



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:55 am BST

PDB ID : 1LGR  
Title : INTERACTIONS OF NUCLEOTIDES WITH FULLY UNADENYLYLATED  
GLUTAMINE SYNTHETASE FROM SALMONELLA TYPHIMURIUM  
Authors : Liaw, S.-H.; Eisenberg, D.  
Deposited on : 1994-08-05  
Resolution : 2.79 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

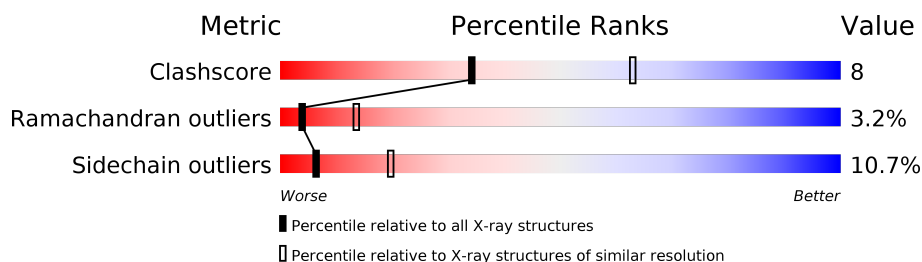
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	468	65% 24% . . 5%
1	B	468	65% 24% . . 5%
1	C	468	64% 25% . . 5%
1	D	468	66% 24% 5% . 5%
1	E	468	66% 24% . . 5%
1	F	468	66% 24% . . 5%
1	G	468	66% 24% . . 5%
1	H	468	66% 23% . . 5%

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Mol	Chain	Length	Quality of chain
1	I	468	<div><div></div><div>65%</div><div>25%</div><div>• • 5%</div></div>
1	J	468	<div><div></div><div>66%</div><div>23%</div><div>• • 5%</div></div>
1	K	468	<div><div></div><div>65%</div><div>24%</div><div>5% • 5%</div></div>
1	L	468	<div><div></div><div>66%</div><div>24%</div><div>• • 5%</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41760 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	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	B	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	C	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	D	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	E	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	F	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	G	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	H	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	I	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	J	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	K	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			
1	L	445	Total	C	N	O	S	0	0	0
			3455	2187	596	652	20			

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

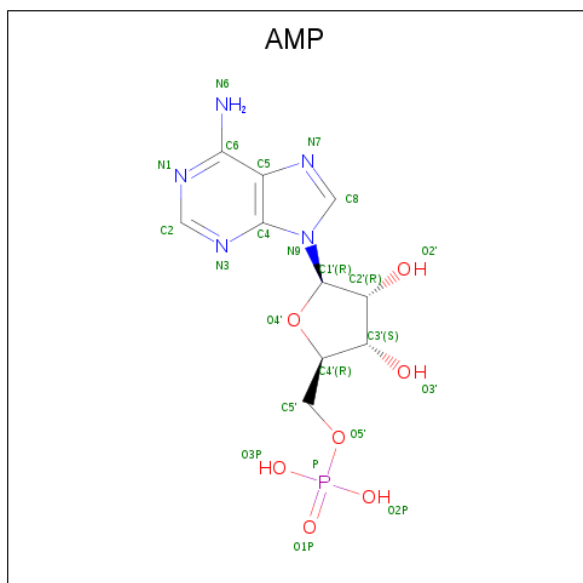
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Mn	0	0
			2	2		
2	J	2	Total	Mn	0	0
			2	2		

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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 MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

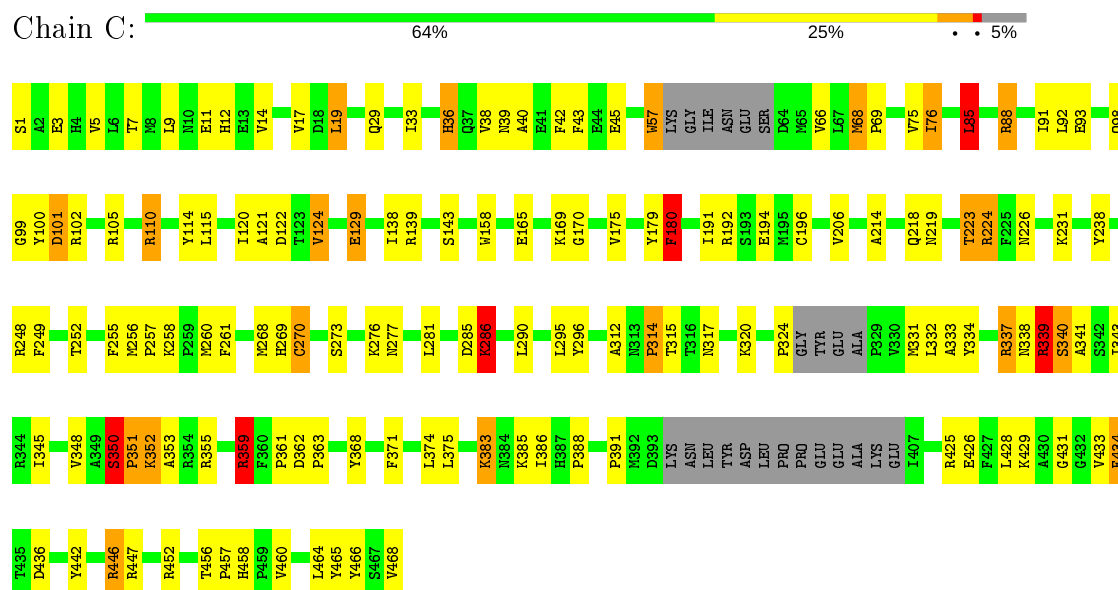
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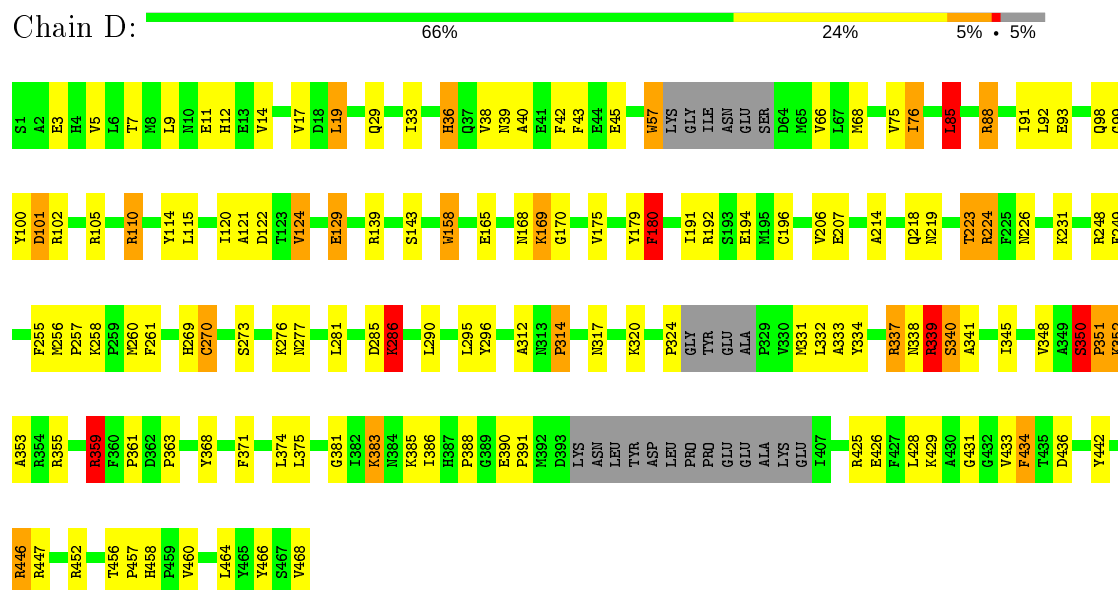
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	I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



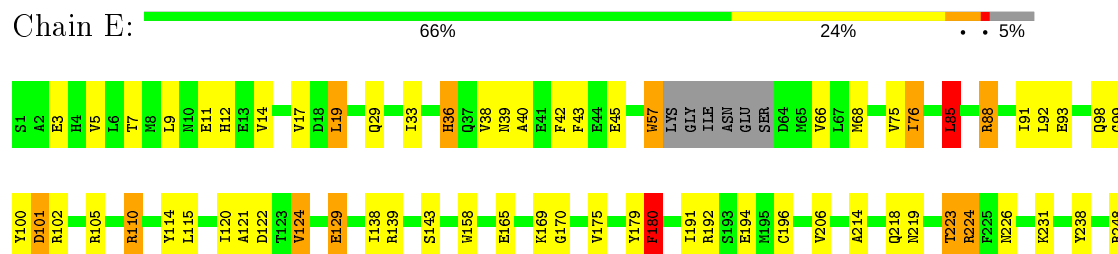
• Molecule 1: GLUTAMINE SYNTHETASE



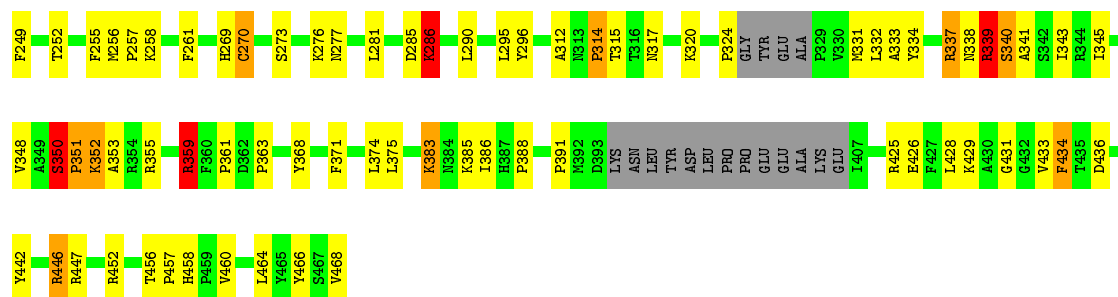
• Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE

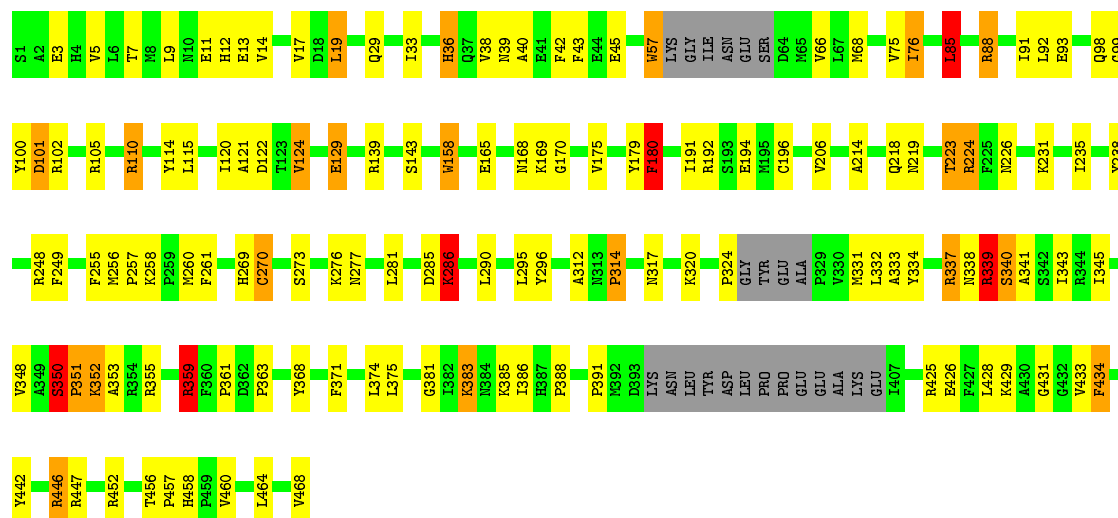






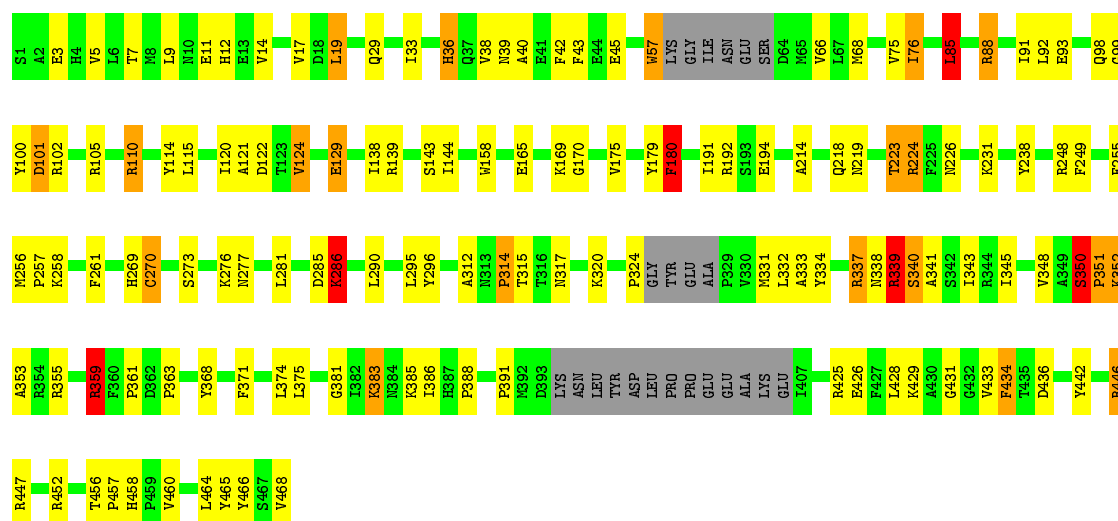
• Molecule 1: GLUTAMINE SYNTHETASE

Chain F: 66% 24% 5%



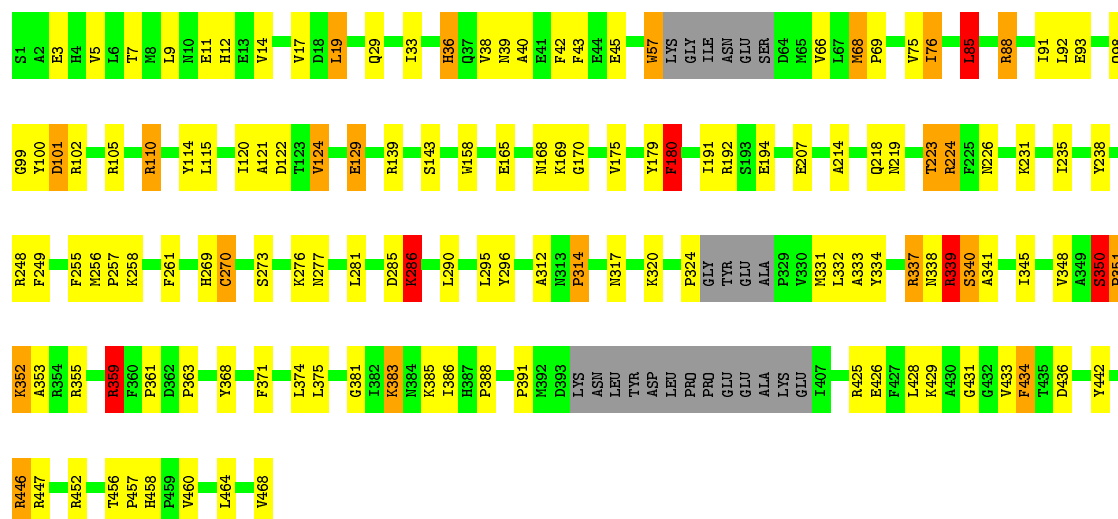
• Molecule 1: GLUTAMINE SYNTHETASE

Chain G: 66% 24% 5%



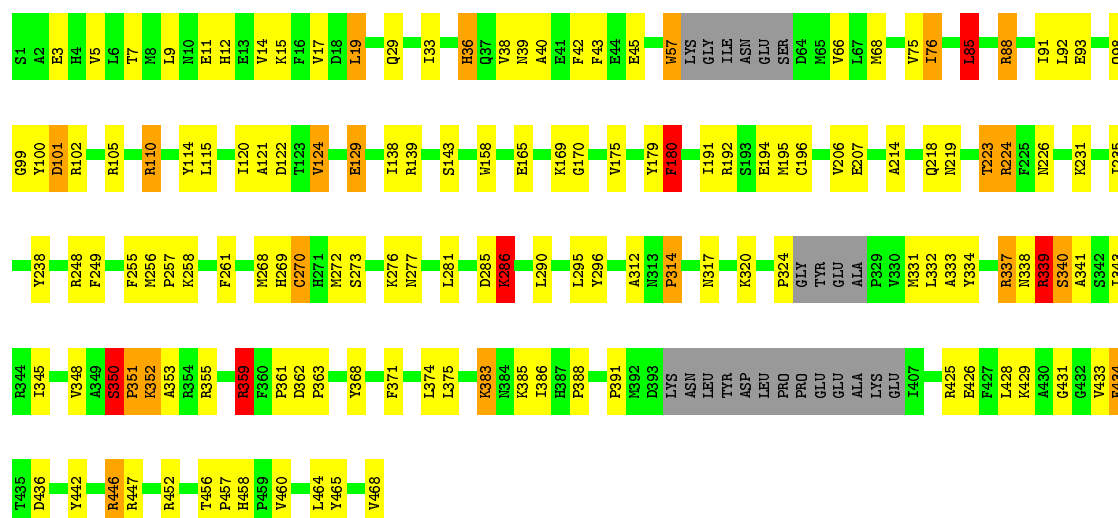
• Molecule 1: GLUTAMINE SYNTHETASE

Chain H:  66% 23% 5%



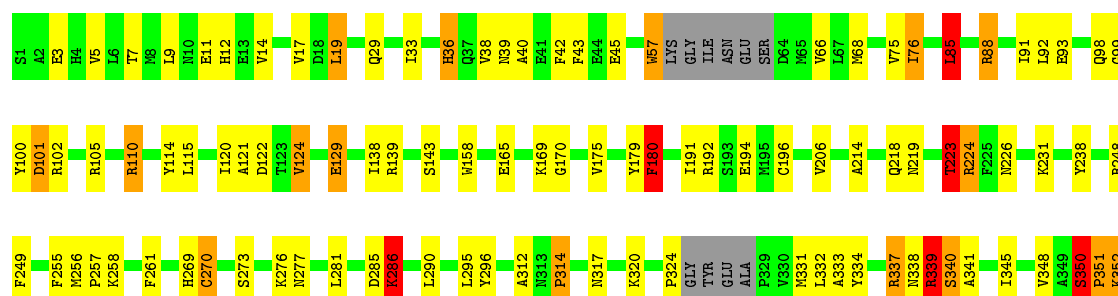
• Molecule 1: GLUTAMINE SYNTHETASE

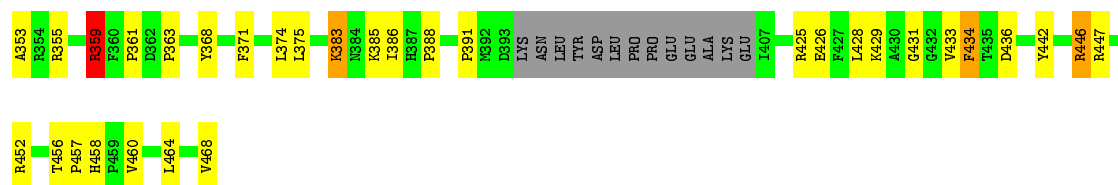
Chain I:  65% 25% 5%



• Molecule 1: GLUTAMINE SYNTHETASE

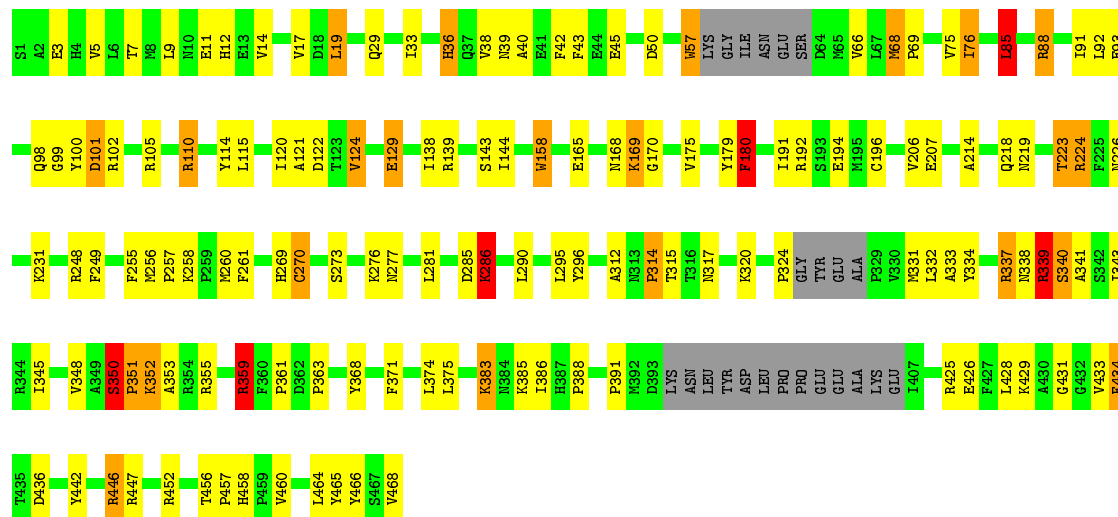
Chain J:  66% 23% 5%





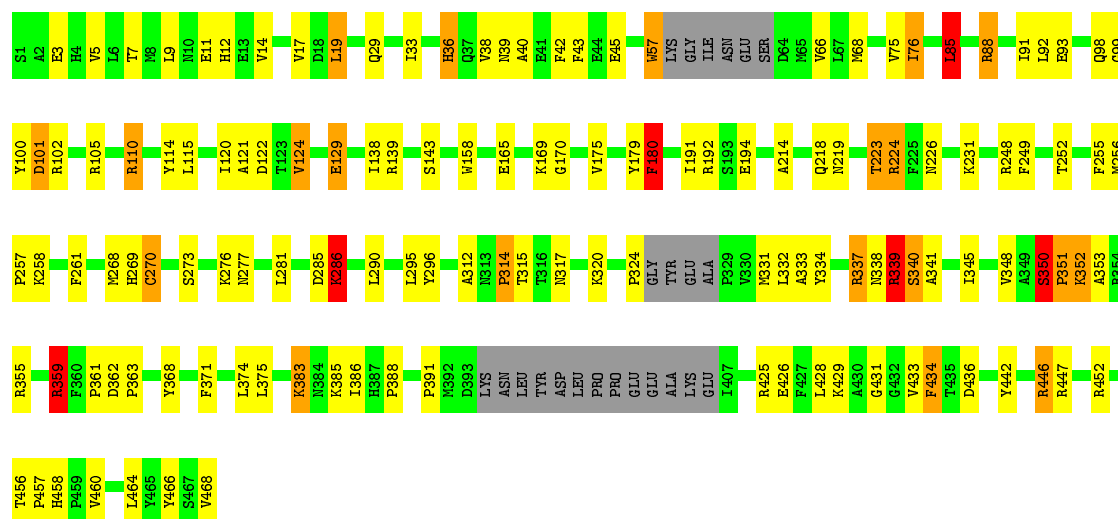
- Molecule 1: GLUTAMINE SYNTHETASE

Chain K:  65% 24% 5% • 5%



- Molecule 1: GLUTAMINE SYNTHETASE

Chain L:  66% 24% . . 5%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	235.50 Å   134.50 Å   200.10 Å 90.00°   102.80°   90.00°	Depositor
Resolution (Å)	8.00 – 2.79	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.79)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.233 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	41760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.74	0/3535	1.51	39/4782 (0.8%)
1	B	0.74	0/3535	1.51	38/4782 (0.8%)
1	C	0.74	0/3535	1.51	39/4782 (0.8%)
1	D	0.74	0/3535	1.51	38/4782 (0.8%)
1	E	0.74	0/3535	1.51	39/4782 (0.8%)
1	F	0.74	0/3535	1.51	39/4782 (0.8%)
1	G	0.74	0/3535	1.51	39/4782 (0.8%)
1	H	0.74	0/3535	1.51	39/4782 (0.8%)
1	I	0.74	0/3535	1.51	40/4782 (0.8%)
1	J	0.74	0/3535	1.51	39/4782 (0.8%)
1	K	0.74	0/3535	1.51	38/4782 (0.8%)
1	L	0.74	0/3535	1.51	38/4782 (0.8%)
All	All	0.74	0/42420	1.51	465/57384 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	24

There are no bond length outliers.

All (465) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	88	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	C	88	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	L	158	TRP	CD1-CG-CD2	9.69	114.05	106.30
1	C	158	TRP	CD1-CG-CD2	9.69	114.05	106.30
1	J	158	TRP	CD1-CG-CD2	9.68	114.05	106.30
1	K	158	TRP	CD1-CG-CD2	9.68	114.04	106.30
1	F	158	TRP	CD1-CG-CD2	9.67	114.04	106.30
1	L	88	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	H	158	TRP	CD1-CG-CD2	9.66	114.03	106.30
1	D	158	TRP	CD1-CG-CD2	9.66	114.03	106.30
1	I	158	TRP	CD1-CG-CD2	9.66	114.03	106.30
1	H	88	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	D	452	ARG	NE-CZ-NH1	9.65	125.12	120.30
1	J	452	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	B	158	TRP	CD1-CG-CD2	9.64	114.01	106.30
1	A	158	TRP	CD1-CG-CD2	9.64	114.01	106.30
1	I	88	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	E	88	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	G	88	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	D	88	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	88	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	E	158	TRP	CD1-CG-CD2	9.61	113.99	106.30
1	G	158	TRP	CD1-CG-CD2	9.60	113.98	106.30
1	B	452	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	B	88	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	K	88	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	A	452	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	J	88	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	L	452	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	E	452	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	G	452	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	F	452	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	I	452	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	H	452	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	K	452	ARG	NE-CZ-NH1	9.49	125.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	452	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	88	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	K	88	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	H	88	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	I	88	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	F	88	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	G	88	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	J	88	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	L	88	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	D	88	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	A	88	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	B	88	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	E	88	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	I	359	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	D	359	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	E	359	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	K	359	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	F	359	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	L	359	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	A	359	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	359	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	J	359	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	C	359	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	H	359	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	D	248	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	K	248	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	I	248	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	G	359	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	D	179	TYR	CA-C-N	-8.58	98.32	117.20
1	G	248	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	K	179	TYR	CA-C-N	-8.57	98.34	117.20
1	B	179	TYR	CA-C-N	-8.57	98.36	117.20
1	F	179	TYR	CA-C-N	-8.56	98.36	117.20
1	J	179	TYR	CA-C-N	-8.56	98.36	117.20
1	B	248	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	C	179	TYR	CA-C-N	-8.56	98.36	117.20
1	G	179	TYR	CA-C-N	-8.56	98.37	117.20
1	A	179	TYR	CA-C-N	-8.56	98.37	117.20
1	A	248	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	I	179	TYR	CA-C-N	-8.56	98.37	117.20
1	L	179	TYR	CA-C-N	-8.55	98.38	117.20
1	E	248	ARG	NE-CZ-NH1	8.55	124.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	179	TYR	CA-C-N	-8.55	98.39	117.20
1	E	179	TYR	CA-C-N	-8.55	98.39	117.20
1	H	248	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	L	248	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	C	248	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	F	248	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	J	248	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	L	158	TRP	CE2-CD2-CG	-8.35	100.62	107.30
1	G	158	TRP	CE2-CD2-CG	-8.31	100.65	107.30
1	H	158	TRP	CE2-CD2-CG	-8.31	100.65	107.30
1	J	158	TRP	CE2-CD2-CG	-8.31	100.65	107.30
1	I	158	TRP	CE2-CD2-CG	-8.30	100.66	107.30
1	D	158	TRP	CE2-CD2-CG	-8.30	100.66	107.30
1	A	158	TRP	CE2-CD2-CG	-8.29	100.67	107.30
1	K	158	TRP	CE2-CD2-CG	-8.29	100.67	107.30
1	E	158	TRP	CE2-CD2-CG	-8.28	100.68	107.30
1	F	158	TRP	CE2-CD2-CG	-8.28	100.68	107.30
1	B	158	TRP	CE2-CD2-CG	-8.27	100.68	107.30
1	C	158	TRP	CE2-CD2-CG	-8.27	100.68	107.30
1	F	68	MET	CG-SD-CE	-6.92	89.13	100.20
1	D	68	MET	CG-SD-CE	-6.91	89.14	100.20
1	L	68	MET	CG-SD-CE	-6.91	89.14	100.20
1	I	68	MET	CG-SD-CE	-6.91	89.15	100.20
1	J	68	MET	CG-SD-CE	-6.90	89.15	100.20
1	C	68	MET	CG-SD-CE	-6.90	89.16	100.20
1	A	68	MET	CG-SD-CE	-6.90	89.16	100.20
1	B	68	MET	CG-SD-CE	-6.90	89.16	100.20
1	G	68	MET	CG-SD-CE	-6.90	89.16	100.20
1	E	68	MET	CG-SD-CE	-6.89	89.18	100.20
1	K	68	MET	CG-SD-CE	-6.88	89.18	100.20
1	H	68	MET	CG-SD-CE	-6.88	89.19	100.20
1	F	57	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	D	180	PHE	N-CA-C	6.86	129.53	111.00
1	C	180	PHE	N-CA-C	6.86	129.53	111.00
1	K	180	PHE	N-CA-C	6.86	129.53	111.00
1	G	180	PHE	N-CA-C	6.86	129.52	111.00
1	L	180	PHE	N-CA-C	6.86	129.52	111.00
1	A	180	PHE	N-CA-C	6.85	129.50	111.00
1	B	180	PHE	N-CA-C	6.85	129.50	111.00
1	C	57	TRP	CE2-CD2-CG	-6.85	101.82	107.30
1	I	180	PHE	N-CA-C	6.85	129.50	111.00
1	J	180	PHE	N-CA-C	6.85	129.50	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	180	PHE	N-CA-C	6.84	129.48	111.00
1	H	180	PHE	N-CA-C	6.84	129.48	111.00
1	F	180	PHE	N-CA-C	6.84	129.47	111.00
1	E	57	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	B	57	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	I	57	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	J	57	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	A	57	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	G	57	TRP	CE2-CD2-CG	-6.83	101.84	107.30
1	H	57	TRP	CE2-CD2-CG	-6.82	101.84	107.30
1	L	57	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	K	57	TRP	CE2-CD2-CG	-6.82	101.85	107.30
1	D	57	TRP	CE2-CD2-CG	-6.78	101.88	107.30
1	F	57	TRP	CD1-CG-CD2	6.72	111.67	106.30
1	E	57	TRP	CD1-CG-CD2	6.69	111.65	106.30
1	B	57	TRP	CD1-CG-CD2	6.68	111.65	106.30
1	H	57	TRP	CD1-CG-CD2	6.68	111.64	106.30
1	C	57	TRP	CD1-CG-CD2	6.66	111.63	106.30
1	A	57	TRP	CD1-CG-CD2	6.65	111.62	106.30
1	I	57	TRP	CD1-CG-CD2	6.65	111.62	106.30
1	J	57	TRP	CD1-CG-CD2	6.65	111.62	106.30
1	K	57	TRP	CD1-CG-CD2	6.63	111.60	106.30
1	D	57	TRP	CD1-CG-CD2	6.61	111.58	106.30
1	G	57	TRP	CD1-CG-CD2	6.61	111.59	106.30
1	L	57	TRP	CD1-CG-CD2	6.58	111.56	106.30
1	J	139	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	K	124	VAL	CB-CA-C	-6.38	99.28	111.40
1	F	124	VAL	CB-CA-C	-6.37	99.29	111.40
1	L	124	VAL	CB-CA-C	-6.36	99.32	111.40
1	B	124	VAL	CB-CA-C	-6.36	99.32	111.40
1	I	124	VAL	CB-CA-C	-6.36	99.32	111.40
1	A	124	VAL	CB-CA-C	-6.36	99.33	111.40
1	J	124	VAL	CB-CA-C	-6.36	99.33	111.40
1	H	124	VAL	CB-CA-C	-6.35	99.33	111.40
1	C	124	VAL	CB-CA-C	-6.35	99.34	111.40
1	G	124	VAL	CB-CA-C	-6.35	99.34	111.40
1	D	124	VAL	CB-CA-C	-6.34	99.35	111.40
1	E	124	VAL	CB-CA-C	-6.33	99.36	111.40
1	G	139	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	K	139	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	139	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	E	139	ARG	NE-CZ-NH2	-6.30	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	447	ARG	CA-CB-CG	-6.30	99.54	113.40
1	K	447	ARG	CA-CB-CG	-6.30	99.54	113.40
1	F	447	ARG	CA-CB-CG	-6.30	99.55	113.40
1	H	447	ARG	CA-CB-CG	-6.30	99.55	113.40
1	J	447	ARG	CA-CB-CG	-6.30	99.55	113.40
1	G	447	ARG	CA-CB-CG	-6.29	99.56	113.40
1	B	447	ARG	CA-CB-CG	-6.29	99.56	113.40
1	I	447	ARG	CA-CB-CG	-6.29	99.56	113.40
1	A	447	ARG	CA-CB-CG	-6.29	99.57	113.40
1	L	447	ARG	CA-CB-CG	-6.28	99.58	113.40
1	D	447	ARG	CA-CB-CG	-6.28	99.59	113.40
1	E	447	ARG	CA-CB-CG	-6.27	99.61	113.40
1	A	139	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	F	139	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	L	139	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	139	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	139	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	H	139	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	I	139	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	223	THR	N-CA-CB	-6.14	98.63	110.30
1	L	223	THR	N-CA-CB	-6.14	98.64	110.30
1	G	223	THR	N-CA-CB	-6.13	98.64	110.30
1	I	110	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	K	223	THR	N-CA-CB	-6.13	98.66	110.30
1	D	223	THR	N-CA-CB	-6.13	98.66	110.30
1	H	223	THR	N-CA-CB	-6.13	98.66	110.30
1	A	223	THR	N-CA-CB	-6.12	98.67	110.30
1	E	223	THR	N-CA-CB	-6.12	98.67	110.30
1	I	223	THR	N-CA-CB	-6.12	98.67	110.30
1	J	223	THR	N-CA-CB	-6.12	98.68	110.30
1	F	223	THR	N-CA-CB	-6.11	98.69	110.30
1	B	223	THR	N-CA-CB	-6.10	98.70	110.30
1	L	179	TYR	O-C-N	6.10	132.46	122.70
1	H	110	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	K	179	TYR	O-C-N	6.10	132.46	122.70
1	D	179	TYR	O-C-N	6.09	132.45	122.70
1	H	179	TYR	O-C-N	6.09	132.44	122.70
1	B	179	TYR	O-C-N	6.09	132.44	122.70
1	B	110	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	179	TYR	O-C-N	6.08	132.43	122.70
1	C	179	TYR	O-C-N	6.08	132.43	122.70
1	G	179	TYR	O-C-N	6.08	132.43	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	TYR	O-C-N	6.07	132.41	122.70
1	I	179	TYR	O-C-N	6.07	132.40	122.70
1	D	337	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	J	110	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	E	179	TYR	O-C-N	6.06	132.39	122.70
1	L	110	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	J	179	TYR	O-C-N	6.05	132.38	122.70
1	I	337	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	J	337	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	F	110	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	110	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	F	337	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	110	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	G	110	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	K	337	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	337	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	E	110	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	H	337	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	G	158	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	A	337	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	110	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	337	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	L	158	TRP	CG-CD2-CE3	5.99	139.29	133.90
1	K	110	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	H	158	TRP	CG-CD2-CE3	5.99	139.29	133.90
1	J	158	TRP	CG-CD2-CE3	5.99	139.29	133.90
1	I	158	TRP	CG-CD2-CE3	5.97	139.28	133.90
1	C	158	TRP	CG-CD2-CE3	5.97	139.27	133.90
1	K	158	TRP	CG-CD2-CE3	5.96	139.27	133.90
1	A	158	TRP	CG-CD2-CE3	5.95	139.26	133.90
1	D	158	TRP	CG-CD2-CE3	5.95	139.25	133.90
1	B	158	TRP	CG-CD2-CE3	5.95	139.25	133.90
1	J	452	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	337	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	F	158	TRP	CG-CD2-CE3	5.94	139.25	133.90
1	G	337	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	E	158	TRP	CG-CD2-CE3	5.93	139.24	133.90
1	L	339	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	L	337	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	452	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	L	452	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	E	447	ARG	NE-CZ-NH2	-5.90	117.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	339	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	D	447	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	K	447	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	L	447	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	K	452	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	K	339	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	F	339	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	452	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	339	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	G	447	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	D	339	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	339	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	447	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	339	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	F	447	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	E	339	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	H	452	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	452	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	H	339	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	447	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	D	350	SER	N-CA-CB	-5.81	101.78	110.50
1	E	350	SER	N-CA-CB	-5.81	101.78	110.50
1	C	447	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	350	SER	N-CA-CB	-5.80	101.80	110.50
1	G	350	SER	N-CA-CB	-5.80	101.80	110.50
1	F	350	SER	N-CA-CB	-5.80	101.80	110.50
1	L	350	SER	N-CA-CB	-5.80	101.80	110.50
1	B	350	SER	N-CA-CB	-5.80	101.81	110.50
1	F	452	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	350	SER	N-CA-CB	-5.79	101.81	110.50
1	G	339	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	I	339	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	K	350	SER	N-CA-CB	-5.79	101.81	110.50
1	I	350	SER	N-CA-CB	-5.79	101.82	110.50
1	I	447	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	J	447	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	C	452	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	F	158	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	C	158	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	G	452	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	H	447	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	J	350	SER	N-CA-CB	-5.78	101.84	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	158	TRP	CG-CD1-NE1	-5.78	104.33	110.10
1	J	158	TRP	CG-CD1-NE1	-5.77	104.33	110.10
1	H	350	SER	N-CA-CB	-5.77	101.85	110.50
1	E	452	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	D	158	TRP	CG-CD1-NE1	-5.76	104.34	110.10
1	I	452	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	E	355	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	L	158	TRP	CG-CD1-NE1	-5.75	104.35	110.10
1	B	158	TRP	CG-CD1-NE1	-5.75	104.35	110.10
1	I	158	TRP	CG-CD1-NE1	-5.75	104.36	110.10
1	F	355	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	E	158	TRP	CG-CD1-NE1	-5.73	104.37	110.10
1	C	355	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	158	TRP	CG-CD1-NE1	-5.73	104.37	110.10
1	C	368	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	K	355	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	355	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	G	158	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	H	158	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	A	355	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	I	368	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	D	355	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	F	368	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	G	355	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	J	355	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	L	355	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	E	368	TYR	CB-CG-CD2	-5.62	117.62	121.00
1	K	368	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	L	368	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	368	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	H	368	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	G	368	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	B	368	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	D	368	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	H	355	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	I	355	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	K	248	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	J	368	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	D	248	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	E	248	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	H	248	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	K	433	VAL	CA-C-N	5.52	129.34	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	85	LEU	CA-CB-CG	5.52	127.99	115.30
1	B	433	VAL	CA-C-N	5.51	129.33	117.20
1	H	433	VAL	CA-C-N	5.51	129.33	117.20
1	I	433	VAL	CA-C-N	5.51	129.33	117.20
1	A	433	VAL	CA-C-N	5.51	129.31	117.20
1	D	85	LEU	CA-CB-CG	5.51	127.97	115.30
1	E	85	LEU	CA-CB-CG	5.51	127.96	115.30
1	G	85	LEU	CA-CB-CG	5.51	127.97	115.30
1	C	85	LEU	CA-CB-CG	5.50	127.96	115.30
1	J	85	LEU	CA-CB-CG	5.50	127.96	115.30
1	A	85	LEU	CA-CB-CG	5.50	127.95	115.30
1	F	433	VAL	CA-C-N	5.50	129.30	117.20
1	G	433	VAL	CA-C-N	5.50	129.30	117.20
1	J	433	VAL	CA-C-N	5.50	129.30	117.20
1	B	85	LEU	CA-CB-CG	5.50	127.94	115.30
1	L	433	VAL	CA-C-N	5.50	129.29	117.20
1	I	85	LEU	CA-CB-CG	5.49	127.94	115.30
1	D	433	VAL	CA-C-N	5.49	129.28	117.20
1	C	224	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	L	248	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	K	85	LEU	CA-CB-CG	5.49	127.92	115.30
1	F	85	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	248	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	C	433	VAL	CA-C-N	5.48	129.26	117.20
1	E	433	VAL	CA-C-N	5.48	129.26	117.20
1	L	85	LEU	CA-CB-CG	5.48	127.91	115.30
1	I	248	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	G	248	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	B	248	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	F	248	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	E	224	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	J	248	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	I	224	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	224	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	F	224	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	G	224	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	F	434	PHE	CB-CA-C	-5.39	99.62	110.40
1	L	224	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	E	442	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	E	434	PHE	CB-CA-C	-5.38	99.64	110.40
1	I	434	PHE	CB-CA-C	-5.38	99.64	110.40
1	J	434	PHE	CB-CA-C	-5.38	99.64	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	PHE	CB-CA-C	-5.38	99.64	110.40
1	K	434	PHE	CB-CA-C	-5.38	99.64	110.40
1	H	434	PHE	CB-CA-C	-5.38	99.65	110.40
1	A	434	PHE	CB-CA-C	-5.37	99.65	110.40
1	C	248	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	D	434	PHE	CB-CA-C	-5.37	99.66	110.40
1	G	434	PHE	CB-CA-C	-5.37	99.67	110.40
1	C	434	PHE	CB-CA-C	-5.36	99.67	110.40
1	L	434	PHE	CB-CA-C	-5.36	99.67	110.40
1	I	442	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	B	224	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	J	224	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	D	224	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	D	442	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	H	224	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	442	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	H	442	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	B	442	TYR	CB-CG-CD1	-5.31	117.82	121.00
1	L	442	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	K	224	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	L	175	VAL	CA-C-N	5.29	128.84	117.20
1	F	442	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	J	442	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	C	442	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	E	175	VAL	CA-C-N	5.28	128.81	117.20
1	F	175	VAL	CA-C-N	5.28	128.81	117.20
1	C	175	VAL	CA-C-N	5.27	128.80	117.20
1	H	175	VAL	CA-C-N	5.27	128.80	117.20
1	I	175	VAL	CA-C-N	5.27	128.79	117.20
1	A	175	VAL	CA-C-N	5.27	128.79	117.20
1	C	256	MET	CA-CB-CG	5.27	122.25	113.30
1	F	256	MET	CA-CB-CG	5.27	122.25	113.30
1	D	175	VAL	CA-C-N	5.27	128.78	117.20
1	E	256	MET	CA-CB-CG	5.26	122.25	113.30
1	K	175	VAL	CA-C-N	5.26	128.78	117.20
1	A	256	MET	CA-CB-CG	5.26	122.25	113.30
1	B	175	VAL	CA-C-N	5.26	128.78	117.20
1	G	256	MET	CA-CB-CG	5.26	122.24	113.30
1	G	442	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	D	256	MET	CA-CB-CG	5.26	122.24	113.30
1	K	256	MET	CA-CB-CG	5.26	122.24	113.30
1	H	256	MET	CA-CB-CG	5.26	122.24	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	256	MET	CA-CB-CG	5.26	122.24	113.30
1	I	256	MET	CA-CB-CG	5.25	122.23	113.30
1	J	175	VAL	CA-C-N	5.25	128.76	117.20
1	G	175	VAL	CA-C-N	5.25	128.75	117.20
1	J	256	MET	CA-CB-CG	5.25	122.22	113.30
1	B	256	MET	CA-CB-CG	5.24	122.21	113.30
1	K	442	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	C	158	TRP	CB-CG-CD1	-5.15	120.30	127.00
1	K	158	TRP	CB-CG-CD1	-5.15	120.30	127.00
1	F	158	TRP	CB-CG-CD1	-5.15	120.30	127.00
1	E	158	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	I	158	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	D	158	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	B	158	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	A	158	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	J	158	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	L	158	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	C	129	GLU	CA-CB-CG	5.11	124.64	113.40
1	H	129	GLU	CA-CB-CG	5.11	124.63	113.40
1	I	270	CYS	CA-CB-SG	-5.10	104.82	114.00
1	E	270	CYS	CA-CB-SG	-5.10	104.82	114.00
1	I	129	GLU	CA-CB-CG	5.10	124.62	113.40
1	G	129	GLU	CA-CB-CG	5.10	124.61	113.40
1	H	158	TRP	CB-CG-CD1	-5.10	120.37	127.00
1	K	129	GLU	CA-CB-CG	5.10	124.61	113.40
1	D	129	GLU	CA-CB-CG	5.09	124.61	113.40
1	E	129	GLU	CA-CB-CG	5.09	124.61	113.40
1	G	270	CYS	CA-CB-SG	-5.09	104.83	114.00
1	A	129	GLU	CA-CB-CG	5.09	124.60	113.40
1	J	129	GLU	CA-CB-CG	5.09	124.60	113.40
1	F	129	GLU	CA-CB-CG	5.09	124.59	113.40
1	A	270	CYS	CA-CB-SG	-5.08	104.85	114.00
1	L	270	CYS	CA-CB-SG	-5.08	104.85	114.00
1	L	129	GLU	CA-CB-CG	5.08	124.58	113.40
1	D	270	CYS	CA-CB-SG	-5.08	104.85	114.00
1	F	270	CYS	CA-CB-SG	-5.08	104.86	114.00
1	G	158	TRP	CB-CG-CD1	-5.08	120.40	127.00
1	H	270	CYS	CA-CB-SG	-5.08	104.86	114.00
1	J	270	CYS	CA-CB-SG	-5.08	104.86	114.00
1	K	270	CYS	CA-CB-SG	-5.08	104.86	114.00
1	B	270	CYS	CA-CB-SG	-5.07	104.87	114.00
1	B	129	GLU	CA-CB-CG	5.07	124.56	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	270	CYS	CA-CB-SG	-5.06	104.89	114.00
1	J	238	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	I	238	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	C	238	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	E	238	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	G	238	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	A	238	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	F	238	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	H	238	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	I	15	LYS	CA-CB-CG	-5.00	102.39	113.40

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	350	SER	Peptide
1	B	224	ARG	Sidechain
1	B	350	SER	Peptide
1	C	224	ARG	Sidechain
1	C	350	SER	Peptide
1	D	224	ARG	Sidechain
1	D	350	SER	Peptide
1	E	224	ARG	Sidechain
1	E	350	SER	Peptide
1	F	224	ARG	Sidechain
1	F	350	SER	Peptide
1	G	224	ARG	Sidechain
1	G	350	SER	Peptide
1	H	224	ARG	Sidechain
1	H	350	SER	Peptide
1	I	224	ARG	Sidechain
1	I	350	SER	Peptide
1	J	224	ARG	Sidechain
1	J	350	SER	Peptide
1	K	224	ARG	Sidechain
1	K	350	SER	Peptide
1	L	224	ARG	Sidechain
1	L	350	SER	Peptide

## 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	3455	0	3371	64	0
1	B	3455	0	3371	64	0
1	C	3455	0	3371	68	2
1	D	3455	0	3371	63	0
1	E	3455	0	3371	62	0
1	F	3455	0	3371	59	2
1	G	3455	0	3371	62	0
1	H	3455	0	3371	58	0
1	I	3455	0	3371	65	0
1	J	3455	0	3371	59	0
1	K	3455	0	3371	69	0
1	L	3455	0	3371	61	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	23	0	12	2	0
3	B	23	0	12	2	0
3	C	23	0	12	2	0
3	D	23	0	12	3	0
3	E	23	0	12	2	0
3	F	23	0	12	2	0
3	G	23	0	12	2	0
3	H	23	0	12	3	0
3	I	23	0	12	3	0
3	J	23	0	12	2	0
3	K	23	0	12	3	0
3	L	23	0	12	2	0
All	All	41760	0	40596	689	2

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 8.

All (689) 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:H:192:ARG:HD3	1:H:219:ASN:HD22	1.57	0.70
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.57	0.70
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.57	0.70
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.57	0.70
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.57	0.69
1:F:192:ARG:HD3	1:F:219:ASN:HD22	1.57	0.69
1:K:192:ARG:HD3	1:K:219:ASN:HD22	1.57	0.69
1:B:425:ARG:HG2	1:B:429:LYS:HD2	1.75	0.69
1:G:192:ARG:HD3	1:G:219:ASN:HD22	1.57	0.69
1:J:425:ARG:HG2	1:J:429:LYS:HD2	1.75	0.69
1:L:425:ARG:HG2	1:L:429:LYS:HD2	1.75	0.69
1:F:425:ARG:HG2	1:F:429:LYS:HD2	1.75	0.69
1:C:192:ARG:HD3	1:C:219:ASN:HD22	1.57	0.69
1:H:425:ARG:HG2	1:H:429:LYS:HD2	1.75	0.69
1:D:425:ARG:HG2	1:D:429:LYS:HD2	1.75	0.68
1:C:425:ARG:HG2	1:C:429:LYS:HD2	1.75	0.68
1:L:192:ARG:HD3	1:L:219:ASN:HD22	1.57	0.68
1:I:192:ARG:HD3	1:I:219:ASN:HD22	1.57	0.68
1:I:425:ARG:HG2	1:I:429:LYS:HD2	1.75	0.68
1:B:192:ARG:HD3	1:B:219:ASN:HD22	1.57	0.68
1:E:425:ARG:HG2	1:E:429:LYS:HD2	1.75	0.68
1:A:425:ARG:HG2	1:A:429:LYS:HD2	1.75	0.67
1:G:425:ARG:HG2	1:G:429:LYS:HD2	1.75	0.67
1:K:425:ARG:HG2	1:K:429:LYS:HD2	1.75	0.66
1:J:180:PHE:HB3	1:K:29:GLN:HB3	1.76	0.66
1:D:180:PHE:HB3	1:E:29:GLN:HB3	1.78	0.65
1:C:258:LYS:HG2	1:C:320:LYS:HB3	1.80	0.64
1:E:258:LYS:HG2	1:E:320:LYS:HB3	1.80	0.64
1:B:258:LYS:HG2	1:B:320:LYS:HB3	1.80	0.64
1:F:258:LYS:HG2	1:F:320:LYS:HB3	1.80	0.64
1:K:258:LYS:HG2	1:K:320:LYS:HB3	1.80	0.64
1:G:258:LYS:HG2	1:G:320:LYS:HB3	1.80	0.63
1:L:258:LYS:HG2	1:L:320:LYS:HB3	1.80	0.63
1:H:214:ALA:HB3	1:H:218:GLN:HB2	1.81	0.63
1:I:258:LYS:HG2	1:I:320:LYS:HB3	1.80	0.63
1:C:214:ALA:HB3	1:C:218:GLN:HB2	1.81	0.63
1:F:214:ALA:HB3	1:F:218:GLN:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ALA:HB3	1:A:218:GLN:HB2	1.81	0.63
1:J:214:ALA:HB3	1:J:218:GLN:HB2	1.81	0.62
1:D:214:ALA:HB3	1:D:218:GLN:HB2	1.81	0.62
1:I:214:ALA:HB3	1:I:218:GLN:HB2	1.81	0.62
1:K:214:ALA:HB3	1:K:218:GLN:HB2	1.81	0.62
1:A:383:LYS:NZ	1:A:383:LYS:HB3	2.15	0.62
1:E:214:ALA:HB3	1:E:218:GLN:HB2	1.81	0.62
1:H:258:LYS:HG2	1:H:320:LYS:HB3	1.80	0.62
1:I:383:LYS:HB3	1:I:383:LYS:NZ	2.15	0.62
1:J:258:LYS:HG2	1:J:320:LYS:HB3	1.80	0.62
1:L:214:ALA:HB3	1:L:218:GLN:HB2	1.81	0.62
1:G:214:ALA:HB3	1:G:218:GLN:HB2	1.81	0.62
1:C:383:LYS:HB3	1:C:383:LYS:NZ	2.15	0.62
1:B:214:ALA:HB3	1:B:218:GLN:HB2	1.81	0.62
1:B:458:HIS:HD2	1:B:460:VAL:H	1.48	0.62
1:A:258:LYS:HG2	1:A:320:LYS:HB3	1.80	0.61
1:D:258:LYS:HG2	1:D:320:LYS:HB3	1.80	0.61
1:G:383:LYS:NZ	1:G:383:LYS:HB3	2.15	0.61
1:K:458:HIS:HD2	1:K:460:VAL:H	1.48	0.61
1:D:383:LYS:NZ	1:D:383:LYS:HB3	2.15	0.61
1:F:458:HIS:HD2	1:F:460:VAL:H	1.48	0.61
1:H:383:LYS:HB3	1:H:383:LYS:NZ	2.15	0.61
1:I:458:HIS:HD2	1:I:460:VAL:H	1.48	0.61
1:D:458:HIS:HD2	1:D:460:VAL:H	1.48	0.61
1:J:458:HIS:HD2	1:J:460:VAL:H	1.48	0.61
1:K:383:LYS:HB3	1:K:383:LYS:NZ	2.15	0.61
1:L:383:LYS:HB3	1:L:383:LYS:NZ	2.15	0.61
1:C:458:HIS:HD2	1:C:460:VAL:H	1.48	0.61
1:B:383:LYS:NZ	1:B:383:LYS:HB3	2.15	0.61
1:G:458:HIS:HD2	1:G:460:VAL:H	1.49	0.61
1:F:383:LYS:NZ	1:F:383:LYS:HB3	2.15	0.60
1:H:180:PHE:HB3	1:I:29:GLN:HB3	1.83	0.60
1:E:383:LYS:HB3	1:E:383:LYS:NZ	2.15	0.60
1:J:383:LYS:NZ	1:J:383:LYS:HB3	2.15	0.60
1:I:66:VAL:HG13	1:I:92:LEU:HB2	1.84	0.60
1:E:458:HIS:HD2	1:E:460:VAL:H	1.48	0.59
1:H:66:VAL:HG13	1:H:92:LEU:HB2	1.84	0.59
1:K:66:VAL:HG13	1:K:92:LEU:HB2	1.85	0.59
1:L:66:VAL:HG13	1:L:92:LEU:HB2	1.84	0.59
1:A:66:VAL:HG13	1:A:92:LEU:HB2	1.84	0.59
1:L:458:HIS:HD2	1:L:460:VAL:H	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:HIS:HD2	1:A:460:VAL:H	1.48	0.59
1:C:261:PHE:HB2	1:K:457:PRO:HD2	1.82	0.59
1:C:180:PHE:HB3	1:D:29:GLN:HB3	1.83	0.59
1:D:66:VAL:HG13	1:D:92:LEU:HB2	1.84	0.59
1:E:66:VAL:HG13	1:E:92:LEU:HB2	1.84	0.59
1:B:66:VAL:HG13	1:B:92:LEU:HB2	1.84	0.59
1:B:180:PHE:HB3	1:C:29:GLN:HB3	1.84	0.59
1:C:66:VAL:HG13	1:C:92:LEU:HB2	1.84	0.59
1:C:92:LEU:HA	1:C:99:GLY:HA2	1.85	0.59
1:E:92:LEU:HA	1:E:99:GLY:HA2	1.85	0.59
1:F:66:VAL:HG13	1:F:92:LEU:HB2	1.84	0.59
1:H:92:LEU:HA	1:H:99:GLY:HA2	1.85	0.59
1:E:76:ILE:HD12	1:E:85:LEU:HD23	1.85	0.59
1:A:29:GLN:HB3	1:F:180:PHE:HB3	1.84	0.59
1:I:92:LEU:HA	1:I:99:GLY:HA2	1.85	0.59
1:K:92:LEU:HA	1:K:99:GLY:HA2	1.85	0.59
1:L:92:LEU:HA	1:L:99:GLY:HA2	1.85	0.59
1:L:76:ILE:HD12	1:L:85:LEU:HD23	1.85	0.59
1:A:92:LEU:HA	1:A:99:GLY:HA2	1.85	0.58
1:H:458:HIS:HD2	1:H:460:VAL:H	1.48	0.58
1:I:76:ILE:HD12	1:I:85:LEU:HD23	1.85	0.58
1:B:76:ILE:HD12	1:B:85:LEU:HD23	1.85	0.58
1:C:76:ILE:HD12	1:C:85:LEU:HD23	1.85	0.58
1:G:76:ILE:HD12	1:G:85:LEU:HD23	1.85	0.58
1:G:66:VAL:HG13	1:G:92:LEU:HB2	1.84	0.58
1:J:76:ILE:HD12	1:J:85:LEU:HD23	1.85	0.58
1:J:66:VAL:HG13	1:J:92:LEU:HB2	1.84	0.58
1:A:76:ILE:HD12	1:A:85:LEU:HD23	1.85	0.58
1:A:180:PHE:HB3	1:B:29:GLN:HB3	1.84	0.58
1:D:76:ILE:HD12	1:D:85:LEU:HD23	1.85	0.58
1:D:92:LEU:HA	1:D:99:GLY:HA2	1.85	0.58
1:F:76:ILE:HD12	1:F:85:LEU:HD23	1.85	0.58
1:F:92:LEU:HA	1:F:99:GLY:HA2	1.85	0.58
1:C:192:ARG:HD3	1:C:219:ASN:ND2	2.19	0.58
1:B:92:LEU:HA	1:B:99:GLY:HA2	1.85	0.58
1:G:192:ARG:HD3	1:G:219:ASN:ND2	2.19	0.58
1:G:92:LEU:HA	1:G:99:GLY:HA2	1.85	0.58
1:I:192:ARG:HD3	1:I:219:ASN:ND2	2.19	0.58
1:J:92:LEU:HA	1:J:99:GLY:HA2	1.85	0.58
1:F:192:ARG:HD3	1:F:219:ASN:ND2	2.19	0.57
1:D:192:ARG:HD3	1:D:219:ASN:ND2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:ILE:HD12	1:H:85:LEU:HD23	1.85	0.57
1:J:192:ARG:HD3	1:J:219:ASN:ND2	2.19	0.57
1:E:192:ARG:HD3	1:E:219:ASN:ND2	2.19	0.57
1:K:76:ILE:HD12	1:K:85:LEU:HD23	1.85	0.57
1:K:180:PHE:HB3	1:L:29:GLN:HB3	1.85	0.57
1:A:192:ARG:HD3	1:A:219:ASN:ND2	2.19	0.57
1:G:29:GLN:HB3	1:L:180:PHE:HB3	1.87	0.57
1:H:192:ARG:HD3	1:H:219:ASN:ND2	2.19	0.57
1:I:180:PHE:HB3	1:J:29:GLN:HB3	1.87	0.57
1:K:192:ARG:HD3	1:K:219:ASN:ND2	2.19	0.57
1:L:192:ARG:HD3	1:L:219:ASN:ND2	2.19	0.57
1:B:457:PRO:HD2	1:L:261:PHE:HB2	1.87	0.56
1:K:5:VAL:HG11	1:K:43:PHE:HZ	1.71	0.56
1:D:456:THR:O	1:J:458:HIS:HE1	1.87	0.56
1:B:192:ARG:HD3	1:B:219:ASN:ND2	2.19	0.56
1:B:5:VAL:HG11	1:B:43:PHE:HZ	1.71	0.56
1:C:457:PRO:HD2	1:K:261:PHE:HB2	1.86	0.56
1:F:5:VAL:HG11	1:F:43:PHE:HZ	1.71	0.56
1:E:5:VAL:HG11	1:E:43:PHE:HZ	1.71	0.56
1:I:5:VAL:HG11	1:I:43:PHE:HZ	1.71	0.56
1:C:5:VAL:HG11	1:C:43:PHE:HZ	1.71	0.56
1:G:5:VAL:HG11	1:G:43:PHE:HZ	1.71	0.56
1:H:5:VAL:HG11	1:H:43:PHE:HZ	1.71	0.56
1:J:5:VAL:HG11	1:J:43:PHE:HZ	1.71	0.56
1:D:5:VAL:HG11	1:D:43:PHE:HZ	1.71	0.55
1:E:457:PRO:HD2	1:I:261:PHE:HB2	1.89	0.55
1:D:458:HIS:HE1	1:J:456:THR:O	1.89	0.55
1:B:19:LEU:HD11	1:B:42:PHE:HZ	1.72	0.55
1:F:458:HIS:HE1	1:H:456:THR:O	1.90	0.55
1:J:19:LEU:HD11	1:J:42:PHE:HZ	1.72	0.55
1:H:19:LEU:HD11	1:H:42:PHE:HZ	1.72	0.55
1:G:19:LEU:HD11	1:G:42:PHE:HZ	1.72	0.55
1:E:19:LEU:HD11	1:E:42:PHE:HZ	1.72	0.55
1:F:456:THR:O	1:H:458:HIS:HE1	1.88	0.55
1:F:19:LEU:HD11	1:F:42:PHE:HZ	1.72	0.55
1:E:456:THR:O	1:I:458:HIS:HE1	1.90	0.55
1:K:19:LEU:HD11	1:K:42:PHE:HZ	1.72	0.55
1:L:19:LEU:HD11	1:L:42:PHE:HZ	1.72	0.55
1:D:19:LEU:HD11	1:D:42:PHE:HZ	1.72	0.54
1:B:261:PHE:HB2	1:L:457:PRO:HD2	1.88	0.54
1:C:19:LEU:HD11	1:C:42:PHE:HZ	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:PHE:HB3	1:H:29:GLN:HB3	1.87	0.54
1:A:5:VAL:HG11	1:A:43:PHE:HZ	1.71	0.54
1:L:5:VAL:HG11	1:L:43:PHE:HZ	1.71	0.54
1:B:333:ALA:O	1:B:341:ALA:HB1	2.08	0.54
1:H:333:ALA:O	1:H:341:ALA:HB1	2.08	0.54
1:K:333:ALA:O	1:K:341:ALA:HB1	2.08	0.54
1:E:333:ALA:O	1:E:341:ALA:HB1	2.08	0.54
1:I:19:LEU:HD11	1:I:42:PHE:HZ	1.72	0.54
1:F:333:ALA:O	1:F:341:ALA:HB1	2.08	0.54
1:A:19:LEU:HD11	1:A:42:PHE:HZ	1.72	0.53
1:G:333:ALA:O	1:G:341:ALA:HB1	2.08	0.53
1:J:333:ALA:O	1:J:341:ALA:HB1	2.08	0.53
1:C:333:ALA:O	1:C:341:ALA:HB1	2.08	0.53
1:G:286:LYS:HB2	1:G:290:LEU:O	2.09	0.53
1:H:458:HIS:CD2	1:H:460:VAL:H	2.27	0.53
1:I:286:LYS:HB2	1:I:290:LEU:O	2.09	0.53
1:I:333:ALA:O	1:I:341:ALA:HB1	2.08	0.53
1:L:333:ALA:O	1:L:341:ALA:HB1	2.08	0.53
1:C:286:LYS:HB2	1:C:290:LEU:O	2.09	0.53
1:E:180:PHE:HB3	1:F:29:GLN:HB3	1.90	0.53
1:E:458:HIS:CD2	1:E:460:VAL:H	2.27	0.53
1:H:286:LYS:HB2	1:H:290:LEU:O	2.09	0.53
1:L:286:LYS:HB2	1:L:290:LEU:O	2.09	0.53
1:A:286:LYS:HB2	1:A:290:LEU:O	2.09	0.53
1:D:286:LYS:HB2	1:D:290:LEU:O	2.09	0.53
1:B:458:HIS:CD2	1:B:460:VAL:H	2.27	0.53
1:A:261:PHE:HB2	1:G:457:PRO:HD2	1.91	0.53
1:D:458:HIS:CD2	1:D:460:VAL:H	2.27	0.53
1:F:286:LYS:HB2	1:F:290:LEU:O	2.09	0.53
1:J:458:HIS:CD2	1:J:460:VAL:H	2.27	0.53
1:K:286:LYS:HB2	1:K:290:LEU:O	2.09	0.53
1:A:457:PRO:HD2	1:G:261:PHE:HB2	1.90	0.53
1:A:456:THR:O	1:G:458:HIS:HE1	1.91	0.53
1:L:191:ILE:HG12	1:L:249:PHE:CD2	2.44	0.53
1:B:191:ILE:HG12	1:B:249:PHE:CD2	2.45	0.52
1:D:191:ILE:HG12	1:D:249:PHE:CD2	2.44	0.52
1:E:261:PHE:HB2	1:I:457:PRO:HD2	1.91	0.52
1:G:314:PRO:HB2	1:G:446:ARG:NH1	2.24	0.52
1:I:191:ILE:HG12	1:I:249:PHE:CD2	2.44	0.52
1:J:286:LYS:HB2	1:J:290:LEU:O	2.09	0.52
1:K:191:ILE:HG12	1:K:249:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:314:PRO:HB2	1:K:446:ARG:NH1	2.24	0.52
1:A:458:HIS:CD2	1:A:460:VAL:H	2.27	0.52
1:D:333:ALA:O	1:D:341:ALA:HB1	2.08	0.52
1:E:191:ILE:HG12	1:E:249:PHE:CD2	2.45	0.52
1:G:458:HIS:CD2	1:G:460:VAL:H	2.27	0.52
1:H:191:ILE:HG12	1:H:249:PHE:CD2	2.45	0.52
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.45	0.52
1:L:314:PRO:HB2	1:L:446:ARG:NH1	2.24	0.52
1:A:333:ALA:O	1:A:341:ALA:HB1	2.08	0.52
1:E:286:LYS:HB2	1:E:290:LEU:O	2.09	0.52
1:E:314:PRO:HB2	1:E:446:ARG:NH1	2.24	0.52
1:H:168:ASN:HB3	1:I:138:ILE:O	2.09	0.52
1:K:458:HIS:CD2	1:K:460:VAL:H	2.27	0.52
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.45	0.52
1:A:191:ILE:HG12	1:A:249:PHE:CD2	2.44	0.52
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.45	0.52
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.45	0.52
1:J:314:PRO:HB2	1:J:446:ARG:NH1	2.24	0.52
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.45	0.52
1:I:314:PRO:HB2	1:I:446:ARG:NH1	2.24	0.52
1:A:314:PRO:HB2	1:A:446:ARG:NH1	2.24	0.52
1:D:314:PRO:HB2	1:D:446:ARG:NH1	2.24	0.52
1:A:458:HIS:HE1	1:G:456:THR:O	1.92	0.52
1:B:286:LYS:HB2	1:B:290:LEU:O	2.09	0.52
1:J:191:ILE:HG12	1:J:249:PHE:CD2	2.45	0.52
1:C:314:PRO:HB2	1:C:446:ARG:NH1	2.24	0.52
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.45	0.52
1:B:314:PRO:HB2	1:B:446:ARG:NH1	2.24	0.51
1:C:191:ILE:HG12	1:C:249:PHE:CD2	2.44	0.51
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.45	0.51
1:I:458:HIS:CD2	1:I:460:VAL:H	2.27	0.51
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.45	0.51
1:L:458:HIS:CD2	1:L:460:VAL:H	2.27	0.51
1:G:191:ILE:HG12	1:G:249:PHE:CD2	2.44	0.51
1:H:314:PRO:HB2	1:H:446:ARG:NH1	2.24	0.51
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.45	0.51
1:B:456:THR:O	1:L:458:HIS:HE1	1.94	0.51
1:C:93:GLU:HB3	1:C:98:GLN:OE1	2.11	0.51
1:D:93:GLU:HB3	1:D:98:GLN:OE1	2.11	0.51
1:F:458:HIS:CD2	1:F:460:VAL:H	2.27	0.51
1:H:93:GLU:HB3	1:H:98:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:GLU:HB3	1:E:98:GLN:OE1	2.11	0.51
1:F:314:PRO:HB2	1:F:446:ARG:NH1	2.24	0.51
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.45	0.51
1:B:458:HIS:HE1	1:L:456:THR:O	1.94	0.51
1:C:458:HIS:CD2	1:C:460:VAL:H	2.27	0.51
1:F:191:ILE:HG12	1:F:249:PHE:CD2	2.45	0.51
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.45	0.51
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.45	0.51
1:L:93:GLU:HB3	1:L:98:GLN:OE1	2.11	0.51
1:A:93:GLU:HB3	1:A:98:GLN:OE1	2.11	0.50
1:D:261:PHE:HB2	1:J:457:PRO:HD2	1.93	0.50
1:F:93:GLU:HB3	1:F:98:GLN:OE1	2.11	0.50
1:D:457:PRO:HD2	1:J:261:PHE:HB2	1.92	0.50
1:B:93:GLU:HB3	1:B:98:GLN:OE1	2.11	0.50
1:E:458:HIS:HE1	1:I:456:THR:O	1.93	0.50
1:I:93:GLU:HB3	1:I:98:GLN:OE1	2.11	0.50
1:C:273:SER:HB2	3:C:473:AMP:N1	2.27	0.50
1:J:93:GLU:HB3	1:J:98:GLN:OE1	2.11	0.50
1:K:312:ALA:HB1	1:K:361:PRO:HB3	1.94	0.50
1:D:273:SER:HB2	3:D:474:AMP:N1	2.27	0.50
1:G:93:GLU:HB3	1:G:98:GLN:OE1	2.11	0.50
1:E:273:SER:HB2	3:E:475:AMP:N1	2.27	0.50
1:K:93:GLU:HB3	1:K:98:GLN:OE1	2.11	0.50
1:A:312:ALA:HB1	1:A:361:PRO:HB3	1.94	0.50
1:H:312:ALA:HB1	1:H:361:PRO:HB3	1.94	0.50
1:D:312:ALA:HB1	1:D:361:PRO:HB3	1.94	0.49
1:H:273:SER:HB2	3:H:478:AMP:N1	2.27	0.49
1:I:312:ALA:HB1	1:I:361:PRO:HB3	1.94	0.49
1:J:273:SER:HB2	3:J:480:AMP:N1	2.27	0.49
1:K:273:SER:HB2	3:K:481:AMP:N1	2.27	0.49
1:F:273:SER:HB2	3:F:476:AMP:N1	2.27	0.49
1:G:312:ALA:HB1	1:G:361:PRO:HB3	1.94	0.49
1:A:273:SER:HB2	3:A:471:AMP:N1	2.27	0.49
1:B:273:SER:HB2	3:B:472:AMP:N1	2.27	0.49
1:I:273:SER:HB2	3:I:479:AMP:N1	2.27	0.49
1:L:273:SER:HB2	3:L:482:AMP:N1	2.27	0.49
1:C:312:ALA:HB1	1:C:361:PRO:HB3	1.94	0.49
1:E:312:ALA:HB1	1:E:361:PRO:HB3	1.94	0.49
1:E:192:ARG:HH11	1:E:219:ASN:ND2	2.11	0.49
1:F:192:ARG:HH11	1:F:219:ASN:ND2	2.11	0.49
1:A:192:ARG:HH11	1:A:219:ASN:ND2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:457:PRO:HD2	1:H:261:PHE:HB2	1.93	0.49
1:B:192:ARG:HH11	1:B:219:ASN:ND2	2.11	0.49
1:D:192:ARG:HH11	1:D:219:ASN:ND2	2.11	0.49
1:K:17:VAL:HG21	1:K:38:VAL:HG21	1.95	0.49
1:E:17:VAL:HG21	1:E:38:VAL:HG21	1.95	0.49
1:G:17:VAL:HG21	1:G:38:VAL:HG21	1.95	0.49
1:F:17:VAL:HG21	1:F:38:VAL:HG21	1.95	0.48
1:L:192:ARG:HH11	1:L:219:ASN:ND2	2.11	0.48
1:D:17:VAL:HG21	1:D:38:VAL:HG21	1.95	0.48
1:L:312:ALA:HB1	1:L:361:PRO:HB3	1.94	0.48
1:G:273:SER:HB2	3:G:477:AMP:N1	2.27	0.48
1:H:17:VAL:HG21	1:H:38:VAL:HG21	1.95	0.48
1:J:312:ALA:HB1	1:J:361:PRO:HB3	1.94	0.48
1:C:17:VAL:HG21	1:C:38:VAL:HG21	1.95	0.48
1:F:12:HIS:HB2	1:F:14:VAL:HG23	1.96	0.48
1:F:312:ALA:HB1	1:F:361:PRO:HB3	1.94	0.48
1:C:458:HIS:HE1	1:K:456:THR:O	1.96	0.48
1:A:12:HIS:HB2	1:A:14:VAL:HG23	1.96	0.48
1:C:12:HIS:HB2	1:C:14:VAL:HG23	1.96	0.48
1:G:12:HIS:HB2	1:G:14:VAL:HG23	1.96	0.48
1:H:192:ARG:HH11	1:H:219:ASN:ND2	2.11	0.48
1:K:12:HIS:HB2	1:K:14:VAL:HG23	1.96	0.48
1:L:57:TRP:CH2	1:L:91:ILE:HG13	2.49	0.48
1:D:101:ASP:HB3	1:D:110:ARG:HH22	1.78	0.48
1:H:12:HIS:HB2	1:H:14:VAL:HG23	1.96	0.48
1:I:101:ASP:HB3	1:I:110:ARG:HH22	1.78	0.48
1:B:312:ALA:HB1	1:B:361:PRO:HB3	1.94	0.48
1:D:121:ALA:HA	1:D:276:LYS:HD2	1.96	0.48
1:J:17:VAL:HG21	1:J:38:VAL:HG21	1.95	0.48
1:C:192:ARG:HH11	1:C:219:ASN:ND2	2.11	0.48
1:C:57:TRP:CH2	1:C:91:ILE:HG13	2.49	0.48
1:D:12:HIS:HB2	1:D:14:VAL:HG23	1.96	0.48
1:D:57:TRP:CH2	1:D:91:ILE:HG13	2.49	0.48
1:E:57:TRP:CH2	1:E:91:ILE:HG13	2.49	0.48
1:F:121:ALA:HA	1:F:276:LYS:HD2	1.96	0.48
1:I:192:ARG:HH11	1:I:219:ASN:ND2	2.11	0.48
1:J:12:HIS:HB2	1:J:14:VAL:HG23	1.96	0.48
1:B:17:VAL:HG21	1:B:38:VAL:HG21	1.95	0.48
1:F:57:TRP:CH2	1:F:91:ILE:HG13	2.49	0.48
1:G:101:ASP:HB3	1:G:110:ARG:HH22	1.78	0.48
1:H:121:ALA:HA	1:H:276:LYS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:269:HIS:HE1	1:I:359:ARG:NH1	2.12	0.48
1:J:101:ASP:HB3	1:J:110:ARG:HH22	1.78	0.48
1:J:192:ARG:HH11	1:J:219:ASN:ND2	2.11	0.48
1:K:121:ALA:HA	1:K:276:LYS:HD2	1.96	0.48
1:K:192:ARG:HH11	1:K:219:ASN:ND2	2.11	0.48
1:B:121:ALA:HA	1:B:276:LYS:HD2	1.96	0.48
1:B:12:HIS:HB2	1:B:14:VAL:HG23	1.96	0.48
1:G:192:ARG:HH11	1:G:219:ASN:ND2	2.11	0.48
1:G:269:HIS:HE1	1:G:359:ARG:NH1	2.12	0.48
1:B:269:HIS:HE1	1:B:359:ARG:NH1	2.12	0.47
1:G:121:ALA:HA	1:G:276:LYS:HD2	1.96	0.47
1:G:57:TRP:CH2	1:G:91:ILE:HG13	2.49	0.47
1:K:101:ASP:HB3	1:K:110:ARG:HH22	1.78	0.47
1:F:101:ASP:HB3	1:F:110:ARG:HH22	1.78	0.47
1:G:231:LYS:HD2	1:G:231:LYS:HA	1.65	0.47
1:H:101:ASP:HB3	1:H:110:ARG:HH22	1.78	0.47
1:I:57:TRP:CH2	1:I:91:ILE:HG13	2.49	0.47
1:L:12:HIS:HB2	1:L:14:VAL:HG23	1.96	0.47
1:C:101:ASP:HB3	1:C:110:ARG:HH22	1.78	0.47
1:G:120:ILE:O	1:G:281:LEU:HD21	2.15	0.47
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.65	0.47
1:H:120:ILE:O	1:H:281:LEU:HD21	2.15	0.47
1:H:57:TRP:CH2	1:H:91:ILE:HG13	2.49	0.47
1:I:12:HIS:HB2	1:I:14:VAL:HG23	1.96	0.47
1:J:121:ALA:HA	1:J:276:LYS:HD2	1.96	0.47
1:C:315:THR:HB	1:K:465:TYR:CZ	2.49	0.47
1:E:121:ALA:HA	1:E:276:LYS:HD2	1.96	0.47
1:E:120:ILE:O	1:E:281:LEU:HD21	2.15	0.47
1:E:269:HIS:HE1	1:E:359:ARG:NH1	2.12	0.47
1:F:261:PHE:HB2	1:H:457:PRO:HD2	1.95	0.47
1:I:121:ALA:HA	1:I:276:LYS:HD2	1.96	0.47
1:I:17:VAL:HG21	1:I:38:VAL:HG21	1.95	0.47
1:L:101:ASP:HB3	1:L:110:ARG:HH22	1.78	0.47
1:L:17:VAL:HG21	1:L:38:VAL:HG21	1.95	0.47
1:A:269:HIS:HE1	1:A:359:ARG:NH1	2.12	0.47
1:A:120:ILE:O	1:A:281:LEU:HD21	2.15	0.47
1:E:101:ASP:HB3	1:E:110:ARG:HH22	1.78	0.47
1:J:269:HIS:HE1	1:J:359:ARG:NH1	2.12	0.47
1:K:120:ILE:O	1:K:281:LEU:HD21	2.15	0.47
1:A:101:ASP:HB3	1:A:110:ARG:HH22	1.78	0.47
1:B:120:ILE:O	1:B:281:LEU:HD21	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:HIS:HE1	1:C:359:ARG:NH1	2.12	0.47
1:E:12:HIS:HB2	1:E:14:VAL:HG23	1.96	0.47
1:F:120:ILE:O	1:F:281:LEU:HD21	2.15	0.47
1:J:57:TRP:CH2	1:J:91:ILE:HG13	2.49	0.47
1:K:269:HIS:HE1	1:K:359:ARG:NH1	2.12	0.47
1:L:121:ALA:HA	1:L:276:LYS:HD2	1.96	0.47
1:D:120:ILE:O	1:D:281:LEU:HD21	2.15	0.47
1:I:207:GLU:OE1	3:I:479:AMP:O3'	2.26	0.47
1:A:17:VAL:HG21	1:A:38:VAL:HG21	1.95	0.47
1:B:101:ASP:HB3	1:B:110:ARG:HH22	1.78	0.47
1:F:231:LYS:HD2	1:F:231:LYS:HA	1.65	0.47
1:K:57:TRP:CH2	1:K:91:ILE:HG13	2.49	0.47
1:D:269:HIS:HE1	1:D:359:ARG:NH1	2.12	0.47
1:B:57:TRP:CH2	1:B:91:ILE:HG13	2.49	0.47
1:C:120:ILE:O	1:C:281:LEU:HD21	2.15	0.47
1:C:348:VAL:HG21	1:C:353:ALA:HB3	1.97	0.47
1:H:348:VAL:HG21	1:H:353:ALA:HB3	1.97	0.47
1:H:269:HIS:HE1	1:H:359:ARG:NH1	2.12	0.47
1:F:348:VAL:HG21	1:F:353:ALA:HB3	1.97	0.47
1:L:269:HIS:HE1	1:L:359:ARG:NH1	2.12	0.47
1:L:348:VAL:HG21	1:L:353:ALA:HB3	1.97	0.47
1:C:121:ALA:HA	1:C:276:LYS:HD2	1.96	0.46
1:C:290:LEU:HD11	1:C:345:ILE:HD12	1.97	0.46
1:D:231:LYS:HD2	1:D:231:LYS:HA	1.65	0.46
1:F:269:HIS:HE1	1:F:359:ARG:NH1	2.12	0.46
1:I:348:VAL:HG21	1:I:353:ALA:HB3	1.97	0.46
1:J:120:ILE:O	1:J:281:LEU:HD21	2.15	0.46
1:A:57:TRP:CH2	1:A:91:ILE:HG13	2.49	0.46
1:I:290:LEU:HD11	1:I:345:ILE:HD12	1.97	0.46
1:K:348:VAL:HG21	1:K:353:ALA:HB3	1.97	0.46
1:C:456:THR:O	1:K:458:HIS:HE1	1.99	0.46
1:A:290:LEU:HD11	1:A:345:ILE:HD12	1.97	0.46
1:D:348:VAL:HG21	1:D:353:ALA:HB3	1.97	0.46
1:F:296:TYR:CZ	1:F:385:LYS:HG2	2.51	0.46
1:A:348:VAL:HG21	1:A:353:ALA:HB3	1.97	0.46
1:B:296:TYR:CZ	1:B:385:LYS:HG2	2.51	0.46
1:C:273:SER:CB	3:C:473:AMP:N1	2.79	0.46
1:C:315:THR:HB	1:K:465:TYR:CE2	2.50	0.46
1:F:334:TYR:CE1	1:F:388:PRO:HB2	2.51	0.46
1:G:296:TYR:CZ	1:G:385:LYS:HG2	2.51	0.46
1:I:334:TYR:CE1	1:I:388:PRO:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:348:VAL:HG21	1:J:353:ALA:HB3	1.97	0.46
1:L:273:SER:CB	3:L:482:AMP:N1	2.79	0.46
1:E:296:TYR:CZ	1:E:385:LYS:HG2	2.51	0.46
1:G:334:TYR:CE1	1:G:388:PRO:HB2	2.51	0.46
1:I:296:TYR:CZ	1:I:385:LYS:HG2	2.51	0.46
1:E:273:SER:CB	3:E:475:AMP:N1	2.79	0.46
1:G:273:SER:CB	3:G:477:AMP:N1	2.79	0.46
1:I:120:ILE:O	1:I:281:LEU:HD21	2.15	0.46
1:J:290:LEU:HD11	1:J:345:ILE:HD12	1.97	0.46
1:K:296:TYR:CZ	1:K:385:LYS:HG2	2.51	0.46
1:L:296:TYR:CZ	1:L:385:LYS:HG2	2.51	0.46
1:A:273:SER:CB	3:A:471:AMP:N1	2.79	0.46
1:A:121:ALA:HA	1:A:276:LYS:HD2	1.96	0.46
1:E:290:LEU:HD11	1:E:345:ILE:HD12	1.97	0.46
1:H:334:TYR:CE1	1:H:388:PRO:HB2	2.51	0.46
1:J:296:TYR:CZ	1:J:385:LYS:HG2	2.51	0.46
1:B:334:TYR:CE1	1:B:388:PRO:HB2	2.51	0.46
1:J:334:TYR:CE1	1:J:388:PRO:HB2	2.51	0.46
1:K:273:SER:CB	3:K:481:AMP:N1	2.79	0.46
1:L:120:ILE:O	1:L:281:LEU:HD21	2.15	0.46
1:B:290:LEU:HD11	1:B:345:ILE:HD12	1.97	0.45
1:C:334:TYR:CE1	1:C:388:PRO:HB2	2.51	0.45
1:L:290:LEU:HD11	1:L:345:ILE:HD12	1.97	0.45
1:B:348:VAL:HG21	1:B:353:ALA:HB3	1.97	0.45
1:D:296:TYR:CZ	1:D:385:LYS:HG2	2.51	0.45
1:D:334:TYR:CE1	1:D:388:PRO:HB2	2.51	0.45
1:E:334:TYR:CE1	1:E:388:PRO:HB2	2.51	0.45
1:F:290:LEU:HD11	1:F:345:ILE:HD12	1.97	0.45
1:H:290:LEU:HD11	1:H:345:ILE:HD12	1.97	0.45
1:I:458:HIS:HD2	1:I:460:VAL:N	2.14	0.45
1:K:334:TYR:CE1	1:K:388:PRO:HB2	2.51	0.45
1:L:334:TYR:CE1	1:L:388:PRO:HB2	2.51	0.45
1:C:383:LYS:HZ3	1:C:383:LYS:HB3	1.81	0.45
1:E:348:VAL:HG21	1:E:353:ALA:HB3	1.97	0.45
1:F:273:SER:CB	3:F:476:AMP:N1	2.79	0.45
1:G:290:LEU:HD11	1:G:345:ILE:HD12	1.97	0.45
1:H:296:TYR:CZ	1:H:385:LYS:HG2	2.51	0.45
1:J:273:SER:CB	3:J:480:AMP:N1	2.79	0.45
1:L:231:LYS:HD2	1:L:231:LYS:HA	1.65	0.45
1:C:296:TYR:CZ	1:C:385:LYS:HG2	2.51	0.45
1:D:273:SER:CB	3:D:474:AMP:N1	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:231:LYS:HA	1:K:231:LYS:HD2	1.65	0.45
1:B:273:SER:CB	3:B:472:AMP:N1	2.79	0.45
1:E:231:LYS:HA	1:E:231:LYS:HD2	1.65	0.45
1:H:273:SER:CB	3:H:478:AMP:N1	2.79	0.45
1:A:334:TYR:CE1	1:A:388:PRO:HB2	2.51	0.45
1:C:138:ILE:HG21	1:K:466:TYR:CZ	2.52	0.45
1:D:290:LEU:HD11	1:D:345:ILE:HD12	1.97	0.45
1:D:458:HIS:HD2	1:D:460:VAL:N	2.14	0.45
1:F:158:TRP:HZ3	1:F:260:MET:HE3	1.82	0.45
1:L:458:HIS:HD2	1:L:460:VAL:N	2.14	0.45
1:A:296:TYR:CZ	1:A:385:LYS:HG2	2.51	0.45
1:E:270:CYS:HG	1:E:371:PHE:HE1	1.65	0.45
1:I:231:LYS:HD2	1:I:231:LYS:HA	1.65	0.45
1:J:270:CYS:HG	1:J:371:PHE:HE1	1.65	0.45
1:K:290:LEU:HD11	1:K:345:ILE:HD12	1.97	0.45
1:A:295:LEU:O	1:A:388:PRO:HD3	2.17	0.45
1:A:458:HIS:HD2	1:A:460:VAL:N	2.14	0.45
1:B:295:LEU:O	1:B:388:PRO:HD3	2.17	0.45
1:B:383:LYS:HZ3	1:B:383:LYS:HB3	1.82	0.45
1:G:348:VAL:HG21	1:G:353:ALA:HB3	1.97	0.45
1:H:295:LEU:O	1:H:388:PRO:HD3	2.17	0.44
1:H:458:HIS:HD2	1:H:460:VAL:N	2.14	0.44
1:I:273:SER:CB	3:I:479:AMP:N1	2.79	0.44
1:J:255:PHE:HB3	1:J:363:PRO:HB2	1.99	0.44
1:C:465:TYR:CE2	1:K:315:THR:HB	2.52	0.44
1:C:295:LEU:O	1:C:388:PRO:HD3	2.18	0.44
1:G:255:PHE:HB3	1:G:363:PRO:HB2	2.00	0.44
1:D:466:TYR:CZ	1:J:138:ILE:HG21	2.52	0.44
1:J:339:ARG:NH2	1:K:50:ASP:CG	2.70	0.44
1:I:295:LEU:O	1:I:388:PRO:HD3	2.17	0.44
1:F:255:PHE:HB3	1:F:363:PRO:HB2	2.00	0.44
1:G:270:CYS:HG	1:G:371:PHE:HE1	1.66	0.44
1:B:255:PHE:HB3	1:B:363:PRO:HB2	1.99	0.44
1:F:295:LEU:O	1:F:388:PRO:HD3	2.17	0.44
1:J:129:GLU:OE1	1:J:269:HIS:HB2	2.18	0.44
1:L:295:LEU:O	1:L:388:PRO:HD3	2.17	0.44
1:C:231:LYS:HA	1:C:231:LYS:HD2	1.65	0.44
1:C:270:CYS:HG	1:C:371:PHE:HE1	1.66	0.44
1:K:168:ASN:HB3	1:L:138:ILE:O	2.18	0.44
1:C:129:GLU:OE1	1:C:269:HIS:HB2	2.18	0.43
1:J:458:HIS:HD2	1:J:460:VAL:N	2.14	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLU:OE1	1:B:269:HIS:HB2	2.18	0.43
1:C:255:PHE:HB3	1:C:363:PRO:HB2	2.00	0.43
1:D:295:LEU:O	1:D:388:PRO:HD3	2.17	0.43
1:E:295:LEU:O	1:E:388:PRO:HD3	2.18	0.43
1:F:129:GLU:OE1	1:F:269:HIS:HB2	2.18	0.43
1:J:295:LEU:O	1:J:388:PRO:HD3	2.17	0.43
1:K:295:LEU:O	1:K:388:PRO:HD3	2.18	0.43
1:A:129:GLU:OE1	1:A:269:HIS:HB2	2.18	0.43
1:E:458:HIS:HD2	1:E:460:VAL:N	2.14	0.43
1:F:235:ILE:HD13	1:F:235:ILE:HA	1.83	0.43
1:F:458:HIS:HD2	1:F:460:VAL:N	2.14	0.43
1:H:129:GLU:OE1	1:H:269:HIS:HB2	2.18	0.43
1:I:235:ILE:HD13	1:I:235:ILE:HA	1.84	0.43
1:L:255:PHE:HB3	1:L:363:PRO:HB2	2.00	0.43
1:D:255:PHE:HB3	1:D:363:PRO:HB2	1.99	0.43
1:G:295:LEU:O	1:G:388:PRO:HD3	2.17	0.43
1:H:255:PHE:HB3	1:H:363:PRO:HB2	2.00	0.43
1:I:255:PHE:HB3	1:I:363:PRO:HB2	1.99	0.43
1:K:129:GLU:OE1	1:K:269:HIS:HB2	2.18	0.43
1:L:129:GLU:OE1	1:L:269:HIS:HB2	2.18	0.43
1:G:129:GLU:OE1	1:G:269:HIS:HB2	2.18	0.43
1:A:231:LYS:HD2	1:A:231:LYS:HA	1.65	0.43
1:B:458:HIS:HD2	1:B:460:VAL:N	2.14	0.43
1:D:129:GLU:OE1	1:D:269:HIS:HB2	2.18	0.43
1:E:129:GLU:OE1	1:E:269:HIS:HB2	2.18	0.43
1:E:255:PHE:HB3	1:E:363:PRO:HB2	2.00	0.43
1:A:255:PHE:HB3	1:A:363:PRO:HB2	2.00	0.43
1:B:270:CYS:HG	1:B:371:PHE:HE1	1.67	0.43
1:A:383:LYS:HB3	1:A:383:LYS:HZ2	1.82	0.43
1:D:351:PRO:HB2	1:D:352:LYS:HG3	2.01	0.43
1:H:270:CYS:HG	1:H:371:PHE:HE1	1.66	0.43
1:I:351:PRO:HB2	1:I:352:LYS:HG3	2.01	0.43
1:C:466:TYR:CZ	1:K:138:ILE:HG21	2.53	0.43
1:K:351:PRO:HB2	1:K:352:LYS:HG3	2.01	0.43
1:B:351:PRO:HB2	1:B:352:LYS:HG3	2.01	0.42
1:D:207:GLU:OE1	3:D:474:AMP:O3'	2.26	0.42
1:G:351:PRO:HB2	1:G:352:LYS:HG3	2.01	0.42
1:K:255:PHE:HB3	1:K:363:PRO:HB2	1.99	0.42
1:B:465:TYR:CE2	1:L:315:THR:HB	2.54	0.42
1:F:351:PRO:HB2	1:F:352:LYS:HG3	2.01	0.42
1:G:383:LYS:HZ3	1:G:383:LYS:HB3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:351:PRO:HB2	1:E:352:LYS:HG3	2.01	0.42
1:D:270:CYS:HG	1:D:371:PHE:HE1	1.68	0.42
1:H:339:ARG:CZ	1:H:359:ARG:NH2	2.83	0.42
1:I:129:GLU:OE1	1:I:269:HIS:HB2	2.18	0.42
1:K:270:CYS:HG	1:K:371:PHE:HE1	1.66	0.42
1:A:138:ILE:O	1:F:168:ASN:HB3	2.19	0.42
1:A:270:CYS:HG	1:A:371:PHE:HE1	1.65	0.42
1:C:351:PRO:HB2	1:C:352:LYS:HG3	2.01	0.42
1:H:207:GLU:OE1	3:H:478:AMP:O3'	2.26	0.42
1:H:68:MET:HA	1:H:69:PRO:HD2	1.93	0.42
1:I:339:ARG:CZ	1:I:359:ARG:NH2	2.83	0.42
1:B:339:ARG:CZ	1:B:359:ARG:NH2	2.83	0.42
1:E:339:ARG:CZ	1:E:359:ARG:NH2	2.83	0.42
1:G:339:ARG:CZ	1:G:359:ARG:NH2	2.83	0.42
1:C:458:HIS:HD2	1:C:460:VAL:N	2.14	0.42
1:F:339:ARG:CZ	1:F:359:ARG:NH2	2.83	0.42
1:G:458:HIS:HD2	1:G:460:VAL:N	2.14	0.42
1:D:158:TRP:HZ3	1:D:260:MET:HE3	1.85	0.42
1:J:223:THR:HG23	1:J:231:LYS:HZ1	1.85	0.42
1:J:231:LYS:HA	1:J:231:LYS:HD2	1.65	0.42
1:K:339:ARG:CZ	1:K:359:ARG:NH2	2.83	0.42
1:L:339:ARG:CZ	1:L:359:ARG:NH2	2.83	0.42
1:A:351:PRO:HB2	1:A:352:LYS:HG3	2.01	0.42
1:C:465:TYR:CZ	1:K:315:THR:HB	2.55	0.42
1:F:257:PRO:HD2	1:F:317:ASN:OD1	2.20	0.42
1:F:270:CYS:HG	1:F:371:PHE:HE1	1.66	0.42
1:E:466:TYR:CZ	1:I:138:ILE:HG21	2.54	0.42
1:J:339:ARG:CZ	1:J:359:ARG:NH2	2.83	0.42
1:J:351:PRO:HB2	1:J:352:LYS:HG3	2.01	0.42
1:L:100:TYR:CE2	1:L:102:ARG:HB3	2.55	0.42
1:L:351:PRO:HB2	1:L:352:LYS:HG3	2.01	0.42
1:B:138:ILE:HG21	1:L:466:TYR:CZ	2.54	0.42
1:C:257:PRO:HD2	1:C:317:ASN:OD1	2.21	0.41
1:E:100:TYR:CE2	1:E:102:ARG:HB3	2.55	0.41
1:K:207:GLU:OE1	3:K:481:AMP:O3'	2.26	0.41
1:B:466:TYR:CZ	1:L:138:ILE:HG21	2.55	0.41
1:C:339:ARG:CZ	1:C:359:ARG:NH2	2.83	0.41
1:A:466:TYR:CZ	1:G:138:ILE:HG21	2.54	0.41
1:K:169:LYS:HA	1:L:252:THR:HB	2.02	0.41
1:D:339:ARG:CZ	1:D:359:ARG:NH2	2.83	0.41
1:F:100:TYR:CE2	1:F:102:ARG:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:257:PRO:HD2	1:H:317:ASN:OD1	2.20	0.41
1:I:257:PRO:HD2	1:I:317:ASN:OD1	2.20	0.41
1:I:270:CYS:HG	1:I:371:PHE:HE1	1.66	0.41
1:I:3:GLU:O	1:I:7:THR:HG23	2.21	0.41
1:J:100:TYR:CE2	1:J:102:ARG:HB3	2.55	0.41
1:K:100:TYR:CE2	1:K:102:ARG:HB3	2.55	0.41
1:K:257:PRO:HD2	1:K:317:ASN:OD1	2.20	0.41
1:K:158:TRP:HZ3	1:K:260:MET:HE3	1.85	0.41
1:K:3:GLU:O	1:K:7:THR:HG23	2.21	0.41
1:L:257:PRO:HD2	1:L:317:ASN:OD1	2.20	0.41
1:L:383:LYS:HB3	1:L:383:LYS:HZ3	1.84	0.41
1:A:339:ARG:CZ	1:A:359:ARG:NH2	2.83	0.41
1:H:235:ILE:HD13	1:H:235:ILE:HA	1.83	0.41
1:H:351:PRO:HB2	1:H:352:LYS:HG3	2.01	0.41
1:L:3:GLU:O	1:L:7:THR:HG23	2.21	0.41
1:A:100:TYR:CE2	1:A:102:ARG:HB3	2.55	0.41
1:C:100:TYR:CE2	1:C:102:ARG:HB3	2.55	0.41
1:C:3:GLU:O	1:C:7:THR:HG23	2.21	0.41
1:G:100:TYR:CE2	1:G:102:ARG:HB3	2.55	0.41
1:G:257:PRO:HD2	1:G:317:ASN:OD1	2.20	0.41
1:J:3:GLU:O	1:J:7:THR:HG23	2.21	0.41
1:G:3:GLU:O	1:G:7:THR:HG23	2.21	0.41
1:A:138:ILE:HG21	1:G:466:TYR:CZ	2.55	0.41
1:A:315:THR:HB	1:G:465:TYR:CE2	2.56	0.41
1:C:114:TYR:CD1	1:C:431:GLY:HA3	2.56	0.41
1:D:100:TYR:CE2	1:D:102:ARG:HB3	2.55	0.41
1:D:66:VAL:CG1	1:D:92:LEU:HB2	2.51	0.41
1:F:3:GLU:O	1:F:7:THR:HG23	2.21	0.41
1:B:334:TYR:HA	1:B:343:ILE:O	2.21	0.41
1:E:257:PRO:HD2	1:E:317:ASN:OD1	2.20	0.41
1:F:334:TYR:HA	1:F:343:ILE:O	2.21	0.41
1:G:114:TYR:CD1	1:G:431:GLY:HA3	2.56	0.41
1:I:334:TYR:HA	1:I:343:ILE:O	2.21	0.41
1:B:114:TYR:CD1	1:B:431:GLY:HA3	2.56	0.41
1:B:196:CYS:SG	1:B:206:VAL:HG11	2.61	0.41
1:B:425:ARG:HD3	1:B:436:ASP:OD1	2.21	0.41
1:C:425:ARG:HD3	1:C:436:ASP:OD1	2.21	0.41
1:D:257:PRO:HD2	1:D:317:ASN:OD1	2.20	0.41
1:D:169:LYS:HA	1:E:252:THR:HB	2.03	0.41
1:A:465:TYR:CE2	1:G:315:THR:HB	2.56	0.41
1:G:334:TYR:HA	1:G:343:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:VAL:CG1	1:G:92:LEU:HB2	2.51	0.41
1:H:100:TYR:CE2	1:H:102:ARG:HB3	2.55	0.41
1:I:196:CYS:SG	1:I:206:VAL:HG11	2.61	0.41
1:K:458:HIS:HD2	1:K:460:VAL:N	2.14	0.41
1:A:196:CYS:SG	1:A:206:VAL:HG11	2.61	0.41
1:A:425:ARG:HD3	1:A:436:ASP:OD1	2.21	0.41
1:E:114:TYR:CD1	1:E:431:GLY:HA3	2.56	0.41
1:H:114:TYR:CD1	1:H:431:GLY:HA3	2.56	0.41
1:H:3:GLU:O	1:H:7:THR:HG23	2.21	0.41
1:I:272:MET:HB2	1:I:272:MET:HE3	2.00	0.41
1:A:257:PRO:HD2	1:A:317:ASN:OD1	2.20	0.41
1:A:350:SER:OG	1:A:351:PRO:HD3	2.21	0.41
1:B:257:PRO:HD2	1:B:317:ASN:OD1	2.20	0.41
1:B:3:GLU:O	1:B:7:THR:HG23	2.21	0.41
1:C:260:MET:HE3	1:K:144:ILE:HG12	2.03	0.41
1:D:196:CYS:SG	1:D:206:VAL:HG11	2.61	0.41
1:D:3:GLU:O	1:D:7:THR:HG23	2.21	0.41
1:E:315:THR:HB	1:I:465:TYR:CE2	2.56	0.41
1:E:334:TYR:HA	1:E:343:ILE:O	2.21	0.41
1:E:3:GLU:O	1:E:7:THR:HG23	2.21	0.41
1:F:114:TYR:CD1	1:F:431:GLY:HA3	2.56	0.41
1:I:100:TYR:CE2	1:I:102:ARG:HB3	2.55	0.41
1:J:257:PRO:HD2	1:J:317:ASN:OD1	2.20	0.41
1:J:114:TYR:CD1	1:J:431:GLY:HA3	2.56	0.41
1:J:425:ARG:HD3	1:J:436:ASP:OD1	2.21	0.41
1:K:114:TYR:CD1	1:K:431:GLY:HA3	2.56	0.41
1:L:270:CYS:HG	1:L:371:PHE:HE1	1.67	0.41
1:C:196:CYS:SG	1:C:206:VAL:HG11	2.61	0.40
1:C:334:TYR:HA	1:C:343:ILE:O	2.21	0.40
1:D:114:TYR:CD1	1:D:431:GLY:HA3	2.56	0.40
1:E:196:CYS:SG	1:E:206:VAL:HG11	2.61	0.40
1:H:296:TYR:O	1:H:381:GLY:HA3	2.22	0.40
1:J:269:HIS:HE1	1:J:359:ARG:CZ	2.35	0.40
1:K:196:CYS:SG	1:K:206:VAL:HG11	2.61	0.40
1:K:334:TYR:HA	1:K:343:ILE:O	2.21	0.40
1:K:425:ARG:HD3	1:K:436:ASP:OD1	2.21	0.40
1:L:425:ARG:HD3	1:L:436:ASP:OD1	2.21	0.40
1:B:100:TYR:CE2	1:B:102:ARG:HB3	2.55	0.40
1:B:296:TYR:O	1:B:381:GLY:HA3	2.22	0.40
1:B:169:LYS:HA	1:C:252:THR:HB	2.03	0.40
1:C:268:MET:H	1:C:362:ASP:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:MET:HA	1:C:69:PRO:HD2	1.93	0.40
1:D:425:ARG:HD3	1:D:436:ASP:OD1	2.21	0.40
1:E:269:HIS:HE1	1:E:359:ARG:CZ	2.35	0.40
1:E:425:ARG:HD3	1:E:436:ASP:OD1	2.21	0.40
1:F:196:CYS:SG	1:F:206:VAL:HG11	2.61	0.40
1:I:191:ILE:O	1:I:195:MET:HG3	2.22	0.40
1:I:268:MET:H	1:I:362:ASP:HA	1.86	0.40
1:L:114:TYR:CD1	1:L:431:GLY:HA3	2.56	0.40
1:B:350:SER:OG	1:B:351:PRO:HD3	2.21	0.40
1:B:268:MET:H	1:B:362:ASP:HA	1.86	0.40
1:D:350:SER:OG	1:D:351:PRO:HD3	2.21	0.40
1:G:425:ARG:HD3	1:G:436:ASP:OD1	2.21	0.40
1:I:425:ARG:HD3	1:I:436:ASP:OD1	2.21	0.40
1:K:350:SER:OG	1:K:351:PRO:HD3	2.21	0.40
1:A:3:GLU:O	1:A:7:THR:HG23	2.21	0.40
1:C:350:SER:OG	1:C:351:PRO:HD3	2.22	0.40
1:D:168:ASN:HB3	1:E:138:ILE:O	2.22	0.40
1:E:320:LYS:HE2	1:I:457:PRO:HA	2.04	0.40
1:E:350:SER:OG	1:E:351:PRO:HD3	2.21	0.40
1:F:350:SER:OG	1:F:351:PRO:HD3	2.21	0.40
1:F:296:TYR:O	1:F:381:GLY:HA3	2.22	0.40
1:A:260:MET:HE3	1:G:144:ILE:HG12	2.04	0.40
1:G:296:TYR:O	1:G:381:GLY:HA3	2.22	0.40
1:J:350:SER:OG	1:J:351:PRO:HD3	2.21	0.40
1:A:191:ILE:O	1:A:195:MET:HG3	2.22	0.40
1:A:269:HIS:HE1	1:A:359:ARG:CZ	2.35	0.40
1:A:114:TYR:CD1	1:A:431:GLY:HA3	2.56	0.40
1:B:168:ASN:HB3	1:C:138:ILE:O	2.21	0.40
1:D:296:TYR:O	1:D:381:GLY:HA3	2.22	0.40
1:D:390:GLU:HA	1:D:391:PRO:HD3	1.95	0.40
1:H:425:ARG:HD3	1:H:436:ASP:OD1	2.21	0.40
1:I:114:TYR:CD1	1:I:431:GLY:HA3	2.56	0.40
1:I:350:SER:OG	1:I:351:PRO:HD3	2.21	0.40
1:J:196:CYS:SG	1:J:206:VAL:HG11	2.61	0.40
1:K:68:MET:HA	1:K:69:PRO:HD2	1.93	0.40
1:L:268:MET:H	1:L:362:ASP:HA	1.86	0.40
1:B:465:TYR:CZ	1:L:315:THR:HB	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:SER:OG	1:F:13:GLU:OE2[4_454]	1.08	1.12
1:C:1:SER:OG	1:F:13:GLU:CD[4_454]	2.11	0.09

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	B	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	C	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	D	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	E	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	F	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	G	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	H	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	I	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	J	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	K	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
1	L	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	4	13
All	All	5244/5616 (93%)	4704 (90%)	372 (7%)	168 (3%)	4	13

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	A	286	LYS
1	B	180	PHE
1	B	286	LYS
1	C	180	PHE
1	C	286	LYS

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Mol	Chain	Res	Type
1	D	180	PHE
1	D	286	LYS
1	E	180	PHE
1	E	286	LYS
1	F	180	PHE
1	F	286	LYS
1	G	180	PHE
1	G	286	LYS
1	H	180	PHE
1	H	286	LYS
1	I	180	PHE
1	I	286	LYS
1	J	180	PHE
1	J	286	LYS
1	K	180	PHE
1	K	286	LYS
1	L	180	PHE
1	L	286	LYS
1	A	40	ALA
1	A	338	ASN
1	B	40	ALA
1	C	40	ALA
1	C	338	ASN
1	D	40	ALA
1	D	338	ASN
1	E	40	ALA
1	F	40	ALA
1	F	338	ASN
1	G	40	ALA
1	G	338	ASN
1	H	40	ALA
1	H	338	ASN
1	I	40	ALA
1	I	338	ASN
1	J	40	ALA
1	J	338	ASN
1	K	40	ALA
1	K	338	ASN
1	L	40	ALA
1	L	338	ASN
1	A	36	HIS
1	A	340	SER

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Mol	Chain	Res	Type
1	A	351	PRO
1	B	36	HIS
1	B	170	GLY
1	B	338	ASN
1	B	340	SER
1	B	351	PRO
1	C	36	HIS
1	C	170	GLY
1	C	340	SER
1	C	351	PRO
1	D	36	HIS
1	D	170	GLY
1	D	340	SER
1	D	351	PRO
1	E	36	HIS
1	E	338	ASN
1	E	340	SER
1	E	351	PRO
1	F	36	HIS
1	F	340	SER
1	F	351	PRO
1	G	36	HIS
1	G	170	GLY
1	G	340	SER
1	G	351	PRO
1	H	36	HIS
1	H	170	GLY
1	H	340	SER
1	H	351	PRO
1	I	36	HIS
1	I	170	GLY
1	I	340	SER
1	I	351	PRO
1	J	36	HIS
1	J	170	GLY
1	J	340	SER
1	J	351	PRO
1	K	36	HIS
1	K	340	SER
1	K	351	PRO
1	L	36	HIS
1	L	340	SER

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Mol	Chain	Res	Type
1	L	351	PRO
1	A	170	GLY
1	E	170	GLY
1	F	170	GLY
1	K	170	GLY
1	L	170	GLY
1	A	169	LYS
1	A	277	ASN
1	A	386	ILE
1	B	169	LYS
1	B	277	ASN
1	B	386	ILE
1	C	169	LYS
1	C	277	ASN
1	C	386	ILE
1	D	169	LYS
1	D	277	ASN
1	D	386	ILE
1	E	169	LYS
1	E	277	ASN
1	E	386	ILE
1	F	169	LYS
1	F	277	ASN
1	F	386	ILE
1	G	169	LYS
1	G	277	ASN
1	G	386	ILE
1	H	169	LYS
1	H	277	ASN
1	H	386	ILE
1	I	169	LYS
1	I	277	ASN
1	I	386	ILE
1	J	169	LYS
1	J	277	ASN
1	J	386	ILE
1	K	169	LYS
1	K	277	ASN
1	K	386	ILE
1	L	169	LYS
1	L	277	ASN
1	L	386	ILE

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Mol	Chain	Res	Type
1	A	285	ASP
1	A	350	SER
1	A	434	PHE
1	B	285	ASP
1	B	350	SER
1	B	434	PHE
1	C	285	ASP
1	C	350	SER
1	C	434	PHE
1	D	285	ASP
1	D	350	SER
1	D	434	PHE
1	E	285	ASP
1	E	350	SER
1	E	434	PHE
1	F	285	ASP
1	F	350	SER
1	F	434	PHE
1	G	285	ASP
1	G	350	SER
1	G	434	PHE
1	H	285	ASP
1	H	350	SER
1	H	434	PHE
1	I	285	ASP
1	I	350	SER
1	I	434	PHE
1	J	285	ASP
1	J	350	SER
1	J	434	PHE
1	K	285	ASP
1	K	350	SER
1	K	434	PHE
1	L	285	ASP
1	L	350	SER
1	L	434	PHE

### 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	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	B	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	C	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	D	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	E	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	F	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	G	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	H	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	I	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	J	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	K	365/384 (95%)	326 (89%)	39 (11%)	6	20
1	L	365/384 (95%)	326 (89%)	39 (11%)	6	20
All	All	4380/4608 (95%)	3912 (89%)	468 (11%)	6	20

All (468) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	GLU
1	A	19	LEU
1	A	33	ILE
1	A	36	HIS
1	A	39	ASN
1	A	45	GLU
1	A	75	VAL
1	A	76	ILE
1	A	85	LEU
1	A	88	ARG
1	A	101	ASP
1	A	105	ARG
1	A	115	LEU
1	A	122	ASP
1	A	124	VAL
1	A	143	SER
1	A	165	GLU
1	A	194	GLU

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Mol	Chain	Res	Type
1	A	223	THR
1	A	226	ASN
1	A	286	LYS
1	A	314	PRO
1	A	324	PRO
1	A	331	MET
1	A	332	LEU
1	A	337	ARG
1	A	339	ARG
1	A	340	SER
1	A	352	LYS
1	A	359	ARG
1	A	374	LEU
1	A	375	LEU
1	A	383	LYS
1	A	426	GLU
1	A	428	LEU
1	A	446	ARG
1	A	464	LEU
1	A	468	VAL
1	B	9	LEU
1	B	11	GLU
1	B	19	LEU
1	B	33	ILE
1	B	36	HIS
1	B	39	ASN
1	B	45	GLU
1	B	75	VAL
1	B	76	ILE
1	B	85	LEU
1	B	88	ARG
1	B	101	ASP
1	B	105	ARG
1	B	115	LEU
1	B	122	ASP
1	B	124	VAL
1	B	143	SER
1	B	165	GLU
1	B	194	GLU
1	B	223	THR
1	B	226	ASN
1	B	286	LYS

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Mol	Chain	Res	Type
1	B	314	PRO
1	B	324	PRO
1	B	331	MET
1	B	332	LEU
1	B	337	ARG
1	B	339	ARG
1	B	340	SER
1	B	352	LYS
1	B	359	ARG
1	B	374	LEU
1	B	375	LEU
1	B	383	LYS
1	B	426	GLU
1	B	428	LEU
1	B	446	ARG
1	B	464	LEU
1	B	468	VAL
1	C	9	LEU
1	C	11	GLU
1	C	19	LEU
1	C	33	ILE
1	C	36	HIS
1	C	39	ASN
1	C	45	GLU
1	C	75	VAL
1	C	76	ILE
1	C	85	LEU
1	C	88	ARG
1	C	101	ASP
1	C	105	ARG
1	C	115	LEU
1	C	122	ASP
1	C	124	VAL
1	C	143	SER
1	C	165	GLU
1	C	194	GLU
1	C	223	THR
1	C	226	ASN
1	C	286	LYS
1	C	314	PRO
1	C	324	PRO
1	C	331	MET

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Mol	Chain	Res	Type
1	C	332	LEU
1	C	337	ARG
1	C	339	ARG
1	C	340	SER
1	C	352	LYS
1	C	359	ARG
1	C	374	LEU
1	C	375	LEU
1	C	383	LYS
1	C	426	GLU
1	C	428	LEU
1	C	446	ARG
1	C	464	LEU
1	C	468	VAL
1	D	9	LEU
1	D	11	GLU
1	D	19	LEU
1	D	33	ILE
1	D	36	HIS
1	D	39	ASN
1	D	45	GLU
1	D	75	VAL
1	D	76	ILE
1	D	85	LEU
1	D	88	ARG
1	D	101	ASP
1	D	105	ARG
1	D	115	LEU
1	D	122	ASP
1	D	124	VAL
1	D	143	SER
1	D	165	GLU
1	D	194	GLU
1	D	223	THR
1	D	226	ASN
1	D	286	LYS
1	D	314	PRO
1	D	324	PRO
1	D	331	MET
1	D	332	LEU
1	D	337	ARG
1	D	339	ARG

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Mol	Chain	Res	Type
1	D	340	SER
1	D	352	LYS
1	D	359	ARG
1	D	374	LEU
1	D	375	LEU
1	D	383	LYS
1	D	426	GLU
1	D	428	LEU
1	D	446	ARG
1	D	464	LEU
1	D	468	VAL
1	E	9	LEU
1	E	11	GLU
1	E	19	LEU
1	E	33	ILE
1	E	36	HIS
1	E	39	ASN
1	E	45	GLU
1	E	75	VAL
1	E	76	ILE
1	E	85	LEU
1	E	88	ARG
1	E	101	ASP
1	E	105	ARG
1	E	115	LEU
1	E	122	ASP
1	E	124	VAL
1	E	143	SER
1	E	165	GLU
1	E	194	GLU
1	E	223	THR
1	E	226	ASN
1	E	286	LYS
1	E	314	PRO
1	E	324	PRO
1	E	331	MET
1	E	332	LEU
1	E	337	ARG
1	E	339	ARG
1	E	340	SER
1	E	352	LYS
1	E	359	ARG

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Mol	Chain	Res	Type
1	E	374	LEU
1	E	375	LEU
1	E	383	LYS
1	E	426	GLU
1	E	428	LEU
1	E	446	ARG
1	E	464	LEU
1	E	468	VAL
1	F	9	LEU
1	F	11	GLU
1	F	19	LEU
1	F	33	ILE
1	F	36	HIS
1	F	39	ASN
1	F	45	GLU
1	F	75	VAL
1	F	76	ILE
1	F	85	LEU
1	F	88	ARG
1	F	101	ASP
1	F	105	ARG
1	F	115	LEU
1	F	122	ASP
1	F	124	VAL
1	F	143	SER
1	F	165	GLU
1	F	194	GLU
1	F	223	THR
1	F	226	ASN
1	F	286	LYS
1	F	314	PRO
1	F	324	PRO
1	F	331	MET
1	F	332	LEU
1	F	337	ARG
1	F	339	ARG
1	F	340	SER
1	F	352	LYS
1	F	359	ARG
1	F	374	LEU
1	F	375	LEU
1	F	383	LYS

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Mol	Chain	Res	Type
1	F	426	GLU
1	F	428	LEU
1	F	446	ARG
1	F	464	LEU
1	F	468	VAL
1	G	9	LEU
1	G	11	GLU
1	G	19	LEU
1	G	33	ILE
1	G	36	HIS
1	G	39	ASN
1	G	45	GLU
1	G	75	VAL
1	G	76	ILE
1	G	85	LEU
1	G	88	ARG
1	G	101	ASP
1	G	105	ARG
1	G	115	LEU
1	G	122	ASP
1	G	124	VAL
1	G	143	SER
1	G	165	GLU
1	G	194	GLU
1	G	223	THR
1	G	226	ASN
1	G	286	LYS
1	G	314	PRO
1	G	324	PRO
1	G	331	MET
1	G	332	LEU
1	G	337	ARG
1	G	339	ARG
1	G	340	SER
1	G	352	LYS
1	G	359	ARG
1	G	374	LEU
1	G	375	LEU
1	G	383	LYS
1	G	426	GLU
1	G	428	LEU
1	G	446	ARG

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Mol	Chain	Res	Type
1	G	464	LEU
1	G	468	VAL
1	H	9	LEU
1	H	11	GLU
1	H	19	LEU
1	H	33	ILE
1	H	36	HIS
1	H	39	ASN
1	H	45	GLU
1	H	75	VAL
1	H	76	ILE
1	H	85	LEU
1	H	88	ARG
1	H	101	ASP
1	H	105	ARG
1	H	115	LEU
1	H	122	ASP
1	H	124	VAL
1	H	143	SER
1	H	165	GLU
1	H	194	GLU
1	H	223	THR
1	H	226	ASN
1	H	286	LYS
1	H	314	PRO
1	H	324	PRO
1	H	331	MET
1	H	332	LEU
1	H	337	ARG
1	H	339	ARG
1	H	340	SER
1	H	352	LYS
1	H	359	ARG
1	H	374	LEU
1	H	375	LEU
1	H	383	LYS
1	H	426	GLU
1	H	428	LEU
1	H	446	ARG
1	H	464	LEU
1	H	468	VAL
1	I	9	LEU

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Mol	Chain	Res	Type
1	I	11	GLU
1	I	19	LEU
1	I	33	ILE
1	I	36	HIS
1	I	39	ASN
1	I	45	GLU
1	I	75	VAL
1	I	76	ILE
1	I	85	LEU
1	I	88	ARG
1	I	101	ASP
1	I	105	ARG
1	I	115	LEU
1	I	122	ASP
1	I	124	VAL
1	I	143	SER
1	I	165	GLU
1	I	194	GLU
1	I	223	THR
1	I	226	ASN
1	I	286	LYS
1	I	314	PRO
1	I	324	PRO
1	I	331	MET
1	I	332	LEU
1	I	337	ARG
1	I	339	ARG
1	I	340	SER
1	I	352	LYS
1	I	359	ARG
1	I	374	LEU
1	I	375	LEU
1	I	383	LYS
1	I	426	GLU
1	I	428	LEU
1	I	446	ARG
1	I	464	LEU
1	I	468	VAL
1	J	9	LEU
1	J	11	GLU
1	J	19	LEU
1	J	33	ILE

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Mol	Chain	Res	Type
1	J	36	HIS
1	J	39	ASN
1	J	45	GLU
1	J	75	VAL
1	J	76	ILE
1	J	85	LEU
1	J	88	ARG
1	J	101	ASP
1	J	105	ARG
1	J	115	LEU
1	J	122	ASP
1	J	124	VAL
1	J	143	SER
1	J	165	GLU
1	J	194	GLU
1	J	223	THR
1	J	226	ASN
1	J	286	LYS
1	J	314	PRO
1	J	324	PRO
1	J	331	MET
1	J	332	LEU
1	J	337	ARG
1	J	339	ARG
1	J	340	SER
1	J	352	LYS
1	J	359	ARG
1	J	374	LEU
1	J	375	LEU
1	J	383	LYS
1	J	426	GLU
1	J	428	LEU
1	J	446	ARG
1	J	464	LEU
1	J	468	VAL
1	K	9	LEU
1	K	11	GLU
1	K	19	LEU
1	K	33	ILE
1	K	36	HIS
1	K	39	ASN
1	K	45	GLU

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Mol	Chain	Res	Type
1	K	75	VAL
1	K	76	ILE
1	K	85	LEU
1	K	88	ARG
1	K	101	ASP
1	K	105	ARG
1	K	115	LEU
1	K	122	ASP
1	K	124	VAL
1	K	143	SER
1	K	165	GLU
1	K	194	GLU
1	K	223	THR
1	K	226	ASN
1	K	286	LYS
1	K	314	PRO
1	K	324	PRO
1	K	331	MET
1	K	332	LEU
1	K	337	ARG
1	K	339	ARG
1	K	340	SER
1	K	352	LYS
1	K	359	ARG
1	K	374	LEU
1	K	375	LEU
1	K	383	LYS
1	K	426	GLU
1	K	428	LEU
1	K	446	ARG
1	K	464	LEU
1	K	468	VAL
1	L	9	LEU
1	L	11	GLU
1	L	19	LEU
1	L	33	ILE
1	L	36	HIS
1	L	39	ASN
1	L	45	GLU
1	L	75	VAL
1	L	76	ILE
1	L	85	LEU

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Mol	Chain	Res	Type
1	L	88	ARG
1	L	101	ASP
1	L	105	ARG
1	L	115	LEU
1	L	122	ASP
1	L	124	VAL
1	L	143	SER
1	L	165	GLU
1	L	194	GLU
1	L	223	THR
1	L	226	ASN
1	L	286	LYS
1	L	314	PRO
1	L	324	PRO
1	L	331	MET
1	L	332	LEU
1	L	337	ARG
1	L	339	ARG
1	L	340	SER
1	L	352	LYS
1	L	359	ARG
1	L	374	LEU
1	L	375	LEU
1	L	383	LYS
1	L	426	GLU
1	L	428	LEU
1	L	446	ARG
1	L	464	LEU
1	L	468	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	159	ASN
1	A	189	GLN
1	A	219	ASN
1	A	269	HIS
1	A	458	HIS
1	B	30	HIS
1	B	159	ASN
1	B	189	GLN

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Mol	Chain	Res	Type
1	B	219	ASN
1	B	269	HIS
1	B	458	HIS
1	C	30	HIS
1	C	159	ASN
1	C	189	GLN
1	C	219	ASN
1	C	269	HIS
1	C	458	HIS
1	D	30	HIS
1	D	159	ASN
1	D	189	GLN
1	D	219	ASN
1	D	269	HIS
1	D	458	HIS
1	E	30	HIS
1	E	159	ASN
1	E	189	GLN
1	E	219	ASN
1	E	269	HIS
1	E	458	HIS
1	F	30	HIS
1	F	159	ASN
1	F	189	GLN
1	F	219	ASN
1	F	269	HIS
1	F	458	HIS
1	G	30	HIS
1	G	159	ASN
1	G	189	GLN
1	G	219	ASN
1	G	269	HIS
1	G	458	HIS
1	H	30	HIS
1	H	189	GLN
1	H	219	ASN
1	H	269	HIS
1	H	458	HIS
1	I	30	HIS
1	I	159	ASN
1	I	189	GLN
1	I	219	ASN

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Mol	Chain	Res	Type
1	I	269	HIS
1	I	458	HIS
1	J	30	HIS
1	J	159	ASN
1	J	189	GLN
1	J	219	ASN
1	J	269	HIS
1	J	458	HIS
1	K	30	HIS
1	K	159	ASN
1	K	189	GLN
1	K	219	ASN
1	K	269	HIS
1	K	458	HIS
1	L	30	HIS
1	L	159	ASN
1	L	189	GLN
1	L	219	ASN
1	L	269	HIS
1	L	458	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	AMP	B	472	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	F	476	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	K	481	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	C	473	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	H	478	-	22,25,25	1.17	3 (13%)	25,38,38	1.11	2 (8%)
3	AMP	J	480	-	22,25,25	1.17	2 (9%)	25,38,38	1.10	2 (8%)
3	AMP	I	479	-	22,25,25	1.17	2 (9%)	25,38,38	1.10	2 (8%)
3	AMP	D	474	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	G	477	-	22,25,25	1.18	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	A	471	-	22,25,25	1.17	3 (13%)	25,38,38	1.10	2 (8%)
3	AMP	L	482	-	22,25,25	1.17	2 (9%)	25,38,38	1.11	2 (8%)
3	AMP	E	475	-	22,25,25	1.18	3 (13%)	25,38,38	1.11	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	B	472	-	-	5/6/26/26	0/3/3/3
3	AMP	F	476	-	-	5/6/26/26	0/3/3/3
3	AMP	K	481	-	-	5/6/26/26	0/3/3/3
3	AMP	C	473	-	-	5/6/26/26	0/3/3/3
3	AMP	H	478	-	-	5/6/26/26	0/3/3/3
3	AMP	J	480	-	-	5/6/26/26	0/3/3/3
3	AMP	I	479	-	-	5/6/26/26	0/3/3/3
3	AMP	D	474	-	-	5/6/26/26	0/3/3/3
3	AMP	G	477	-	-	5/6/26/26	0/3/3/3
3	AMP	A	471	-	-	5/6/26/26	0/3/3/3
3	AMP	L	482	-	-	5/6/26/26	0/3/3/3
3	AMP	E	475	-	-	5/6/26/26	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	478	AMP	P-O1P	2.89	1.59	1.50
3	L	482	AMP	P-O1P	2.88	1.59	1.50
3	F	476	AMP	P-O1P	2.88	1.59	1.50
3	E	475	AMP	P-O1P	2.88	1.59	1.50
3	I	479	AMP	P-O1P	2.88	1.59	1.50
3	A	471	AMP	P-O1P	2.88	1.59	1.50
3	B	472	AMP	P-O1P	2.87	1.59	1.50
3	C	473	AMP	P-O1P	2.87	1.59	1.50
3	K	481	AMP	P-O1P	2.87	1.59	1.50
3	D	474	AMP	P-O1P	2.86	1.59	1.50
3	J	480	AMP	P-O1P	2.86	1.59	1.50
3	G	477	AMP	P-O1P	2.86	1.59	1.50
3	J	480	AMP	C8-N7	-2.49	1.30	1.34
3	G	477	AMP	C8-N7	-2.48	1.30	1.34
3	I	479	AMP	C8-N7	-2.47	1.30	1.34
3	D	474	AMP	C8-N7	-2.47	1.30	1.34
3	F	476	AMP	C8-N7	-2.47	1.30	1.34
3	L	482	AMP	C8-N7	-2.46	1.30	1.34
3	A	471	AMP	C8-N7	-2.46	1.30	1.34
3	H	478	AMP	C8-N7	-2.46	1.30	1.34
3	E	475	AMP	C8-N7	-2.45	1.30	1.34
3	K	481	AMP	C8-N7	-2.45	1.30	1.34
3	C	473	AMP	C8-N7	-2.44	1.30	1.34
3	B	472	AMP	C8-N7	-2.43	1.30	1.34
3	E	475	AMP	O3'-C3'	-2.06	1.38	1.43
3	G	477	AMP	O3'-C3'	-2.04	1.38	1.43
3	B	472	AMP	O3'-C3'	-2.03	1.38	1.43
3	H	478	AMP	O3'-C3'	-2.02	1.38	1.43
3	A	471	AMP	O3'-C3'	-2.02	1.38	1.43
3	D	474	AMP	O3'-C3'	-2.02	1.38	1.43
3	F	476	AMP	O3'-C3'	-2.01	1.38	1.43
3	C	473	AMP	O3'-C3'	-2.01	1.38	1.43
3	K	481	AMP	O3'-C3'	-2.00	1.38	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	482	AMP	O3'-C3'-C4'	-2.11	104.94	111.05
3	J	480	AMP	O3'-C3'-C4'	-2.10	104.96	111.05
3	H	478	AMP	O3'-C3'-C4'	-2.10	104.97	111.05
3	B	472	AMP	O3'-C3'-C4'	-2.10	104.97	111.05
3	C	473	AMP	O3'-C3'-C4'	-2.10	104.99	111.05
3	A	471	AMP	O3'-C3'-C4'	-2.10	104.99	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	475	AMP	O3'-C3'-C4'	-2.10	104.99	111.05
3	G	477	AMP	O3'-C3'-C4'	-2.10	104.99	111.05
3	D	474	AMP	O3'-C3'-C4'	-2.09	104.99	111.05
3	K	481	AMP	O3'-C3'-C4'	-2.09	105.00	111.05
3	I	479	AMP	O3'-C3'-C4'	-2.09	105.00	111.05
3	F	476	AMP	O3'-C3'-C4'	-2.08	105.03	111.05
3	F	476	AMP	O3P-P-O2P	2.06	115.52	107.64
3	L	482	AMP	O3P-P-O2P	2.06	115.52	107.64
3	I	479	AMP	O3P-P-O2P	2.06	115.51	107.64
3	A	471	AMP	O3P-P-O2P	2.06	115.51	107.64
3	H	478	AMP	O3P-P-O2P	2.06	115.51	107.64
3	C	473	AMP	O3P-P-O2P	2.06	115.51	107.64
3	J	480	AMP	O3P-P-O2P	2.06	115.50	107.64
3	G	477	AMP	O3P-P-O2P	2.06	115.50	107.64
3	D	474	AMP	O3P-P-O2P	2.05	115.49	107.64
3	B	472	AMP	O3P-P-O2P	2.05	115.48	107.64
3	E	475	AMP	O3P-P-O2P	2.05	115.48	107.64
3	K	481	AMP	O3P-P-O2P	2.05	115.48	107.64

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	473	AMP	C5'-O5'-P-O1P
3	C	473	AMP	C5'-O5'-P-O2P
3	C	473	AMP	C5'-O5'-P-O3P
3	C	473	AMP	O4'-C4'-C5'-O5'
3	C	473	AMP	C3'-C4'-C5'-O5'
3	L	482	AMP	C5'-O5'-P-O1P
3	L	482	AMP	C5'-O5'-P-O2P
3	L	482	AMP	C5'-O5'-P-O3P
3	L	482	AMP	O4'-C4'-C5'-O5'
3	L	482	AMP	C3'-C4'-C5'-O5'
3	I	479	AMP	C5'-O5'-P-O1P
3	I	479	AMP	C5'-O5'-P-O2P
3	I	479	AMP	C5'-O5'-P-O3P
3	I	479	AMP	O4'-C4'-C5'-O5'
3	I	479	AMP	C3'-C4'-C5'-O5'
3	B	472	AMP	C5'-O5'-P-O1P
3	B	472	AMP	C5'-O5'-P-O2P
3	B	472	AMP	C5'-O5'-P-O3P
3	B	472	AMP	O4'-C4'-C5'-O5'

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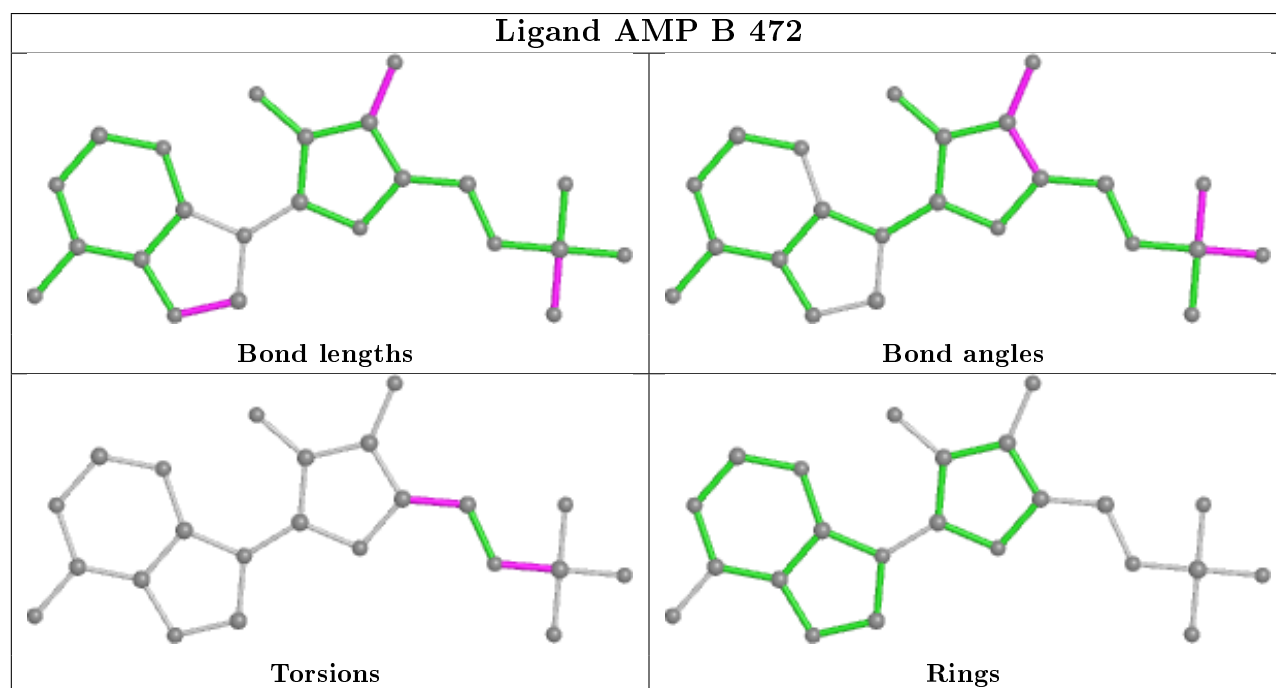
Mol	Chain	Res	Type	Atoms
3	B	472	AMP	C3'-C4'-C5'-O5'
3	K	481	AMP	C5'-O5'-P-O1P
3	K	481	AMP	C5'-O5'-P-O2P
3	K	481	AMP	C5'-O5'-P-O3P
3	K	481	AMP	O4'-C4'-C5'-O5'
3	K	481	AMP	C3'-C4'-C5'-O5'
3	G	477	AMP	C5'-O5'-P-O1P
3	G	477	AMP	C5'-O5'-P-O2P
3	G	477	AMP	C5'-O5'-P-O3P
3	G	477	AMP	O4'-C4'-C5'-O5'
3	G	477	AMP	C3'-C4'-C5'-O5'
3	F	476	AMP	C5'-O5'-P-O1P
3	F	476	AMP	C5'-O5'-P-O2P
3	F	476	AMP	C5'-O5'-P-O3P
3	F	476	AMP	O4'-C4'-C5'-O5'
3	F	476	AMP	C3'-C4'-C5'-O5'
3	D	474	AMP	C5'-O5'-P-O1P
3	D	474	AMP	C5'-O5'-P-O2P
3	D	474	AMP	C5'-O5'-P-O3P
3	D	474	AMP	O4'-C4'-C5'-O5'
3	D	474	AMP	C3'-C4'-C5'-O5'
3	A	471	AMP	C5'-O5'-P-O1P
3	A	471	AMP	C5'-O5'-P-O2P
3	A	471	AMP	C5'-O5'-P-O3P
3	A	471	AMP	O4'-C4'-C5'-O5'
3	A	471	AMP	C3'-C4'-C5'-O5'
3	H	478	AMP	C5'-O5'-P-O1P
3	H	478	AMP	C5'-O5'-P-O2P
3	H	478	AMP	C5'-O5'-P-O3P
3	H	478	AMP	O4'-C4'-C5'-O5'
3	H	478	AMP	C3'-C4'-C5'-O5'
3	J	480	AMP	C5'-O5'-P-O1P
3	J	480	AMP	C5'-O5'-P-O2P
3	J	480	AMP	C5'-O5'-P-O3P
3	J	480	AMP	O4'-C4'-C5'-O5'
3	J	480	AMP	C3'-C4'-C5'-O5'
3	E	475	AMP	C5'-O5'-P-O1P
3	E	475	AMP	C5'-O5'-P-O2P
3	E	475	AMP	C5'-O5'-P-O3P
3	E	475	AMP	O4'-C4'-C5'-O5'
3	E	475	AMP	C3'-C4'-C5'-O5'

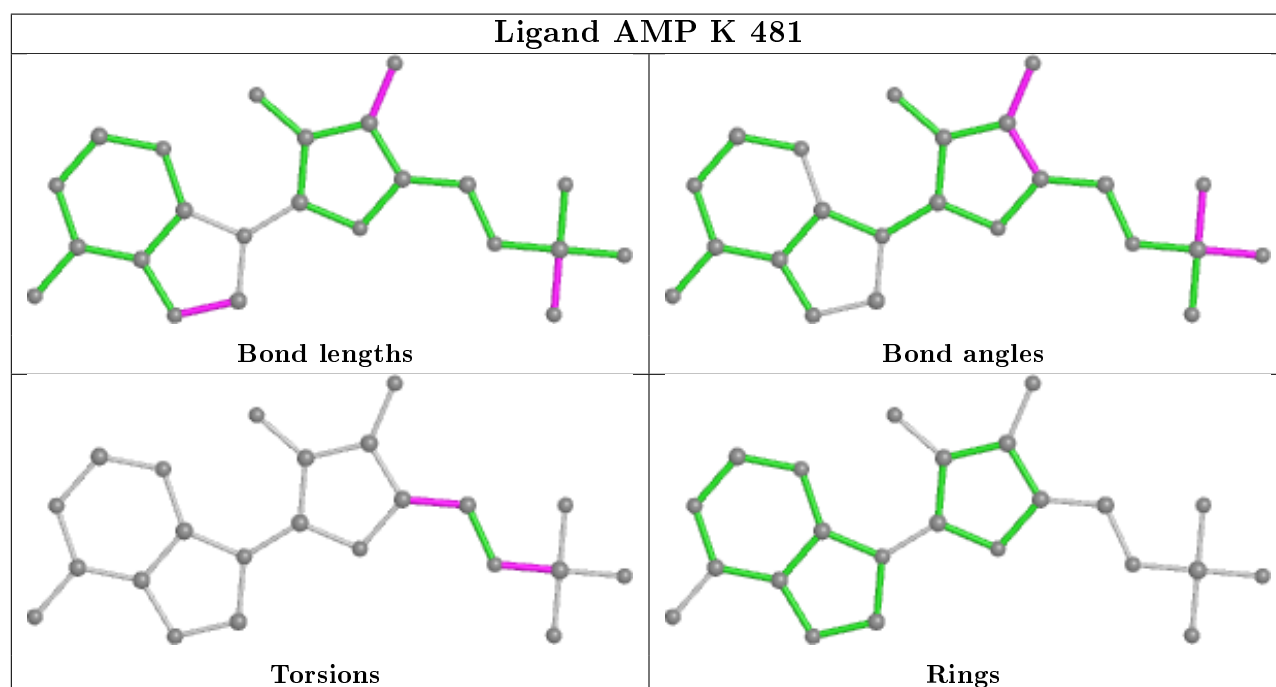
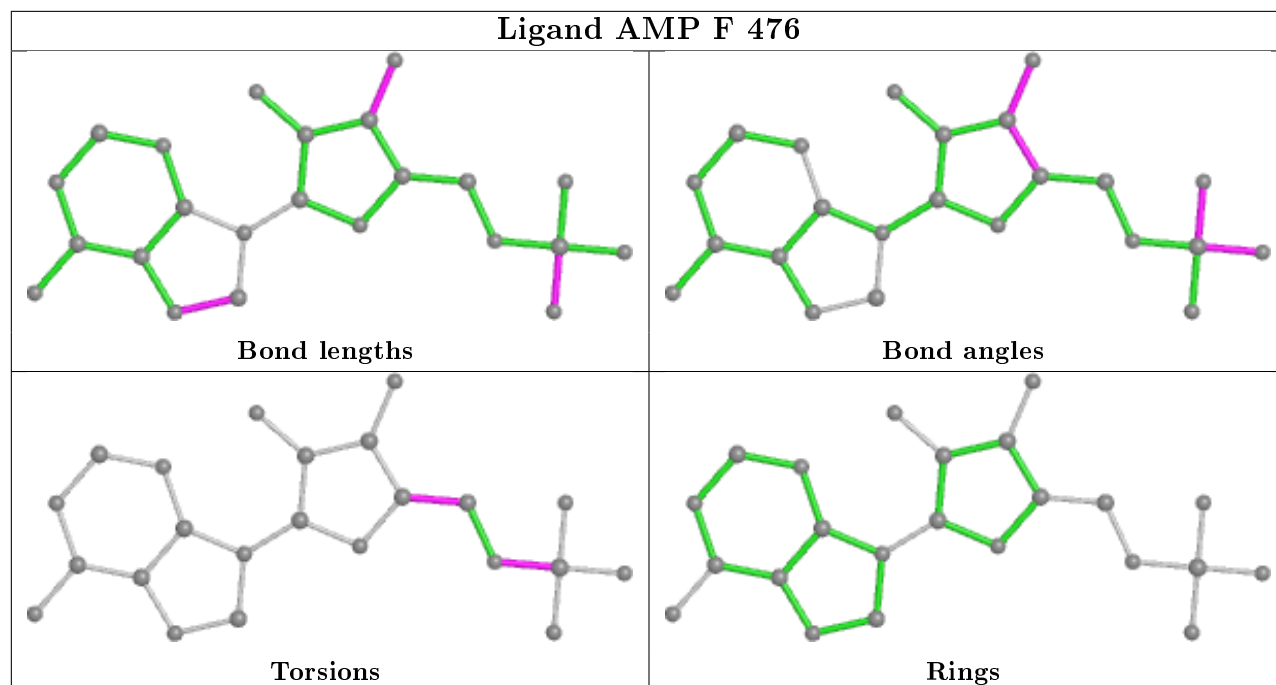
There are no ring outliers.

12 monomers are involved in 28 short contacts:

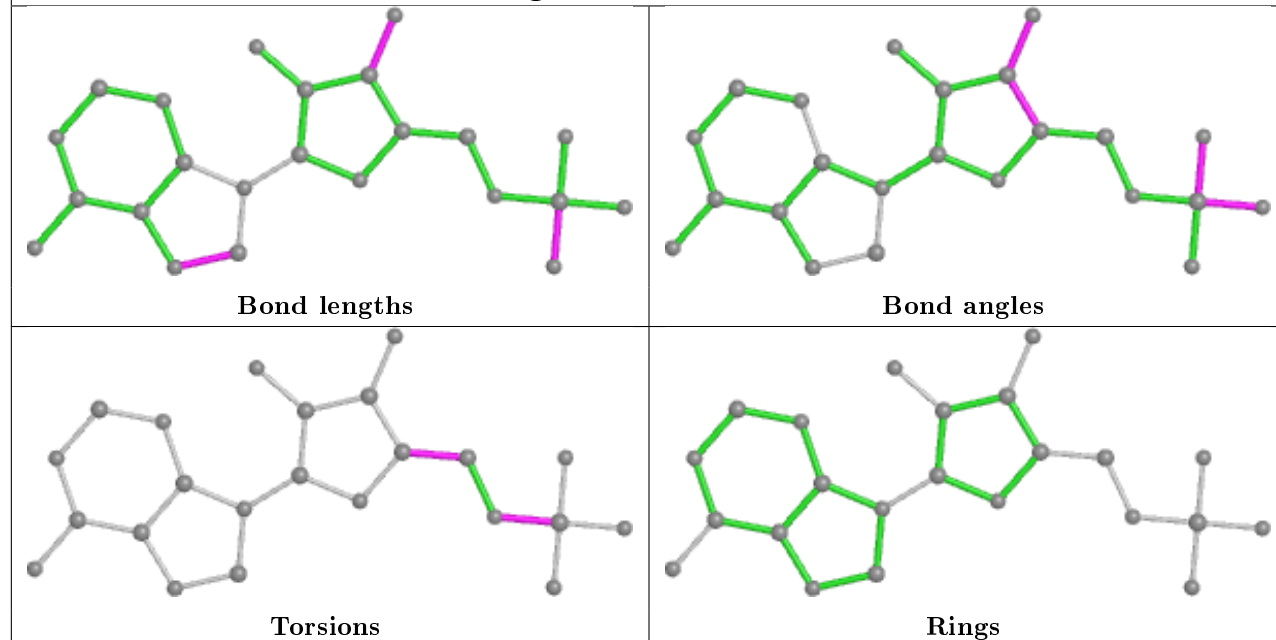
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	472	AMP	2	0
3	F	476	AMP	2	0
3	K	481	AMP	3	0
3	C	473	AMP	2	0
3	H	478	AMP	3	0
3	J	480	AMP	2	0
3	I	479	AMP	3	0
3	D	474	AMP	3	0
3	G	477	AMP	2	0
3	A	471	AMP	2	0
3	L	482	AMP	2	0
3	E	475	AMP	2	0

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

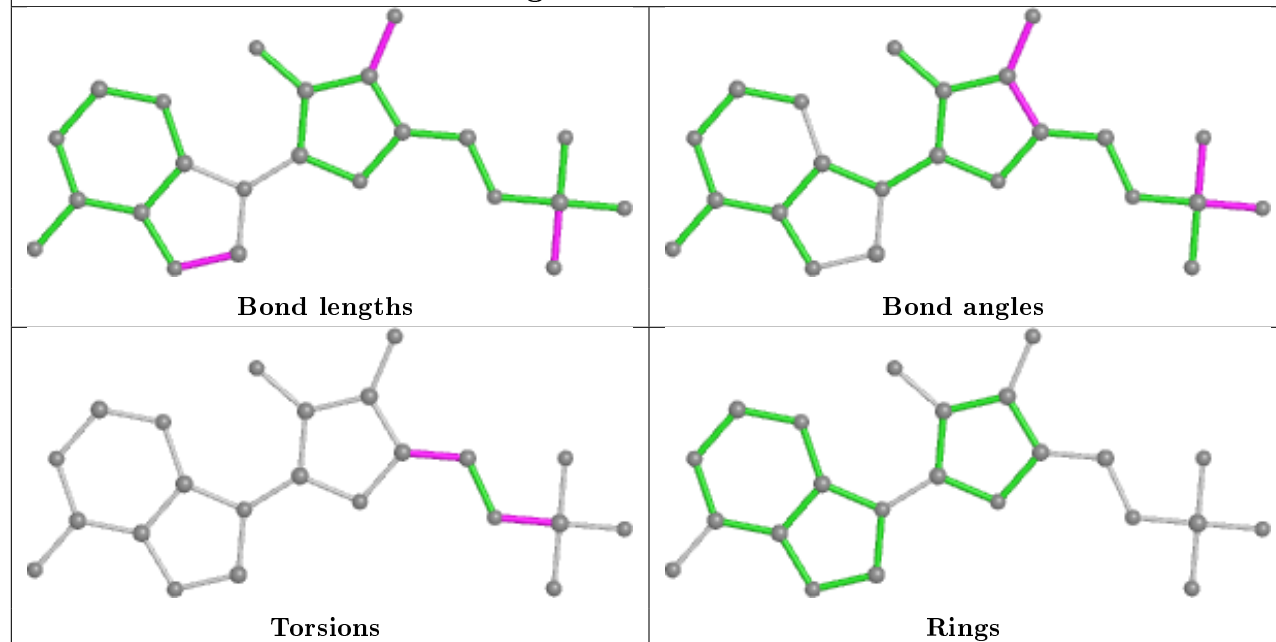




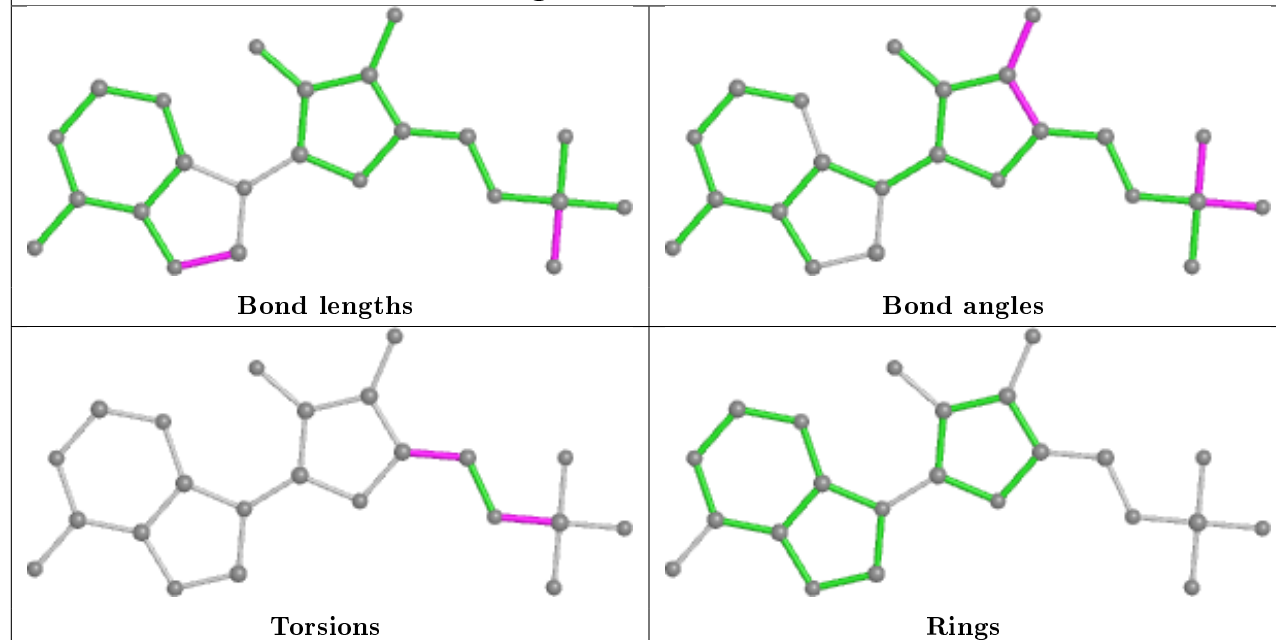
## Ligand AMP C 473



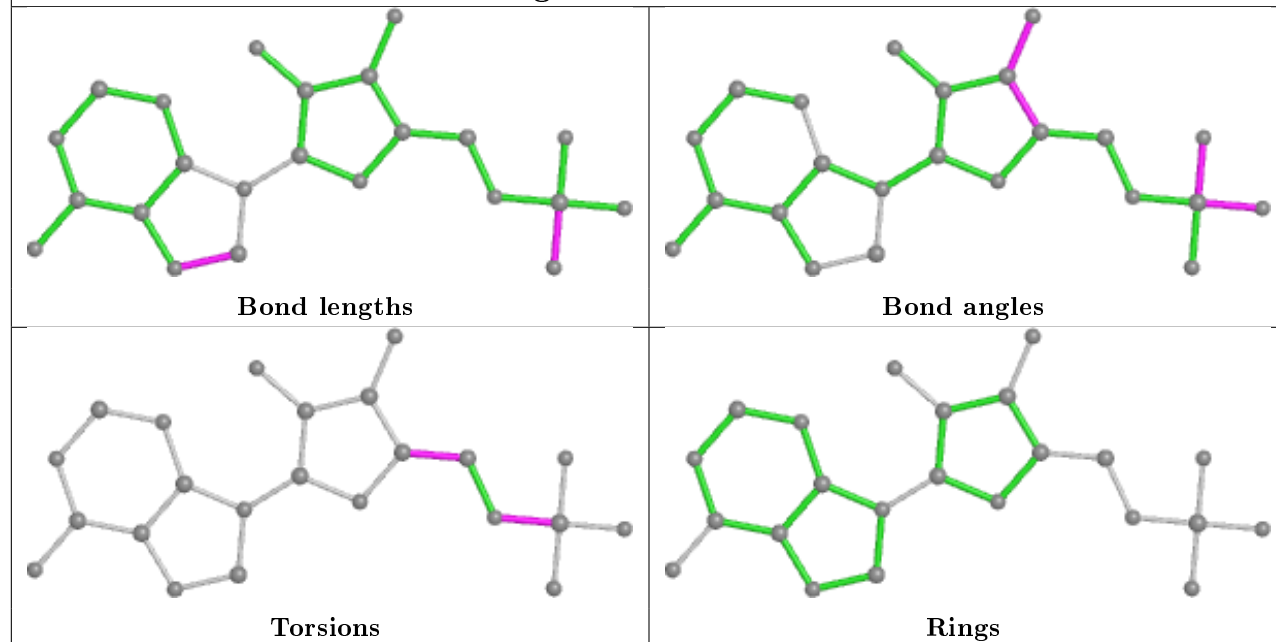
## Ligand AMP H 478



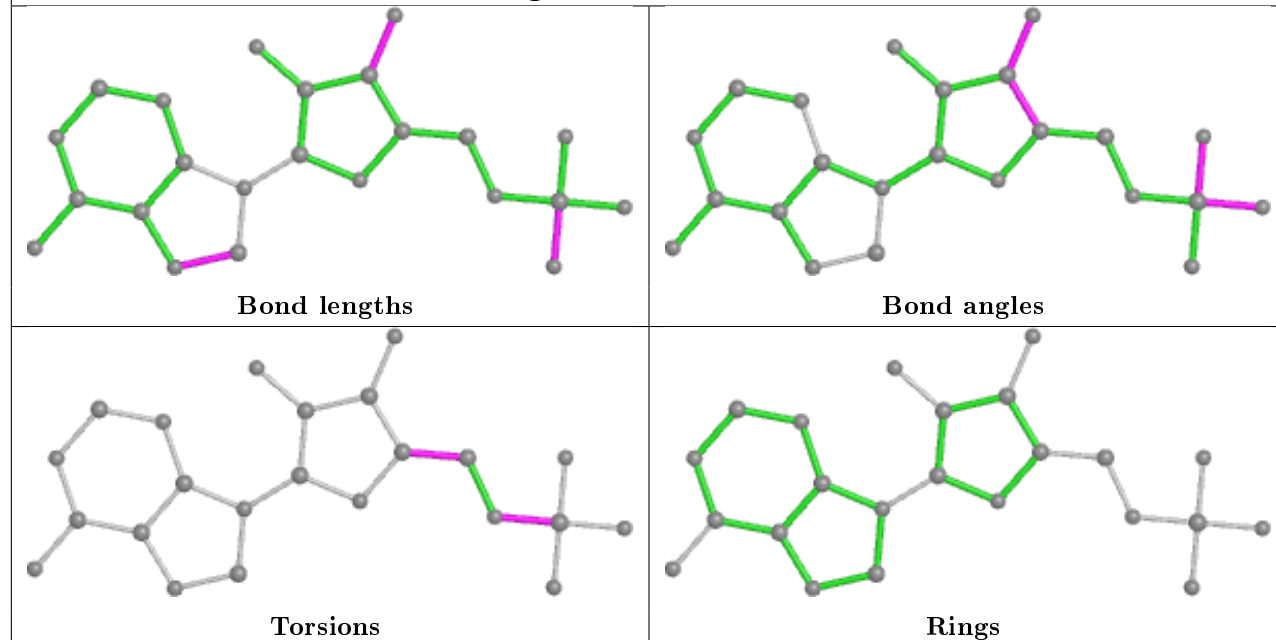
## Ligand AMP J 480



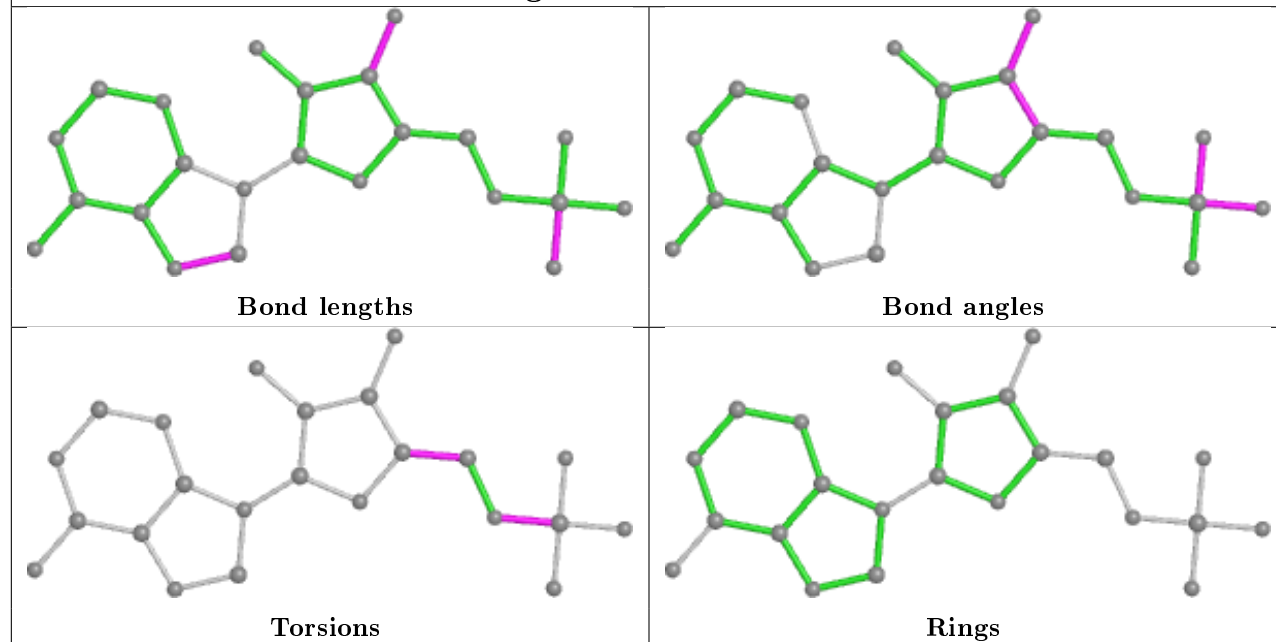
## Ligand AMP I 479



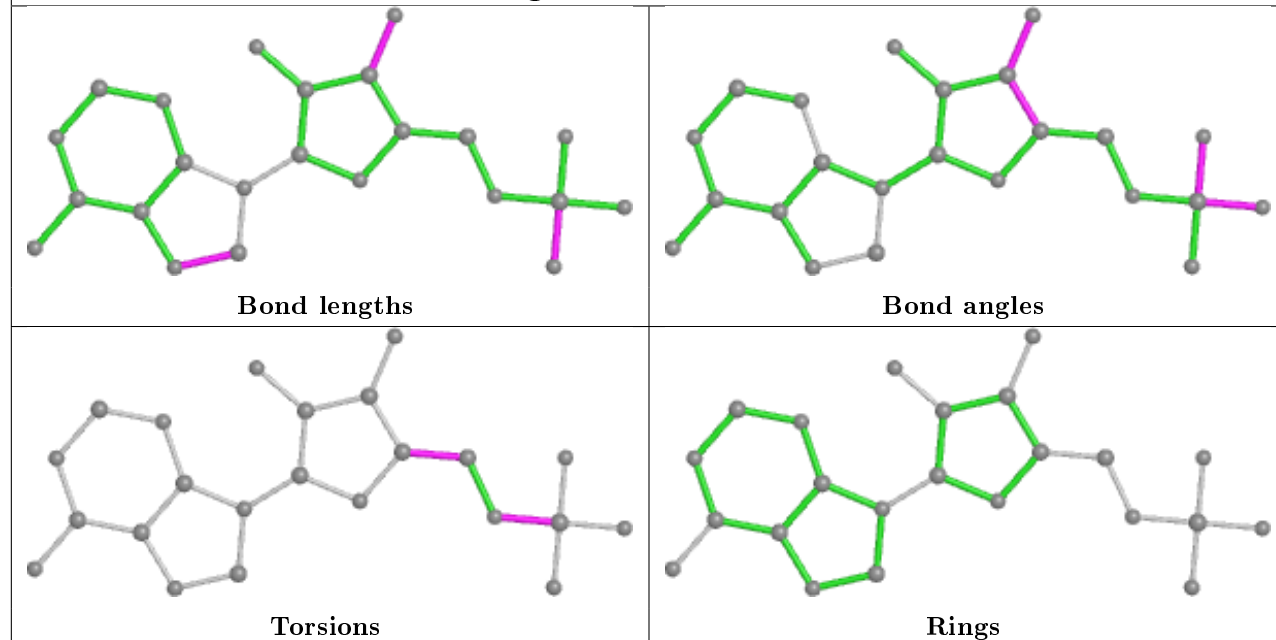
## Ligand AMP D 474



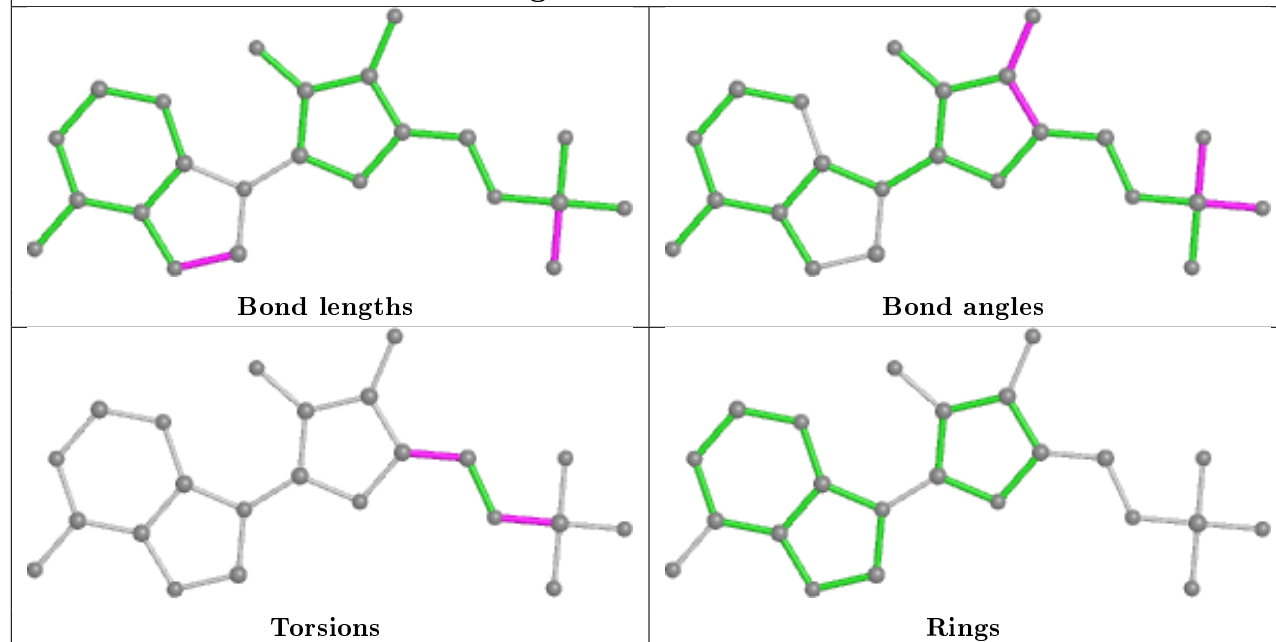
## Ligand AMP G 477



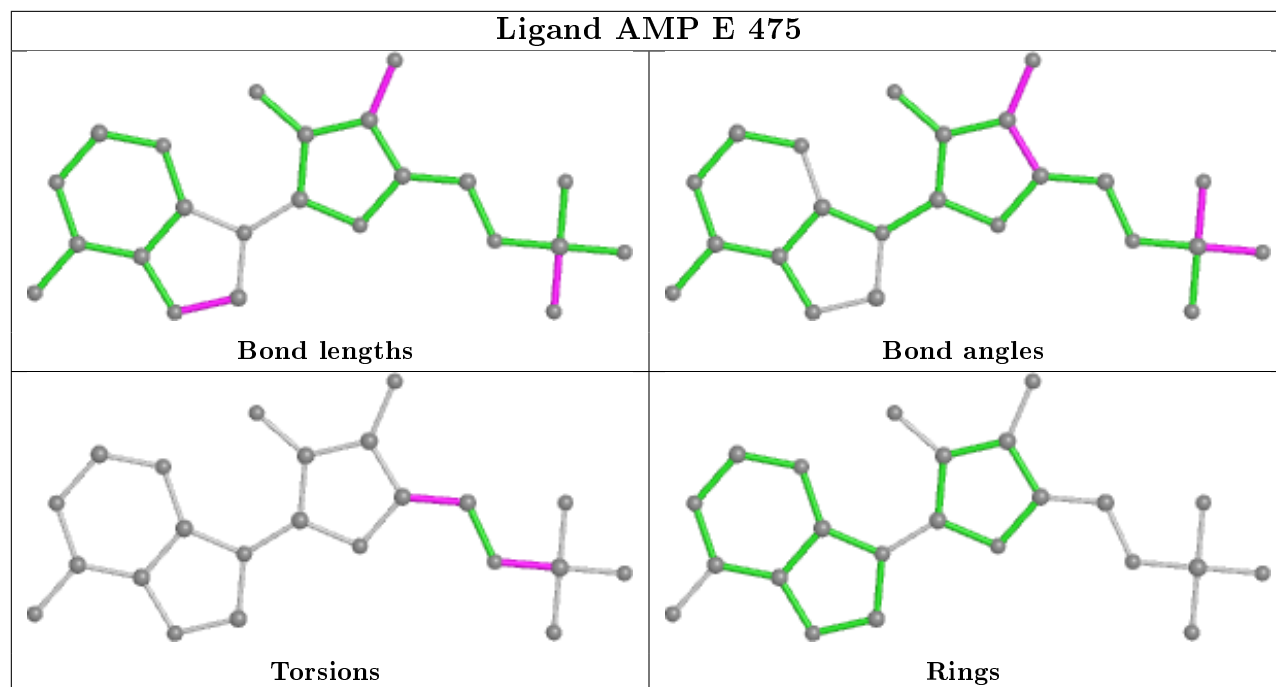
## Ligand AMP A 471



## Ligand AMP L 482







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.