1
1	C	352	LYS	2.1
1	E	275	ALA	2.1
1	G	58	LYS	2.1
1	L	361	PRO	2.1
1	B	434	PHE	2.1
1	E	119	GLY	2.1
1	A	468	VAL	2.1
1	D	407	ILE	2.1
1	H	390	GLU	2.1
1	B	56	GLY	2.1
1	F	278	GLY	2.1
1	C	8	MET	2.1
1	I	392	MET	2.1
1	A	301	VAL	2.1
1	B	38	VAL	2.1
1	E	296	TYR	2.1
1	A	4	HIS	2.1
1	I	370	CYS	2.1
1	J	132	PHE	2.1
1	D	277	ASN	2.1
1	B	59	GLY	2.1
1	C	95	GLY	2.1
1	L	45	GLU	2.1
1	F	5	VAL	2.1
1	B	382	ILE	2.1
1	L	180	PHE	2.1
1	B	46	GLY	2.1
1	D	3	GLU	2.1
1	A	388	PRO	2.0
1	I	367	PRO	2.0
1	L	365	ALA	2.0
1	A	433	VAL	2.0
1	D	468	VAL	2.0
1	I	7	THR	2.0
1	D	11	GLU	2.0
1	J	9	LEU	2.0
1	L	97	LEU	2.0
1	K	344	ARG	2.0
1	E	8	MET	2.0
1	L	370	CYS	2.0
1	L	392	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	205	VAL	2.0
1	A	435	THR	2.0
1	D	327	GLU	2.0
1	A	55	GLY	2.0
1	A	166	GLY	2.0
1	L	238	TYR	2.0
1	L	389	GLY	2.0
1	D	337	ARG	2.0
1	G	359	ARG	2.0
1	I	270	CYS	2.0
1	K	270	CYS	2.0
1	A	66	VAL	2.0
1	B	340	SER	2.0
1	B	281	LEU	2.0
1	F	179	TYR	2.0
1	G	296	TYR	2.0
1	A	176	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
3	ADP	A	4471	27/27	0.51	0.54	38,77,100,100	27
4	MPD	B	5474	8/8	0.58	0.47	63,68,75,98	8
4	MPD	C	5476	8/8	0.59	0.45	63,68,75,98	8
4	MPD	A	5472	8/8	0.63	0.48	63,68,75,98	8
3	ADP	B	4472	27/27	0.64	0.45	38,77,100,100	27
4	MPD	H	5486	8/8	0.65	0.52	63,68,75,98	8

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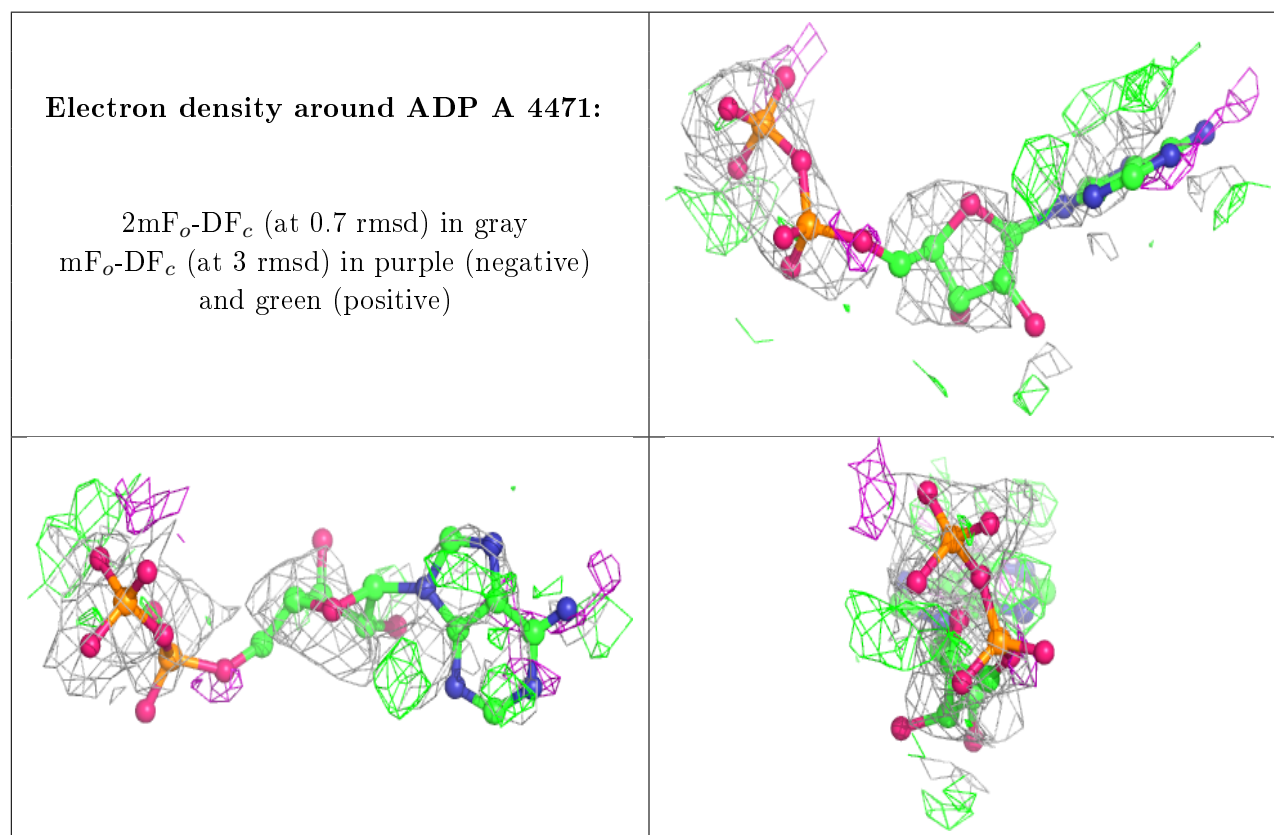
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ADP	F	4476	27/27	0.70	0.41	38,77,100,100	27
3	ADP	E	4475	27/27	0.71	0.36	38,77,100,100	27
3	ADP	L	4482	27/27	0.71	0.44	38,77,100,100	27
3	ADP	K	4481	27/27	0.73	0.40	38,77,100,100	27
3	ADP	I	4479	27/27	0.73	0.41	38,77,100,100	27
4	MPD	B	5471	8/8	0.74	0.46	37,50,65,66	8
4	MPD	G	5484	8/8	0.74	0.51	63,68,75,98	8
4	MPD	J	5490	8/8	0.75	0.49	63,68,75,98	8
3	ADP	G	4477	27/27	0.75	0.39	38,77,100,100	27
3	ADP	D	4474	27/27	0.75	0.34	38,77,100,100	27
4	MPD	E	5480	8/8	0.76	0.48	63,68,75,98	8
4	MPD	I	5488	8/8	0.77	0.55	63,68,75,98	8
3	ADP	C	4473	27/27	0.77	0.34	38,77,100,100	27
4	MPD	D	5478	8/8	0.78	0.49	63,68,75,98	8
4	MPD	F	5482	8/8	0.78	0.36	63,68,75,98	8
3	ADP	H	4478	27/27	0.80	0.33	38,77,100,100	27
4	MPD	K	5492	8/8	0.80	0.50	63,68,75,98	8
3	ADP	J	4480	27/27	0.81	0.39	38,77,100,100	27
4	MPD	L	5494	8/8	0.82	0.52	63,68,75,98	8
4	MPD	A	5481	8/8	0.82	0.38	37,50,65,66	8
4	MPD	D	5475	8/8	0.83	0.36	37,50,65,66	8
4	MPD	F	5479	8/8	0.83	0.45	37,50,65,66	8
2	MN	A	470	1/1	0.87	0.07	46,46,46,46	0
4	MPD	E	5477	8/8	0.87	0.40	37,50,65,66	8
4	MPD	I	5489	8/8	0.88	0.40	37,50,65,66	8
4	MPD	C	5473	8/8	0.88	0.39	37,50,65,66	8
4	MPD	H	5487	8/8	0.88	0.44	37,50,65,66	8
4	MPD	L	5483	8/8	0.89	0.42	37,50,65,66	8
4	MPD	G	5485	8/8	0.89	0.44	37,50,65,66	8
2	MN	A	469	1/1	0.91	0.07	47,47,47,47	0
4	MPD	J	5491	8/8	0.92	0.43	37,50,65,66	8
2	MN	L	469	1/1	0.92	0.16	47,47,47,47	0
2	MN	C	469	1/1	0.93	0.07	47,47,47,47	0
4	MPD	K	5493	8/8	0.93	0.43	37,50,65,66	8
2	MN	D	470	1/1	0.93	0.04	46,46,46,46	0
2	MN	E	470	1/1	0.94	0.06	46,46,46,46	0
2	MN	B	470	1/1	0.94	0.07	46,46,46,46	0
2	MN	H	469	1/1	0.95	0.15	47,47,47,47	0
2	MN	F	469	1/1	0.95	0.07	47,47,47,47	0
2	MN	B	469	1/1	0.96	0.06	47,47,47,47	0
2	MN	H	470	1/1	0.96	0.08	46,46,46,46	0
2	MN	K	469	1/1	0.97	0.15	47,47,47,47	0

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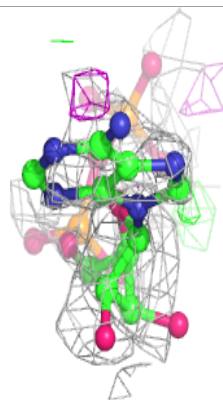
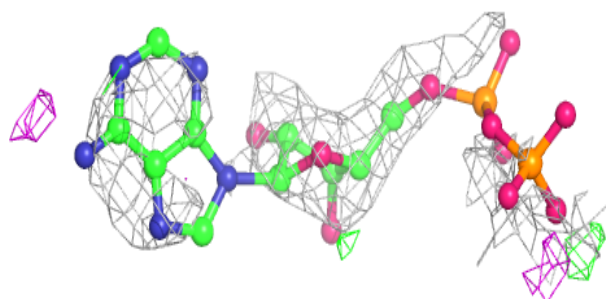
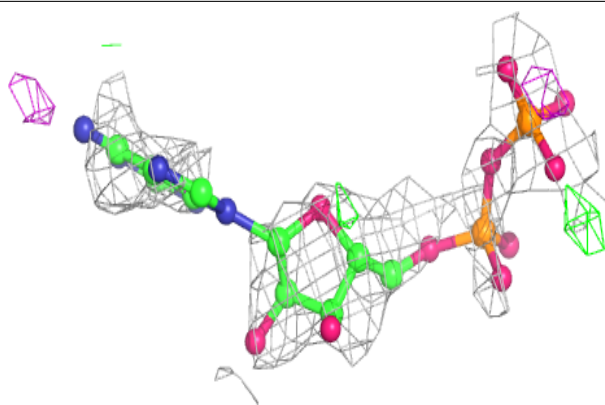
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	I	470	1/1	0.97	0.08	46,46,46,46	0
2	MN	G	470	1/1	0.97	0.10	46,46,46,46	0
2	MN	J	469	1/1	0.97	0.16	47,47,47,47	0
2	MN	C	470	1/1	0.97	0.04	46,46,46,46	0
2	MN	E	469	1/1	0.97	0.03	47,47,47,47	0
2	MN	I	469	1/1	0.97	0.12	47,47,47,47	0
2	MN	J	470	1/1	0.98	0.10	46,46,46,46	0
2	MN	F	470	1/1	0.98	0.04	46,46,46,46	0
2	MN	L	470	1/1	0.98	0.13	46,46,46,46	0
2	MN	D	469	1/1	0.98	0.09	47,47,47,47	0
2	MN	K	470	1/1	0.99	0.12	46,46,46,46	0
2	MN	G	469	1/1	0.99	0.10	47,47,47,47	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.

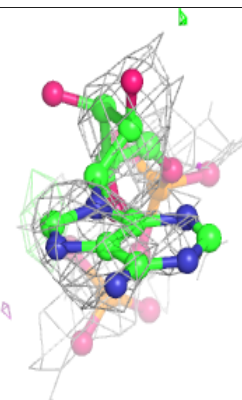
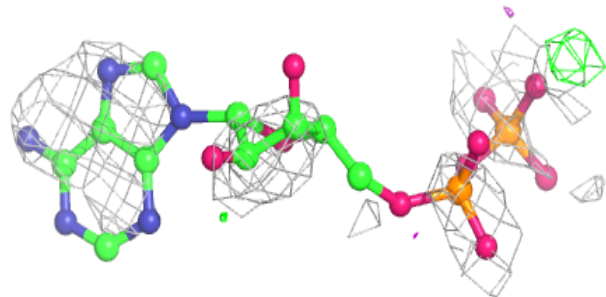
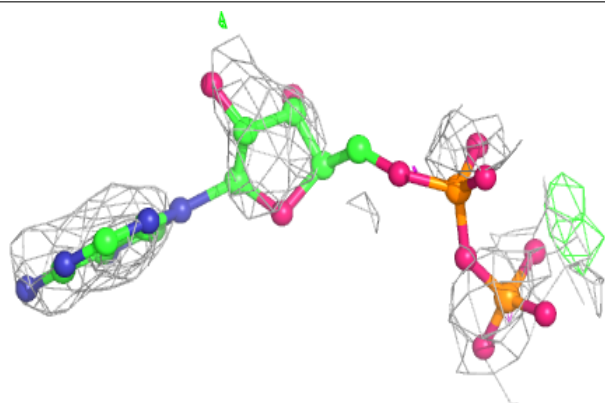


**Electron density around ADP B 4472:**

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

**Electron density around ADP F 4476:**

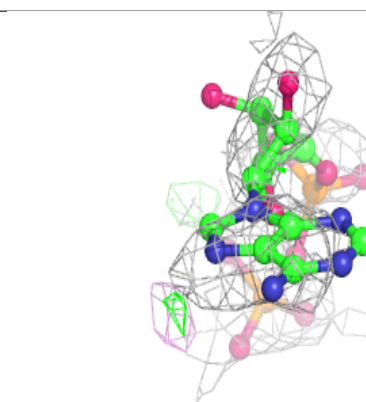
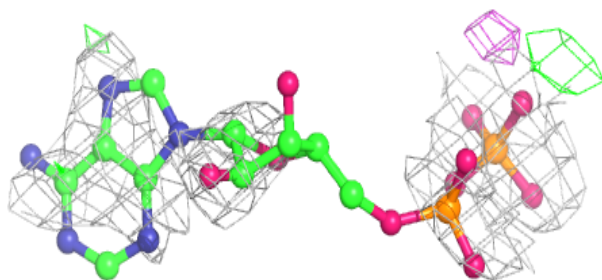
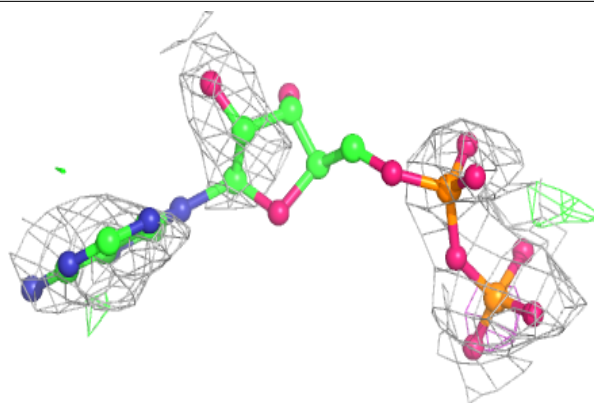
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



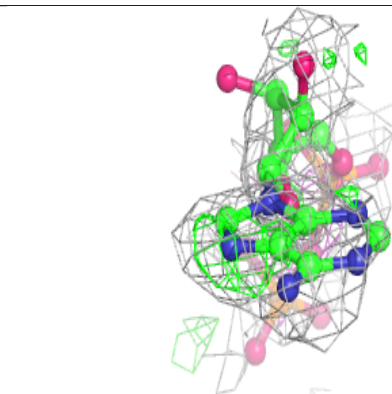
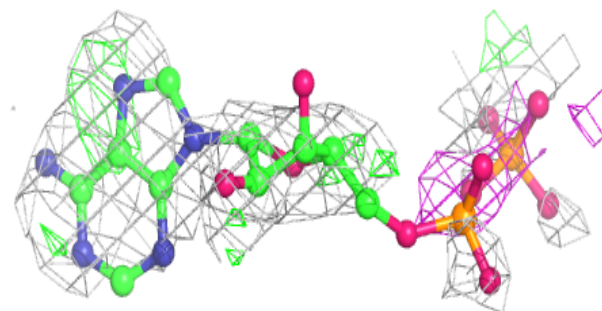
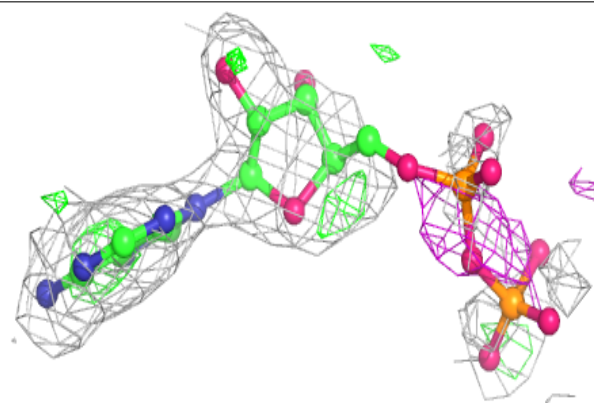


**Electron density around ADP E 4475:**

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

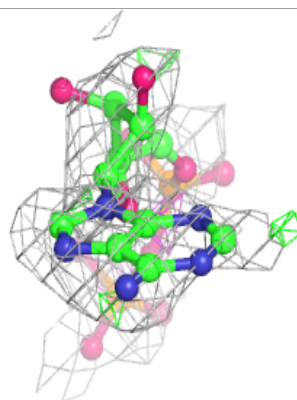
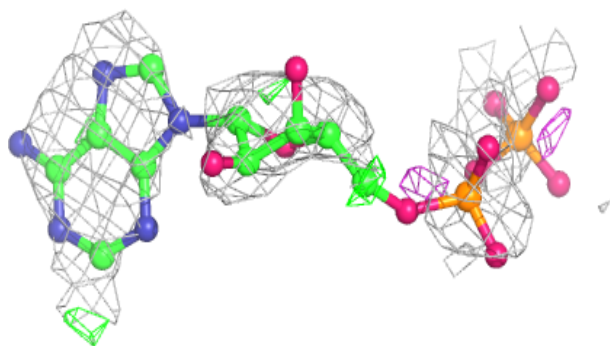
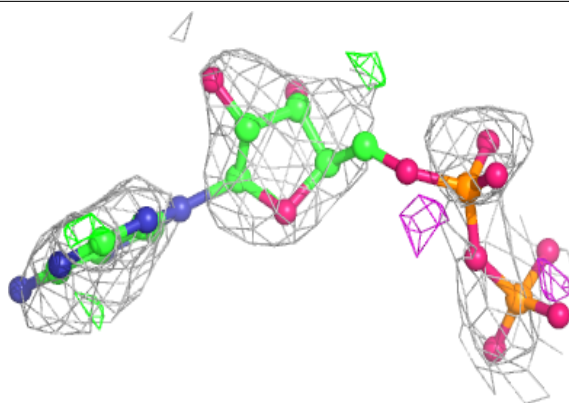
**Electron density around ADP L 4482:**

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

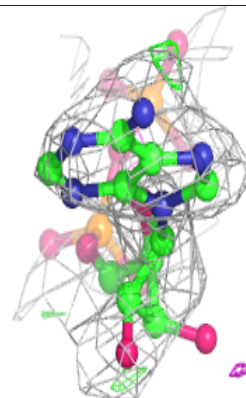
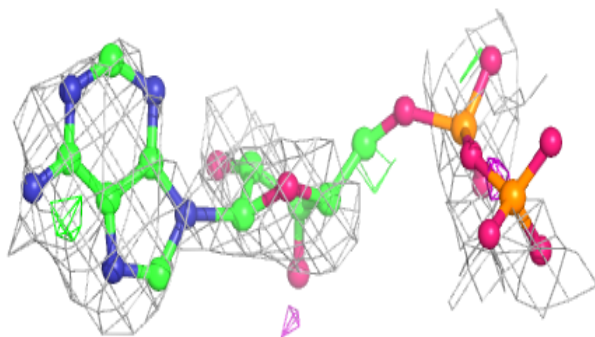
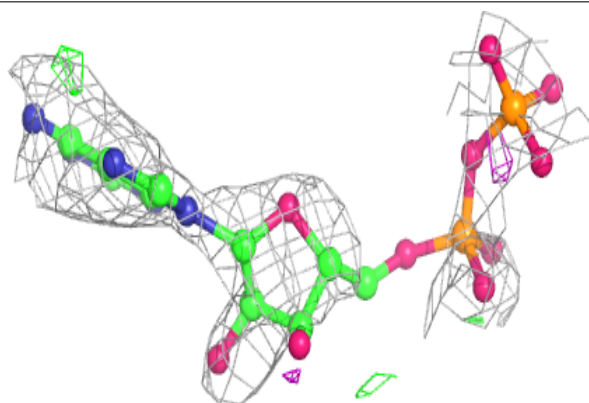


**Electron density around ADP K 4481:**

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

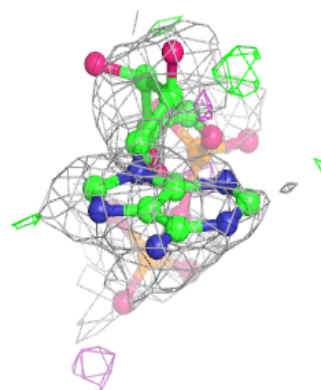
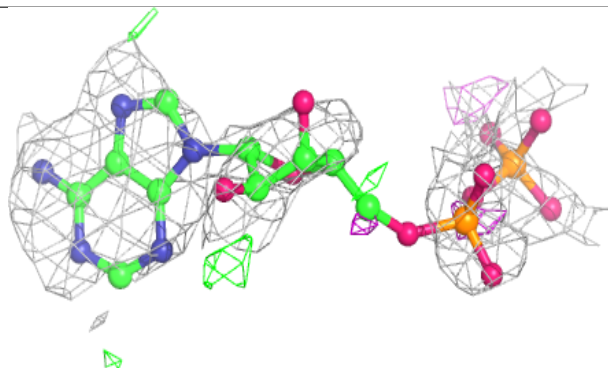
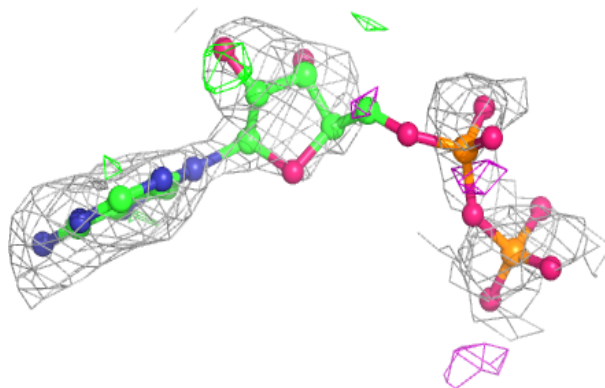
**Electron density around ADP I 4479:**

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

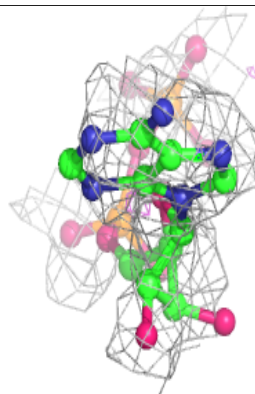
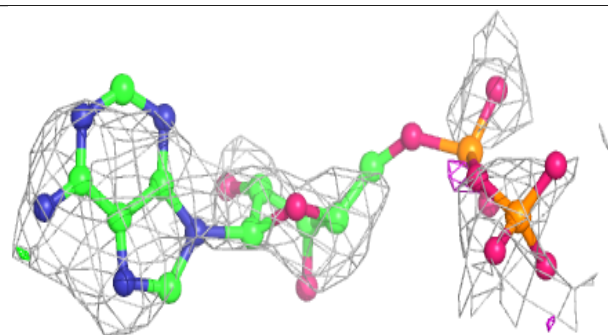
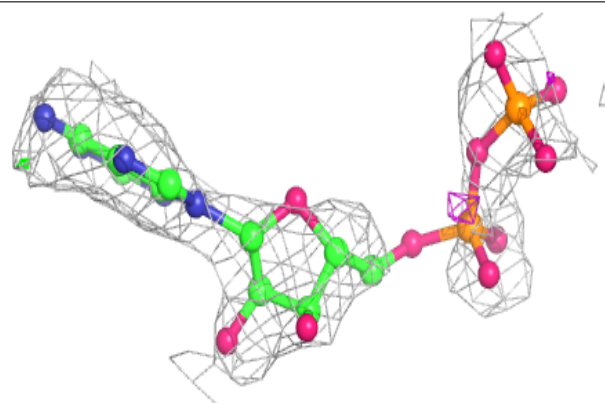


**Electron density around ADP G 4477:**

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

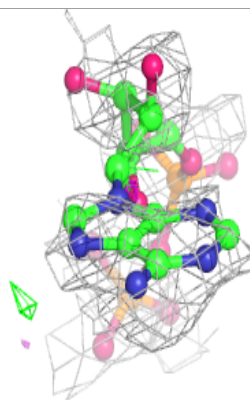
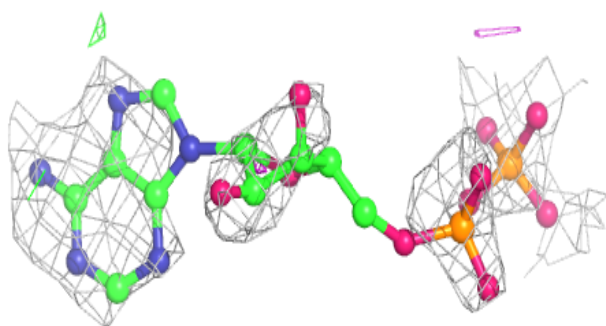
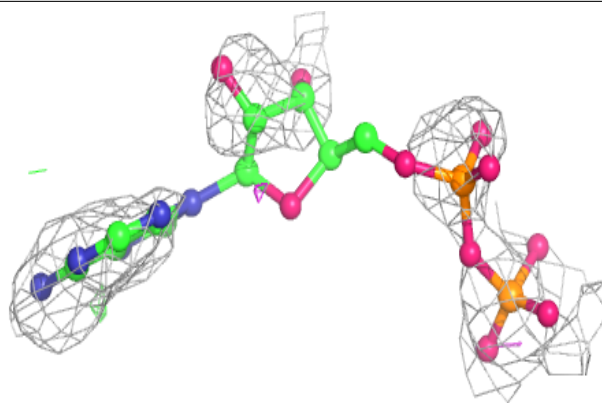
**Electron density around ADP D 4474:**

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

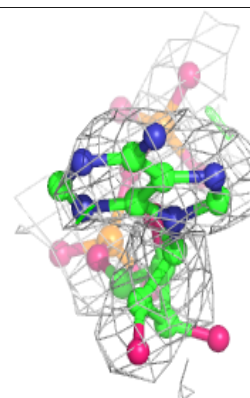
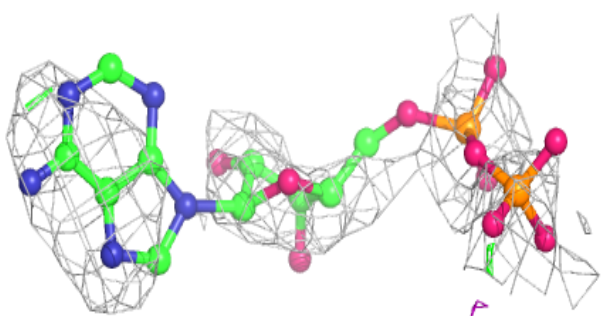
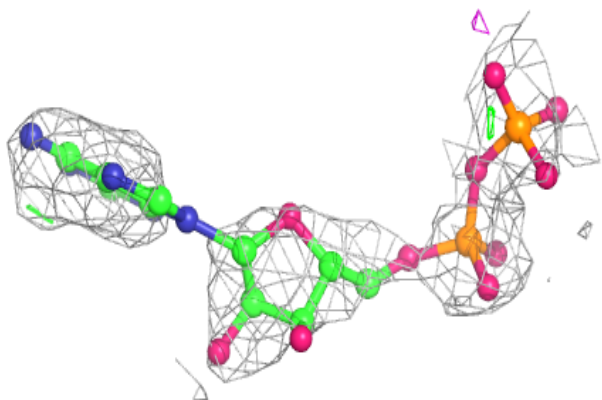


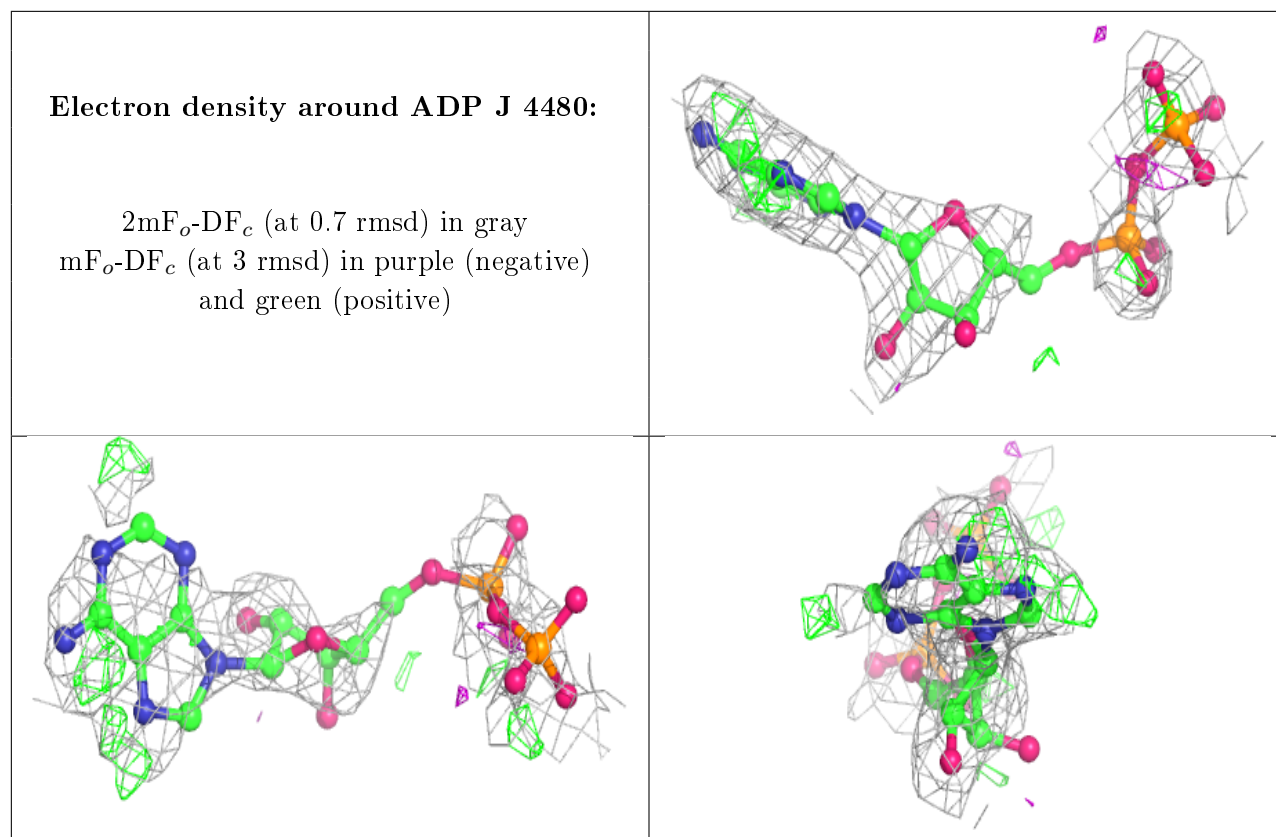
**Electron density around ADP C 4473:**

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

**Electron density around ADP H 4478:**

$2mF_o - DF_c$  (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.