



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:57 AM UTC

PDB ID : 1LGR / pdb_00001lgr
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

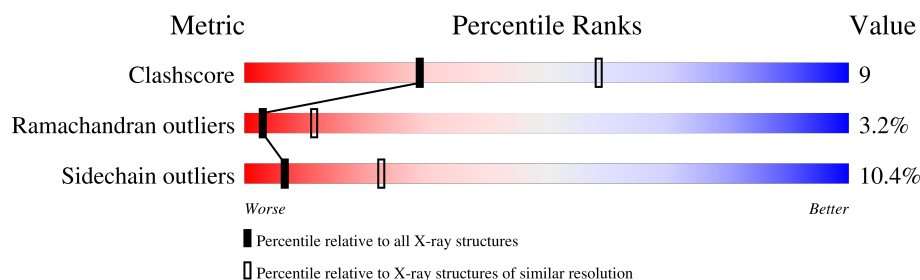
1 Overall quality at a glance

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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	468	56% 30% 8% • 5%
1	B	468	55% 29% 9% • 5%
1	C	468	55% 30% 9% • 5%
1	D	468	56% 29% 9% • 5%
1	E	468	56% 30% 8% • 5%
1	F	468	56% 29% 8% • 5%
1	G	468	56% 29% 8% • 5%
1	H	468	56% 29% 9% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	468	55%30%8%• 5%
1	J	468	56%29%8%• 5%
1	K	468	55%29%9%• 5%
1	L	468	56%29%9%• 5%

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 (CCD ID: MN) (formula: Mn).

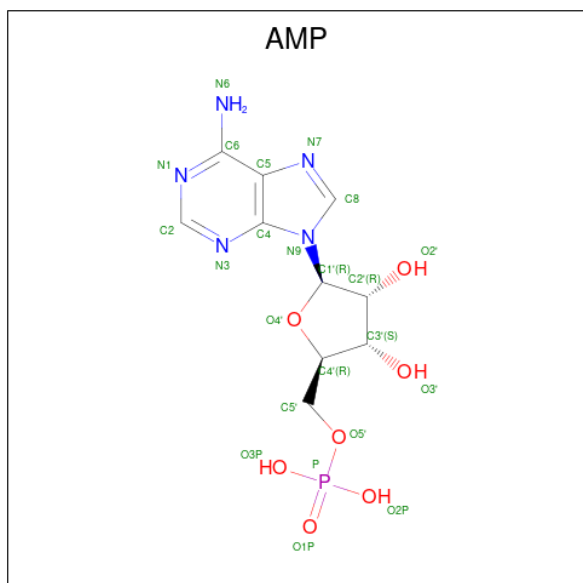
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

Continued on next page...

Continued from previous page...

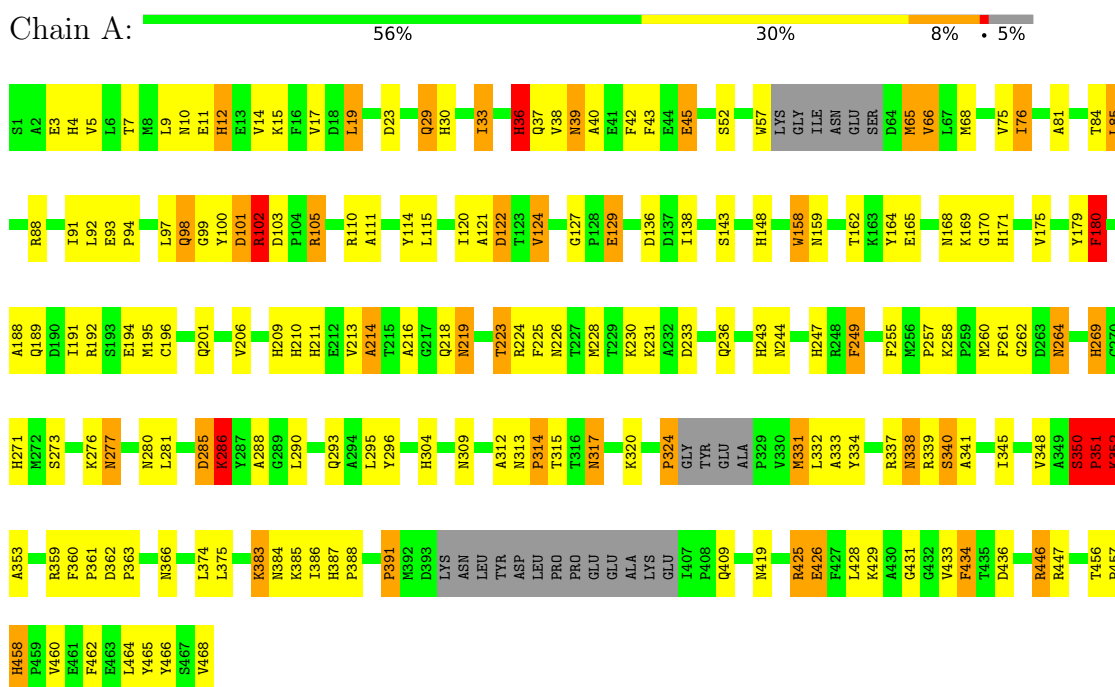
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	H	1	Total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

3 Residue-property plots

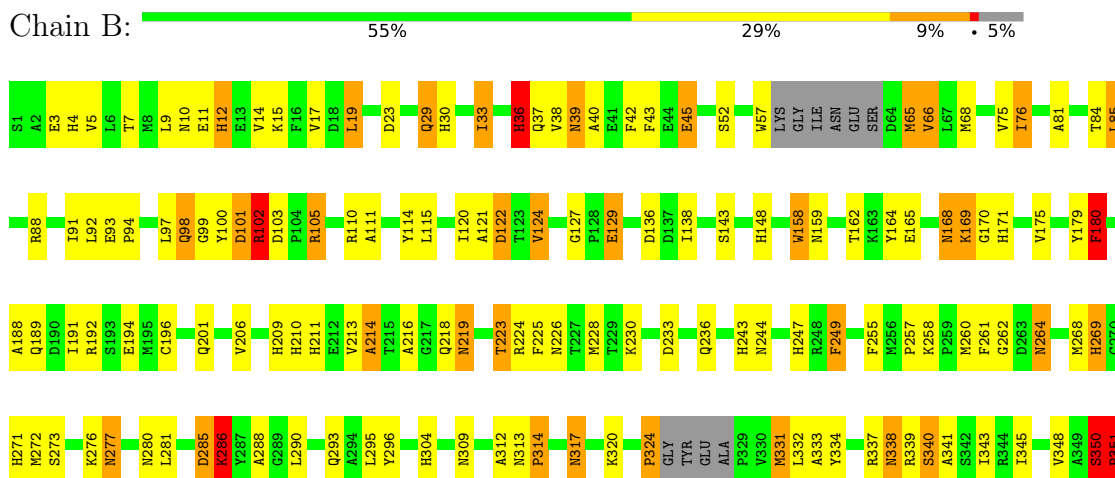
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

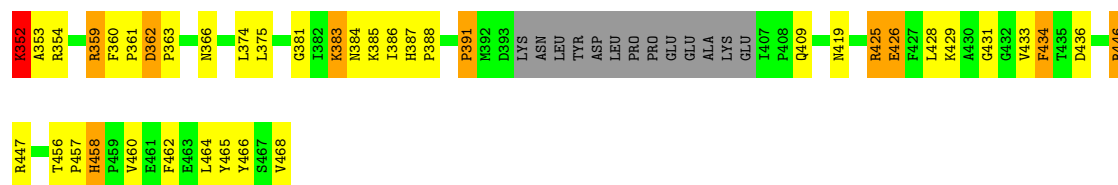
Note EDS was not executed.

• Molecule 1: GLUTAMINE SYNTHETASE

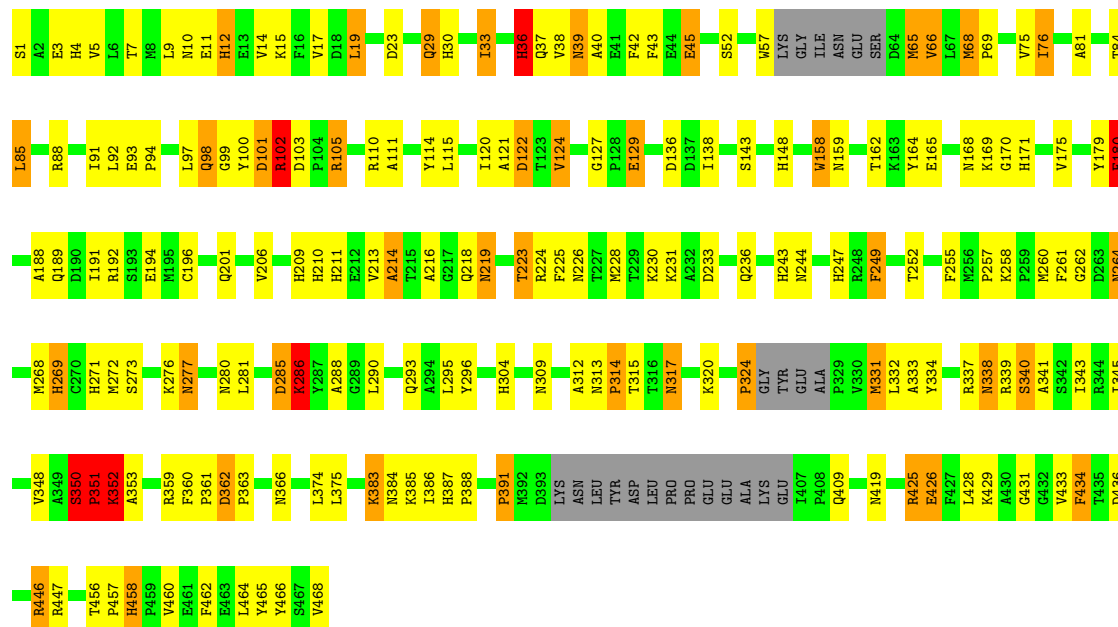


• Molecule 1: GLUTAMINE SYNTHETASE

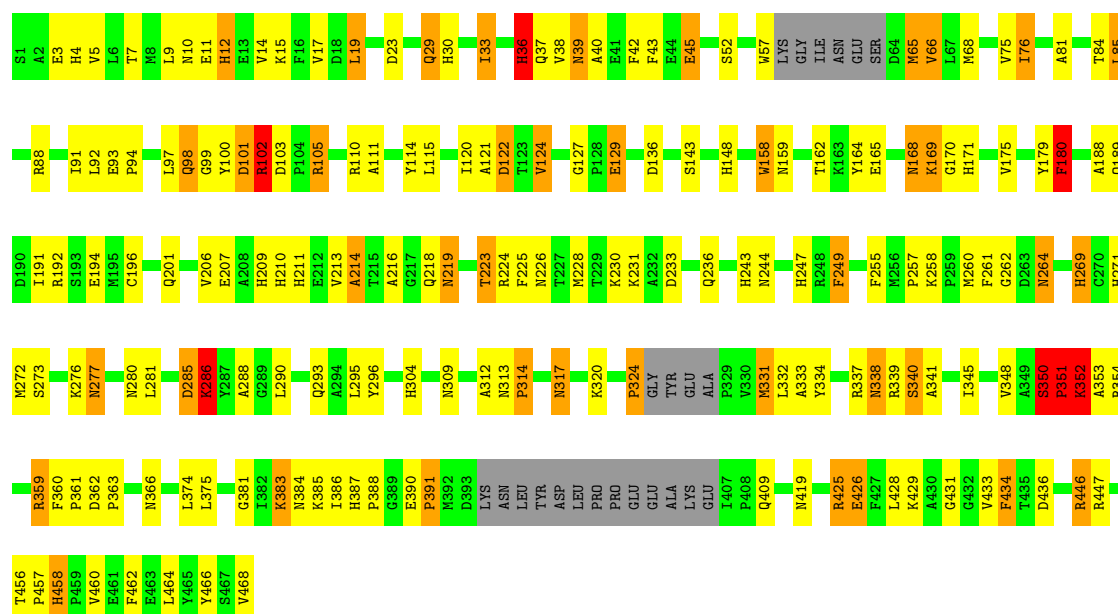




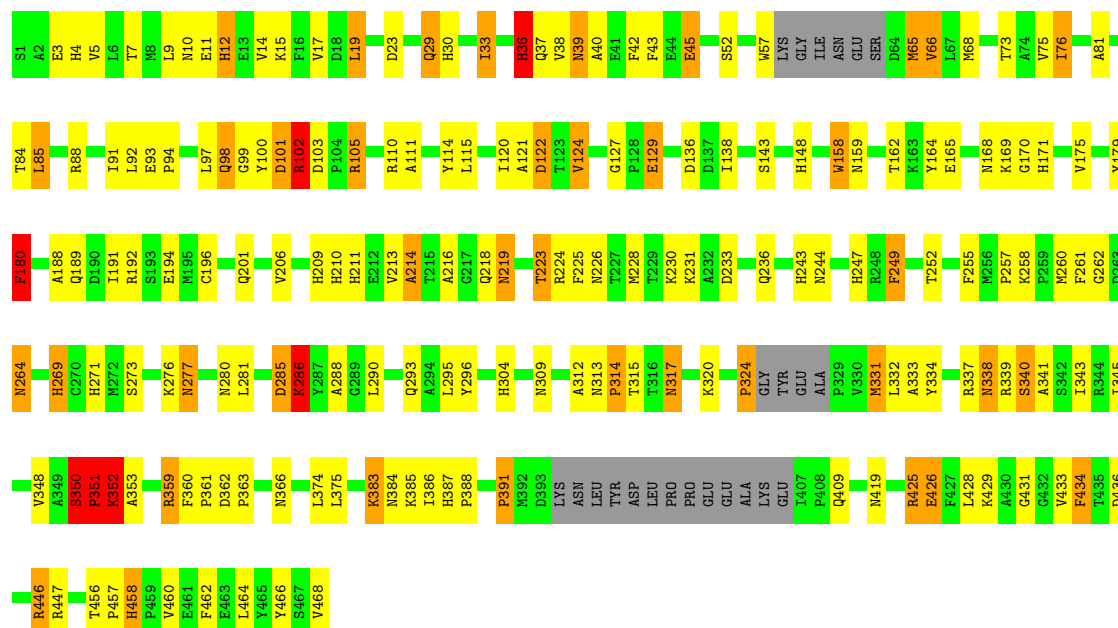
Molecule 1: GLUTAMINE SYNTHETASE



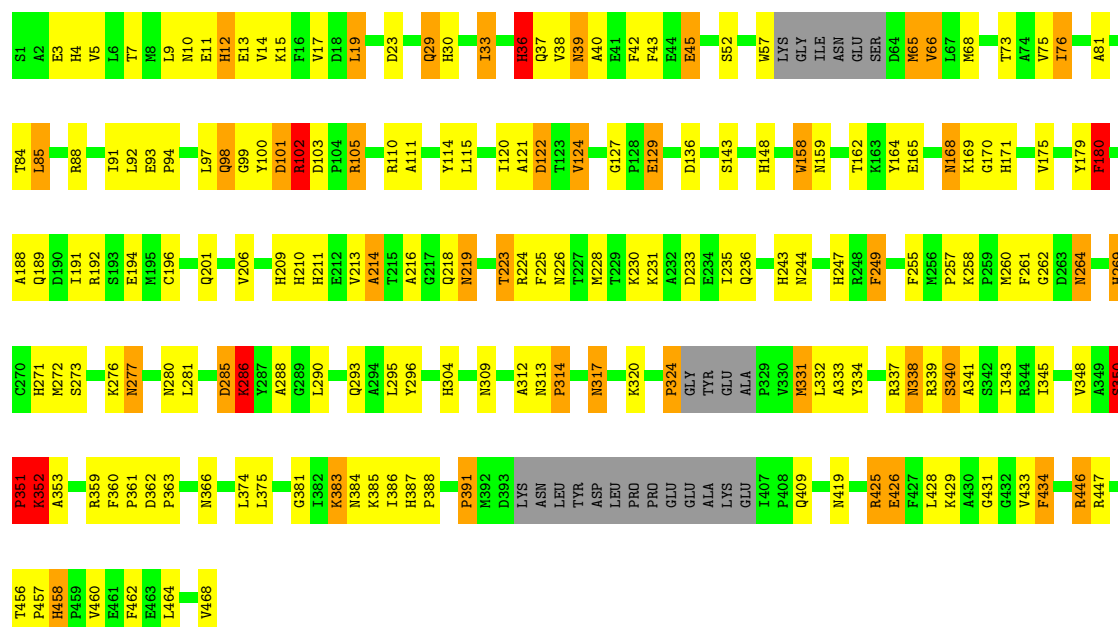
Molecule 1: GLUTAMINE SYNTHETASE



• Molecule 1: GLUTAMINE SYNTHETASE

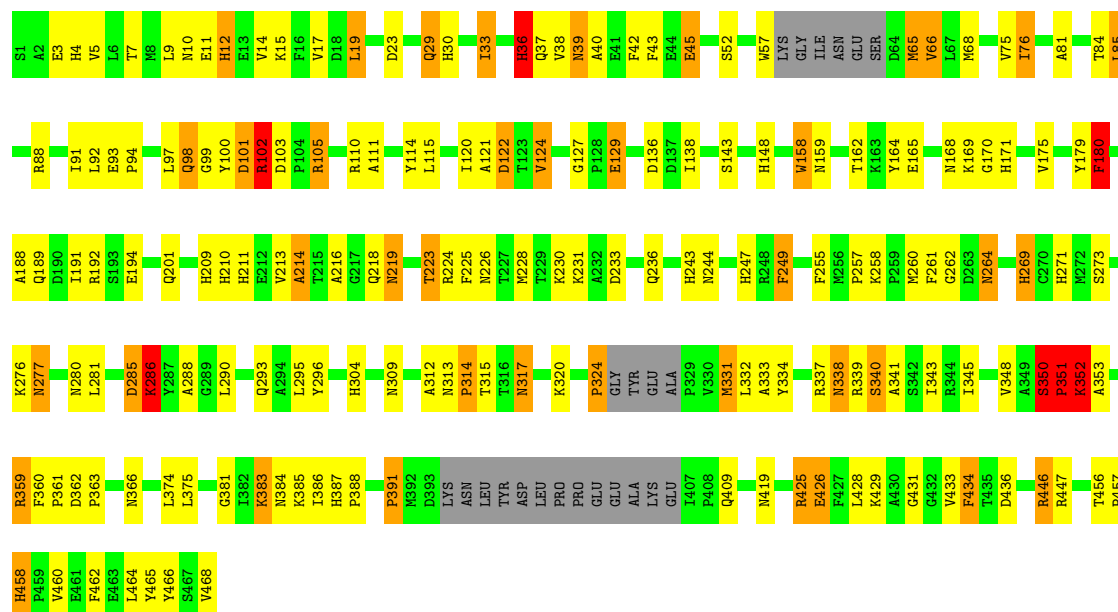
Chain E: 

• Molecule 1: GLUTAMINE SYNTHETASE

Chain F: 

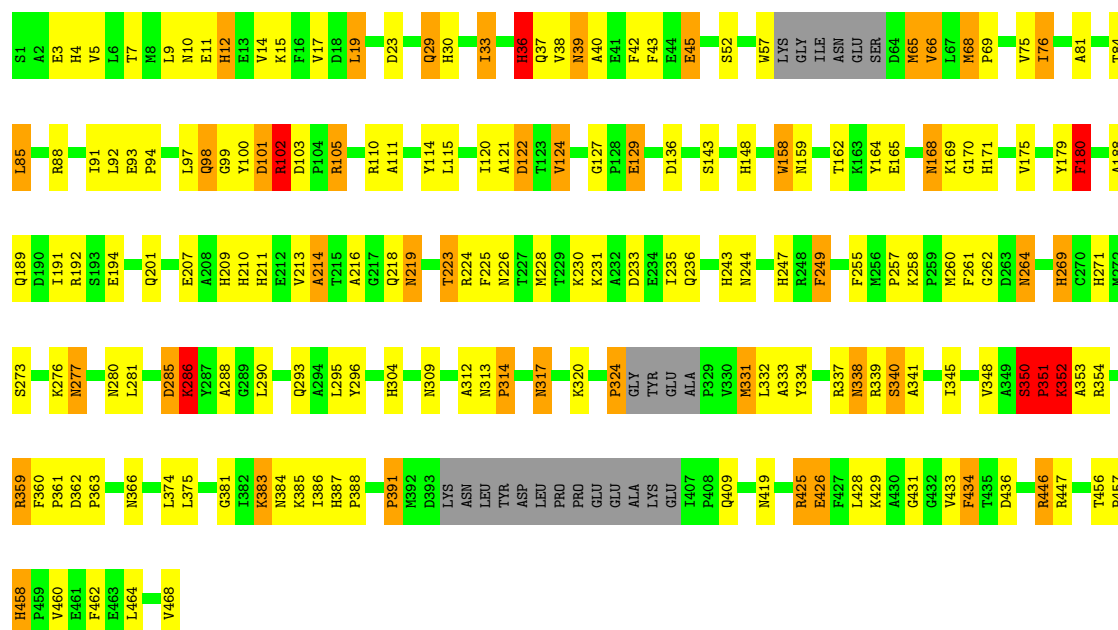
• Molecule 1: GLUTAMINE SYNTHETASE

Chain G: 



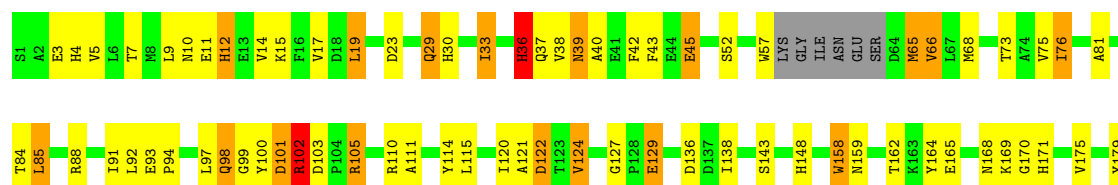
• Molecule 1: GLUTAMINE SYNTHETASE

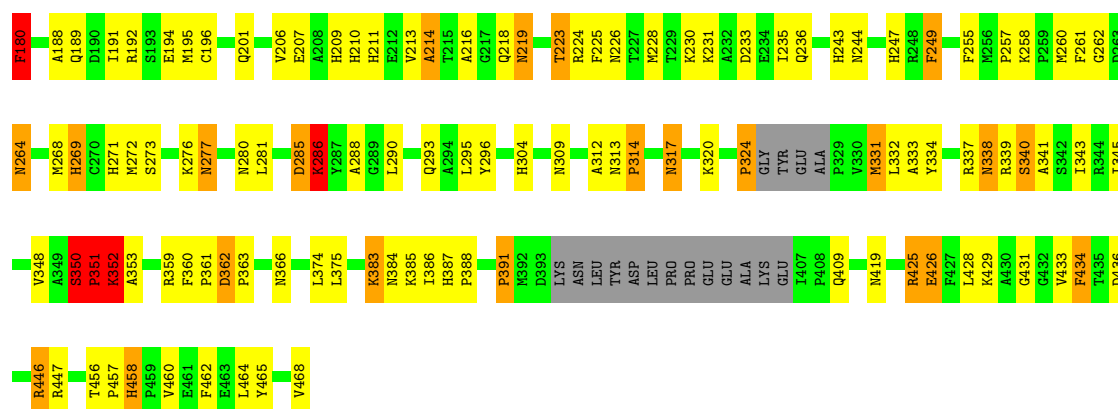
Chain H: 56% 29% 9% 5%



• Molecule 1: GLUTAMINE SYNTHETASE

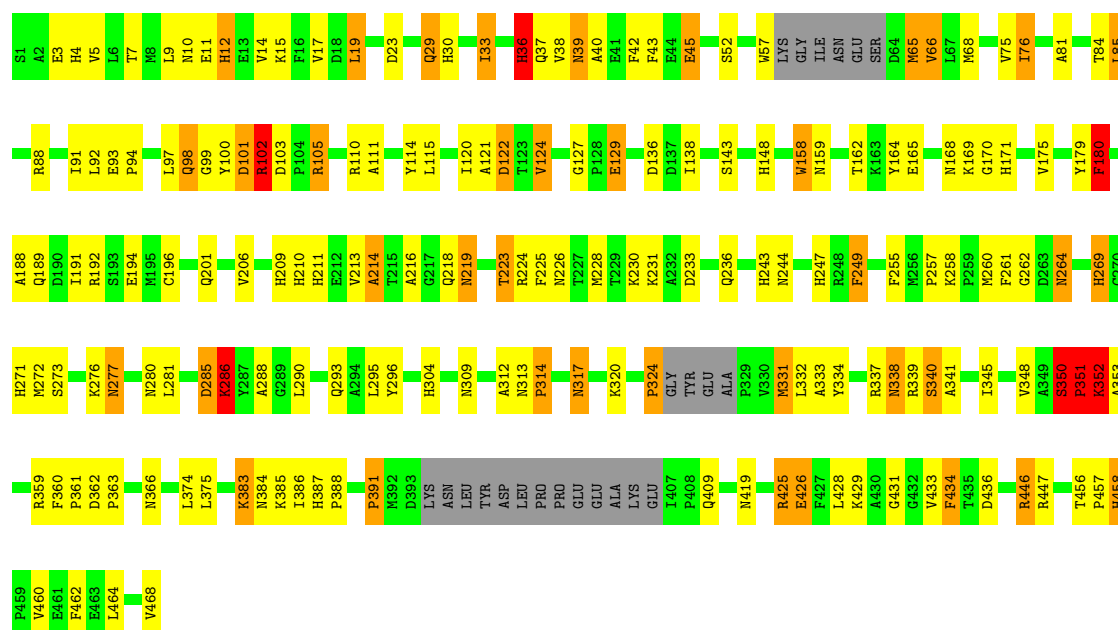
Chain I: 55% 30% 8% 5%





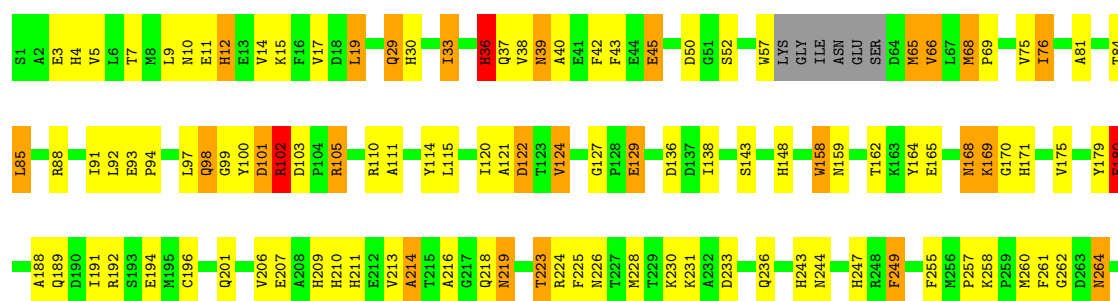
• Molecule 1: GLUTAMINE SYNTHETASE

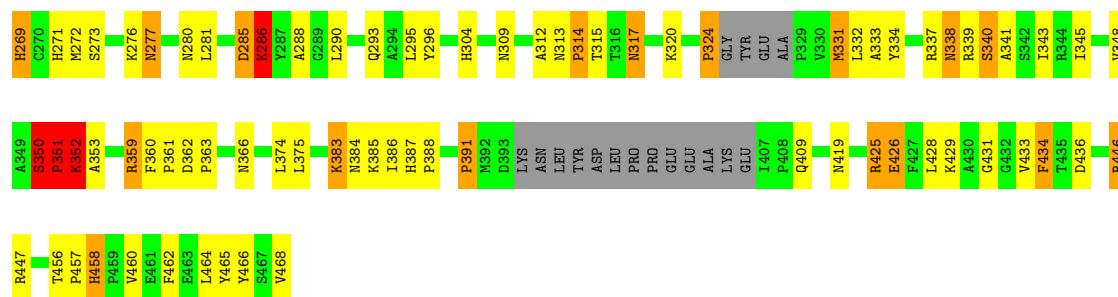
Chain J: 56% 29% 8% • 5%



• Molecule 1: GLUTAMINE SYNTHETASE

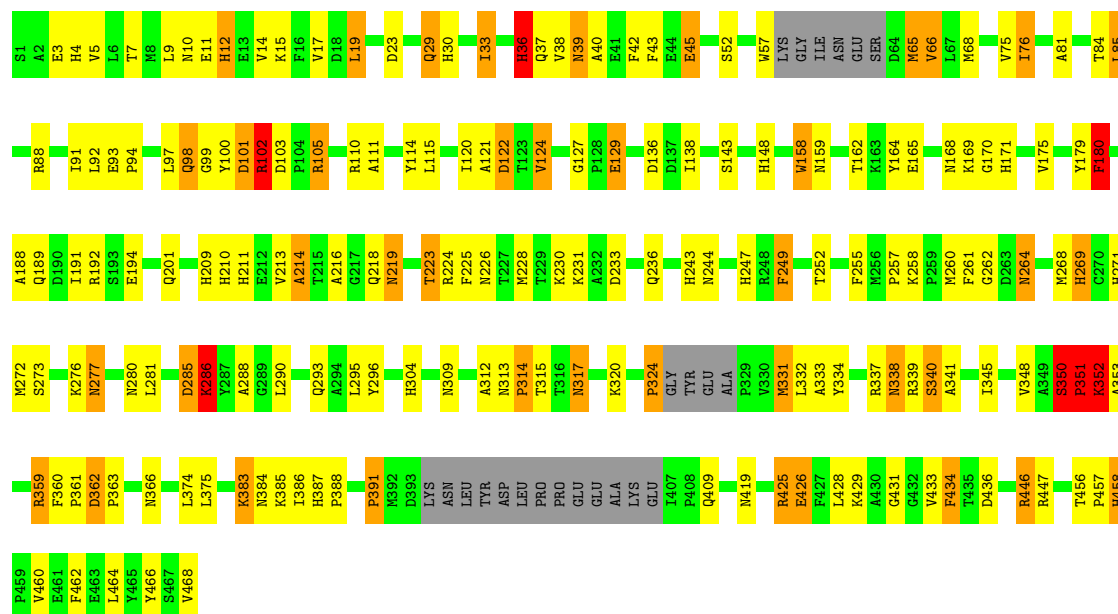
Chain K: 55% 29% 9% • 5%





• Molecule 1: GLUTAMINE SYNTHETASE

Chain L: 56% 29% 9% 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, α , β , γ	235.50Å 134.50Å 200.10Å 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 ²)	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	0.97	19/3535 (0.5%)	1.90	115/4782 (2.4%)
1	B	0.97	19/3535 (0.5%)	1.90	116/4782 (2.4%)
1	C	0.97	19/3535 (0.5%)	1.90	115/4782 (2.4%)
1	D	0.97	19/3535 (0.5%)	1.90	114/4782 (2.4%)
1	E	0.97	19/3535 (0.5%)	1.90	117/4782 (2.4%)
1	F	0.97	19/3535 (0.5%)	1.90	115/4782 (2.4%)
1	G	0.97	19/3535 (0.5%)	1.90	115/4782 (2.4%)
1	H	0.97	19/3535 (0.5%)	1.90	116/4782 (2.4%)
1	I	0.97	19/3535 (0.5%)	1.90	116/4782 (2.4%)
1	J	0.97	19/3535 (0.5%)	1.90	114/4782 (2.4%)
1	K	0.97	19/3535 (0.5%)	1.90	114/4782 (2.4%)
1	L	0.97	19/3535 (0.5%)	1.90	115/4782 (2.4%)
All	All	0.97	228/42420 (0.5%)	1.90	1382/57384 (2.4%)

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

Continued on next page...

Continued from previous page...

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

All (228) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	210	HIS	CD2-NE2	-7.46	1.29	1.37
1	F	210	HIS	CD2-NE2	-7.44	1.29	1.37
1	B	210	HIS	CD2-NE2	-7.42	1.29	1.37
1	I	210	HIS	CD2-NE2	-7.41	1.29	1.37
1	K	210	HIS	CD2-NE2	-7.41	1.29	1.37
1	A	210	HIS	CD2-NE2	-7.39	1.29	1.37
1	J	210	HIS	CD2-NE2	-7.39	1.29	1.37
1	H	210	HIS	CD2-NE2	-7.39	1.29	1.37
1	E	210	HIS	CD2-NE2	-7.38	1.29	1.37
1	D	269	HIS	CD2-NE2	-7.36	1.29	1.37
1	G	210	HIS	CD2-NE2	-7.36	1.29	1.37
1	D	210	HIS	CD2-NE2	-7.36	1.29	1.37
1	I	269	HIS	CD2-NE2	-7.35	1.29	1.37
1	B	269	HIS	CD2-NE2	-7.35	1.29	1.37
1	E	269	HIS	CD2-NE2	-7.34	1.29	1.37
1	A	269	HIS	CD2-NE2	-7.34	1.29	1.37
1	K	269	HIS	CD2-NE2	-7.34	1.29	1.37
1	L	210	HIS	CD2-NE2	-7.33	1.29	1.37
1	G	269	HIS	CD2-NE2	-7.33	1.29	1.37
1	F	269	HIS	CD2-NE2	-7.33	1.29	1.37
1	J	269	HIS	CD2-NE2	-7.33	1.29	1.37
1	H	269	HIS	CD2-NE2	-7.32	1.29	1.37
1	L	269	HIS	CD2-NE2	-7.32	1.29	1.37
1	C	269	HIS	CD2-NE2	-7.32	1.29	1.37
1	J	30	HIS	CD2-NE2	-7.28	1.29	1.37
1	K	30	HIS	CD2-NE2	-7.28	1.29	1.37
1	L	30	HIS	CD2-NE2	-7.28	1.29	1.37
1	D	30	HIS	CD2-NE2	-7.27	1.29	1.37
1	G	30	HIS	CD2-NE2	-7.25	1.29	1.37
1	I	30	HIS	CD2-NE2	-7.24	1.29	1.37
1	H	30	HIS	CD2-NE2	-7.23	1.29	1.37
1	A	30	HIS	CD2-NE2	-7.23	1.29	1.37
1	E	30	HIS	CD2-NE2	-7.23	1.29	1.37
1	B	30	HIS	CD2-NE2	-7.22	1.29	1.37
1	C	30	HIS	CD2-NE2	-7.21	1.29	1.37
1	G	211	HIS	CD2-NE2	-7.21	1.29	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	30	HIS	CD2-NE2	-7.21	1.29	1.37
1	L	211	HIS	CD2-NE2	-7.21	1.29	1.37
1	D	211	HIS	CD2-NE2	-7.18	1.29	1.37
1	H	211	HIS	CD2-NE2	-7.18	1.29	1.37
1	I	211	HIS	CD2-NE2	-7.18	1.29	1.37
1	E	211	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	211	HIS	CD2-NE2	-7.17	1.29	1.37
1	B	211	HIS	CD2-NE2	-7.16	1.29	1.37
1	F	211	HIS	CD2-NE2	-7.16	1.29	1.37
1	K	211	HIS	CD2-NE2	-7.16	1.29	1.37
1	J	211	HIS	CD2-NE2	-7.15	1.29	1.37
1	C	211	HIS	CD2-NE2	-7.12	1.30	1.37
1	F	458	HIS	CD2-NE2	-6.88	1.30	1.37
1	E	458	HIS	CD2-NE2	-6.86	1.30	1.37
1	I	458	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	458	HIS	CD2-NE2	-6.80	1.30	1.37
1	L	458	HIS	CD2-NE2	-6.80	1.30	1.37
1	H	304	HIS	CD2-NE2	-6.80	1.30	1.37
1	H	458	HIS	CD2-NE2	-6.80	1.30	1.37
1	B	458	HIS	CD2-NE2	-6.79	1.30	1.37
1	G	458	HIS	CD2-NE2	-6.79	1.30	1.37
1	C	458	HIS	CD2-NE2	-6.78	1.30	1.37
1	G	304	HIS	CD2-NE2	-6.78	1.30	1.37
1	J	458	HIS	CD2-NE2	-6.78	1.30	1.37
1	K	458	HIS	CD2-NE2	-6.77	1.30	1.37
1	F	304	HIS	CD2-NE2	-6.76	1.30	1.37
1	J	304	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	304	HIS	CD2-NE2	-6.75	1.30	1.37
1	D	458	HIS	CD2-NE2	-6.75	1.30	1.37
1	I	304	HIS	CD2-NE2	-6.74	1.30	1.37
1	C	304	HIS	CD2-NE2	-6.74	1.30	1.37
1	E	304	HIS	CD2-NE2	-6.74	1.30	1.37
1	K	304	HIS	CD2-NE2	-6.73	1.30	1.37
1	B	304	HIS	CD2-NE2	-6.73	1.30	1.37
1	D	304	HIS	CD2-NE2	-6.73	1.30	1.37
1	L	304	HIS	CD2-NE2	-6.71	1.30	1.37
1	G	36	HIS	CD2-NE2	-6.58	1.30	1.37
1	H	12	HIS	CD2-NE2	-6.58	1.30	1.37
1	C	12	HIS	CD2-NE2	-6.58	1.30	1.37
1	E	12	HIS	CD2-NE2	-6.58	1.30	1.37
1	K	12	HIS	CD2-NE2	-6.57	1.30	1.37
1	B	12	HIS	CD2-NE2	-6.56	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	12	HIS	CD2-NE2	-6.56	1.30	1.37
1	D	12	HIS	CD2-NE2	-6.56	1.30	1.37
1	F	36	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	36	HIS	CD2-NE2	-6.56	1.30	1.37
1	H	36	HIS	CD2-NE2	-6.56	1.30	1.37
1	I	36	HIS	CD2-NE2	-6.56	1.30	1.37
1	F	12	HIS	CD2-NE2	-6.55	1.30	1.37
1	A	12	HIS	CD2-NE2	-6.55	1.30	1.37
1	D	36	HIS	CD2-NE2	-6.54	1.30	1.37
1	C	36	HIS	CD2-NE2	-6.53	1.30	1.37
1	G	12	HIS	CD2-NE2	-6.52	1.30	1.37
1	L	36	HIS	CD2-NE2	-6.52	1.30	1.37
1	J	12	HIS	CD2-NE2	-6.52	1.30	1.37
1	J	36	HIS	CD2-NE2	-6.52	1.30	1.37
1	B	36	HIS	CD2-NE2	-6.51	1.30	1.37
1	E	36	HIS	CD2-NE2	-6.51	1.30	1.37
1	L	12	HIS	CD2-NE2	-6.48	1.30	1.37
1	K	36	HIS	CD2-NE2	-6.46	1.30	1.37
1	I	4	HIS	CD2-NE2	-6.44	1.30	1.37
1	D	4	HIS	CD2-NE2	-6.42	1.30	1.37
1	K	4	HIS	CD2-NE2	-6.42	1.30	1.37
1	H	148	HIS	CD2-NE2	-6.41	1.30	1.37
1	L	271	HIS	CD2-NE2	-6.41	1.30	1.37
1	J	4	HIS	CD2-NE2	-6.41	1.30	1.37
1	G	148	HIS	CD2-NE2	-6.40	1.30	1.37
1	J	148	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	148	HIS	CD2-NE2	-6.38	1.30	1.37
1	F	148	HIS	CD2-NE2	-6.38	1.30	1.37
1	C	4	HIS	CD2-NE2	-6.38	1.30	1.37
1	G	271	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	4	HIS	CD2-NE2	-6.37	1.30	1.37
1	C	148	HIS	CD2-NE2	-6.37	1.30	1.37
1	L	4	HIS	CD2-NE2	-6.37	1.30	1.37
1	F	271	HIS	CD2-NE2	-6.36	1.30	1.37
1	H	271	HIS	CD2-NE2	-6.36	1.30	1.37
1	H	4	HIS	CD2-NE2	-6.36	1.30	1.37
1	B	148	HIS	CD2-NE2	-6.36	1.30	1.37
1	L	148	HIS	CD2-NE2	-6.35	1.30	1.37
1	B	4	HIS	CD2-NE2	-6.35	1.30	1.37
1	K	148	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	271	HIS	CD2-NE2	-6.35	1.30	1.37
1	G	4	HIS	CD2-NE2	-6.35	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	271	HIS	CD2-NE2	-6.35	1.30	1.37
1	C	271	HIS	CD2-NE2	-6.34	1.30	1.37
1	I	148	HIS	CD2-NE2	-6.34	1.30	1.37
1	B	271	HIS	CD2-NE2	-6.33	1.30	1.37
1	E	4	HIS	CD2-NE2	-6.32	1.30	1.37
1	F	4	HIS	CD2-NE2	-6.32	1.30	1.37
1	D	148	HIS	CD2-NE2	-6.31	1.30	1.37
1	J	209	HIS	CD2-NE2	-6.30	1.30	1.37
1	I	271	HIS	CD2-NE2	-6.30	1.30	1.37
1	E	148	HIS	CD2-NE2	-6.29	1.30	1.37
1	J	271	HIS	CD2-NE2	-6.28	1.30	1.37
1	D	271	HIS	CD2-NE2	-6.28	1.30	1.37
1	D	209	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	209	HIS	CD2-NE2	-6.27	1.30	1.37
1	K	271	HIS	CD2-NE2	-6.26	1.30	1.37
1	C	209	HIS	CD2-NE2	-6.26	1.30	1.37
1	G	387	HIS	CD2-NE2	-6.25	1.30	1.37
1	I	209	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	209	HIS	CD2-NE2	-6.25	1.30	1.37
1	E	209	HIS	CD2-NE2	-6.25	1.30	1.37
1	E	387	HIS	CD2-NE2	-6.24	1.30	1.37
1	K	387	HIS	CD2-NE2	-6.24	1.30	1.37
1	F	209	HIS	CD2-NE2	-6.24	1.30	1.37
1	H	209	HIS	CD2-NE2	-6.23	1.30	1.37
1	D	387	HIS	CD2-NE2	-6.22	1.31	1.37
1	F	387	HIS	CD2-NE2	-6.21	1.31	1.37
1	L	209	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	387	HIS	CD2-NE2	-6.20	1.31	1.37
1	B	387	HIS	CD2-NE2	-6.20	1.31	1.37
1	J	387	HIS	CD2-NE2	-6.18	1.31	1.37
1	G	209	HIS	CD2-NE2	-6.18	1.31	1.37
1	I	387	HIS	CD2-NE2	-6.18	1.31	1.37
1	C	387	HIS	CD2-NE2	-6.17	1.31	1.37
1	K	209	HIS	CD2-NE2	-6.17	1.31	1.37
1	L	387	HIS	CD2-NE2	-6.17	1.31	1.37
1	H	387	HIS	CD2-NE2	-6.15	1.31	1.37
1	I	243	HIS	CD2-NE2	-6.05	1.31	1.37
1	L	243	HIS	CD2-NE2	-6.05	1.31	1.37
1	D	243	HIS	CD2-NE2	-6.04	1.31	1.37
1	J	243	HIS	CD2-NE2	-6.04	1.31	1.37
1	H	243	HIS	CD2-NE2	-6.00	1.31	1.37
1	K	243	HIS	CD2-NE2	-6.00	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	HIS	CD2-NE2	-5.98	1.31	1.37
1	E	247	HIS	CD2-NE2	-5.98	1.31	1.37
1	F	243	HIS	CD2-NE2	-5.97	1.31	1.37
1	C	243	HIS	CD2-NE2	-5.97	1.31	1.37
1	B	243	HIS	CD2-NE2	-5.96	1.31	1.37
1	G	243	HIS	CD2-NE2	-5.96	1.31	1.37
1	G	247	HIS	CD2-NE2	-5.94	1.31	1.37
1	I	247	HIS	CD2-NE2	-5.93	1.31	1.37
1	K	247	HIS	CD2-NE2	-5.92	1.31	1.37
1	C	247	HIS	CD2-NE2	-5.91	1.31	1.37
1	E	243	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	247	HIS	CD2-NE2	-5.90	1.31	1.37
1	H	247	HIS	CD2-NE2	-5.90	1.31	1.37
1	J	247	HIS	CD2-NE2	-5.87	1.31	1.37
1	B	247	HIS	CD2-NE2	-5.85	1.31	1.37
1	F	247	HIS	CD2-NE2	-5.85	1.31	1.37
1	L	247	HIS	CD2-NE2	-5.85	1.31	1.37
1	D	247	HIS	CD2-NE2	-5.84	1.31	1.37
1	B	271	HIS	CG-ND1	-5.53	1.32	1.38
1	F	271	HIS	CG-ND1	-5.51	1.32	1.38
1	E	271	HIS	CG-ND1	-5.50	1.32	1.38
1	D	271	HIS	CG-ND1	-5.49	1.32	1.38
1	L	271	HIS	CG-ND1	-5.49	1.32	1.38
1	C	271	HIS	CG-ND1	-5.49	1.32	1.38
1	K	271	HIS	CG-ND1	-5.49	1.32	1.38
1	A	271	HIS	CG-ND1	-5.48	1.32	1.38
1	I	271	HIS	CG-ND1	-5.47	1.32	1.38
1	G	271	HIS	CG-ND1	-5.46	1.32	1.38
1	J	271	HIS	CG-ND1	-5.45	1.32	1.38
1	H	271	HIS	CG-ND1	-5.44	1.32	1.38
1	G	171	HIS	CD2-NE2	-5.39	1.31	1.37
1	H	271	HIS	CA-CB	-5.38	1.45	1.53
1	K	171	HIS	CD2-NE2	-5.38	1.31	1.37
1	E	171	HIS	CD2-NE2	-5.37	1.31	1.37
1	C	171	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	171	HIS	CD2-NE2	-5.35	1.31	1.37
1	H	171	HIS	CD2-NE2	-5.35	1.31	1.37
1	B	171	HIS	CD2-NE2	-5.34	1.31	1.37
1	E	271	HIS	CA-CB	-5.34	1.45	1.53
1	I	171	HIS	CD2-NE2	-5.34	1.31	1.37
1	D	171	HIS	CD2-NE2	-5.34	1.31	1.37
1	D	271	HIS	CA-CB	-5.33	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	271	HIS	CA-CB	-5.33	1.45	1.53
1	A	271	HIS	CA-CB	-5.33	1.45	1.53
1	G	271	HIS	CA-CB	-5.33	1.45	1.53
1	J	171	HIS	CD2-NE2	-5.32	1.32	1.37
1	L	271	HIS	CA-CB	-5.32	1.45	1.53
1	L	171	HIS	CD2-NE2	-5.32	1.32	1.37
1	B	271	HIS	CA-CB	-5.31	1.45	1.53
1	G	210	HIS	CG-ND1	-5.31	1.32	1.38
1	I	271	HIS	CA-CB	-5.31	1.45	1.53
1	F	171	HIS	CD2-NE2	-5.31	1.32	1.37
1	F	271	HIS	CA-CB	-5.30	1.45	1.53
1	J	271	HIS	CA-CB	-5.30	1.45	1.53
1	I	210	HIS	CG-ND1	-5.30	1.32	1.38
1	C	271	HIS	CA-CB	-5.30	1.45	1.53
1	J	210	HIS	CG-ND1	-5.29	1.32	1.38
1	K	210	HIS	CG-ND1	-5.27	1.32	1.38
1	C	210	HIS	CG-ND1	-5.26	1.32	1.38
1	A	210	HIS	CG-ND1	-5.26	1.32	1.38
1	B	210	HIS	CG-ND1	-5.25	1.32	1.38
1	D	210	HIS	CG-ND1	-5.25	1.32	1.38
1	F	210	HIS	CG-ND1	-5.25	1.32	1.38
1	L	210	HIS	CG-ND1	-5.23	1.32	1.38
1	H	210	HIS	CG-ND1	-5.20	1.32	1.38
1	E	210	HIS	CG-ND1	-5.18	1.32	1.38

All (1382) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	ASN	OD1-CG-ND2	-11.59	111.01	122.60
1	B	39	ASN	OD1-CG-ND2	-11.58	111.02	122.60
1	G	39	ASN	OD1-CG-ND2	-11.55	111.05	122.60
1	L	39	ASN	OD1-CG-ND2	-11.54	111.06	122.60
1	J	39	ASN	OD1-CG-ND2	-11.54	111.06	122.60
1	A	39	ASN	OD1-CG-ND2	-11.53	111.07	122.60
1	K	39	ASN	OD1-CG-ND2	-11.53	111.07	122.60
1	F	39	ASN	OD1-CG-ND2	-11.52	111.08	122.60
1	E	39	ASN	OD1-CG-ND2	-11.50	111.10	122.60
1	H	39	ASN	OD1-CG-ND2	-11.50	111.10	122.60
1	I	39	ASN	OD1-CG-ND2	-11.50	111.10	122.60
1	C	39	ASN	OD1-CG-ND2	-11.49	111.11	122.60
1	E	189	GLN	OE1-CD-NE2	-10.54	112.06	122.60
1	C	189	GLN	OE1-CD-NE2	-10.53	112.07	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	189	GLN	OE1-CD-NE2	-10.53	112.07	122.60
1	L	189	GLN	OE1-CD-NE2	-10.53	112.07	122.60
1	F	189	GLN	OE1-CD-NE2	-10.53	112.07	122.60
1	D	189	GLN	OE1-CD-NE2	-10.52	112.08	122.60
1	J	189	GLN	OE1-CD-NE2	-10.52	112.08	122.60
1	A	189	GLN	OE1-CD-NE2	-10.51	112.09	122.60
1	B	189	GLN	OE1-CD-NE2	-10.51	112.09	122.60
1	I	189	GLN	OE1-CD-NE2	-10.50	112.10	122.60
1	H	189	GLN	OE1-CD-NE2	-10.49	112.11	122.60
1	K	189	GLN	OE1-CD-NE2	-10.49	112.11	122.60
1	L	98	GLN	OE1-CD-NE2	-9.61	112.99	122.60
1	I	98	GLN	OE1-CD-NE2	-9.60	113.00	122.60
1	F	98	GLN	OE1-CD-NE2	-9.59	113.01	122.60
1	J	98	GLN	OE1-CD-NE2	-9.58	113.02	122.60
1	A	98	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	G	98	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	D	98	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	E	98	GLN	OE1-CD-NE2	-9.56	113.04	122.60
1	K	98	GLN	OE1-CD-NE2	-9.55	113.05	122.60
1	B	98	GLN	OE1-CD-NE2	-9.53	113.07	122.60
1	C	98	GLN	OE1-CD-NE2	-9.53	113.08	122.60
1	H	98	GLN	OE1-CD-NE2	-9.51	113.09	122.60
1	K	159	ASN	OD1-CG-ND2	-9.47	113.13	122.60
1	G	159	ASN	OD1-CG-ND2	-9.44	113.16	122.60
1	E	159	ASN	OD1-CG-ND2	-9.44	113.16	122.60
1	B	159	ASN	OD1-CG-ND2	-9.43	113.17	122.60
1	C	159	ASN	OD1-CG-ND2	-9.43	113.17	122.60
1	J	159	ASN	OD1-CG-ND2	-9.43	113.17	122.60
1	A	159	ASN	OD1-CG-ND2	-9.42	113.18	122.60
1	F	159	ASN	OD1-CG-ND2	-9.42	113.18	122.60
1	H	159	ASN	OD1-CG-ND2	-9.41	113.19	122.60
1	I	159	ASN	OD1-CG-ND2	-9.41	113.19	122.60
1	D	159	ASN	OD1-CG-ND2	-9.40	113.20	122.60
1	L	159	ASN	OD1-CG-ND2	-9.40	113.20	122.60
1	F	426	GLU	N-CA-C	9.11	120.82	111.07
1	L	426	GLU	N-CA-C	9.11	120.81	111.07
1	E	426	GLU	N-CA-C	9.07	120.78	111.07
1	I	426	GLU	N-CA-C	9.07	120.77	111.07
1	A	426	GLU	N-CA-C	9.06	120.77	111.07
1	B	426	GLU	N-CA-C	9.06	120.77	111.07
1	J	426	GLU	N-CA-C	9.05	120.75	111.07
1	C	426	GLU	N-CA-C	9.04	120.75	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	426	GLU	N-CA-C	9.04	120.75	111.07
1	D	426	GLU	N-CA-C	9.04	120.74	111.07
1	K	426	GLU	N-CA-C	9.04	120.74	111.07
1	G	426	GLU	N-CA-C	9.01	120.72	111.07
1	D	180	PHE	N-CA-C	8.92	129.53	109.81
1	C	180	PHE	N-CA-C	8.92	129.53	109.81
1	K	180	PHE	N-CA-C	8.92	129.53	109.81
1	G	180	PHE	N-CA-C	8.92	129.52	109.81
1	L	180	PHE	N-CA-C	8.92	129.52	109.81
1	A	180	PHE	N-CA-C	8.91	129.50	109.81
1	B	180	PHE	N-CA-C	8.91	129.50	109.81
1	I	180	PHE	N-CA-C	8.91	129.50	109.81
1	J	180	PHE	N-CA-C	8.91	129.50	109.81
1	E	180	PHE	N-CA-C	8.90	129.48	109.81
1	H	180	PHE	N-CA-C	8.90	129.48	109.81
1	F	180	PHE	N-CA-C	8.90	129.47	109.81
1	K	236	GLN	OE1-CD-NE2	-8.68	113.92	122.60
1	H	236	GLN	OE1-CD-NE2	-8.66	113.94	122.60
1	J	236	GLN	OE1-CD-NE2	-8.62	113.97	122.60
1	L	236	GLN	OE1-CD-NE2	-8.62	113.98	122.60
1	F	236	GLN	OE1-CD-NE2	-8.62	113.98	122.60
1	A	236	GLN	OE1-CD-NE2	-8.62	113.98	122.60
1	B	236	GLN	OE1-CD-NE2	-8.62	113.98	122.60
1	E	236	GLN	OE1-CD-NE2	-8.61	113.99	122.60
1	I	236	GLN	OE1-CD-NE2	-8.61	113.99	122.60
1	D	236	GLN	OE1-CD-NE2	-8.61	113.99	122.60
1	C	236	GLN	OE1-CD-NE2	-8.57	114.03	122.60
1	G	236	GLN	OE1-CD-NE2	-8.54	114.06	122.60
1	F	97	LEU	N-CA-C	8.52	123.12	111.54
1	K	124	VAL	CB-CA-C	-8.50	99.28	110.84
1	B	97	LEU	N-CA-C	8.49	123.09	111.54
1	F	124	VAL	CB-CA-C	-8.49	99.29	110.84
1	C	97	LEU	N-CA-C	8.49	123.08	111.54
1	I	97	LEU	N-CA-C	8.49	123.08	111.54
1	A	97	LEU	N-CA-C	8.48	123.07	111.54
1	L	97	LEU	N-CA-C	8.48	123.07	111.54
1	J	97	LEU	N-CA-C	8.47	123.06	111.54
1	L	124	VAL	CB-CA-C	-8.47	99.32	110.84
1	B	124	VAL	CB-CA-C	-8.47	99.32	110.84
1	E	97	LEU	N-CA-C	8.47	123.06	111.54
1	H	97	LEU	N-CA-C	8.47	123.06	111.54
1	I	124	VAL	CB-CA-C	-8.47	99.32	110.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	124	VAL	CB-CA-C	-8.47	99.33	110.84
1	A	124	VAL	CB-CA-C	-8.47	99.33	110.84
1	H	124	VAL	CB-CA-C	-8.47	99.33	110.84
1	D	97	LEU	N-CA-C	8.46	123.05	111.54
1	C	124	VAL	CB-CA-C	-8.46	99.34	110.84
1	K	97	LEU	N-CA-C	8.46	123.04	111.54
1	G	124	VAL	CB-CA-C	-8.46	99.34	110.84
1	D	124	VAL	CB-CA-C	-8.45	99.35	110.84
1	E	124	VAL	CB-CA-C	-8.44	99.36	110.84
1	G	97	LEU	N-CA-C	8.44	123.01	111.54
1	B	309	ASN	OD1-CG-ND2	-8.40	114.20	122.60
1	C	309	ASN	OD1-CG-ND2	-8.36	114.24	122.60
1	J	309	ASN	OD1-CG-ND2	-8.36	114.24	122.60
1	L	309	ASN	OD1-CG-ND2	-8.36	114.24	122.60
1	F	309	ASN	OD1-CG-ND2	-8.34	114.26	122.60
1	A	309	ASN	OD1-CG-ND2	-8.34	114.26	122.60
1	H	309	ASN	OD1-CG-ND2	-8.34	114.26	122.60
1	I	309	ASN	OD1-CG-ND2	-8.33	114.27	122.60
1	D	309	ASN	OD1-CG-ND2	-8.32	114.28	122.60
1	E	309	ASN	OD1-CG-ND2	-8.31	114.29	122.60
1	K	309	ASN	OD1-CG-ND2	-8.30	114.30	122.60
1	G	309	ASN	OD1-CG-ND2	-8.29	114.31	122.60
1	B	188	ALA	N-CA-C	8.23	122.10	112.72
1	K	188	ALA	N-CA-C	8.23	122.10	112.72
1	I	188	ALA	N-CA-C	8.22	122.09	112.72
1	E	188	ALA	N-CA-C	8.21	122.08	112.72
1	G	188	ALA	N-CA-C	8.20	122.07	112.72
1	A	188	ALA	N-CA-C	8.20	122.07	112.72
1	J	188	ALA	N-CA-C	8.19	122.06	112.72
1	C	188	ALA	N-CA-C	8.19	122.05	112.72
1	L	188	ALA	N-CA-C	8.19	122.05	112.72
1	H	188	ALA	N-CA-C	8.18	122.05	112.72
1	D	188	ALA	N-CA-C	8.18	122.05	112.72
1	F	188	ALA	N-CA-C	8.17	122.04	112.72
1	F	277	ASN	OD1-CG-ND2	-7.92	114.68	122.60
1	K	277	ASN	OD1-CG-ND2	-7.91	114.69	122.60
1	E	277	ASN	OD1-CG-ND2	-7.91	114.69	122.60
1	J	277	ASN	OD1-CG-ND2	-7.89	114.71	122.60
1	B	277	ASN	OD1-CG-ND2	-7.89	114.71	122.60
1	H	277	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	G	277	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	L	277	ASN	OD1-CG-ND2	-7.88	114.72	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	ASN	OD1-CG-ND2	-7.88	114.72	122.60
1	I	277	ASN	OD1-CG-ND2	-7.87	114.73	122.60
1	A	277	ASN	OD1-CG-ND2	-7.86	114.74	122.60
1	C	277	ASN	OD1-CG-ND2	-7.84	114.76	122.60
1	I	409	GLN	OE1-CD-NE2	-7.82	114.78	122.60
1	D	409	GLN	OE1-CD-NE2	-7.81	114.79	122.60
1	C	409	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	D	39	ASN	CB-CG-ND2	7.79	128.09	116.40
1	K	409	GLN	OE1-CD-NE2	-7.79	114.81	122.60
1	F	39	ASN	CB-CG-ND2	7.79	128.08	116.40
1	H	409	GLN	OE1-CD-NE2	-7.78	114.82	122.60
1	A	409	GLN	OE1-CD-NE2	-7.78	114.82	122.60
1	B	39	ASN	CB-CG-ND2	7.78	128.07	116.40
1	E	39	ASN	CB-CG-ND2	7.77	128.06	116.40
1	L	39	ASN	CB-CG-ND2	7.77	128.06	116.40
1	A	39	ASN	CB-CG-ND2	7.77	128.05	116.40
1	J	39	ASN	CB-CG-ND2	7.77	128.05	116.40
1	H	39	ASN	CB-CG-ND2	7.76	128.04	116.40
1	E	409	GLN	OE1-CD-NE2	-7.76	114.84	122.60
1	G	409	GLN	OE1-CD-NE2	-7.76	114.84	122.60
1	L	409	GLN	OE1-CD-NE2	-7.76	114.84	122.60
1	B	409	GLN	OE1-CD-NE2	-7.76	114.84	122.60
1	C	39	ASN	CB-CG-ND2	7.76	128.04	116.40
1	G	39	ASN	CB-CG-ND2	7.76	128.03	116.40
1	K	39	ASN	CB-CG-ND2	7.75	128.03	116.40
1	I	39	ASN	CB-CG-ND2	7.75	128.02	116.40
1	J	409	GLN	OE1-CD-NE2	-7.74	114.86	122.60
1	F	409	GLN	OE1-CD-NE2	-7.71	114.89	122.60
1	J	179	TYR	CA-C-O	7.61	129.20	120.98
1	D	179	TYR	CA-C-O	7.59	129.18	120.98
1	F	179	TYR	CA-C-O	7.58	129.16	120.98
1	I	179	TYR	CA-C-O	7.58	129.16	120.98
1	E	179	TYR	CA-C-O	7.57	129.15	120.98
1	B	179	TYR	CA-C-O	7.56	129.15	120.98
1	C	179	TYR	CA-C-O	7.56	129.15	120.98
1	A	179	TYR	CA-C-O	7.56	129.14	120.98
1	G	179	TYR	CA-C-O	7.56	129.14	120.98
1	K	179	TYR	CA-C-O	7.55	129.14	120.98
1	H	179	TYR	CA-C-O	7.53	129.11	120.98
1	L	179	TYR	CA-C-O	7.51	129.10	120.98
1	L	293	GLN	OE1-CD-NE2	-7.40	115.20	122.60
1	E	293	GLN	OE1-CD-NE2	-7.39	115.21	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	293	GLN	OE1-CD-NE2	-7.39	115.21	122.60
1	L	179	TYR	O-C-N	7.38	132.46	122.57
1	K	179	TYR	O-C-N	7.38	132.46	122.57
1	C	293	GLN	OE1-CD-NE2	-7.38	115.22	122.60
1	D	179	TYR	O-C-N	7.37	132.45	122.57
1	H	179	TYR	O-C-N	7.37	132.44	122.57
1	B	179	TYR	O-C-N	7.37	132.44	122.57
1	B	293	GLN	OE1-CD-NE2	-7.36	115.24	122.60
1	C	179	TYR	O-C-N	7.36	132.43	122.57
1	G	179	TYR	O-C-N	7.36	132.43	122.57
1	A	179	TYR	O-C-N	7.36	132.43	122.57
1	A	293	GLN	OE1-CD-NE2	-7.36	115.25	122.60
1	J	293	GLN	OE1-CD-NE2	-7.35	115.25	122.60
1	I	293	GLN	OE1-CD-NE2	-7.35	115.25	122.60
1	F	179	TYR	O-C-N	7.35	132.41	122.57
1	D	293	GLN	OE1-CD-NE2	-7.34	115.26	122.60
1	I	179	TYR	O-C-N	7.34	132.40	122.57
1	G	293	GLN	OE1-CD-NE2	-7.34	115.26	122.60
1	I	280	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	H	293	GLN	OE1-CD-NE2	-7.33	115.27	122.60
1	E	179	TYR	O-C-N	7.33	132.39	122.57
1	B	280	ASN	OD1-CG-ND2	-7.33	115.27	122.60
1	J	179	TYR	O-C-N	7.32	132.38	122.57
1	L	280	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	D	280	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	G	280	ASN	OD1-CG-ND2	-7.31	115.29	122.60
1	K	293	GLN	OE1-CD-NE2	-7.31	115.29	122.60
1	K	280	ASN	OD1-CG-ND2	-7.31	115.29	122.60
1	J	280	ASN	OD1-CG-ND2	-7.31	115.29	122.60
1	A	280	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	F	280	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	C	280	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	C	447	ARG	CA-CB-CG	-7.28	99.54	114.10
1	F	447	ARG	CA-CB-CG	-7.28	99.55	114.10
1	J	447	ARG	CA-CB-CG	-7.28	99.55	114.10
1	K	447	ARG	CA-CB-CG	-7.28	99.54	114.10
1	H	447	ARG	CA-CB-CG	-7.28	99.55	114.10
1	E	280	ASN	OD1-CG-ND2	-7.27	115.33	122.60
1	G	447	ARG	CA-CB-CG	-7.27	99.56	114.10
1	B	447	ARG	CA-CB-CG	-7.27	99.56	114.10
1	H	280	ASN	OD1-CG-ND2	-7.27	115.33	122.60
1	I	447	ARG	CA-CB-CG	-7.27	99.56	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	ARG	CA-CB-CG	-7.26	99.57	114.10
1	L	447	ARG	CA-CB-CG	-7.26	99.58	114.10
1	D	447	ARG	CA-CB-CG	-7.25	99.59	114.10
1	E	447	ARG	CA-CB-CG	-7.25	99.61	114.10
1	D	219	ASN	OD1-CG-ND2	-7.22	115.38	122.60
1	J	219	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	C	219	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	L	219	ASN	OD1-CG-ND2	-7.21	115.39	122.60
1	F	219	ASN	OD1-CG-ND2	-7.20	115.40	122.60
1	G	219	ASN	OD1-CG-ND2	-7.18	115.42	122.60
1	H	219	ASN	OD1-CG-ND2	-7.18	115.42	122.60
1	A	219	ASN	OD1-CG-ND2	-7.17	115.42	122.60
1	I	219	ASN	OD1-CG-ND2	-7.17	115.43	122.60
1	E	219	ASN	OD1-CG-ND2	-7.16	115.44	122.60
1	K	219	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	B	219	ASN	OD1-CG-ND2	-7.13	115.47	122.60
1	E	264	ASN	N-CA-C	7.13	120.29	110.24
1	K	124	VAL	N-CA-CB	7.12	119.53	110.99
1	F	264	ASN	N-CA-C	7.12	120.28	110.24
1	H	124	VAL	N-CA-CB	7.11	119.53	110.99
1	C	124	VAL	N-CA-CB	7.11	119.52	110.99
1	L	124	VAL	N-CA-CB	7.11	119.52	110.99
1	E	124	VAL	N-CA-CB	7.10	119.51	110.99
1	A	124	VAL	N-CA-CB	7.10	119.51	110.99
1	B	124	VAL	N-CA-CB	7.10	119.51	110.99
1	B	264	ASN	N-CA-C	7.10	120.25	110.24
1	I	264	ASN	N-CA-C	7.10	120.25	110.24
1	D	124	VAL	N-CA-CB	7.09	119.50	110.99
1	J	124	VAL	N-CA-CB	7.09	119.50	110.99
1	G	124	VAL	N-CA-CB	7.09	119.50	110.99
1	J	264	ASN	N-CA-C	7.09	120.24	110.24
1	F	124	VAL	N-CA-CB	7.08	119.49	110.99
1	E	213	VAL	N-CA-C	7.08	117.87	110.72
1	A	264	ASN	N-CA-C	7.08	120.22	110.24
1	C	264	ASN	N-CA-C	7.08	120.22	110.24
1	F	213	VAL	N-CA-C	7.07	117.86	110.72
1	D	264	ASN	N-CA-C	7.07	120.21	110.24
1	G	264	ASN	N-CA-C	7.07	120.21	110.24
1	I	124	VAL	N-CA-CB	7.07	119.47	110.99
1	L	264	ASN	N-CA-C	7.06	120.20	110.24
1	K	264	ASN	N-CA-C	7.05	120.19	110.24
1	G	213	VAL	N-CA-C	7.05	117.84	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	213	VAL	N-CA-C	7.05	117.84	110.72
1	L	213	VAL	N-CA-C	7.04	117.83	110.72
1	C	213	VAL	N-CA-C	7.04	117.83	110.72
1	A	213	VAL	N-CA-C	7.04	117.83	110.72
1	H	264	ASN	N-CA-C	7.04	120.16	110.24
1	B	213	VAL	N-CA-C	7.03	117.82	110.72
1	H	213	VAL	N-CA-C	7.02	117.81	110.72
1	K	213	VAL	N-CA-C	7.02	117.81	110.72
1	D	213	VAL	N-CA-C	7.01	117.81	110.72
1	I	213	VAL	N-CA-C	7.00	117.80	110.72
1	L	366	ASN	OD1-CG-ND2	-6.89	115.71	122.60
1	H	366	ASN	OD1-CG-ND2	-6.84	115.76	122.60
1	C	223	THR	N-CA-CB	-6.84	98.63	111.00
1	I	366	ASN	OD1-CG-ND2	-6.83	115.77	122.60
1	L	223	THR	N-CA-CB	-6.83	98.64	111.00
1	G	223	THR	N-CA-CB	-6.83	98.64	111.00
1	C	366	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	K	223	THR	N-CA-CB	-6.82	98.66	111.00
1	K	366	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	D	223	THR	N-CA-CB	-6.82	98.66	111.00
1	H	223	THR	N-CA-CB	-6.82	98.66	111.00
1	A	223	THR	N-CA-CB	-6.81	98.67	111.00
1	D	366	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	E	223	THR	N-CA-CB	-6.81	98.67	111.00
1	I	223	THR	N-CA-CB	-6.81	98.67	111.00
1	A	366	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	J	223	THR	N-CA-CB	-6.81	98.68	111.00
1	J	366	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	F	223	THR	N-CA-CB	-6.80	98.69	111.00
1	G	366	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	B	366	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	B	223	THR	N-CA-CB	-6.79	98.70	111.00
1	F	366	ASN	OD1-CG-ND2	-6.79	115.81	122.60
1	E	366	ASN	OD1-CG-ND2	-6.78	115.82	122.60
1	E	159	ASN	CA-CB-CG	-6.76	105.84	112.60
1	B	201	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	C	159	ASN	CA-CB-CG	-6.74	105.86	112.60
1	B	159	ASN	CA-CB-CG	-6.73	105.87	112.60
1	D	201	GLN	OE1-CD-NE2	-6.72	115.88	122.60
1	H	201	GLN	OE1-CD-NE2	-6.72	115.88	122.60
1	D	159	ASN	CA-CB-CG	-6.72	105.88	112.60
1	G	101	ASP	N-CA-C	6.72	121.15	113.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	101	ASP	N-CA-C	6.72	121.14	113.15
1	C	101	ASP	N-CA-C	6.72	121.14	113.15
1	I	101	ASP	N-CA-C	6.71	121.14	113.15
1	I	159	ASN	CA-CB-CG	-6.71	105.89	112.60
1	H	101	ASP	N-CA-C	6.71	121.13	113.15
1	F	159	ASN	CA-CB-CG	-6.70	105.90	112.60
1	K	159	ASN	CA-CB-CG	-6.70	105.90	112.60
1	A	159	ASN	CA-CB-CG	-6.70	105.90	112.60
1	H	159	ASN	CA-CB-CG	-6.70	105.90	112.60
1	L	201	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	201	GLN	OE1-CD-NE2	-6.70	115.91	122.60
1	K	201	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	F	101	ASP	N-CA-C	6.69	121.11	113.15
1	A	101	ASP	N-CA-C	6.69	121.11	113.15
1	I	201	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	L	159	ASN	CA-CB-CG	-6.69	105.91	112.60
1	G	159	ASN	CA-CB-CG	-6.69	105.91	112.60
1	D	101	ASP	N-CA-C	6.69	121.11	113.15
1	J	201	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	J	159	ASN	CA-CB-CG	-6.69	105.91	112.60
1	F	201	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	J	101	ASP	N-CA-C	6.68	121.10	113.15
1	K	101	ASP	N-CA-C	6.68	121.10	113.15
1	L	103	ASP	CA-CB-CG	6.68	119.28	112.60
1	E	101	ASP	N-CA-C	6.67	121.09	113.15
1	E	201	GLN	OE1-CD-NE2	-6.67	115.93	122.60
1	G	201	GLN	OE1-CD-NE2	-6.67	115.94	122.60
1	J	103	ASP	CA-CB-CG	6.67	119.27	112.60
1	C	201	GLN	OE1-CD-NE2	-6.66	115.94	122.60
1	D	103	ASP	CA-CB-CG	6.66	119.26	112.60
1	L	338	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	B	101	ASP	N-CA-C	6.66	121.07	113.15
1	G	103	ASP	CA-CB-CG	6.65	119.25	112.60
1	H	103	ASP	CA-CB-CG	6.65	119.25	112.60
1	H	338	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	F	338	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	A	103	ASP	CA-CB-CG	6.65	119.25	112.60
1	C	338	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	E	338	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	I	338	ASN	OD1-CG-ND2	-6.63	115.97	122.60
1	C	211	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	K	29	GLN	OE1-CD-NE2	-6.63	115.97	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	ASP	CA-CB-CG	6.62	119.22	112.60
1	D	29	GLN	OE1-CD-NE2	-6.62	115.97	122.60
1	I	211	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	A	338	ASN	OD1-CG-ND2	-6.62	115.98	122.60
1	K	211	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	B	103	ASP	CA-CB-CG	6.61	119.21	112.60
1	K	103	ASP	CA-CB-CG	6.61	119.21	112.60
1	E	211	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	A	211	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	E	103	ASP	CA-CB-CG	6.60	119.20	112.60
1	G	211	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	J	338	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	B	211	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	H	211	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	F	103	ASP	CA-CB-CG	6.60	119.20	112.60
1	G	29	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	H	419	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	C	419	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	D	338	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	J	211	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	C	29	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	K	338	ASN	OD1-CG-ND2	-6.59	116.01	122.60
1	L	29	GLN	OE1-CD-NE2	-6.59	116.01	122.60
1	I	103	ASP	CA-CB-CG	6.58	119.19	112.60
1	L	211	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	B	29	GLN	OE1-CD-NE2	-6.58	116.02	122.60
1	B	338	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	D	211	HIS	CB-CG-CD2	-6.58	122.64	131.20
1	I	419	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	E	29	GLN	OE1-CD-NE2	-6.58	116.02	122.60
1	J	29	GLN	OE1-CD-NE2	-6.58	116.02	122.60
1	F	211	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	G	338	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	F	419	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	A	29	GLN	OE1-CD-NE2	-6.57	116.03	122.60
1	L	419	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	D	419	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	K	350	SER	O-C-N	-6.56	113.77	121.32
1	G	419	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	H	29	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	A	419	ASN	OD1-CG-ND2	-6.55	116.05	122.60
1	B	419	ASN	OD1-CG-ND2	-6.55	116.05	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	350	SER	O-C-N	-6.54	113.80	121.32
1	B	350	SER	O-C-N	-6.54	113.80	121.32
1	C	236	GLN	CG-CD-NE2	6.54	126.21	116.40
1	J	350	SER	O-C-N	-6.54	113.80	121.32
1	K	236	GLN	CG-CD-NE2	6.54	126.21	116.40
1	F	29	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	F	350	SER	O-C-N	-6.54	113.81	121.32
1	E	419	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	E	350	SER	O-C-N	-6.53	113.81	121.32
1	A	350	SER	O-C-N	-6.52	113.82	121.32
1	B	236	GLN	CG-CD-NE2	6.52	126.19	116.40
1	I	29	GLN	OE1-CD-NE2	-6.52	116.08	122.60
1	K	419	ASN	OD1-CG-ND2	-6.52	116.08	122.60
1	H	236	GLN	CG-CD-NE2	6.52	126.18	116.40
1	H	350	SER	O-C-N	-6.52	113.83	121.32
1	G	350	SER	O-C-N	-6.51	113.83	121.32
1	C	350	SER	O-C-N	-6.51	113.83	121.32
1	E	236	GLN	CG-CD-NE2	6.51	126.16	116.40
1	J	419	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	J	236	GLN	CG-CD-NE2	6.51	126.16	116.40
1	A	236	GLN	CG-CD-NE2	6.51	126.16	116.40
1	I	236	GLN	CG-CD-NE2	6.51	126.16	116.40
1	D	236	GLN	CG-CD-NE2	6.50	126.15	116.40
1	L	350	SER	O-C-N	-6.50	113.84	121.32
1	F	236	GLN	CG-CD-NE2	6.49	126.14	116.40
1	G	236	GLN	CG-CD-NE2	6.49	126.13	116.40
1	L	236	GLN	CG-CD-NE2	6.48	126.11	116.40
1	D	350	SER	O-C-N	-6.47	113.87	121.32
1	E	168	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	J	168	ASN	OD1-CG-ND2	-6.45	116.15	122.60
1	H	168	ASN	OD1-CG-ND2	-6.45	116.16	122.60
1	I	285	ASP	CA-CB-CG	6.44	119.04	112.60
1	D	168	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	G	168	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	F	168	ASN	OD1-CG-ND2	-6.42	116.18	122.60
1	F	285	ASP	CA-CB-CG	6.41	119.01	112.60
1	A	168	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	E	285	ASP	CA-CB-CG	6.40	119.00	112.60
1	I	168	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	L	285	ASP	CA-CB-CG	6.39	118.99	112.60
1	G	285	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	285	ASP	CA-CB-CG	6.38	118.98	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	K	168	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	K	285	ASP	CA-CB-CG	6.38	118.98	112.60
1	C	10	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	J	285	ASP	CA-CB-CG	6.37	118.97	112.60
1	C	285	ASP	CA-CB-CG	6.37	118.97	112.60
1	D	285	ASP	CA-CB-CG	6.37	118.97	112.60
1	H	285	ASP	CA-CB-CG	6.36	118.96	112.60
1	L	168	ASN	OD1-CG-ND2	-6.36	116.24	122.60
1	C	168	ASN	OD1-CG-ND2	-6.36	116.25	122.60
1	E	52	SER	N-CA-C	6.35	118.73	111.11
1	B	52	SER	N-CA-C	6.35	118.73	111.11
1	B	285	ASP	CA-CB-CG	6.34	118.94	112.60
1	J	52	SER	N-CA-C	6.34	118.72	111.11
1	L	10	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	D	52	SER	N-CA-C	6.33	118.70	111.11
1	H	52	SER	N-CA-C	6.33	118.70	111.11
1	A	52	SER	N-CA-C	6.32	118.69	111.11
1	C	52	SER	N-CA-C	6.31	118.68	111.11
1	E	10	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	I	52	SER	N-CA-C	6.31	118.69	111.11
1	K	52	SER	N-CA-C	6.31	118.69	111.11
1	F	52	SER	N-CA-C	6.31	118.68	111.11
1	D	175	VAL	O-C-N	-6.30	115.73	121.91
1	G	52	SER	N-CA-C	6.30	118.67	111.11
1	C	244	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	I	462	PHE	CA-CB-CG	-6.30	107.50	113.80
1	D	10	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	L	52	SER	N-CA-C	6.29	118.66	111.11
1	L	175	VAL	O-C-N	-6.29	115.74	121.91
1	J	10	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	10	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	I	175	VAL	O-C-N	-6.29	115.75	121.91
1	A	244	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	J	244	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	K	175	VAL	O-C-N	-6.28	115.75	121.91
1	L	244	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	I	10	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	B	244	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	C	175	VAL	O-C-N	-6.28	115.75	121.91
1	F	244	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	I	244	ASN	OD1-CG-ND2	-6.28	116.32	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	E	175	VAL	O-C-N	-6.28	115.76	121.91
1	G	462	PHE	CA-CB-CG	-6.28	107.53	113.80
1	D	462	PHE	CA-CB-CG	-6.27	107.53	113.80
1	F	10	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	G	10	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	A	175	VAL	O-C-N	-6.27	115.77	121.91
1	K	244	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	B	30	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	E	244	ASN	OD1-CG-ND2	-6.26	116.33	122.60
1	G	175	VAL	O-C-N	-6.26	115.77	121.91
1	B	462	PHE	CA-CB-CG	-6.26	107.54	113.80
1	F	175	VAL	O-C-N	-6.26	115.78	121.91
1	G	30	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	H	244	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	J	175	VAL	O-C-N	-6.26	115.78	121.91
1	G	244	ASN	OD1-CG-ND2	-6.25	116.34	122.60
1	E	30	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	D	244	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	F	462	PHE	CA-CB-CG	-6.25	107.56	113.80
1	K	462	PHE	CA-CB-CG	-6.24	107.56	113.80
1	A	462	PHE	CA-CB-CG	-6.24	107.56	113.80
1	J	462	PHE	CA-CB-CG	-6.24	107.56	113.80
1	K	10	ASN	OD1-CG-ND2	-6.24	116.36	122.60
1	H	175	VAL	O-C-N	-6.24	115.80	121.91
1	C	30	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	A	30	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	C	462	PHE	CA-CB-CG	-6.23	107.57	113.80
1	K	30	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	H	10	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	H	462	PHE	CA-CB-CG	-6.22	107.58	113.80
1	L	462	PHE	CA-CB-CG	-6.22	107.58	113.80
1	F	30	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	B	175	VAL	O-C-N	-6.22	115.81	121.91
1	E	462	PHE	CA-CB-CG	-6.22	107.58	113.80
1	B	233	ASP	CA-CB-CG	6.21	118.81	112.60
1	I	360	PHE	N-CA-C	6.21	123.54	109.81
1	L	214	ALA	N-CA-C	6.21	119.47	110.28
1	C	214	ALA	N-CA-C	6.21	119.47	110.28
1	H	214	ALA	N-CA-C	6.21	119.47	110.28
1	I	214	ALA	N-CA-C	6.21	119.47	110.28
1	I	30	HIS	CB-CG-CD2	-6.21	123.13	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	30	HIS	CB-CG-CD2	-6.21	123.13	131.20
1	J	214	ALA	N-CA-C	6.21	119.46	110.28
1	K	214	ALA	N-CA-C	6.20	119.46	110.28
1	L	30	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	G	360	PHE	N-CA-C	6.20	123.52	109.81
1	B	360	PHE	N-CA-C	6.20	123.51	109.81
1	D	30	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	I	233	ASP	CA-CB-CG	6.20	118.80	112.60
1	D	214	ALA	N-CA-C	6.20	119.45	110.28
1	J	30	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	L	189	GLN	CG-CD-NE2	6.20	125.69	116.40
1	F	214	ALA	N-CA-C	6.19	119.45	110.28
1	H	233	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	214	ALA	N-CA-C	6.19	119.44	110.28
1	A	360	PHE	N-CA-C	6.19	123.49	109.81
1	J	360	PHE	N-CA-C	6.19	123.48	109.81
1	F	233	ASP	CA-CB-CG	6.18	118.78	112.60
1	C	360	PHE	N-CA-C	6.18	123.47	109.81
1	D	360	PHE	N-CA-C	6.18	123.47	109.81
1	L	360	PHE	N-CA-C	6.18	123.47	109.81
1	C	189	GLN	CG-CD-NE2	6.18	125.67	116.40
1	E	214	ALA	N-CA-C	6.18	119.43	110.28
1	E	233	ASP	CA-CB-CG	6.18	118.78	112.60
1	H	360	PHE	N-CA-C	6.18	123.46	109.81
1	K	360	PHE	N-CA-C	6.17	123.46	109.81
1	L	36	HIS	CB-CG-CD2	-6.17	123.17	131.20
1	E	360	PHE	N-CA-C	6.17	123.45	109.81
1	G	214	ALA	N-CA-C	6.17	119.42	110.28
1	F	360	PHE	N-CA-C	6.17	123.45	109.81
1	G	164	TYR	N-CA-C	6.17	121.74	113.72
1	K	233	ASP	CA-CB-CG	6.17	118.77	112.60
1	I	189	GLN	CG-CD-NE2	6.17	125.65	116.40
1	F	164	TYR	N-CA-C	6.17	121.73	113.72
1	A	189	GLN	CG-CD-NE2	6.16	125.64	116.40
1	G	189	GLN	CG-CD-NE2	6.16	125.64	116.40
1	A	233	ASP	CA-CB-CG	6.16	118.76	112.60
1	E	189	GLN	CG-CD-NE2	6.16	125.64	116.40
1	K	189	GLN	CG-CD-NE2	6.16	125.64	116.40
1	F	189	GLN	CG-CD-NE2	6.16	125.64	116.40
1	B	214	ALA	N-CA-C	6.16	119.39	110.28
1	K	164	TYR	N-CA-C	6.16	121.72	113.72
1	L	233	ASP	CA-CB-CG	6.16	118.76	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	189	GLN	CG-CD-NE2	6.15	125.63	116.40
1	H	189	GLN	CG-CD-NE2	6.15	125.62	116.40
1	C	233	ASP	CA-CB-CG	6.15	118.75	112.60
1	B	36	HIS	CB-CG-CD2	-6.15	123.21	131.20
1	C	164	TYR	N-CA-C	6.15	121.71	113.72
1	D	233	ASP	CA-CB-CG	6.15	118.75	112.60
1	J	164	TYR	N-CA-C	6.15	121.71	113.72
1	B	189	GLN	CG-CD-NE2	6.14	125.62	116.40
1	D	189	GLN	CG-CD-NE2	6.14	125.62	116.40
1	K	36	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	E	164	TYR	N-CA-C	6.14	121.70	113.72
1	G	233	ASP	CA-CB-CG	6.14	118.74	112.60
1	I	164	TYR	N-CA-C	6.14	121.70	113.72
1	J	36	HIS	CB-CG-CD2	-6.14	123.22	131.20
1	J	233	ASP	CA-CB-CG	6.13	118.73	112.60
1	F	36	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	G	36	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	A	164	TYR	N-CA-C	6.13	121.69	113.72
1	D	36	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	E	36	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	A	36	HIS	CB-CG-CD2	-6.12	123.25	131.20
1	B	164	TYR	N-CA-C	6.12	121.67	113.72
1	C	36	HIS	CB-CG-CD2	-6.12	123.25	131.20
1	C	66	VAL	N-CA-C	6.11	116.67	108.11
1	D	164	TYR	N-CA-C	6.11	121.67	113.72
1	L	164	TYR	N-CA-C	6.11	121.67	113.72
1	I	36	HIS	CB-CG-CD2	-6.11	123.26	131.20
1	G	66	VAL	N-CA-C	6.10	116.64	108.11
1	D	66	VAL	N-CA-C	6.09	116.64	108.11
1	H	164	TYR	N-CA-C	6.09	121.64	113.72
1	H	36	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	F	66	VAL	N-CA-C	6.08	116.62	108.11
1	E	66	VAL	N-CA-C	6.08	116.62	108.11
1	A	66	VAL	N-CA-C	6.08	116.61	108.11
1	K	66	VAL	N-CA-C	6.08	116.62	108.11
1	I	66	VAL	N-CA-C	6.07	116.61	108.11
1	J	66	VAL	N-CA-C	6.07	116.61	108.11
1	B	66	VAL	N-CA-C	6.07	116.60	108.11
1	H	66	VAL	N-CA-C	6.06	116.60	108.11
1	L	66	VAL	N-CA-C	6.05	116.57	108.11
1	F	317	ASN	OD1-CG-ND2	-6.03	116.57	122.60
1	K	148	HIS	CB-CG-CD2	-6.03	123.37	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	HIS	CB-CG-CD2	-6.01	123.38	131.20
1	G	148	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	E	148	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	F	148	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	B	148	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	D	148	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	A	148	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	H	148	HIS	CB-CG-CD2	-5.99	123.41	131.20
1	I	317	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	L	148	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	I	148	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	C	317	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	J	148	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	E	317	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	H	317	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	A	317	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	B	317	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	L	317	ASN	OD1-CG-ND2	-5.96	116.64	122.60
1	G	317	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	I	304	HIS	CB-CG-CD2	-5.95	123.47	131.20
1	J	317	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	E	304	HIS	CB-CG-CD2	-5.93	123.49	131.20
1	D	317	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	K	209	HIS	CB-CG-CD2	-5.93	123.50	131.20
1	K	317	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	C	209	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	H	304	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	F	209	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	D	304	HIS	CB-CG-CD2	-5.91	123.51	131.20
1	G	304	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	G	209	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	C	304	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	H	209	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	J	209	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	J	304	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	L	209	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	304	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	D	209	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	209	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	G	175	VAL	N-CA-C	5.89	116.08	110.42
1	L	304	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	B	304	HIS	CB-CG-CD2	-5.89	123.54	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	171	HIS	CA-CB-CG	-5.89	107.91	113.80
1	B	209	HIS	CB-CG-CD2	-5.88	123.55	131.20
1	F	175	VAL	N-CA-C	5.88	116.07	110.42
1	K	171	HIS	CA-CB-CG	-5.88	107.92	113.80
1	F	304	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	F	171	HIS	CA-CB-CG	-5.88	107.92	113.80
1	E	209	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	I	209	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	C	171	HIS	CA-CB-CG	-5.87	107.93	113.80
1	D	175	VAL	N-CA-C	5.87	116.05	110.42
1	G	171	HIS	CA-CB-CG	-5.87	107.93	113.80
1	B	171	HIS	CA-CB-CG	-5.87	107.93	113.80
1	A	171	HIS	CA-CB-CG	-5.87	107.94	113.80
1	K	304	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	L	171	HIS	CA-CB-CG	-5.87	107.93	113.80
1	D	171	HIS	CA-CB-CG	-5.86	107.94	113.80
1	H	175	VAL	N-CA-C	5.86	116.05	110.42
1	J	171	HIS	CA-CB-CG	-5.86	107.94	113.80
1	J	175	VAL	N-CA-C	5.86	116.04	110.42
1	I	15	LYS	CA-CB-CG	-5.86	102.39	114.10
1	E	171	HIS	CA-CB-CG	-5.85	107.95	113.80
1	H	171	HIS	CA-CB-CG	-5.84	107.95	113.80
1	J	129	GLU	CA-C-N	5.84	126.04	119.90
1	J	129	GLU	C-N-CA	5.84	126.04	119.90
1	L	129	GLU	CA-C-N	5.84	126.03	119.90
1	L	129	GLU	C-N-CA	5.84	126.03	119.90
1	I	433	VAL	O-C-N	-5.84	116.41	122.66
1	A	175	VAL	N-CA-C	5.84	116.03	110.42
1	B	15	LYS	CA-CB-CG	-5.84	102.42	114.10
1	C	15	LYS	CA-CB-CG	-5.84	102.42	114.10
1	K	15	LYS	CA-CB-CG	-5.84	102.42	114.10
1	E	175	VAL	N-CA-C	5.84	116.02	110.42
1	L	15	LYS	CA-CB-CG	-5.84	102.43	114.10
1	G	15	LYS	CA-CB-CG	-5.83	102.43	114.10
1	I	175	VAL	N-CA-C	5.83	116.02	110.42
1	K	175	VAL	N-CA-C	5.83	116.02	110.42
1	J	15	LYS	CA-CB-CG	-5.83	102.44	114.10
1	A	15	LYS	CA-CB-CG	-5.83	102.44	114.10
1	F	129	GLU	CA-C-N	5.83	126.02	119.90
1	F	129	GLU	C-N-CA	5.83	126.02	119.90
1	G	129	GLU	CA-C-N	5.83	126.02	119.90
1	G	129	GLU	C-N-CA	5.83	126.02	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	15	LYS	CA-CB-CG	-5.83	102.45	114.10
1	C	175	VAL	N-CA-C	5.82	116.01	110.42
1	F	15	LYS	CA-CB-CG	-5.82	102.45	114.10
1	D	15	LYS	CA-CB-CG	-5.82	102.47	114.10
1	L	175	VAL	N-CA-C	5.81	116.00	110.42
1	B	175	VAL	N-CA-C	5.81	115.99	110.42
1	D	129	GLU	CA-C-N	5.81	126.00	119.90
1	D	129	GLU	C-N-CA	5.81	126.00	119.90
1	E	15	LYS	CA-CB-CG	-5.80	102.49	114.10
1	A	129	GLU	CA-C-N	5.80	125.99	119.90
1	A	129	GLU	C-N-CA	5.80	125.99	119.90
1	B	129	GLU	CA-C-N	5.80	125.99	119.90
1	B	129	GLU	C-N-CA	5.80	125.99	119.90
1	B	433	VAL	O-C-N	-5.80	116.46	122.66
1	H	129	GLU	CA-C-N	5.80	125.99	119.90
1	H	129	GLU	C-N-CA	5.80	125.99	119.90
1	H	433	VAL	O-C-N	-5.79	116.46	122.66
1	C	129	GLU	CA-C-N	5.79	125.98	119.90
1	C	129	GLU	C-N-CA	5.79	125.98	119.90
1	E	129	GLU	CA-C-N	5.78	125.97	119.90
1	E	129	GLU	C-N-CA	5.78	125.97	119.90
1	G	433	VAL	O-C-N	-5.78	116.48	122.66
1	K	129	GLU	CA-C-N	5.78	125.96	119.90
1	K	129	GLU	C-N-CA	5.78	125.96	119.90
1	K	433	VAL	O-C-N	-5.77	116.48	122.66
1	D	247	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	I	129	GLU	CA-C-N	5.77	125.96	119.90
1	I	129	GLU	C-N-CA	5.77	125.96	119.90
1	G	247	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	A	433	VAL	O-C-N	-5.77	116.49	122.66
1	F	433	VAL	O-C-N	-5.77	116.49	122.66
1	J	433	VAL	O-C-N	-5.76	116.50	122.66
1	L	433	VAL	O-C-N	-5.76	116.49	122.66
1	C	425	ARG	N-CA-C	5.76	118.33	111.71
1	J	247	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	E	37	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	I	37	GLN	OE1-CD-NE2	-5.75	116.85	122.60
1	E	433	VAL	O-C-N	-5.75	116.51	122.66
1	L	247	HIS	CB-CG-CD2	-5.74	123.73	131.20
1	A	247	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	B	247	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	D	433	VAL	O-C-N	-5.74	116.52	122.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	247	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	I	247	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	L	37	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	C	433	VAL	O-C-N	-5.73	116.53	122.66
1	G	37	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	D	425	ARG	N-CA-C	5.73	118.30	111.71
1	E	244	ASN	N-CA-C	5.73	119.45	112.23
1	F	247	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	F	244	ASN	N-CA-C	5.73	119.44	112.23
1	G	425	ARG	N-CA-C	5.73	118.30	111.71
1	I	244	ASN	N-CA-C	5.72	119.44	112.23
1	J	37	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	A	37	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	C	37	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	K	37	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	H	247	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	C	247	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	A	425	ARG	N-CA-C	5.71	118.28	111.71
1	B	37	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	D	37	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	F	425	ARG	N-CA-C	5.70	118.27	111.71
1	F	37	GLN	OE1-CD-NE2	-5.70	116.90	122.60
1	A	244	ASN	N-CA-C	5.70	119.41	112.23
1	H	244	ASN	N-CA-C	5.70	119.41	112.23
1	D	244	ASN	N-CA-C	5.70	119.41	112.23
1	H	425	ARG	N-CA-C	5.70	118.26	111.71
1	K	247	HIS	CB-CG-CD2	-5.70	123.80	131.20
1	I	425	ARG	N-CA-C	5.69	118.26	111.71
1	G	244	ASN	N-CA-C	5.69	119.40	112.23
1	J	425	ARG	N-CA-C	5.69	118.25	111.71
1	K	244	ASN	N-CA-C	5.69	119.40	112.23
1	B	425	ARG	N-CA-C	5.69	118.25	111.71
1	K	288	ALA	N-CA-C	5.68	119.27	111.54
1	L	244	ASN	N-CA-C	5.68	119.39	112.23
1	K	425	ARG	N-CA-C	5.68	118.24	111.71
1	B	244	ASN	N-CA-C	5.67	119.38	112.23
1	L	425	ARG	N-CA-C	5.67	118.24	111.71
1	E	425	ARG	N-CA-C	5.67	118.23	111.71
1	J	244	ASN	N-CA-C	5.67	119.37	112.23
1	H	136	ASP	CA-C-O	5.67	126.23	119.60
1	B	136	ASP	CA-C-O	5.66	126.23	119.60
1	E	288	ALA	N-CA-C	5.66	119.24	111.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	ILE	N-CA-CB	-5.66	103.29	111.21
1	H	288	ALA	N-CA-C	5.66	119.24	111.54
1	J	288	ALA	N-CA-C	5.66	119.24	111.54
1	G	288	ALA	N-CA-C	5.66	119.23	111.54
1	I	288	ALA	N-CA-C	5.66	119.23	111.54
1	L	288	ALA	N-CA-C	5.65	119.23	111.54
1	C	244	ASN	N-CA-C	5.65	119.35	112.23
1	H	37	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	A	288	ALA	N-CA-C	5.65	119.22	111.54
1	C	288	ALA	N-CA-C	5.65	119.23	111.54
1	K	433	VAL	CA-C-O	-5.65	114.03	120.98
1	F	33	ILE	N-CA-CB	-5.65	103.30	111.21
1	G	211	HIS	CB-CG-ND1	5.65	131.17	122.70
1	H	33	ILE	N-CA-CB	-5.65	103.30	111.21
1	F	136	ASP	CA-C-O	5.65	126.21	119.60
1	K	33	ILE	N-CA-CB	-5.64	103.31	111.21
1	C	136	ASP	CA-C-O	5.64	126.20	119.60
1	D	288	ALA	N-CA-C	5.64	119.21	111.54
1	K	211	HIS	CB-CG-ND1	5.64	131.16	122.70
1	A	136	ASP	CA-C-O	5.64	126.20	119.60
1	I	33	ILE	N-CA-CB	-5.64	103.31	111.21
1	K	136	ASP	CA-C-O	5.64	126.20	119.60
1	B	288	ALA	N-CA-C	5.64	119.21	111.54
1	J	136	ASP	CA-C-O	5.64	126.20	119.60
1	B	33	ILE	N-CA-CB	-5.64	103.32	111.21
1	E	33	ILE	N-CA-CB	-5.64	103.32	111.21
1	E	211	HIS	CB-CG-ND1	5.64	131.16	122.70
1	G	136	ASP	CA-C-O	5.64	126.19	119.60
1	J	33	ILE	N-CA-CB	-5.64	103.32	111.21
1	A	33	ILE	N-CA-CB	-5.63	103.33	111.21
1	A	433	VAL	CA-C-O	-5.63	114.05	120.98
1	D	4	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	F	433	VAL	N-CA-C	-5.63	101.33	108.93
1	C	211	HIS	CB-CG-ND1	5.63	131.15	122.70
1	I	338	ASN	N-CA-C	5.63	122.79	110.80
1	C	33	ILE	N-CA-CB	-5.63	103.33	111.21
1	C	338	ASN	N-CA-C	5.63	122.79	110.80
1	E	338	ASN	N-CA-C	5.63	122.79	110.80
1	L	136	ASP	CA-C-O	5.63	126.19	119.60
1	D	338	ASN	N-CA-C	5.63	122.79	110.80
1	G	433	VAL	N-CA-C	-5.63	101.33	108.93
1	H	433	VAL	CA-C-O	-5.63	114.06	120.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	288	ALA	N-CA-C	5.62	119.19	111.54
1	G	338	ASN	N-CA-C	5.62	122.78	110.80
1	A	211	HIS	CB-CG-ND1	5.62	131.14	122.70
1	B	211	HIS	CB-CG-ND1	5.62	131.14	122.70
1	D	433	VAL	CA-C-O	-5.62	114.06	120.98
1	L	33	ILE	N-CA-CB	-5.62	103.34	111.21
1	J	433	VAL	CA-C-O	-5.62	114.06	120.98
1	C	433	VAL	CA-C-O	-5.62	114.07	120.98
1	F	338	ASN	N-CA-C	5.62	122.77	110.80
1	I	136	ASP	CA-C-O	5.62	126.17	119.60
1	L	338	ASN	N-CA-C	5.62	122.77	110.80
1	L	433	VAL	CA-C-O	-5.62	114.07	120.98
1	A	338	ASN	N-CA-C	5.62	122.76	110.80
1	H	4	HIS	CB-CG-CD2	-5.62	123.90	131.20
1	B	433	VAL	CA-C-O	-5.62	114.07	120.98
1	B	433	VAL	N-CA-C	-5.62	101.35	108.93
1	G	33	ILE	N-CA-CB	-5.62	103.35	111.21
1	L	211	HIS	CB-CG-ND1	5.62	131.12	122.70
1	F	4	HIS	CB-CG-CD2	-5.61	123.90	131.20
1	I	211	HIS	CB-CG-ND1	5.61	131.12	122.70
1	J	338	ASN	N-CA-C	5.61	122.76	110.80
1	D	433	VAL	N-CA-C	-5.61	101.35	108.93
1	H	338	ASN	N-CA-C	5.61	122.75	110.80
1	E	4	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	F	433	VAL	CA-C-O	-5.61	114.08	120.98
1	I	433	VAL	N-CA-C	-5.61	101.36	108.93
1	J	211	HIS	CB-CG-ND1	5.61	131.12	122.70
1	L	4	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	I	4	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	4	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	G	433	VAL	CA-C-O	-5.61	114.08	120.98
1	H	433	VAL	N-CA-C	-5.60	101.36	108.93
1	J	4	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	E	433	VAL	CA-C-O	-5.60	114.09	120.98
1	D	211	HIS	CB-CG-ND1	5.60	131.10	122.70
1	A	433	VAL	N-CA-C	-5.60	101.37	108.93
1	B	338	ASN	N-CA-C	5.60	122.72	110.80
1	F	211	HIS	CB-CG-ND1	5.59	131.09	122.70
1	J	433	VAL	N-CA-C	-5.59	101.38	108.93
1	K	338	ASN	N-CA-C	5.59	122.72	110.80
1	C	433	VAL	N-CA-C	-5.59	101.38	108.93
1	G	4	HIS	CB-CG-CD2	-5.59	123.93	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	433	VAL	N-CA-C	-5.59	101.38	108.93
1	H	211	HIS	CB-CG-ND1	5.59	131.08	122.70
1	L	433	VAL	N-CA-C	-5.59	101.39	108.93
1	D	136	ASP	CA-C-O	5.59	126.14	119.60
1	E	136	ASP	CA-C-O	5.59	126.14	119.60
1	E	433	VAL	N-CA-C	-5.58	101.39	108.93
1	I	433	VAL	CA-C-O	-5.58	114.12	120.98
1	B	4	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	C	4	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	K	4	HIS	CB-CG-CD2	-5.57	123.96	131.20
1	E	351	PRO	N-CA-C	5.57	123.93	112.47
1	H	175	VAL	CA-C-O	-5.56	115.28	121.17
1	F	175	VAL	CA-C-O	-5.55	115.28	121.17
1	B	175	VAL	CA-C-O	-5.55	115.29	121.17
1	B	351	PRO	N-CA-C	5.55	123.89	112.47
1	D	351	PRO	N-CA-C	5.54	123.89	112.47
1	L	175	VAL	CA-C-O	-5.54	115.30	121.17
1	K	351	PRO	N-CA-C	5.54	123.88	112.47
1	A	351	PRO	N-CA-C	5.54	123.87	112.47
1	E	175	VAL	CA-C-O	-5.54	115.30	121.17
1	F	351	PRO	N-CA-C	5.53	123.87	112.47
1	I	351	PRO	N-CA-C	5.53	123.86	112.47
1	J	351	PRO	N-CA-C	5.53	123.86	112.47
1	G	351	PRO	N-CA-C	5.53	123.86	112.47
1	H	351	PRO	N-CA-C	5.53	123.86	112.47
1	L	351	PRO	N-CA-C	5.53	123.86	112.47
1	C	351	PRO	N-CA-C	5.52	123.84	112.47
1	B	313	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	A	175	VAL	CA-C-O	-5.52	115.32	121.17
1	C	175	VAL	CA-C-O	-5.51	115.33	121.17
1	I	313	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	I	175	VAL	CA-C-O	-5.50	115.34	121.17
1	J	175	VAL	CA-C-O	-5.50	115.34	121.17
1	H	313	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	K	175	VAL	CA-C-O	-5.50	115.34	121.17
1	J	210	HIS	CB-CG-CD2	-5.50	124.06	131.20
1	L	352	LYS	CA-C-O	5.50	125.86	118.38
1	C	15	LYS	CG-CD-CE	-5.49	98.66	111.30
1	G	175	VAL	CA-C-O	-5.49	115.35	121.17
1	G	352	LYS	CA-C-O	5.49	125.85	118.38
1	K	15	LYS	CG-CD-CE	-5.49	98.67	111.30
1	A	313	ASN	OD1-CG-ND2	-5.49	117.11	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	210	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	I	15	LYS	CG-CD-CE	-5.49	98.68	111.30
1	J	313	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	G	210	HIS	CB-CG-CD2	-5.49	124.07	131.20
1	I	210	HIS	CB-CG-CD2	-5.49	124.07	131.20
1	J	15	LYS	CG-CD-CE	-5.48	98.69	111.30
1	L	210	HIS	CB-CG-CD2	-5.48	124.07	131.20
1	F	210	HIS	CB-CG-CD2	-5.48	124.07	131.20
1	L	158	TRP	CE2-CD2-CG	-5.48	100.62	107.20
1	A	15	LYS	CG-CD-CE	-5.48	98.70	111.30
1	D	175	VAL	CA-C-O	-5.48	115.36	121.17
1	E	15	LYS	CG-CD-CE	-5.48	98.69	111.30
1	I	352	LYS	CA-C-O	5.48	125.83	118.38
1	K	313	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	G	15	LYS	CG-CD-CE	-5.48	98.70	111.30
1	L	15	LYS	CG-CD-CE	-5.48	98.70	111.30
1	B	352	LYS	CA-C-O	5.47	125.82	118.38
1	F	313	ASN	OD1-CG-ND2	-5.47	117.12	122.60
1	A	352	LYS	CA-C-O	5.47	125.82	118.38
1	E	313	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	F	352	LYS	CA-C-O	5.47	125.82	118.38
1	K	101	ASP	CA-CB-CG	5.47	118.07	112.60
1	E	352	LYS	CA-C-O	5.47	125.82	118.38
1	F	15	LYS	CG-CD-CE	-5.47	98.72	111.30
1	J	352	LYS	CA-C-O	5.47	125.82	118.38
1	F	101	ASP	CA-CB-CG	5.47	118.07	112.60
1	H	12	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	D	45	GLU	N-CA-C	5.47	119.93	112.88
1	C	45	GLU	N-CA-C	5.46	119.93	112.88
1	K	352	LYS	CA-C-O	5.46	125.81	118.38
1	A	210	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	C	352	LYS	CA-C-O	5.46	125.81	118.38
1	F	45	GLU	N-CA-C	5.46	119.93	112.88
1	H	81	ALA	N-CA-C	5.46	117.99	111.71
1	D	15	LYS	CG-CD-CE	-5.46	98.74	111.30
1	E	45	GLU	N-CA-C	5.46	119.93	112.88
1	E	101	ASP	CA-CB-CG	5.46	118.06	112.60
1	H	15	LYS	CG-CD-CE	-5.46	98.74	111.30
1	D	352	LYS	CA-C-O	5.46	125.81	118.38
1	H	158	TRP	CE2-CD2-CG	-5.46	100.65	107.20
1	L	81	ALA	N-CA-C	5.46	117.99	111.71
1	G	45	GLU	N-CA-C	5.46	119.92	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	158	TRP	CE2-CD2-CG	-5.46	100.65	107.20
1	J	158	TRP	CE2-CD2-CG	-5.46	100.65	107.20
1	B	101	ASP	CA-CB-CG	5.46	118.06	112.60
1	E	12	HIS	CB-CG-CD2	-5.46	124.11	131.20
1	H	101	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	15	LYS	CG-CD-CE	-5.46	98.75	111.30
1	K	45	GLU	N-CA-C	5.45	119.92	112.88
1	C	313	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	I	158	TRP	CE2-CD2-CG	-5.45	100.66	107.20
1	C	12	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	D	81	ALA	N-CA-C	5.45	117.98	111.71
1	D	101	ASP	CA-CB-CG	5.45	118.05	112.60
1	D	158	TRP	CE2-CD2-CG	-5.45	100.66	107.20
1	G	12	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	J	101	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	45	GLU	N-CA-C	5.45	119.91	112.88
1	A	101	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	158	TRP	CE2-CD2-CG	-5.44	100.67	107.20
1	J	12	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	J	45	GLU	N-CA-C	5.44	119.90	112.88
1	D	210	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	F	12	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	G	81	ALA	N-CA-C	5.44	117.97	111.71
1	H	210	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	K	12	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	A	12	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	G	313	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	I	81	ALA	N-CA-C	5.44	117.97	111.71
1	K	158	TRP	CE2-CD2-CG	-5.44	100.67	107.20
1	B	12	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	H	352	LYS	CA-C-O	5.44	125.78	118.38
1	C	101	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	12	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	D	249	PHE	CA-CB-CG	-5.44	108.36	113.80
1	E	158	TRP	CE2-CD2-CG	-5.43	100.68	107.20
1	F	158	TRP	CE2-CD2-CG	-5.43	100.68	107.20
1	L	101	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	158	TRP	CE2-CD2-CG	-5.43	100.68	107.20
1	J	81	ALA	N-CA-C	5.43	117.96	111.71
1	B	158	TRP	CE2-CD2-CG	-5.43	100.68	107.20
1	B	210	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	H	45	GLU	N-CA-C	5.43	119.88	112.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	210	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	F	434	PHE	CB-CA-C	-5.43	99.62	110.42
1	A	81	ALA	N-CA-C	5.43	117.95	111.71
1	B	249	PHE	CA-CB-CG	-5.43	108.37	113.80
1	C	81	ALA	N-CA-C	5.43	117.95	111.71
1	E	337	ARG	O-C-N	-5.43	116.52	122.38
1	J	249	PHE	CA-CB-CG	-5.43	108.37	113.80
1	E	81	ALA	N-CA-C	5.42	117.95	111.71
1	H	249	PHE	CA-CB-CG	-5.42	108.38	113.80
1	I	45	GLU	N-CA-C	5.42	119.88	112.88
1	L	313	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	B	179	TYR	N-CA-C	5.42	117.56	108.23
1	G	179	TYR	N-CA-C	5.42	117.56	108.23
1	G	249	PHE	CA-CB-CG	-5.42	108.38	113.80
1	I	12	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	I	101	ASP	CA-CB-CG	5.42	118.02	112.60
1	L	249	PHE	CA-CB-CG	-5.42	108.38	113.80
1	B	45	GLU	N-CA-C	5.42	119.87	112.88
1	C	210	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	E	434	PHE	CB-CA-C	-5.42	99.64	110.42
1	I	434	PHE	CB-CA-C	-5.42	99.64	110.42
1	J	434	PHE	CB-CA-C	-5.42	99.64	110.42
1	I	179	TYR	N-CA-C	5.42	117.55	108.23
1	L	45	GLU	N-CA-C	5.42	119.87	112.88
1	B	434	PHE	CB-CA-C	-5.42	99.64	110.42
1	K	434	PHE	CB-CA-C	-5.42	99.64	110.42
1	L	12	HIS	CB-CG-CD2	-5.42	124.16	131.20
1	E	249	PHE	CA-CB-CG	-5.41	108.39	113.80
1	H	434	PHE	CB-CA-C	-5.41	99.65	110.42
1	A	434	PHE	CB-CA-C	-5.41	99.65	110.42
1	F	81	ALA	N-CA-C	5.41	117.93	111.71
1	I	249	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	179	TYR	N-CA-C	5.41	117.53	108.23
1	C	179	TYR	N-CA-C	5.41	117.53	108.23
1	G	101	ASP	CA-CB-CG	5.41	118.01	112.60
1	K	179	TYR	N-CA-C	5.41	117.53	108.23
1	B	81	ALA	N-CA-C	5.41	117.93	111.71
1	L	179	TYR	N-CA-C	5.41	117.53	108.23
1	A	249	PHE	CA-CB-CG	-5.41	108.39	113.80
1	D	434	PHE	CB-CA-C	-5.41	99.66	110.42
1	G	434	PHE	CB-CA-C	-5.40	99.67	110.42
1	F	179	TYR	N-CA-C	5.40	117.52	108.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	179	TYR	N-CA-C	5.40	117.52	108.23
1	C	434	PHE	CB-CA-C	-5.40	99.67	110.42
1	D	337	ARG	O-C-N	-5.40	116.55	122.38
1	K	81	ALA	N-CA-C	5.40	117.92	111.71
1	L	434	PHE	CB-CA-C	-5.40	99.67	110.42
1	D	179	TYR	N-CA-C	5.40	117.52	108.23
1	G	158	TRP	CG-CD2-CE3	5.40	139.30	133.90
1	J	179	TYR	N-CA-C	5.40	117.52	108.23
1	D	313	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	E	98	GLN	CG-CD-NE2	5.40	124.50	116.40
1	K	249	PHE	CA-CB-CG	-5.39	108.41	113.80
1	I	331	MET	N-CA-C	5.39	116.91	109.15
1	L	158	TRP	CG-CD2-CE3	5.39	139.29	133.90
1	C	249	PHE	CA-CB-CG	-5.39	108.41	113.80
1	D	98	GLN	CG-CD-NE2	5.39	124.48	116.40
1	H	158	TRP	CG-CD2-CE3	5.39	139.29	133.90
1	J	158	TRP	CG-CD2-CE3	5.39	139.29	133.90
1	E	179	TYR	N-CA-C	5.38	117.49	108.23
1	F	249	PHE	CA-CB-CG	-5.38	108.42	113.80
1	C	122	ASP	CA-CB-CG	5.38	117.98	112.60
1	F	331	MET	N-CA-C	5.38	116.90	109.15
1	I	122	ASP	CA-CB-CG	5.38	117.98	112.60
1	E	331	MET	N-CA-C	5.38	116.90	109.15
1	B	122	ASP	CA-CB-CG	5.38	117.98	112.60
1	H	98	GLN	CG-CD-NE2	5.38	124.47	116.40
1	G	337	ARG	O-C-N	-5.38	116.57	122.38
1	I	158	TRP	CG-CD2-CE3	5.38	139.28	133.90
1	J	98	GLN	CG-CD-NE2	5.38	124.46	116.40
1	A	98	GLN	CG-CD-NE2	5.38	124.46	116.40
1	D	331	MET	N-CA-C	5.38	116.89	109.15
1	C	158	TRP	CG-CD2-CE3	5.37	139.27	133.90
1	F	98	GLN	CG-CD-NE2	5.37	124.46	116.40
1	G	331	MET	N-CA-C	5.37	116.89	109.15
1	B	98	GLN	CG-CD-NE2	5.37	124.45	116.40
1	I	98	GLN	CG-CD-NE2	5.37	124.45	116.40
1	K	98	GLN	CG-CD-NE2	5.37	124.45	116.40
1	K	331	MET	N-CA-C	5.37	116.88	109.15
1	L	98	GLN	CG-CD-NE2	5.37	124.45	116.40
1	A	331	MET	N-CA-C	5.37	116.88	109.15
1	F	122	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	331	MET	N-CA-C	5.37	116.88	109.15
1	G	98	GLN	CG-CD-NE2	5.37	124.45	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	158	TRP	CG-CD2-CE3	5.37	139.27	133.90
1	J	337	ARG	O-C-N	-5.36	116.59	122.38
1	L	226	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	L	331	MET	N-CA-C	5.36	116.87	109.15
1	A	122	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	337	ARG	O-C-N	-5.36	116.59	122.38
1	H	331	MET	N-CA-C	5.36	116.87	109.15
1	K	122	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	158	TRP	CG-CD2-CE3	5.36	139.26	133.90
1	B	337	ARG	O-C-N	-5.36	116.59	122.38
1	D	158	TRP	CG-CD2-CE3	5.36	139.25	133.90
1	J	331	MET	N-CA-C	5.36	116.86	109.15
1	H	162	THR	N-CA-C	5.35	117.99	109.96
1	B	158	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	E	122	ASP	CA-CB-CG	5.35	117.95	112.60
1	L	337	ARG	O-C-N	-5.35	116.60	122.38
1	B	162	THR	N-CA-C	5.35	117.99	109.96
1	I	162	THR	N-CA-C	5.35	117.99	109.96
1	C	98	GLN	CG-CD-NE2	5.35	124.42	116.40
1	F	68	MET	CG-SD-CE	-5.35	89.13	100.90
1	F	158	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	C	337	ARG	O-C-N	-5.35	116.61	122.38
1	C	360	PHE	CA-CB-CG	5.35	119.15	113.80
1	E	360	PHE	CA-CB-CG	5.35	119.15	113.80
1	H	122	ASP	CA-CB-CG	5.35	117.95	112.60
1	J	162	THR	N-CA-C	5.35	117.98	109.96
1	L	162	THR	N-CA-C	5.35	117.98	109.96
1	C	331	MET	N-CA-C	5.34	116.85	109.15
1	D	68	MET	CG-SD-CE	-5.34	89.14	100.90
1	G	162	THR	N-CA-C	5.34	117.97	109.96
1	J	384	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	L	68	MET	CG-SD-CE	-5.34	89.14	100.90
1	A	162	THR	N-CA-C	5.34	117.97	109.96
1	I	337	ARG	O-C-N	-5.34	116.61	122.38
1	J	122	ASP	CA-CB-CG	5.34	117.94	112.60
1	E	158	TRP	CG-CD2-CE3	5.34	139.24	133.90
1	I	68	MET	CG-SD-CE	-5.34	89.15	100.90
1	K	337	ARG	O-C-N	-5.34	116.61	122.38
1	J	68	MET	CG-SD-CE	-5.34	89.15	100.90
1	C	68	MET	CG-SD-CE	-5.34	89.16	100.90
1	F	162	THR	N-CA-C	5.34	117.97	109.96
1	J	226	ASN	OD1-CG-ND2	-5.34	117.26	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	337	ARG	O-C-N	-5.34	116.62	122.38
1	H	360	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	68	MET	CG-SD-CE	-5.33	89.16	100.90
1	B	68	MET	CG-SD-CE	-5.33	89.16	100.90
1	G	68	MET	CG-SD-CE	-5.33	89.16	100.90
1	D	122	ASP	CA-CB-CG	5.33	117.93	112.60
1	H	226	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	E	162	THR	N-CA-C	5.33	117.95	109.96
1	J	360	PHE	CA-CB-CG	5.33	119.13	113.80
1	C	162	THR	N-CA-C	5.33	117.95	109.96
1	E	68	MET	CG-SD-CE	-5.33	89.18	100.90
1	L	122	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	162	THR	N-CA-C	5.33	117.95	109.96
1	K	68	MET	CG-SD-CE	-5.33	89.18	100.90
1	L	360	PHE	CA-CB-CG	5.33	119.12	113.80
1	A	360	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	226	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	K	162	THR	N-CA-C	5.32	117.94	109.96
1	H	68	MET	CG-SD-CE	-5.32	89.19	100.90
1	D	360	PHE	CA-CB-CG	5.32	119.12	113.80
1	F	360	PHE	CA-CB-CG	5.32	119.12	113.80
1	F	337	ARG	O-C-N	-5.31	116.64	122.38
1	C	226	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	D	226	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	G	384	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	B	360	PHE	CA-CB-CG	5.31	119.11	113.80
1	E	226	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	G	360	PHE	CA-CB-CG	5.30	119.10	113.80
1	K	360	PHE	CA-CB-CG	5.30	119.11	113.80
1	K	384	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	I	360	PHE	CA-CB-CG	5.30	119.10	113.80
1	I	384	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	H	384	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	L	384	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	C	384	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	D	384	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	F	391	PRO	N-CA-C	5.29	118.81	110.50
1	G	122	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	384	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	F	384	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	226	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	B	384	ASN	OD1-CG-ND2	-5.28	117.32	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	226	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	G	226	ASN	OD1-CG-ND2	-5.28	117.33	122.60
1	K	226	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	C	129	GLU	CA-CB-CG	5.27	124.64	114.10
1	K	391	PRO	N-CA-C	5.27	118.77	110.50
1	H	129	GLU	CA-CB-CG	5.27	124.63	114.10
1	I	129	GLU	CA-CB-CG	5.26	124.62	114.10
1	H	391	PRO	N-CA-C	5.26	118.76	110.50
1	E	384	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	D	102	ARG	N-CA-CB	-5.26	103.63	110.88
1	G	129	GLU	CA-CB-CG	5.26	124.61	114.10
1	K	129	GLU	CA-CB-CG	5.26	124.61	114.10
1	B	391	PRO	N-CA-C	5.25	118.75	110.50
1	D	129	GLU	CA-CB-CG	5.25	124.61	114.10
1	E	129	GLU	CA-CB-CG	5.25	124.61	114.10
1	L	102	ARG	N-CA-CB	-5.25	103.63	110.88
1	A	129	GLU	CA-CB-CG	5.25	124.60	114.10
1	H	102	ARG	N-CA-CB	-5.25	103.64	110.88
1	J	129	GLU	CA-CB-CG	5.25	124.60	114.10
1	A	391	PRO	N-CA-C	5.25	118.74	110.50
1	I	362	ASP	CA-CB-CG	5.25	117.84	112.60
1	E	102	ARG	N-CA-CB	-5.24	103.64	110.88
1	F	129	GLU	CA-CB-CG	5.24	124.59	114.10
1	K	102	ARG	N-CA-CB	-5.24	103.64	110.88
1	F	226	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	J	102	ARG	N-CA-CB	-5.24	103.65	110.88
1	L	129	GLU	CA-CB-CG	5.24	124.58	114.10
1	G	391	PRO	N-CA-C	5.24	118.72	110.50
1	B	102	ARG	N-CA-CB	-5.24	103.65	110.88
1	I	391	PRO	N-CA-C	5.23	118.71	110.50
1	J	391	PRO	N-CA-C	5.23	118.71	110.50
1	L	391	PRO	N-CA-C	5.23	118.71	110.50
1	A	102	ARG	N-CA-CB	-5.23	103.67	110.88
1	B	129	GLU	CA-CB-CG	5.23	124.56	114.10
1	C	391	PRO	N-CA-C	5.23	118.71	110.50
1	E	391	PRO	N-CA-C	5.23	118.71	110.50
1	G	102	ARG	N-CA-CB	-5.23	103.67	110.88
1	D	362	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	391	PRO	N-CA-C	5.22	118.70	110.50
1	F	102	ARG	N-CA-CB	-5.22	103.68	110.88
1	E	362	ASP	CA-CB-CG	5.21	117.81	112.60
1	F	362	ASP	CA-CB-CG	5.21	117.81	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ASP	CA-CB-CG	5.21	117.81	112.60
1	I	225	PHE	N-CA-C	5.21	117.05	110.33
1	J	362	ASP	CA-CB-CG	5.21	117.81	112.60
1	I	102	ARG	N-CA-CB	-5.21	103.69	110.88
1	C	362	ASP	CA-CB-CG	5.21	117.81	112.60
1	H	362	ASP	CA-CB-CG	5.21	117.81	112.60
1	C	102	ARG	N-CA-CB	-5.20	103.70	110.88
1	G	362	ASP	CA-CB-CG	5.20	117.80	112.60
1	L	225	PHE	N-CA-C	5.20	117.04	110.33
1	J	225	PHE	N-CA-C	5.20	117.04	110.33
1	K	362	ASP	CA-CB-CG	5.20	117.80	112.60
1	E	225	PHE	N-CA-C	5.20	117.03	110.33
1	H	225	PHE	N-CA-C	5.20	117.03	110.33
1	B	30	HIS	CB-CG-ND1	5.19	130.49	122.70
1	B	362	ASP	CA-CB-CG	5.19	117.79	112.60
1	K	216	ALA	N-CA-C	5.19	118.60	111.54
1	G	30	HIS	CB-CG-ND1	5.19	130.48	122.70
1	K	30	HIS	CB-CG-ND1	5.19	130.48	122.70
1	L	362	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	101	ASP	CA-C-N	5.18	130.37	122.23
1	C	101	ASP	C-N-CA	5.18	130.37	122.23
1	A	225	PHE	N-CA-C	5.18	117.02	110.33
1	B	225	PHE	N-CA-C	5.18	117.01	110.33
1	E	30	HIS	CB-CG-ND1	5.18	130.46	122.70
1	E	216	ALA	N-CA-C	5.17	118.58	111.54
1	A	30	HIS	CB-CG-ND1	5.17	130.46	122.70
1	C	225	PHE	N-CA-C	5.17	117.00	110.33
1	J	216	ALA	N-CA-C	5.17	118.58	111.54
1	D	225	PHE	N-CA-C	5.17	117.00	110.33
1	L	216	ALA	N-CA-C	5.17	118.57	111.54
1	C	30	HIS	CB-CG-ND1	5.17	130.46	122.70
1	F	30	HIS	CB-CG-ND1	5.17	130.46	122.70
1	A	216	ALA	N-CA-C	5.17	118.57	111.54
1	F	225	PHE	N-CA-C	5.17	116.99	110.33
1	K	225	PHE	N-CA-C	5.16	116.99	110.33
1	L	30	HIS	CB-CG-ND1	5.16	130.45	122.70
1	H	30	HIS	CB-CG-ND1	5.16	130.44	122.70
1	E	101	ASP	CA-C-N	5.16	130.33	122.23
1	E	101	ASP	C-N-CA	5.16	130.33	122.23
1	C	216	ALA	N-CA-C	5.16	118.55	111.54
1	H	216	ALA	N-CA-C	5.16	118.55	111.54
1	I	30	HIS	CB-CG-ND1	5.16	130.43	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	101	ASP	CA-C-N	5.15	130.32	122.23
1	L	101	ASP	C-N-CA	5.15	130.32	122.23
1	D	101	ASP	CA-C-N	5.15	130.32	122.23
1	D	101	ASP	C-N-CA	5.15	130.32	122.23
1	J	30	HIS	CB-CG-ND1	5.15	130.43	122.70
1	J	101	ASP	CA-C-N	5.15	130.32	122.23
1	J	101	ASP	C-N-CA	5.15	130.32	122.23
1	B	216	ALA	N-CA-C	5.15	118.55	111.54
1	D	30	HIS	CB-CG-ND1	5.15	130.43	122.70
1	I	216	ALA	N-CA-C	5.15	118.54	111.54
1	A	101	ASP	CA-C-N	5.14	130.31	122.23
1	A	101	ASP	C-N-CA	5.14	130.31	122.23
1	B	101	ASP	CA-C-N	5.14	130.31	122.23
1	B	101	ASP	C-N-CA	5.14	130.31	122.23
1	F	216	ALA	N-CA-C	5.14	118.54	111.54
1	G	225	PHE	N-CA-C	5.14	116.96	110.33
1	B	105	ARG	CA-CB-CG	-5.14	103.83	114.10
1	H	101	ASP	CA-C-N	5.14	130.29	122.23
1	H	101	ASP	C-N-CA	5.14	130.29	122.23
1	F	105	ARG	CA-CB-CG	-5.13	103.83	114.10
1	G	101	ASP	CA-C-N	5.13	130.29	122.23
1	G	101	ASP	C-N-CA	5.13	130.29	122.23
1	G	105	ARG	CA-CB-CG	-5.13	103.84	114.10
1	K	105	ARG	CA-CB-CG	-5.13	103.83	114.10
1	G	216	ALA	N-CA-C	5.13	118.52	111.54
1	I	101	ASP	CA-C-N	5.13	130.28	122.23
1	I	101	ASP	C-N-CA	5.13	130.28	122.23
1	K	262	GLY	CA-C-O	5.13	124.50	118.96
1	C	105	ARG	CA-CB-CG	-5.13	103.84	114.10
1	D	216	ALA	N-CA-C	5.13	118.51	111.54
1	F	101	ASP	CA-C-N	5.13	130.28	122.23
1	F	101	ASP	C-N-CA	5.13	130.28	122.23
1	D	262	GLY	CA-C-O	5.12	124.50	118.96
1	K	101	ASP	CA-C-N	5.12	130.27	122.23
1	K	101	ASP	C-N-CA	5.12	130.27	122.23
1	A	105	ARG	CA-CB-CG	-5.12	103.86	114.10
1	I	105	ARG	CA-CB-CG	-5.12	103.86	114.10
1	E	262	GLY	CA-C-O	5.12	124.49	118.96
1	E	105	ARG	CA-CB-CG	-5.12	103.87	114.10
1	C	262	GLY	CA-C-O	5.11	124.48	118.96
1	H	262	GLY	CA-C-O	5.11	124.48	118.96
1	I	262	GLY	CA-C-O	5.11	124.47	118.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	105	ARG	CA-CB-CG	-5.10	103.89	114.10
1	D	105	ARG	CA-CB-CG	-5.10	103.89	114.10
1	H	105	ARG	CA-CB-CG	-5.10	103.90	114.10
1	L	105	ARG	CA-CB-CG	-5.10	103.90	114.10
1	H	127	GLY	CA-C-N	5.10	125.50	119.99
1	H	127	GLY	C-N-CA	5.10	125.50	119.99
1	L	23	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	262	GLY	CA-C-O	5.10	124.47	118.96
1	C	324	PRO	N-CA-C	5.09	124.82	112.10
1	D	324	PRO	N-CA-C	5.09	124.82	112.10
1	G	324	PRO	N-CA-C	5.09	124.81	112.10
1	H	324	PRO	N-CA-C	5.09	124.82	112.10
1	J	324	PRO	N-CA-C	5.09	124.82	112.10
1	F	324	PRO	N-CA-C	5.08	124.81	112.10
1	A	324	PRO	N-CA-C	5.08	124.81	112.10
1	A	262	GLY	CA-C-O	5.08	124.45	118.96
1	L	127	GLY	CA-C-N	5.08	125.47	119.99
1	L	127	GLY	C-N-CA	5.08	125.47	119.99
1	G	262	GLY	CA-C-O	5.08	124.44	118.96
1	K	127	GLY	CA-C-N	5.08	125.47	119.99
1	K	127	GLY	C-N-CA	5.08	125.47	119.99
1	K	324	PRO	N-CA-C	5.08	124.79	112.10
1	D	127	GLY	CA-C-N	5.07	125.47	119.99
1	D	127	GLY	C-N-CA	5.07	125.47	119.99
1	F	127	GLY	CA-C-N	5.07	125.47	119.99
1	F	127	GLY	C-N-CA	5.07	125.47	119.99
1	L	324	PRO	N-CA-C	5.07	124.78	112.10
1	B	324	PRO	N-CA-C	5.07	124.78	112.10
1	E	324	PRO	N-CA-C	5.07	124.78	112.10
1	I	324	PRO	N-CA-C	5.07	124.78	112.10
1	J	23	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	36	HIS	CB-CG-ND1	5.07	130.30	122.70
1	I	23	ASP	CA-CB-CG	5.07	117.67	112.60
1	F	262	GLY	CA-C-O	5.06	124.43	118.96
1	E	23	ASP	CA-CB-CG	5.06	117.66	112.60
1	E	84	THR	N-CA-C	5.06	117.15	108.90
1	J	36	HIS	CB-CG-ND1	5.06	130.29	122.70
1	J	127	GLY	CA-C-N	5.06	125.45	119.99
1	J	127	GLY	C-N-CA	5.06	125.45	119.99
1	K	84	THR	N-CA-C	5.05	117.14	108.90
1	A	127	GLY	CA-C-N	5.05	125.45	119.99
1	A	127	GLY	C-N-CA	5.05	125.45	119.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	36	HIS	CB-CG-ND1	5.05	130.28	122.70
1	B	23	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	23	ASP	CA-CB-CG	5.05	117.65	112.60
1	G	84	THR	N-CA-C	5.05	117.13	108.90
1	H	23	ASP	CA-CB-CG	5.05	117.65	112.60
1	E	127	GLY	CA-C-N	5.05	125.44	119.99
1	E	127	GLY	C-N-CA	5.05	125.44	119.99
1	L	84	THR	N-CA-C	5.05	117.13	108.90
1	L	262	GLY	CA-C-O	5.05	124.41	118.96
1	L	36	HIS	CB-CG-ND1	5.05	130.27	122.70
1	G	36	HIS	CB-CG-ND1	5.04	130.27	122.70
1	J	262	GLY	CA-C-O	5.04	124.40	118.96
1	B	244	ASN	CA-CB-CG	-5.04	107.56	112.60
1	D	23	ASP	CA-CB-CG	5.04	117.64	112.60
1	G	23	ASP	CA-CB-CG	5.04	117.64	112.60
1	D	36	HIS	CB-CG-ND1	5.04	130.26	122.70
1	E	36	HIS	CB-CG-ND1	5.04	130.26	122.70
1	A	36	HIS	CB-CG-ND1	5.04	130.25	122.70
1	F	36	HIS	CB-CG-ND1	5.04	130.25	122.70
1	H	244	ASN	CA-CB-CG	-5.04	107.56	112.60
1	E	73	THR	N-CA-C	5.03	119.29	113.20
1	A	84	THR	N-CA-C	5.03	117.10	108.90
1	B	84	THR	N-CA-C	5.03	117.10	108.90
1	F	84	THR	N-CA-C	5.03	117.10	108.90
1	J	84	THR	N-CA-C	5.03	117.10	108.90
1	A	244	ASN	CA-CB-CG	-5.03	107.57	112.60
1	C	36	HIS	CB-CG-ND1	5.03	130.25	122.70
1	C	84	THR	N-CA-C	5.03	117.10	108.90
1	L	359	ARG	N-CA-C	5.03	119.13	112.89
1	F	73	THR	N-CA-C	5.03	119.28	113.20
1	F	226	ASN	CA-CB-CG	-5.03	107.57	112.60
1	B	226	ASN	CA-CB-CG	-5.03	107.57	112.60
1	C	23	ASP	CA-CB-CG	5.03	117.63	112.60
1	E	359	ARG	N-CA-C	5.03	119.12	112.89
1	F	23	ASP	CA-CB-CG	5.03	117.63	112.60
1	G	359	ARG	N-CA-C	5.03	119.12	112.89
1	H	84	THR	N-CA-C	5.02	117.09	108.90
1	C	226	ASN	CA-CB-CG	-5.02	107.58	112.60
1	C	244	ASN	CA-CB-CG	-5.02	107.58	112.60
1	D	84	THR	N-CA-C	5.02	117.08	108.90
1	I	127	GLY	CA-C-N	5.02	125.41	119.99
1	I	127	GLY	C-N-CA	5.02	125.41	119.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	36	HIS	CB-CG-ND1	5.02	130.22	122.70
1	D	359	ARG	N-CA-C	5.02	119.11	112.89
1	B	127	GLY	CA-C-N	5.01	125.41	119.99
1	B	127	GLY	C-N-CA	5.01	125.41	119.99
1	I	226	ASN	CA-CB-CG	-5.01	107.59	112.60
1	K	244	ASN	CA-CB-CG	-5.01	107.59	112.60
1	I	73	THR	N-CA-C	5.01	119.27	113.20
1	E	244	ASN	CA-CB-CG	-5.01	107.59	112.60
1	H	36	HIS	CB-CG-ND1	5.01	130.22	122.70
1	I	84	THR	N-CA-C	5.01	117.07	108.90
1	C	127	GLY	CA-C-N	5.01	125.40	119.99
1	C	127	GLY	C-N-CA	5.01	125.40	119.99
1	G	127	GLY	CA-C-N	5.01	125.40	119.99
1	G	127	GLY	C-N-CA	5.01	125.40	119.99
1	I	244	ASN	CA-CB-CG	-5.01	107.59	112.60
1	L	244	ASN	CA-CB-CG	-5.01	107.59	112.60
1	E	226	ASN	CA-CB-CG	-5.01	107.59	112.60
1	H	226	ASN	CA-CB-CG	-5.01	107.59	112.60
1	K	359	ARG	N-CA-C	5.01	119.10	112.89
1	G	226	ASN	CA-CB-CG	-5.00	107.60	112.60
1	H	359	ARG	N-CA-C	5.00	119.09	112.89
1	J	244	ASN	CA-CB-CG	-5.00	107.60	112.60
1	A	226	ASN	CA-CB-CG	-5.00	107.60	112.60
1	B	359	ARG	N-CA-C	5.00	119.09	112.89

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3455	0	3371	64	0
1	B	3455	0	3371	68	0
1	C	3455	0	3371	70	2
1	D	3455	0	3371	66	0
1	E	3455	0	3371	64	0
1	F	3455	0	3371	62	2
1	G	3455	0	3371	63	0
1	H	3455	0	3371	61	0
1	I	3455	0	3371	67	0
1	J	3455	0	3371	62	0
1	K	3455	0	3371	71	0
1	L	3455	0	3371	64	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	719	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 9.

All (719) 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:C:192:ARG:HD3	1:C:219:ASN:HD22	1.57	0.69
1:F:425:ARG:HG2	1:F:429:LYS:HD2	1.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:NZ	1:I:383:LYS:HB3	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:NZ	1:C:383:LYS:HB3	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:NZ	1:H:383:LYS:HB3	2.15	0.61
1:I:458:HIS:HD2	1:I:460:VAL:H	1.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NZ	1:K:383:LYS:HB3	2.15	0.61
1:L:383:LYS:NZ	1:L:383:LYS:HB3	2.15	0.61
1:C:458:HIS:HD2	1:C:460:VAL:H	1.48	0.61
1:B:383:LYS:HB3	1:B:383:LYS:NZ	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:NZ	1:E:383:LYS:HB3	2.15	0.60
1:J:383:LYS:HB3	1:J:383:LYS:NZ	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
1:A:458:HIS:HD2	1:A:460:VAL:H	1.48	0.59
1:C:180:PHE:HB3	1:D:29:GLN:HB3	1.83	0.59
1:C:261:PHE:HB2	1:K:457:PRO:HD2	1.82	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:A:29:GLN:HB3	1:F:180:PHE:HB3	1.84	0.59
1:E:76:ILE:HD12	1:E:85:LEU:HD23	1.85	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:VAL:HG13	1:G:92:LEU:HB2	1.84	0.58
1:G:76:ILE:HD12	1:G:85:LEU:HD23	1.85	0.58
1:J:66:VAL:HG13	1:J:92:LEU:HB2	1.84	0.58
1:J:76:ILE:HD12	1:J:85:LEU:HD23	1.85	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:92:LEU:HA	1:G:99:GLY:HA2	1.85	0.58
1:G:192:ARG:HD3	1:G:219:ASN:ND2	2.19	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
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:B:192:ARG:HD3	1:B:219:ASN:ND2	2.19	0.56
1:D:456:THR:O	1:J:458:HIS:HE1	1.87	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:65:MET:HE2	1:A:94:PRO:HD3	1.89	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:I:65:MET:HE2	1:I:94:PRO:HD3	1.89	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:65:MET:HE2	1:D:94:PRO:HD3	1.89	0.54
1:C:65:MET:HE2	1:C:94:PRO:HD3	1.89	0.54
1:D:19:LEU:HD11	1:D:42:PHE:HZ	1.72	0.54
1:L:65:MET:HE2	1:L:94:PRO:HD3	1.89	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
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:J:65:MET:HE2	1:J:94:PRO:HD3	1.89	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:K:65:MET:HE2	1:K:94:PRO:HD3	1.89	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:E:65:MET:HE2	1:E:94:PRO:HD3	1.89	0.53
1:G:65:MET:HE2	1:G:94:PRO:HD3	1.89	0.53
1:G:286:LYS:HB2	1:G:290:LEU:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:65:MET:HE2	1:H:94:PRO:HD3	1.89	0.53
1:A:261:PHE:HB2	1:G:457:PRO:HD2	1.91	0.53
1:B:65:MET:HE2	1:B:94:PRO:HD3	1.89	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:F:65:MET:HE2	1:F:94:PRO:HD3	1.89	0.53
1:J:383:LYS:HB3	1:J:383:LYS:HZ3	1.74	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:456:THR:O	1:L:458:HIS:HE1	1.94	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:PHE:HB2	1:J:457:PRO:HD2	1.93	0.50
1:D:457:PRO:HD2	1:J:261:PHE:HB2	1.92	0.50
1:F:93:GLU:HB3	1:F:98:GLN:OE1	2.11	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:111:ALA:HB3	1:B:228:MET:HE1	1.95	0.49
1:B:273:SER:HB2	3:B:472:AMP:N1	2.27	0.49
1:E:111:ALA:HB3	1:E:228:MET:HE1	1.95	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:J:111:ALA:HB3	1:J:228:MET:HE1	1.95	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:G:111:ALA:HB3	1:G:228:MET:HE1	1.95	0.49
1:E:192:ARG:HH11	1:E:219:ASN:ND2	2.11	0.49
1:F:111:ALA:HB3	1:F:228:MET:HE1	1.95	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
1:C:111:ALA:HB3	1:C:228:MET:HE1	1.95	0.49
1:F:457:PRO:HD2	1:H:261:PHE:HB2	1.93	0.49
1:J:339:ARG:NH2	1:K:50:ASP:CG	2.70	0.49
1:B:192:ARG:HH11	1:B:219:ASN:ND2	2.11	0.49
1:B:383:LYS:HB3	1:B:383:LYS:HZ3	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:111:ALA:HB3	1:H:228:MET:HE1	1.95	0.49
1:I:111:ALA:HB3	1:I:228:MET:HE1	1.95	0.49
1:L:111:ALA:HB3	1:L:228:MET:HE1	1.95	0.49
1:F:17:VAL:HG21	1:F:38:VAL:HG21	1.95	0.48
1:K:111:ALA:HB3	1:K:228:MET:HE1	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:E:158:TRP:HZ3	1:E:260:MET:HE3	1.78	0.48
1:L:312:ALA:HB1	1:L:361:PRO:HB3	1.94	0.48
1:F:158:TRP:HZ3	1:F:260:MET:HE3	1.78	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:I:158:TRP:HZ3	1:I:260:MET:HE3	1.78	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:C:458:HIS:HE1	1:K:456:THR:O	1.96	0.48
1:D:158:TRP:HZ3	1:D:260:MET:HE3	1.79	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: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:G:158:TRP:HZ3	1:G:260:MET:HE3	1.78	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:J:158:TRP:HZ3	1:J:260:MET:HE3	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:F:383:LYS:HB3	1:F:383:LYS:HZ3	1.78	0.48
1:J:17:VAL:HG21	1:J:38:VAL:HG21	1.95	0.48
1:C:57:TRP:CH2	1:C:91:ILE:HG13	2.49	0.48
1:C:192:ARG:HH11	1:C:219:ASN:ND2	2.11	0.48
1:D:12:HIS:HB2	1:D:14:VAL:HG23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:TRP:CH2	1:D:91:ILE:HG13	2.49	0.48
1:D:111:ALA:HB3	1:D:228:MET:HE1	1.95	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
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:K:383:LYS:HB3	1:K:383:LYS:HZ3	1.77	0.48
1:A:111:ALA:HB3	1:A:228:MET:HE1	1.95	0.48
1:B:12:HIS:HB2	1:B:14:VAL:HG23	1.96	0.48
1:B:121:ALA:HA	1:B:276:LYS:HD2	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:57:TRP:CH2	1:G:91:ILE:HG13	2.49	0.47
1:G:121:ALA:HA	1:G:276:LYS:HD2	1.96	0.47
1:K:101:ASP:HB3	1:K:110:ARG:HH22	1.78	0.47
1:A:158:TRP:HZ3	1:A:260:MET:HE3	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:L:158:TRP:HZ3	1:L:260:MET:HE3	1.78	0.47
1:C:101:ASP:HB3	1:C:110:ARG:HH22	1.78	0.47
1:C:315:THR:HB	1:K:465:TYR:CZ	2.49	0.47
1:G:120:ILE:O	1:G:281:LEU:HD21	2.15	0.47
1:H:57:TRP:CH2	1:H:91:ILE:HG13	2.49	0.47
1:H:120:ILE:O	1:H:281:LEU:HD21	2.15	0.47
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.65	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:B:158:TRP:HZ3	1:B:260:MET:HE3	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:ILE:O	1:E:281:LEU:HD21	2.15	0.47
1:E:121:ALA:HA	1:E:276:LYS:HD2	1.96	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:17:VAL:HG21	1:I:38:VAL:HG21	1.95	0.47
1:I:121:ALA:HA	1:I:276:LYS:HD2	1.96	0.47
1:L:17:VAL:HG21	1:L:38:VAL:HG21	1.95	0.47
1:L:101:ASP:HB3	1:L:110:ARG:HH22	1.78	0.47
1:A:120:ILE:O	1:A:281:LEU:HD21	2.15	0.47
1:A:269:HIS:HE1	1:A:359:ARG:NH1	2.12	0.47
1:E:101:ASP:HB3	1:E:110:ARG:HH22	1.78	0.47
1:H:158:TRP:HZ3	1:H:260:MET:HE3	1.79	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
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: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:D:120:ILE:O	1:D:281:LEU:HD21	2.15	0.47
1:F:231:LYS:HA	1:F:231:LYS:HD2	1.65	0.47
1:I:207:GLU:OE1	3:I:479:AMP:O3'	2.26	0.47
1:K:57:TRP:CH2	1:K:91:ILE:HG13	2.49	0.47
1:K:158:TRP:HZ3	1:K:260:MET:HE3	1.78	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:269:HIS:HE1	1:H:359:ARG:NH1	2.12	0.47
1:H:348:VAL:HG21	1:H:353:ALA:HB3	1.97	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:HA	1:D:231:LYS:HD2	1.65	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:456:THR:O	1:K:458:HIS:HE1	1.99	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: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:D:272:MET:HE3	1:D:272:MET:HB2	1.81	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
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:121:ALA:HA	1:A:276:LYS:HD2	1.96	0.46
1:A:273:SER:CB	3:A:471:AMP:N1	2.79	0.46
1:C:158:TRP:HZ3	1:C:260:MET:HE3	1.79	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:272:MET:HE3	1:B:272:MET:HB2	1.82	0.45
1:B:290:LEU:HD11	1:B:345:ILE:HD12	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	1:C:383:LYS:HZ3	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
1:K:231:LYS:HD2	1:K:231:LYS:HA	1.65	0.45
1:B:273:SER:CB	3:B:472:AMP:N1	2.79	0.45
1:E:231:LYS:HD2	1:E:231:LYS:HA	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: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:I:231:LYS:HA	1:I:231:LYS:HD2	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: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:C:465:TYR:CE2	1:K:315:THR:HB	2.52	0.44
1:J:255:PHE:HB3	1:J:363:PRO:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:O	1:C:388:PRO:HD3	2.18	0.44
1:D:466:TYR:CZ	1:J:138:ILE:HG21	2.52	0.44
1:G:255:PHE:HB3	1:G:363:PRO:HB2	2.00	0.44
1:I:295:LEU:O	1:I:388:PRO:HD3	2.17	0.44
1:C:272:MET:HE3	1:C:272:MET:HB2	1.82	0.44
1:F:255:PHE:HB3	1:F:363:PRO:HB2	2.00	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:HD2	1:C:231:LYS:HA	1.65	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:PRO:HB2	1:D:352:LYS:HG3	2.01	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:I:272:MET:HB2	1:I:272:MET:HE3	1.81	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:HB3	1:G:383:LYS:HZ3	1.81	0.42
1:E:351:PRO:HB2	1:E:352:LYS:HG3	2.01	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:A:138:ILE:O	1:F:168:ASN:HB3	2.19	0.42
1:C:351:PRO:HB2	1:C:352:LYS:HG3	2.01	0.42
1:H:68:MET:HA	1:H:69:PRO:HD2	1.93	0.42
1:H:207:GLU:OE1	3:H:478:AMP:O3'	2.26	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:272:MET:HE3	1:F:272:MET:HB2	1.82	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:J:231:LYS:HD2	1:J:231:LYS:HA	1.65	0.42
1:K:339:ARG:CZ	1:K:359:ARG:NH2	2.83	0.42
1:L:272:MET:HE3	1:L:272:MET:HB2	1.82	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:B:138:ILE:HG21	1:L:466:TYR:CZ	2.54	0.42
1:C:465:TYR:CZ	1:K:315:THR:HB	2.55	0.42
1:E:466:TYR:CZ	1:I:138:ILE:HG21	2.54	0.42
1:F:257:PRO:HD2	1:F:317:ASN:OD1	2.20	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:C:257:PRO:HD2	1:C:317:ASN:OD1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:466:TYR:CZ	1:G:138:ILE:HG21	2.54	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: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
1:H:257:PRO:HD2	1:H:317:ASN:OD1	2.20	0.41
1:I:3:GLU:O	1:I:7:THR:HG23	2.21	0.41
1:I:257:PRO:HD2	1:I:317:ASN:OD1	2.20	0.41
1:J:100:TYR:CE2	1:J:102:ARG:HB3	2.55	0.41
1:J:272:MET:HE3	1:J:272:MET:HB2	1.82	0.41
1:K:3:GLU:O	1:K:7:THR:HG23	2.21	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: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:3:GLU:O	1:C:7:THR:HG23	2.21	0.41
1:C:100:TYR:CE2	1:C:102:ARG:HB3	2.55	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:66:VAL:CG1	1:D:92:LEU:HB2	2.51	0.41
1:D:100:TYR:CE2	1:D:102:ARG:HB3	2.55	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:A:196:CYS:SG	1:A:206:VAL:HG11	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ARG:HD3	1:A:436:ASP:OD1	2.21	0.41
1:A:465:TYR:CE2	1:G:315:THR:HB	2.56	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:169:LYS:HA	1:E:252:THR:HB	2.03	0.41
1:D:257:PRO:HD2	1:D:317:ASN:OD1	2.20	0.41
1:E:114:TYR:CD1	1:E:431:GLY:HA3	2.56	0.41
1:G:66:VAL:CG1	1:G:92:LEU:HB2	2.51	0.41
1:G:334:TYR:HA	1:G:343:ILE:O	2.21	0.41
1:H:3:GLU:O	1:H:7:THR:HG23	2.21	0.41
1:H:100:TYR:CE2	1:H:102:ARG:HB3	2.55	0.41
1:H:114:TYR:CD1	1:H:431:GLY:HA3	2.56	0.41
1:I:196:CYS:SG	1:I:206:VAL:HG11	2.61	0.41
1:K:272:MET:HE3	1:K:272:MET:HB2	1.82	0.41
1:K:458:HIS:HD2	1:K:460:VAL:N	2.14	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:3:GLU:O	1:B:7:THR:HG23	2.21	0.41
1:B:257:PRO:HD2	1:B:317:ASN:OD1	2.20	0.41
1:D:3:GLU:O	1:D:7:THR:HG23	2.21	0.41
1:D:196:CYS:SG	1:D:206:VAL:HG11	2.61	0.41
1:E:3:GLU:O	1:E: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: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:114:TYR:CD1	1:J:431:GLY:HA3	2.56	0.41
1:J:257:PRO:HD2	1:J:317:ASN:OD1	2.20	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:B:352:LYS:C	1:B:354:ARG:H	2.29	0.40
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:LYS:HA	1:C:252:THR:HB	2.03	0.40
1:B:296:TYR:O	1:B:381:GLY:HA3	2.22	0.40
1:C:68:MET:HA	1:C:69:PRO:HD2	1.93	0.40
1:C:268:MET:H	1:C:362:ASP:HA	1.86	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:268:MET:H	1:B:362:ASP:HA	1.86	0.40
1:B:350:SER:OG	1:B:351:PRO:HD3	2.21	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:D:352:LYS:C	1:D:354:ARG:H	2.29	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:296:TYR:O	1:F:381:GLY:HA3	2.22	0.40
1:F:350:SER:OG	1:F:351:PRO:HD3	2.21	0.40
1:G:296:TYR:O	1:G:381:GLY:HA3	2.22	0.40
1:H:352:LYS:C	1:H:354:ARG:H	2.29	0.40
1:J:350:SER:OG	1:J:351:PRO:HD3	2.21	0.40
1:A:114:TYR:CD1	1:A:431:GLY:HA3	2.56	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:B:168:ASN:HB3	1:C:138:ILE:O	2.21	0.40
1:B:465:TYR:CZ	1:L:315:THR:HB	2.56	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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

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	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	B	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	C	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	D	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	E	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	F	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	G	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	H	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	I	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	J	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	K	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
1	L	437/468 (93%)	392 (90%)	31 (7%)	14 (3%)	3	11
All	All	5244/5616 (93%)	4704 (90%)	372 (7%)	168 (3%)	3	11

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	40	ALA
1	K	338	ASN
1	L	40	ALA
1	L	338	ASN
1	A	36	HIS
1	A	340	SER
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	351	PRO
1	K	36	HIS
1	K	340	SER
1	K	351	PRO
1	L	36	HIS
1	L	340	SER
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	169	LYS
1	K	277	ASN
1	K	386	ILE
1	L	169	LYS
1	L	277	ASN
1	L	386	ILE
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%)	327 (90%)	38 (10%)	7	22
1	B	365/384 (95%)	327 (90%)	38 (10%)	7	22
1	C	365/384 (95%)	327 (90%)	38 (10%)	7	22
1	D	365/384 (95%)	327 (90%)	38 (10%)	7	22
1	E	365/384 (95%)	327 (90%)	38 (10%)	7	22
1	F	365/384 (95%)	327 (90%)	38 (10%)	7	22
1	G	365/384 (95%)	327 (90%)	38 (10%)	7	22
1	H	365/384 (95%)	327 (90%)	38 (10%)	7	22
1	I	365/384 (95%)	327 (90%)	38 (10%)	7	22
1	J	365/384 (95%)	327 (90%)	38 (10%)	7	22
1	K	365/384 (95%)	327 (90%)	38 (10%)	7	22
1	L	365/384 (95%)	327 (90%)	38 (10%)	7	22
All	All	4380/4608 (95%)	3924 (90%)	456 (10%)	7	22

All (456) 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	65	MET
1	A	75	VAL
1	A	76	ILE
1	A	85	LEU
1	A	88	ARG
1	A	102	ARG
1	A	105	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	115	LEU
1	A	122	ASP
1	A	124	VAL
1	A	143	SER
1	A	165	GLU
1	A	194	GLU
1	A	223	THR
1	A	230	LYS
1	A	264	ASN
1	A	286	LYS
1	A	314	PRO
1	A	324	PRO
1	A	331	MET
1	A	332	LEU
1	A	340	SER
1	A	352	LYS
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	65	MET
1	B	75	VAL
1	B	76	ILE
1	B	85	LEU
1	B	88	ARG
1	B	102	ARG
1	B	105	ARG
1	B	115	LEU
1	B	122	ASP
1	B	124	VAL
1	B	143	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	165	GLU
1	B	194	GLU
1	B	223	THR
1	B	230	LYS
1	B	264	ASN
1	B	286	LYS
1	B	314	PRO
1	B	324	PRO
1	B	331	MET
1	B	332	LEU
1	B	340	SER
1	B	352	LYS
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	65	MET
1	C	75	VAL
1	C	76	ILE
1	C	85	LEU
1	C	88	ARG
1	C	102	ARG
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	230	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	264	ASN
1	C	286	LYS
1	C	314	PRO
1	C	324	PRO
1	C	331	MET
1	C	332	LEU
1	C	340	SER
1	C	352	LYS
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	65	MET
1	D	75	VAL
1	D	76	ILE
1	D	85	LEU
1	D	88	ARG
1	D	102	ARG
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	230	LYS
1	D	264	ASN
1	D	286	LYS
1	D	314	PRO
1	D	324	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	331	MET
1	D	332	LEU
1	D	340	SER
1	D	352	LYS
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	65	MET
1	E	75	VAL
1	E	76	ILE
1	E	85	LEU
1	E	88	ARG
1	E	102	ARG
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	230	LYS
1	E	264	ASN
1	E	286	LYS
1	E	314	PRO
1	E	324	PRO
1	E	331	MET
1	E	332	LEU
1	E	340	SER
1	E	352	LYS

Continued on next page...

Continued from previous page...

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	65	MET
1	F	75	VAL
1	F	76	ILE
1	F	85	LEU
1	F	88	ARG
1	F	102	ARG
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	230	LYS
1	F	264	ASN
1	F	286	LYS
1	F	314	PRO
1	F	324	PRO
1	F	331	MET
1	F	332	LEU
1	F	340	SER
1	F	352	LYS
1	F	374	LEU
1	F	375	LEU
1	F	383	LYS
1	F	426	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	65	MET
1	G	75	VAL
1	G	76	ILE
1	G	85	LEU
1	G	88	ARG
1	G	102	ARG
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	230	LYS
1	G	264	ASN
1	G	286	LYS
1	G	314	PRO
1	G	324	PRO
1	G	331	MET
1	G	332	LEU
1	G	340	SER
1	G	352	LYS
1	G	374	LEU
1	G	375	LEU
1	G	383	LYS
1	G	426	GLU
1	G	428	LEU
1	G	446	ARG
1	G	464	LEU
1	G	468	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	65	MET
1	H	75	VAL
1	H	76	ILE
1	H	85	LEU
1	H	88	ARG
1	H	102	ARG
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	230	LYS
1	H	264	ASN
1	H	286	LYS
1	H	314	PRO
1	H	324	PRO
1	H	331	MET
1	H	332	LEU
1	H	340	SER
1	H	352	LYS
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
1	I	11	GLU
1	I	19	LEU
1	I	33	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	36	HIS
1	I	39	ASN
1	I	45	GLU
1	I	65	MET
1	I	75	VAL
1	I	76	ILE
1	I	85	LEU
1	I	88	ARG
1	I	102	ARG
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	230	LYS
1	I	264	ASN
1	I	286	LYS
1	I	314	PRO
1	I	324	PRO
1	I	331	MET
1	I	332	LEU
1	I	340	SER
1	I	352	LYS
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
1	J	36	HIS
1	J	39	ASN
1	J	45	GLU
1	J	65	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	75	VAL
1	J	76	ILE
1	J	85	LEU
1	J	88	ARG
1	J	102	ARG
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	230	LYS
1	J	264	ASN
1	J	286	LYS
1	J	314	PRO
1	J	324	PRO
1	J	331	MET
1	J	332	LEU
1	J	340	SER
1	J	352	LYS
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
1	K	65	MET
1	K	75	VAL
1	K	76	ILE
1	K	85	LEU
1	K	88	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	102	ARG
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	230	LYS
1	K	264	ASN
1	K	286	LYS
1	K	314	PRO
1	K	324	PRO
1	K	331	MET
1	K	332	LEU
1	K	340	SER
1	K	352	LYS
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	65	MET
1	L	75	VAL
1	L	76	ILE
1	L	85	LEU
1	L	88	ARG
1	L	102	ARG
1	L	105	ARG
1	L	115	LEU
1	L	122	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	124	VAL
1	L	143	SER
1	L	165	GLU
1	L	194	GLU
1	L	223	THR
1	L	230	LYS
1	L	264	ASN
1	L	286	LYS
1	L	314	PRO
1	L	324	PRO
1	L	331	MET
1	L	332	LEU
1	L	340	SER
1	L	352	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	A	189	GLN
1	A	219	ASN
1	A	236	GLN
1	A	244	ASN
1	A	264	ASN
1	A	269	HIS
1	A	409	GLN
1	A	458	HIS
1	B	30	HIS
1	B	159	ASN
1	B	219	ASN
1	B	236	GLN
1	B	244	ASN
1	B	269	HIS
1	B	409	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	458	HIS
1	C	159	ASN
1	C	219	ASN
1	C	236	GLN
1	C	244	ASN
1	C	269	HIS
1	C	409	GLN
1	C	458	HIS
1	D	159	ASN
1	D	189	GLN
1	D	219	ASN
1	D	236	GLN
1	D	244	ASN
1	D	264	ASN
1	D	269	HIS
1	D	409	GLN
1	D	458	HIS
1	E	30	HIS
1	E	159	ASN
1	E	219	ASN
1	E	236	GLN
1	E	244	ASN
1	E	264	ASN
1	E	269	HIS
1	E	409	GLN
1	E	458	HIS
1	F	159	ASN
1	F	219	ASN
1	F	236	GLN
1	F	244	ASN
1	F	269	HIS
1	F	409	GLN
1	F	458	HIS
1	G	159	ASN
1	G	219	ASN
1	G	236	GLN
1	G	244	ASN
1	G	264	ASN
1	G	269	HIS
1	G	409	GLN
1	G	458	HIS
1	H	159	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	219	ASN
1	H	236	GLN
1	H	244	ASN
1	H	264	ASN
1	H	269	HIS
1	H	409	GLN
1	H	458	HIS
1	I	159	ASN
1	I	219	ASN
1	I	236	GLN
1	I	244	ASN
1	I	264	ASN
1	I	269	HIS
1	I	409	GLN
1	I	458	HIS
1	J	159	ASN
1	J	219	ASN
1	J	236	GLN
1	J	244	ASN
1	J	264	ASN
1	J	269	HIS
1	J	409	GLN
1	J	458	HIS
1	K	159	ASN
1	K	219	ASN
1	K	236	GLN
1	K	244	ASN
1	K	264	ASN
1	K	269	HIS
1	K	338	ASN
1	K	409	GLN
1	K	458	HIS
1	L	159	ASN
1	L	219	ASN
1	L	236	GLN
1	L	244	ASN
1	L	264	ASN
1	L	269	HIS
1	L	409	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	K	481	-	25,25,25	0.94	1 (4%)	37,38,38	0.79	2 (5%)
3	AMP	B	472	-	25,25,25	0.94	1 (4%)	37,38,38	0.79	2 (5%)
3	AMP	E	475	-	25,25,25	0.95	1 (4%)	37,38,38	0.79	2 (5%)
3	AMP	I	479	-	25,25,25	0.94	1 (4%)	37,38,38	0.80	2 (5%)
3	AMP	G	477	-	25,25,25	0.94	1 (4%)	37,38,38	0.79	2 (5%)
3	AMP	A	471	-	25,25,25	0.94	1 (4%)	37,38,38	0.79	2 (5%)
3	AMP	L	482	-	25,25,25	0.94	1 (4%)	37,38,38	0.79	2 (5%)
3	AMP	H	478	-	25,25,25	0.95	1 (4%)	37,38,38	0.79	2 (5%)
3	AMP	F	476	-	25,25,25	0.94	1 (4%)	37,38,38	0.79	2 (5%)
3	AMP	D	474	-	25,25,25	0.94	1 (4%)	37,38,38	0.79	2 (5%)
3	AMP	C	473	-	25,25,25	0.94	1 (4%)	37,38,38	0.79	2 (5%)
3	AMP	J	480	-	25,25,25	0.93	1 (4%)	37,38,38	0.79	2 (5%)

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	K	481	-	-	5/10/26/26	0/3/3/3
3	AMP	B	472	-	-	5/10/26/26	0/3/3/3
3	AMP	E	475	-	-	5/10/26/26	0/3/3/3
3	AMP	I	479	-	-	5/10/26/26	0/3/3/3
3	AMP	G	477	-	-	5/10/26/26	0/3/3/3
3	AMP	A	471	-	-	5/10/26/26	0/3/3/3
3	AMP	L	482	-	-	5/10/26/26	0/3/3/3
3	AMP	H	478	-	-	5/10/26/26	0/3/3/3
3	AMP	F	476	-	-	5/10/26/26	0/3/3/3
3	AMP	D	474	-	-	5/10/26/26	0/3/3/3
3	AMP	C	473	-	-	5/10/26/26	0/3/3/3
3	AMP	J	480	-	-	5/10/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	478	AMP	P-O1P	3.02	1.59	1.50
3	L	482	AMP	P-O1P	3.01	1.59	1.50
3	F	476	AMP	P-O1P	3.01	1.59	1.50
3	E	475	AMP	P-O1P	3.01	1.59	1.50
3	I	479	AMP	P-O1P	3.01	1.59	1.50
3	A	471	AMP	P-O1P	3.01	1.59	1.50
3	B	472	AMP	P-O1P	3.00	1.59	1.50
3	C	473	AMP	P-O1P	3.00	1.59	1.50
3	K	481	AMP	P-O1P	2.99	1.59	1.50
3	D	474	AMP	P-O1P	2.99	1.59	1.50
3	J	480	AMP	P-O1P	2.99	1.59	1.50
3	G	477	AMP	P-O1P	2.98	1.59	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	482	AMP	O3'-C3'-C4'	-2.14	104.94	111.08
3	J	480	AMP	O3'-C3'-C4'	-2.13	104.96	111.08
3	H	478	AMP	O3'-C3'-C4'	-2.13	104.97	111.08
3	B	472	AMP	O3'-C3'-C4'	-2.13	104.97	111.08
3	A	471	AMP	O3'-C3'-C4'	-2.12	104.99	111.08
3	C	473	AMP	O3'-C3'-C4'	-2.12	104.99	111.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	475	AMP	O3'-C3'-C4'	-2.12	104.99	111.08
3	G	477	AMP	O3'-C3'-C4'	-2.12	104.99	111.08
3	D	474	AMP	O3'-C3'-C4'	-2.12	104.99	111.08
3	K	481	AMP	O3'-C3'-C4'	-2.12	105.00	111.08
3	I	479	AMP	O3'-C3'-C4'	-2.12	105.00	111.08
3	F	476	AMP	O3'-C3'-C4'	-2.11	105.03	111.08
3	F	476	AMP	O3P-P-O2P	2.06	115.52	107.80
3	L	482	AMP	O3P-P-O2P	2.06	115.52	107.80
3	I	479	AMP	O3P-P-O2P	2.06	115.51	107.80
3	A	471	AMP	O3P-P-O2P	2.06	115.51	107.80
3	H	478	AMP	O3P-P-O2P	2.06	115.51	107.80
3	C	473	AMP	O3P-P-O2P	2.06	115.51	107.80
3	J	480	AMP	O3P-P-O2P	2.05	115.50	107.80
3	G	477	AMP	O3P-P-O2P	2.05	115.50	107.80
3	D	474	AMP	O3P-P-O2P	2.05	115.49	107.80
3	B	472	AMP	O3P-P-O2P	2.05	115.48	107.80
3	E	475	AMP	O3P-P-O2P	2.05	115.48	107.80
3	K	481	AMP	O3P-P-O2P	2.05	115.48	107.80

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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'
3	B	472	AMP	C3'-C4'-C5'-O5'
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	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'

Continued on next page...

Continued from previous page...

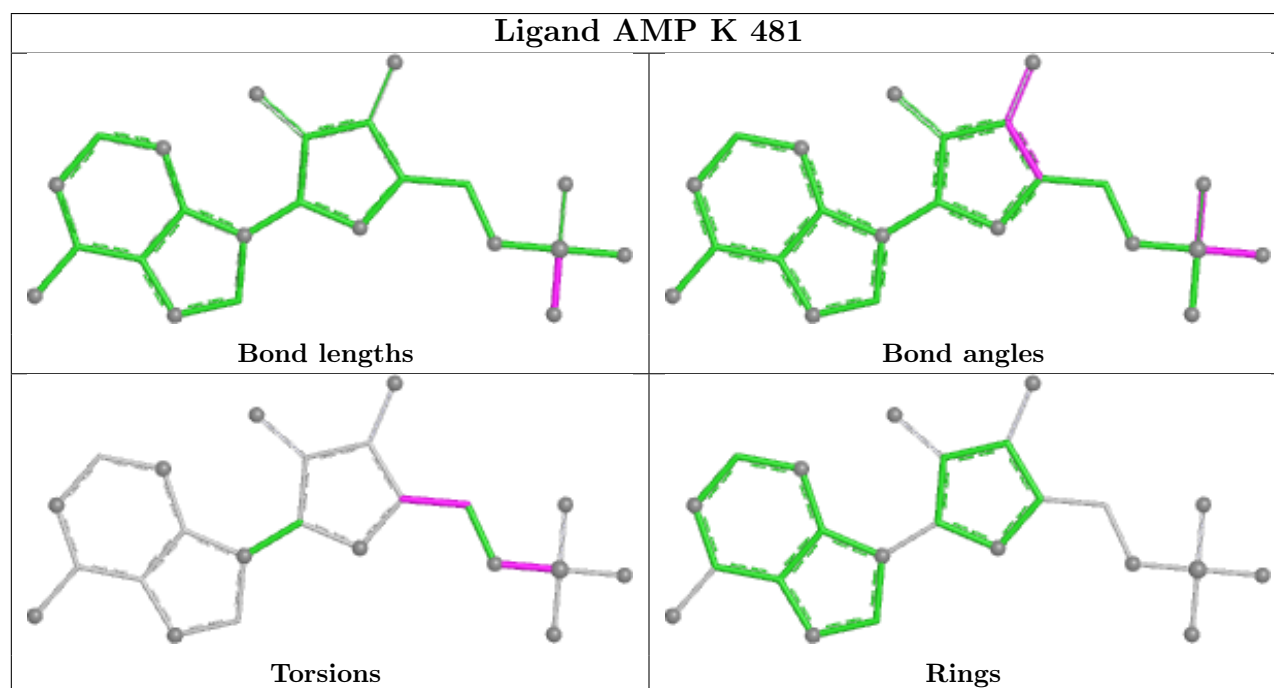
Mol	Chain	Res	Type	Atoms
3	D	474	AMP	C3'-C4'-C5'-O5'
3	E	475	AMP	C5'-O5'-P-O1P
3	E	475	AMP	C5'-O5'-P-O2P
3	E	475	AMP	C5'-O5'-P-O3P
3	E	475	AMP	O4'-C4'-C5'-O5'
3	E	475	AMP	C3'-C4'-C5'-O5'
3	F	476	AMP	C5'-O5'-P-O1P
3	F	476	AMP	C5'-O5'-P-O2P
3	F	476	AMP	C5'-O5'-P-O3P
3	F	476	AMP	O4'-C4'-C5'-O5'
3	F	476	AMP	C3'-C4'-C5'-O5'
3	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	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	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	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	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	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'

There are no ring outliers.

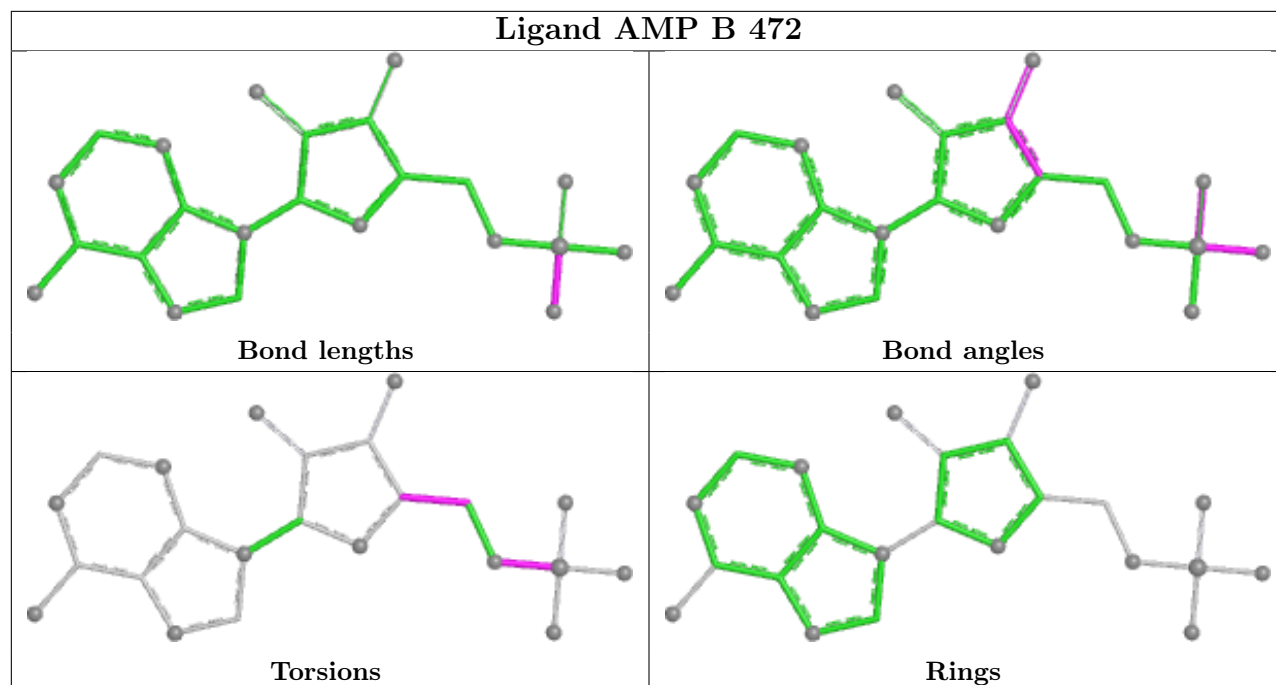
12 monomers are involved in 28 short contacts:

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

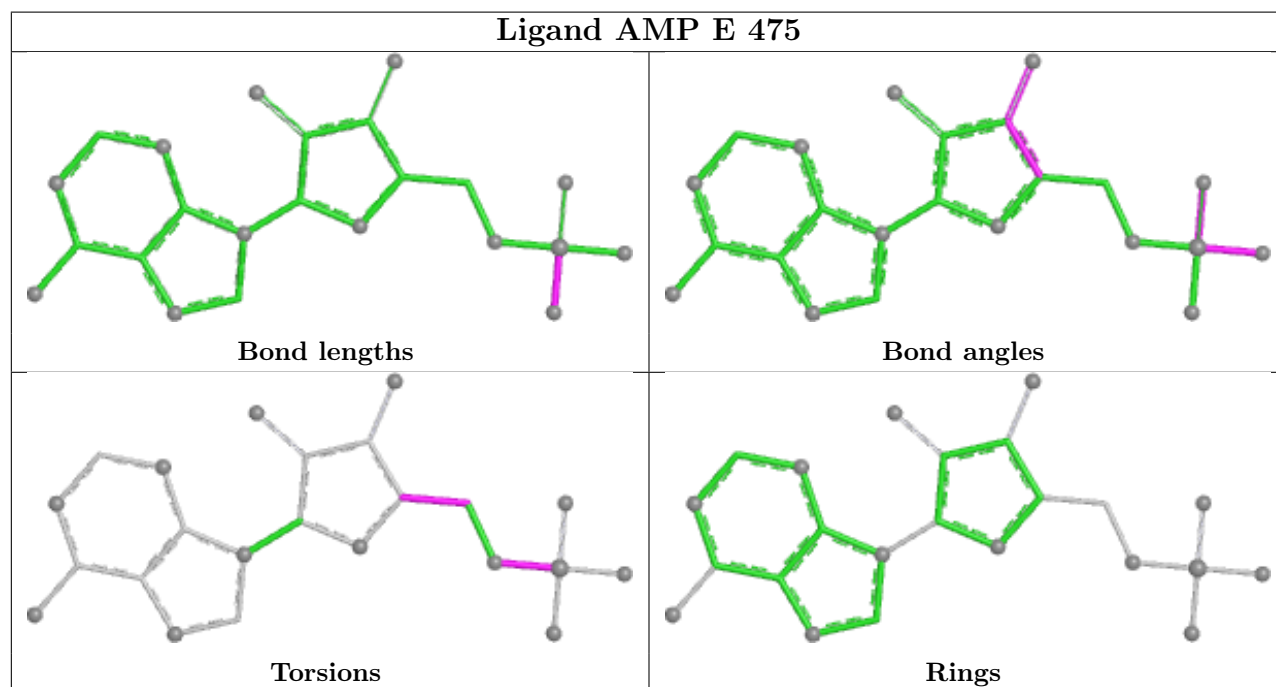
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



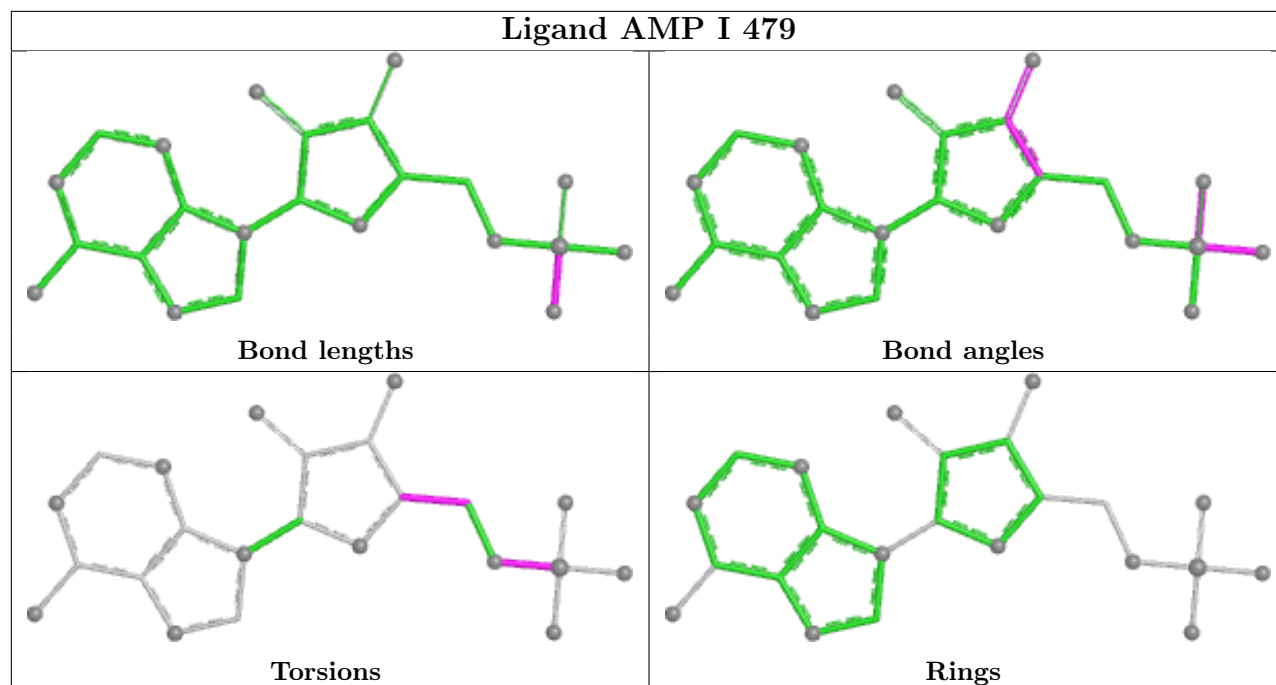
Ligand AMP B 472



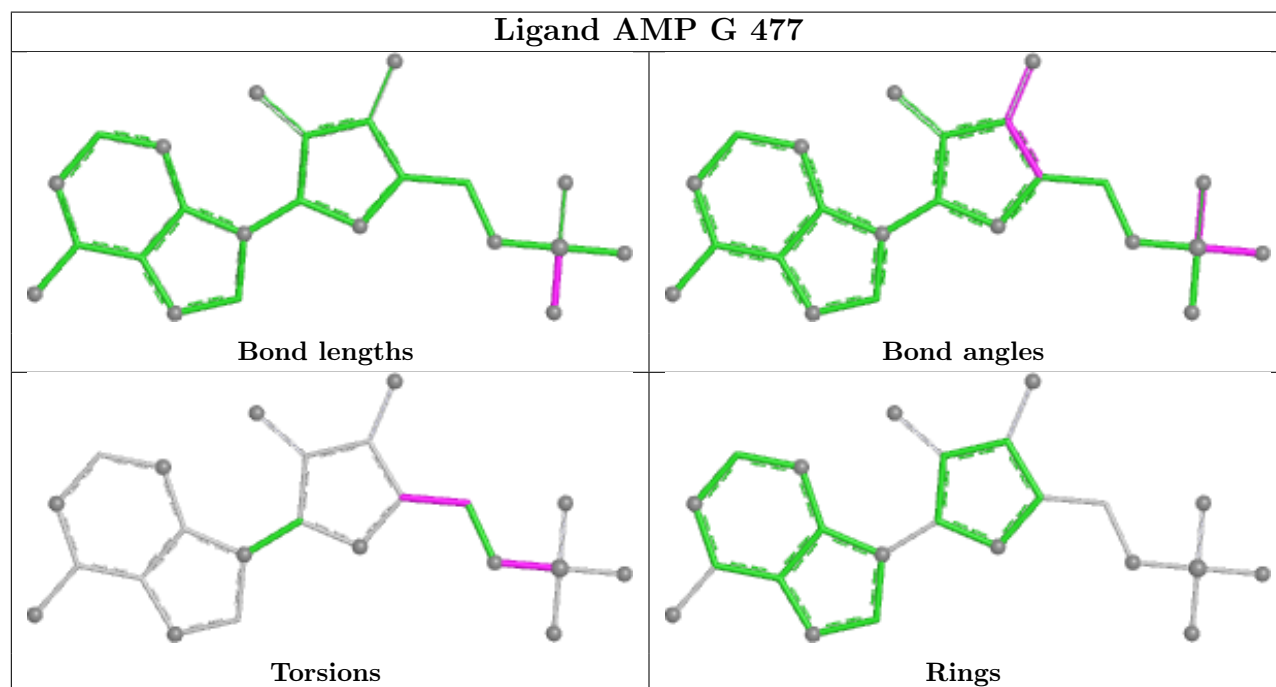
Ligand AMP E 475

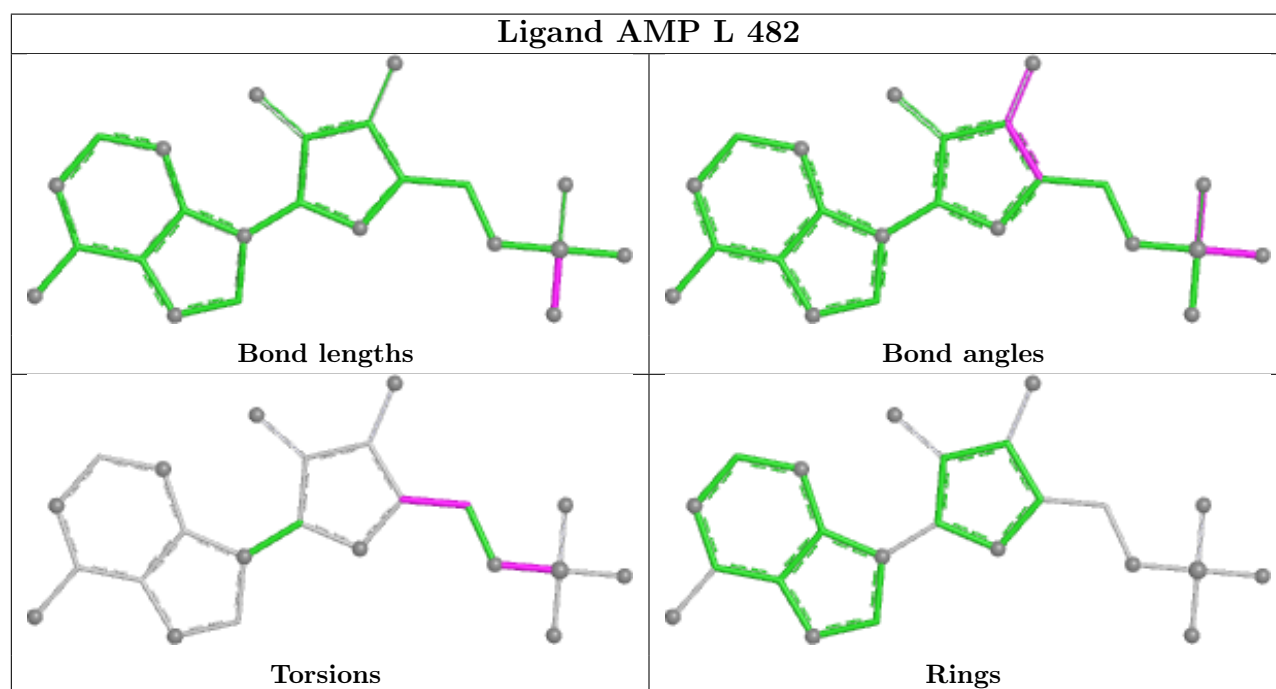
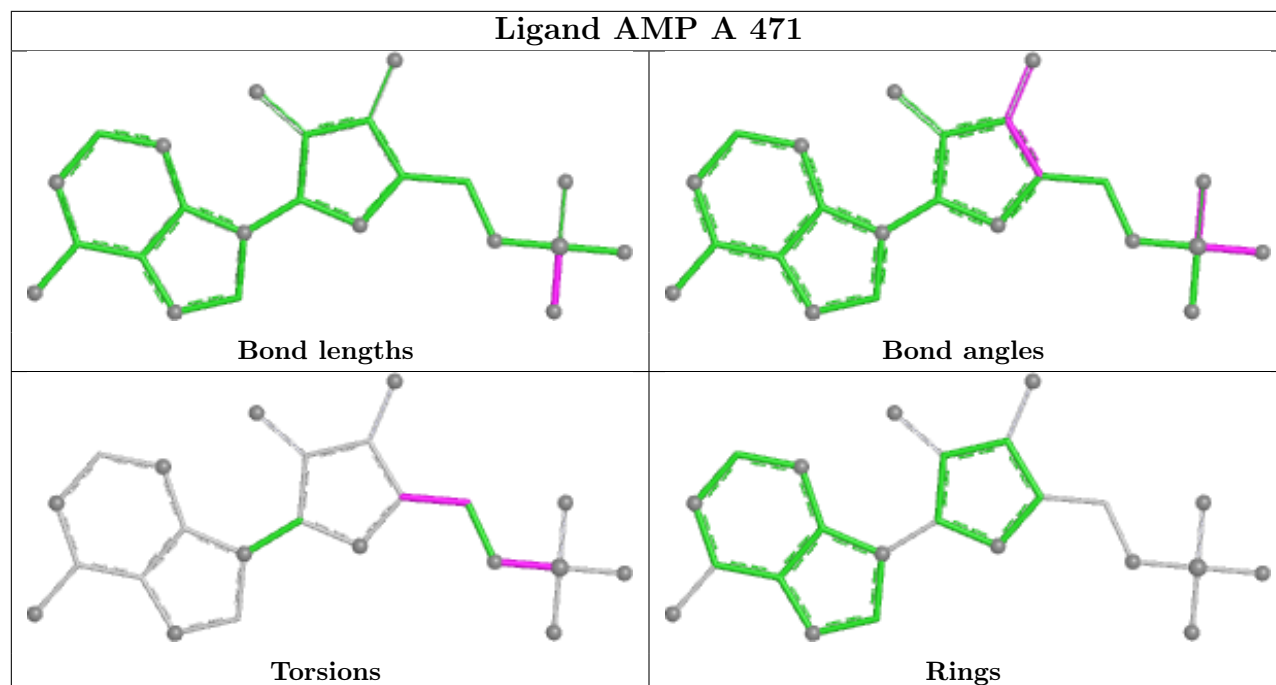


Ligand AMP I 479

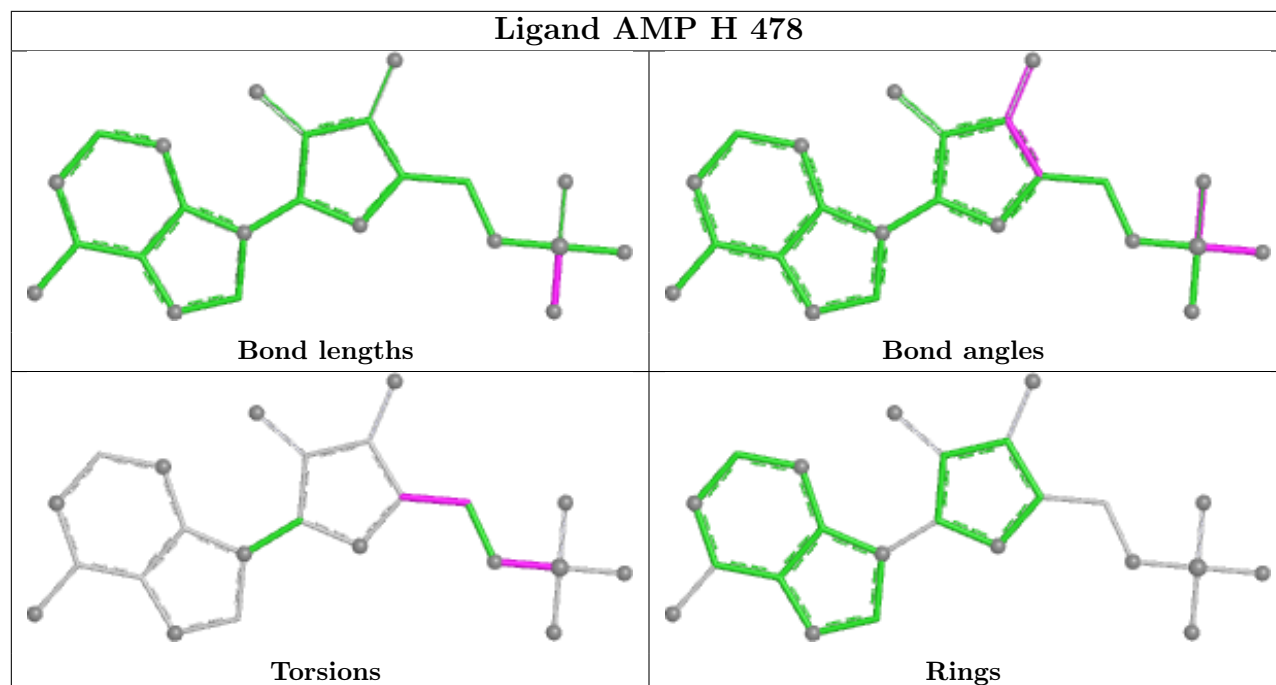


Ligand AMP G 477

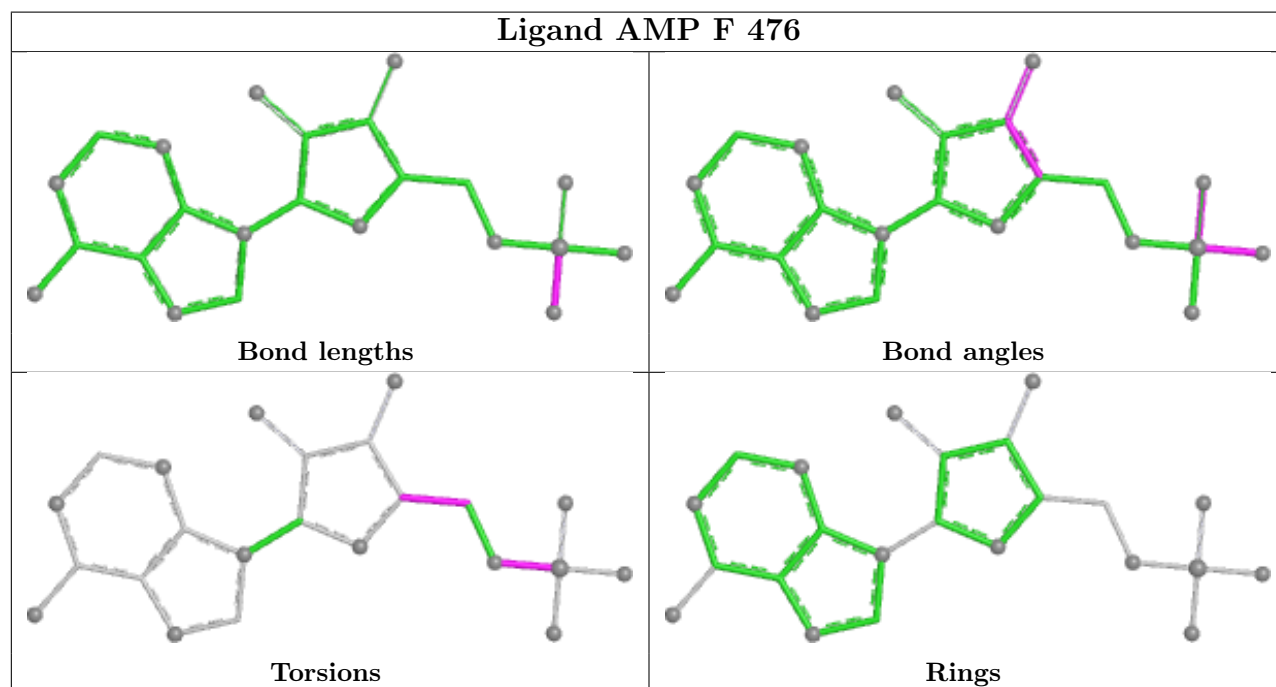




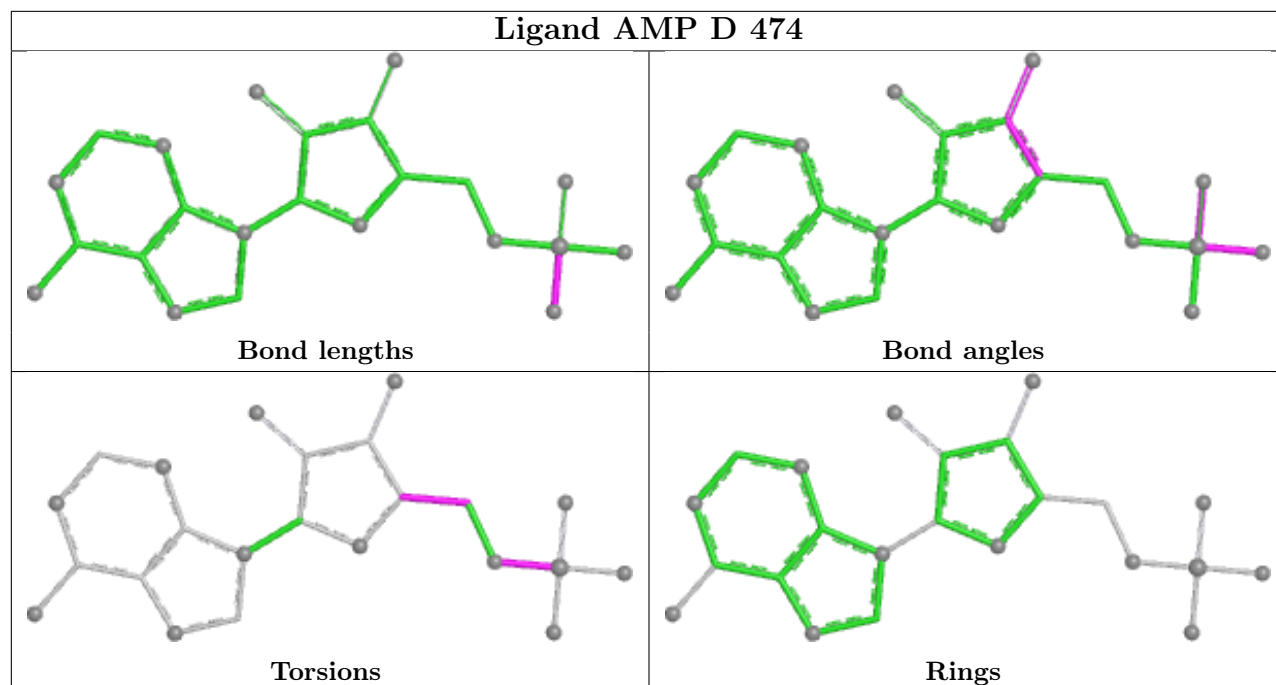
Ligand AMP H 478



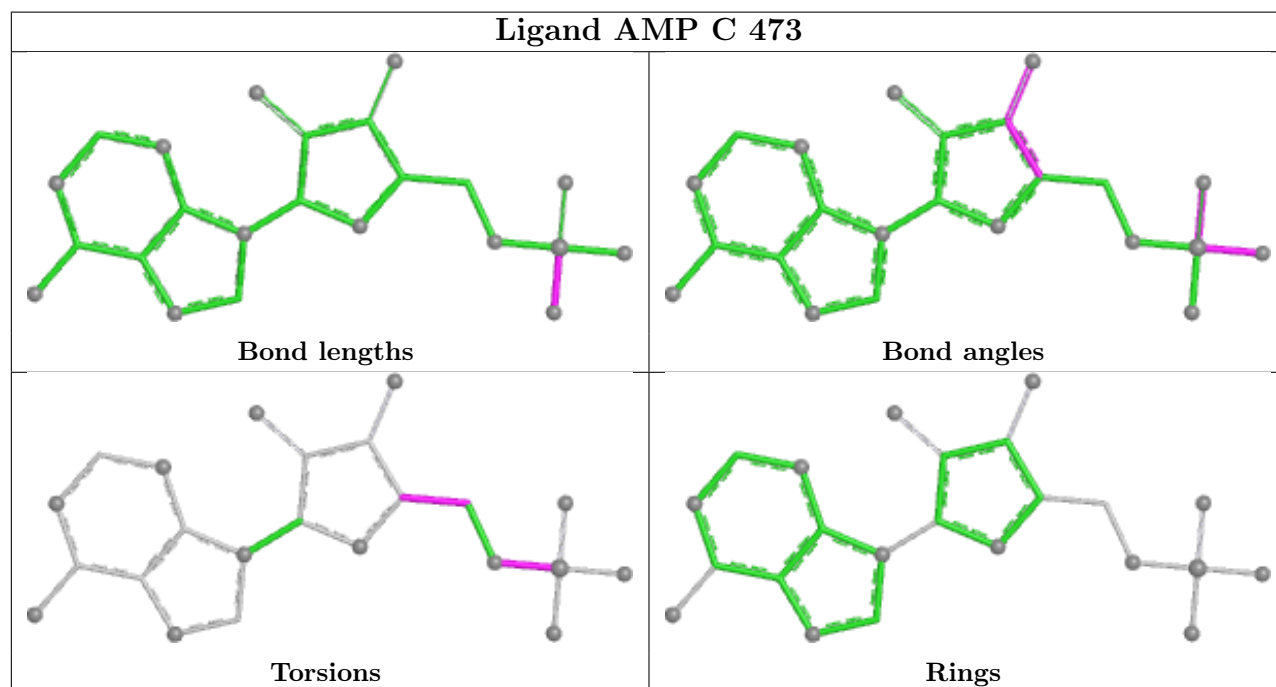
Ligand AMP F 476

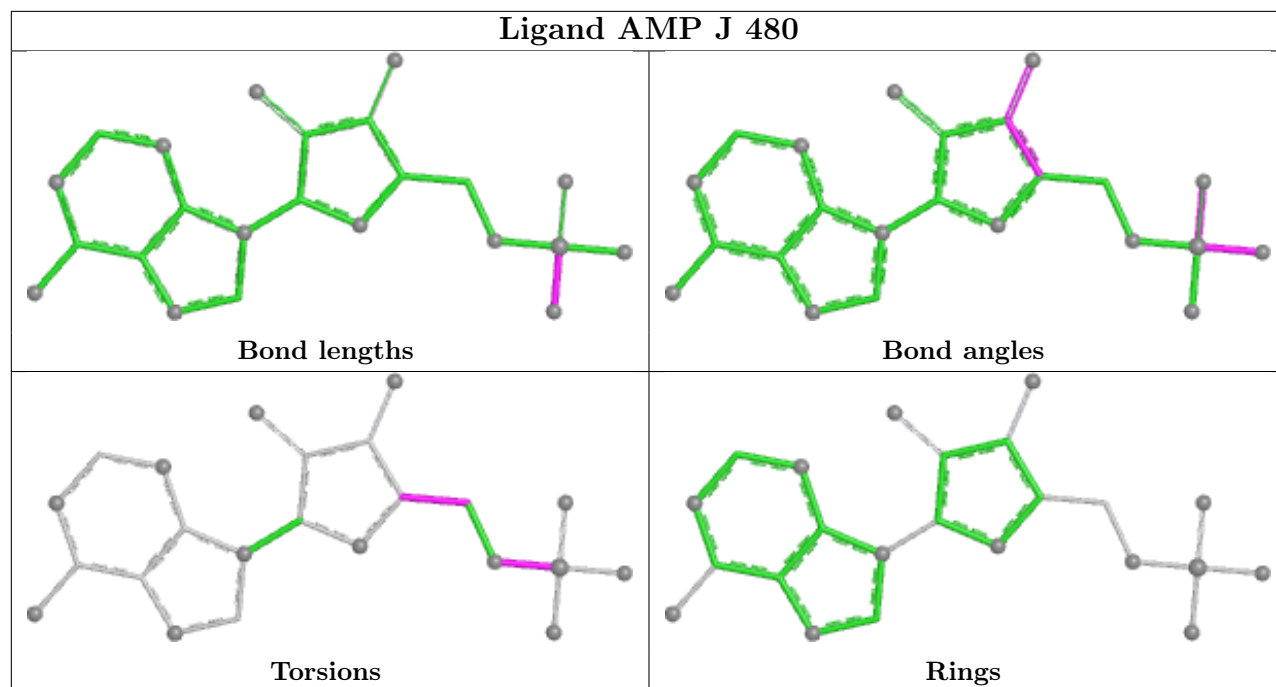


Ligand AMP D 474



Ligand AMP C 473





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.