



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:00 AM UTC

PDB ID : 2LGS / pdb_00002lgs
Title : FEEDBACK INHIBITION OF FULLY UNADENYLYLATED GLUTAMINE
SYNTHETASE FROM SALMONELLA TYPHIMURIUM BY GLYCINE,
ALANINE, AND SERINE
Authors : Liaw, S.-H.; Eisenberg, D.
Deposited on : 1994-08-05
Resolution : 2.80 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
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

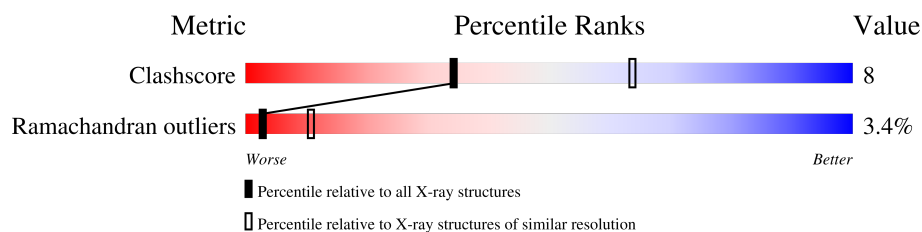
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)

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	 63% 28% . . 5%
1	B	468	 63% 28% . . 5%
1	C	468	 61% 29% . . 5%
1	D	468	 62% 28% . . 5%
1	E	468	 63% 27% . . 5%
1	F	468	 62% 28% . . 5%
1	G	468	 63% 28% . . 5%
1	H	468	 62% 28% . . 5%
1	I	468	 63% 28% . . 5%

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Mol	Chain	Length	Quality of chain
1	J	468	62%28% 5%
1	K	468	61%29% 5%
1	L	468	62%28% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41604 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).

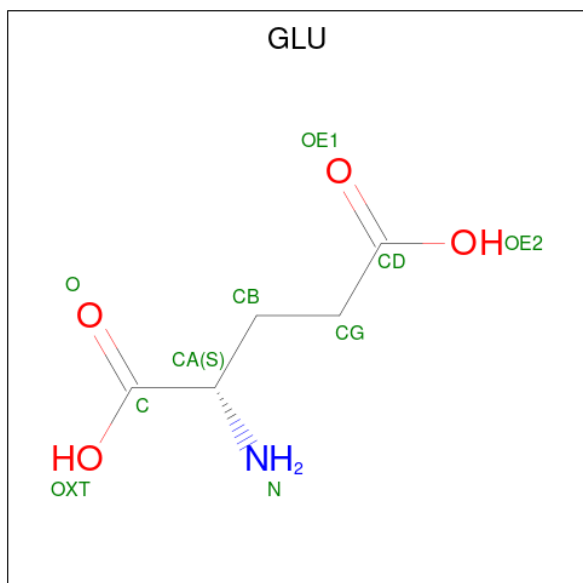
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

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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 GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	5	1	4		

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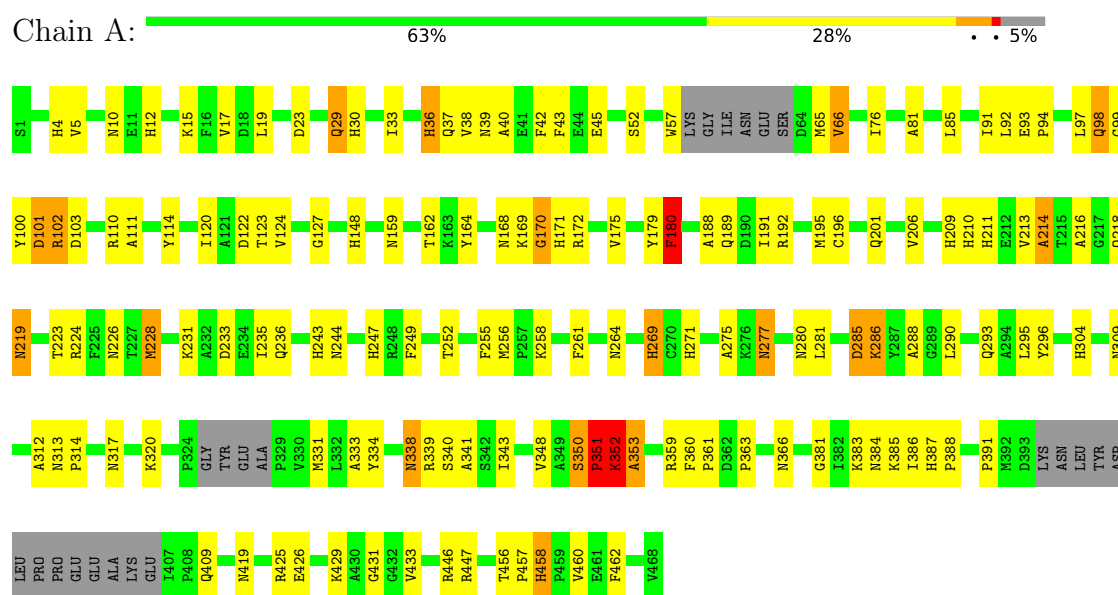
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	5	1	4		
3	C	1	Total	C	N	O	0	0
			10	5	1	4		
3	D	1	Total	C	N	O	0	0
			10	5	1	4		
3	E	1	Total	C	N	O	0	0
			10	5	1	4		
3	F	1	Total	C	N	O	0	0
			10	5	1	4		
3	G	1	Total	C	N	O	0	0
			10	5	1	4		
3	H	1	Total	C	N	O	0	0
			10	5	1	4		
3	I	1	Total	C	N	O	0	0
			10	5	1	4		
3	J	1	Total	C	N	O	0	0
			10	5	1	4		
3	K	1	Total	C	N	O	0	0
			10	5	1	4		
3	L	1	Total	C	N	O	0	0
			10	5	1	4		

3 Residue-property plots

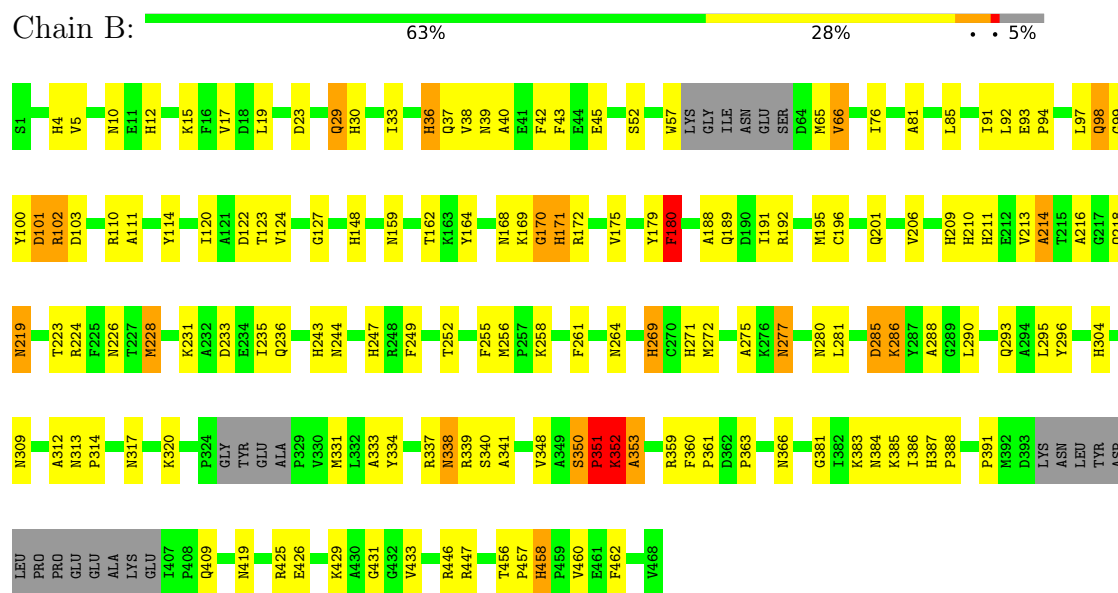
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

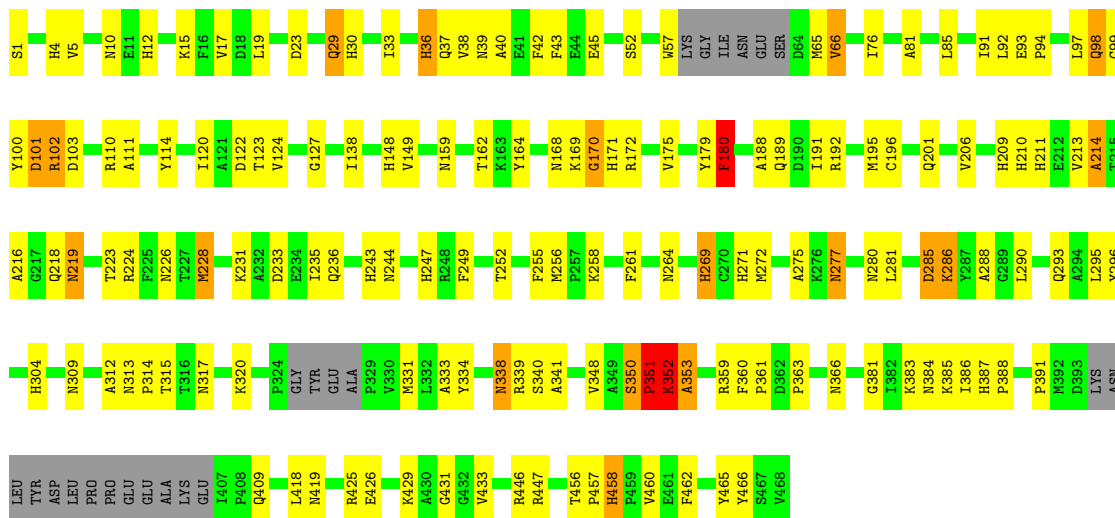


• Molecule 1: GLUTAMINE SYNTHETASE



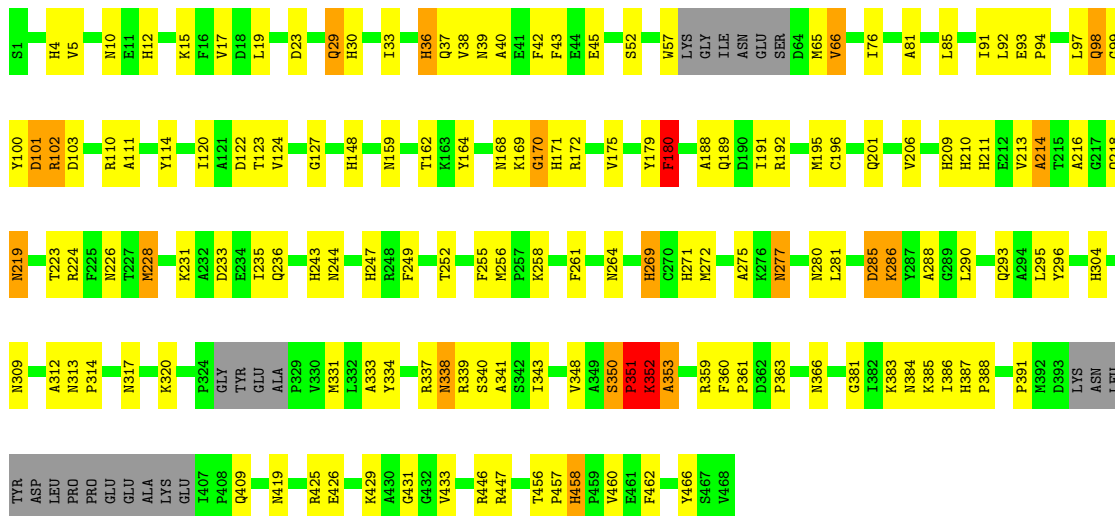
• Molecule 1: GLUTAMINE SYNTHETASE

Chain C:  61% 29% 5%



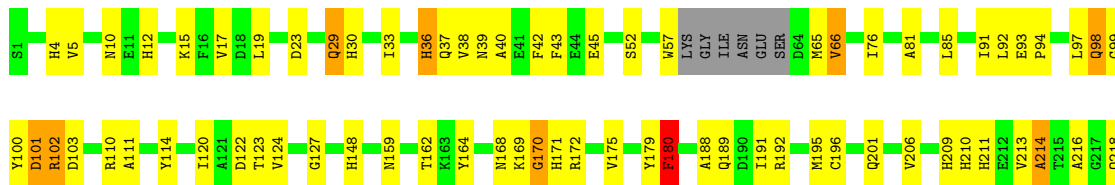
• Molecule 1: GLUTAMINE SYNTHETASE

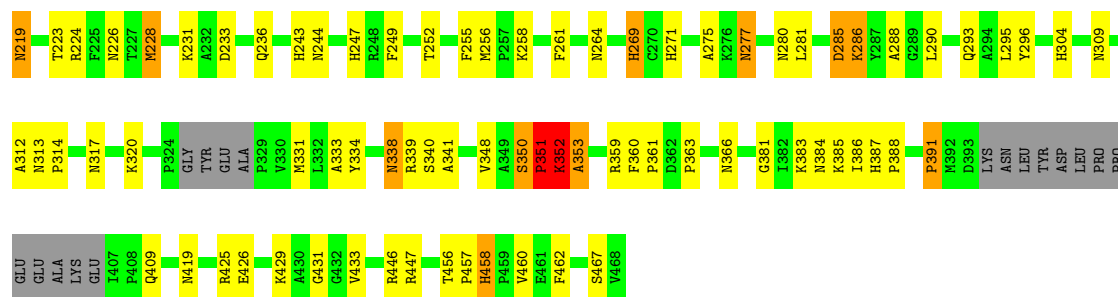
Chain D:  62% 28% 5%



• Molecule 1: GLUTAMINE SYNTHETASE

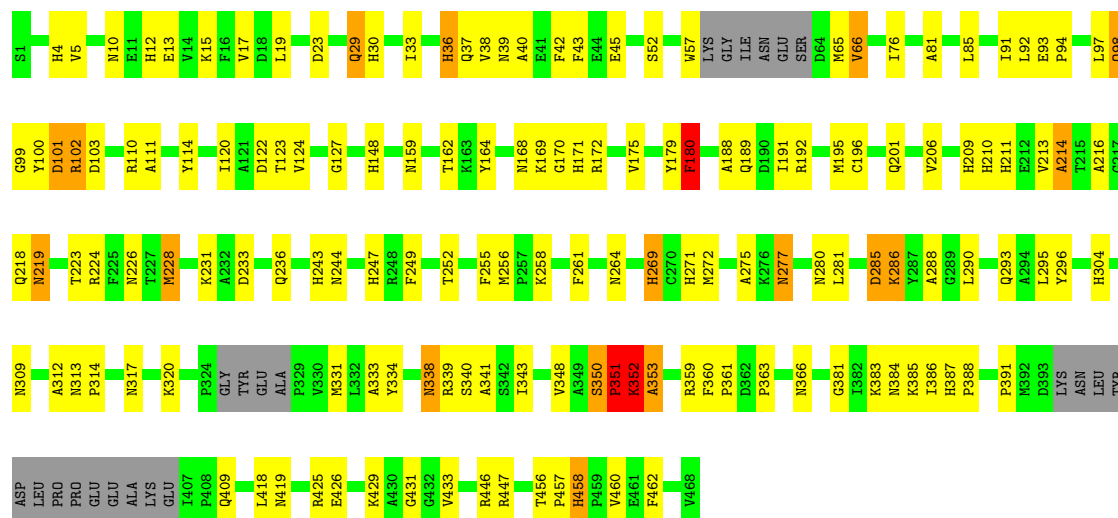
Chain E:  63% 27% 5%





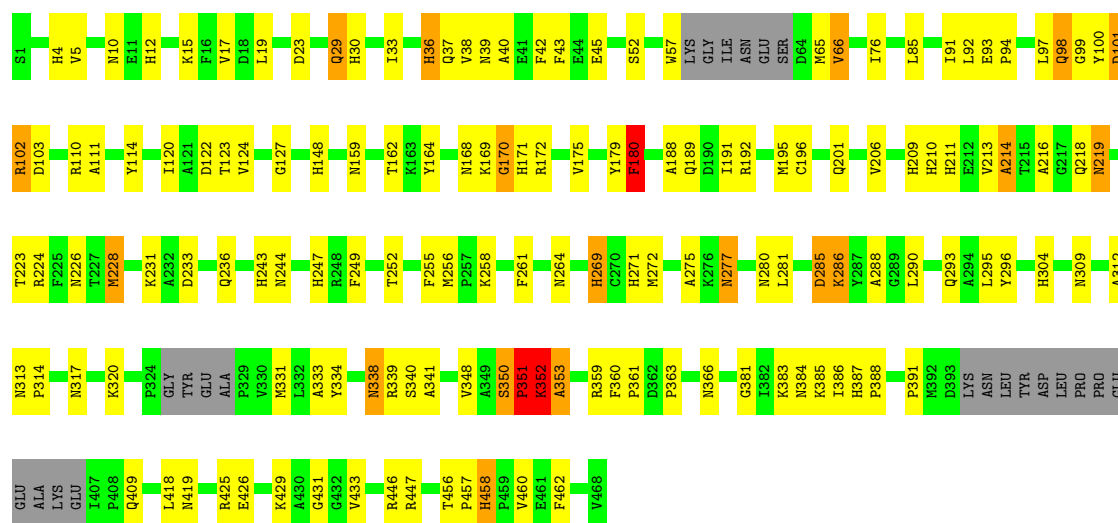
• Molecule 1: GLUTAMINE SYNTHETASE

Chain F: 62% 28% 5%



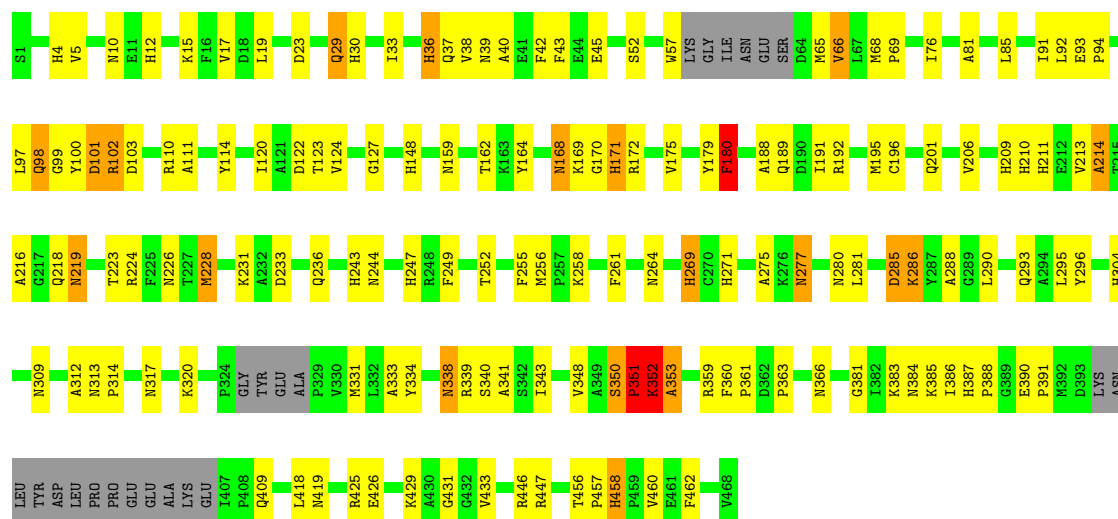
• Molecule 1: GLUTAMINE SYNTHETASE

Chain G: 63% 28% 5%



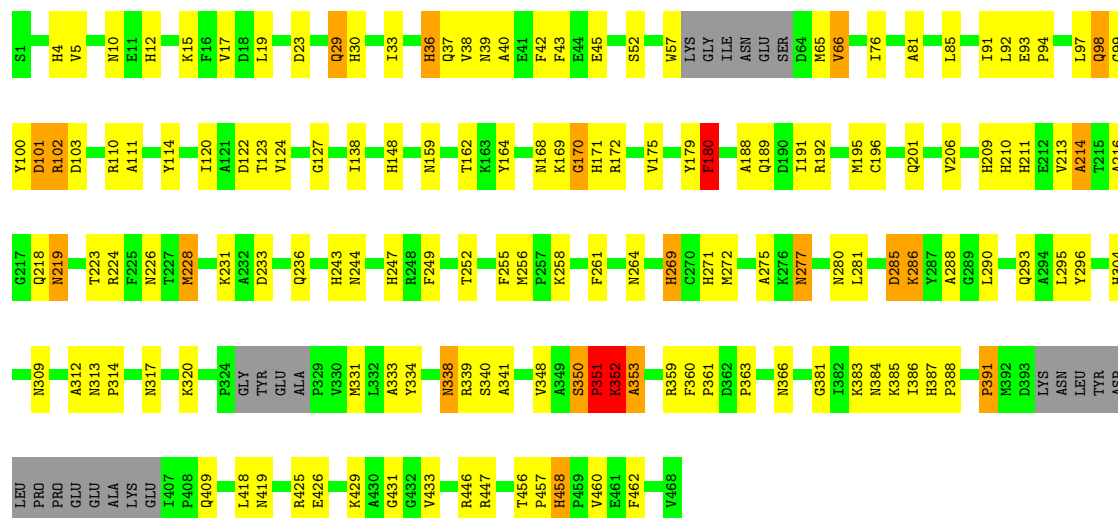
• Molecule 1: GLUTAMINE SYNTHETASE

Chain H:  62% 28% • • 5%



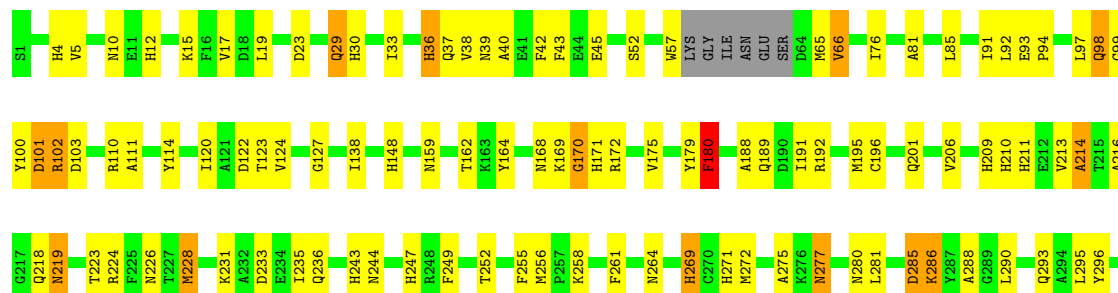
• Molecule 1: GLUTAMINE SYNTHETASE

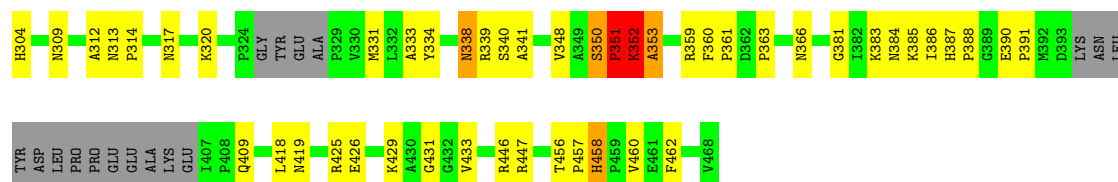
Chain I:  63% 28% • • 5%



• Molecule 1: GLUTAMINE SYNTHETASE

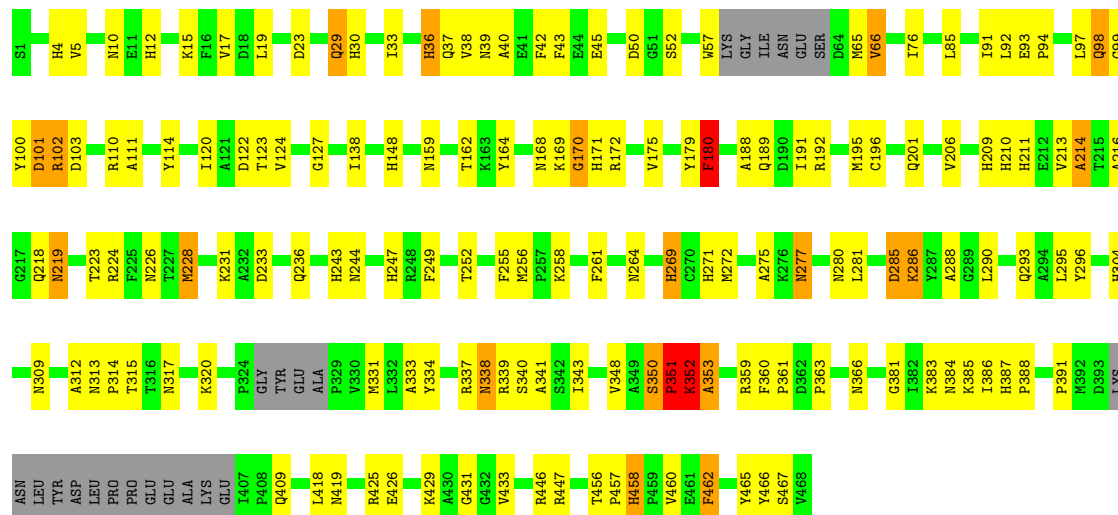
Chain J:  62% 28% • • 5%





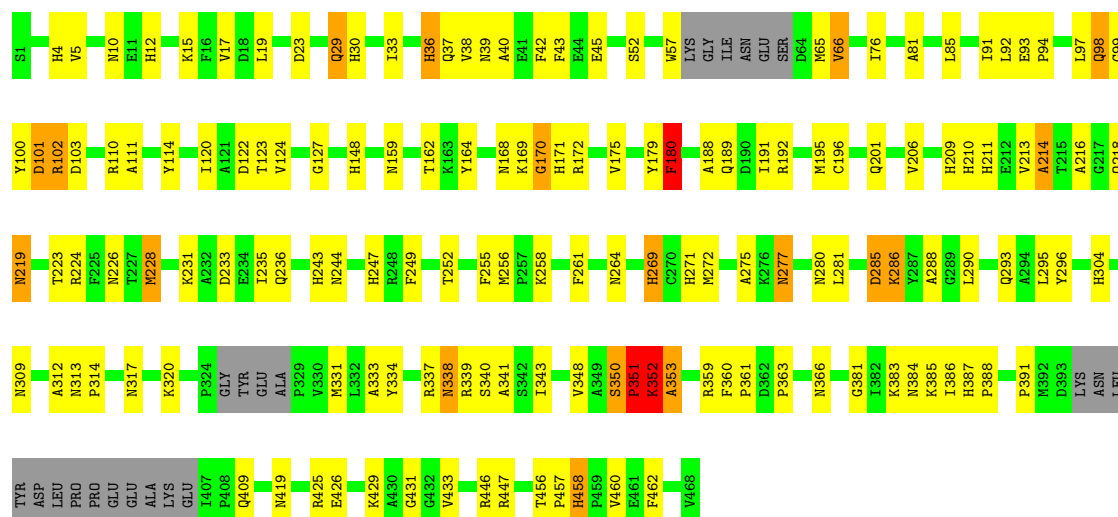
• Molecule 1: GLUTAMINE SYNTHETASE

Chain K: 61% 29% 5%



• Molecule 1: GLUTAMINE SYNTHETASE

Chain L: 62% 28% 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 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.235 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	41604	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: 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	0.96	18/3535 (0.5%)	1.88	100/4782 (2.1%)
1	B	0.96	18/3535 (0.5%)	1.88	101/4782 (2.1%)
1	C	0.96	18/3535 (0.5%)	1.88	100/4782 (2.1%)
1	D	0.96	18/3535 (0.5%)	1.88	101/4782 (2.1%)
1	E	0.96	18/3535 (0.5%)	1.88	101/4782 (2.1%)
1	F	0.96	19/3535 (0.5%)	1.88	99/4782 (2.1%)
1	G	0.96	18/3535 (0.5%)	1.88	99/4782 (2.1%)
1	H	0.96	18/3535 (0.5%)	1.88	99/4782 (2.1%)
1	I	0.96	18/3535 (0.5%)	1.88	101/4782 (2.1%)
1	J	0.96	18/3535 (0.5%)	1.88	100/4782 (2.1%)
1	K	0.96	19/3535 (0.5%)	1.88	100/4782 (2.1%)
1	L	0.96	18/3535 (0.5%)	1.88	101/4782 (2.1%)
All	All	0.96	218/42420 (0.5%)	1.88	1202/57384 (2.1%)

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

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

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

All (218) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	211	HIS	CD2-NE2	-7.37	1.29	1.37
1	G	211	HIS	CD2-NE2	-7.36	1.29	1.37
1	J	211	HIS	CD2-NE2	-7.35	1.29	1.37
1	E	211	HIS	CD2-NE2	-7.34	1.29	1.37
1	H	211	HIS	CD2-NE2	-7.33	1.29	1.37
1	I	211	HIS	CD2-NE2	-7.33	1.29	1.37
1	A	211	HIS	CD2-NE2	-7.33	1.29	1.37
1	L	211	HIS	CD2-NE2	-7.32	1.29	1.37
1	F	211	HIS	CD2-NE2	-7.31	1.29	1.37
1	B	211	HIS	CD2-NE2	-7.31	1.29	1.37
1	K	304	HIS	CD2-NE2	-7.31	1.29	1.37
1	B	304	HIS	CD2-NE2	-7.29	1.29	1.37
1	K	211	HIS	CD2-NE2	-7.29	1.29	1.37
1	F	304	HIS	CD2-NE2	-7.29	1.29	1.37
1	I	304	HIS	CD2-NE2	-7.28	1.29	1.37
1	D	304	HIS	CD2-NE2	-7.27	1.29	1.37
1	D	211	HIS	CD2-NE2	-7.26	1.29	1.37
1	A	304	HIS	CD2-NE2	-7.26	1.29	1.37
1	H	304	HIS	CD2-NE2	-7.25	1.29	1.37
1	G	304	HIS	CD2-NE2	-7.25	1.29	1.37
1	E	304	HIS	CD2-NE2	-7.25	1.29	1.37
1	K	30	HIS	CD2-NE2	-7.24	1.29	1.37
1	L	30	HIS	CD2-NE2	-7.24	1.29	1.37
1	C	304	HIS	CD2-NE2	-7.24	1.29	1.37
1	G	210	HIS	CD2-NE2	-7.22	1.29	1.37
1	D	30	HIS	CD2-NE2	-7.20	1.29	1.37
1	J	304	HIS	CD2-NE2	-7.20	1.29	1.37
1	E	30	HIS	CD2-NE2	-7.20	1.29	1.37
1	L	304	HIS	CD2-NE2	-7.20	1.29	1.37
1	F	30	HIS	CD2-NE2	-7.20	1.29	1.37
1	J	30	HIS	CD2-NE2	-7.19	1.29	1.37
1	F	210	HIS	CD2-NE2	-7.19	1.29	1.37
1	H	210	HIS	CD2-NE2	-7.18	1.29	1.37
1	L	210	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	30	HIS	CD2-NE2	-7.18	1.29	1.37
1	G	30	HIS	CD2-NE2	-7.18	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	HIS	CD2-NE2	-7.17	1.29	1.37
1	A	210	HIS	CD2-NE2	-7.17	1.29	1.37
1	C	30	HIS	CD2-NE2	-7.17	1.29	1.37
1	I	210	HIS	CD2-NE2	-7.17	1.29	1.37
1	K	210	HIS	CD2-NE2	-7.17	1.29	1.37
1	B	210	HIS	CD2-NE2	-7.16	1.29	1.37
1	J	210	HIS	CD2-NE2	-7.16	1.29	1.37
1	E	210	HIS	CD2-NE2	-7.16	1.29	1.37
1	K	269	HIS	CD2-NE2	-7.16	1.29	1.37
1	F	269	HIS	CD2-NE2	-7.15	1.29	1.37
1	L	269	HIS	CD2-NE2	-7.15	1.29	1.37
1	J	269	HIS	CD2-NE2	-7.14	1.29	1.37
1	E	269	HIS	CD2-NE2	-7.13	1.30	1.37
1	H	30	HIS	CD2-NE2	-7.13	1.30	1.37
1	I	30	HIS	CD2-NE2	-7.13	1.30	1.37
1	D	210	HIS	CD2-NE2	-7.12	1.30	1.37
1	C	210	HIS	CD2-NE2	-7.12	1.30	1.37
1	I	269	HIS	CD2-NE2	-7.11	1.30	1.37
1	H	269	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	269	HIS	CD2-NE2	-7.09	1.30	1.37
1	D	269	HIS	CD2-NE2	-7.09	1.30	1.37
1	B	269	HIS	CD2-NE2	-7.08	1.30	1.37
1	C	269	HIS	CD2-NE2	-7.06	1.30	1.37
1	G	269	HIS	CD2-NE2	-7.06	1.30	1.37
1	E	458	HIS	CD2-NE2	-7.04	1.30	1.37
1	D	458	HIS	CD2-NE2	-7.03	1.30	1.37
1	H	458	HIS	CD2-NE2	-7.02	1.30	1.37
1	A	458	HIS	CD2-NE2	-7.01	1.30	1.37
1	J	458	HIS	CD2-NE2	-7.01	1.30	1.37
1	C	458	HIS	CD2-NE2	-7.00	1.30	1.37
1	G	458	HIS	CD2-NE2	-7.00	1.30	1.37
1	F	458	HIS	CD2-NE2	-6.98	1.30	1.37
1	K	458	HIS	CD2-NE2	-6.97	1.30	1.37
1	B	458	HIS	CD2-NE2	-6.97	1.30	1.37
1	I	458	HIS	CD2-NE2	-6.96	1.30	1.37
1	L	458	HIS	CD2-NE2	-6.96	1.30	1.37
1	C	4	HIS	CD2-NE2	-6.39	1.30	1.37
1	B	4	HIS	CD2-NE2	-6.38	1.30	1.37
1	F	243	HIS	CD2-NE2	-6.36	1.30	1.37
1	K	4	HIS	CD2-NE2	-6.36	1.30	1.37
1	I	4	HIS	CD2-NE2	-6.36	1.30	1.37
1	H	4	HIS	CD2-NE2	-6.35	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243	HIS	CD2-NE2	-6.35	1.30	1.37
1	G	4	HIS	CD2-NE2	-6.34	1.30	1.37
1	J	243	HIS	CD2-NE2	-6.33	1.30	1.37
1	D	4	HIS	CD2-NE2	-6.33	1.30	1.37
1	H	243	HIS	CD2-NE2	-6.33	1.30	1.37
1	E	4	HIS	CD2-NE2	-6.33	1.30	1.37
1	A	4	HIS	CD2-NE2	-6.32	1.30	1.37
1	J	4	HIS	CD2-NE2	-6.32	1.30	1.37
1	E	209	HIS	CD2-NE2	-6.32	1.30	1.37
1	F	4	HIS	CD2-NE2	-6.32	1.30	1.37
1	L	4	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	243	HIS	CD2-NE2	-6.31	1.30	1.37
1	E	243	HIS	CD2-NE2	-6.31	1.30	1.37
1	C	12	HIS	CD2-NE2	-6.30	1.30	1.37
1	G	36	HIS	CD2-NE2	-6.30	1.30	1.37
1	I	243	HIS	CD2-NE2	-6.29	1.30	1.37
1	D	243	HIS	CD2-NE2	-6.29	1.30	1.37
1	H	12	HIS	CD2-NE2	-6.29	1.30	1.37
1	D	12	HIS	CD2-NE2	-6.29	1.30	1.37
1	G	243	HIS	CD2-NE2	-6.29	1.30	1.37
1	B	12	HIS	CD2-NE2	-6.29	1.30	1.37
1	L	243	HIS	CD2-NE2	-6.28	1.30	1.37
1	I	209	HIS	CD2-NE2	-6.28	1.30	1.37
1	C	209	HIS	CD2-NE2	-6.28	1.30	1.37
1	F	209	HIS	CD2-NE2	-6.28	1.30	1.37
1	K	243	HIS	CD2-NE2	-6.28	1.30	1.37
1	B	209	HIS	CD2-NE2	-6.27	1.30	1.37
1	K	12	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	36	HIS	CD2-NE2	-6.26	1.30	1.37
1	C	36	HIS	CD2-NE2	-6.26	1.30	1.37
1	D	209	HIS	CD2-NE2	-6.26	1.30	1.37
1	B	243	HIS	CD2-NE2	-6.26	1.30	1.37
1	I	36	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	12	HIS	CD2-NE2	-6.25	1.30	1.37
1	F	36	HIS	CD2-NE2	-6.25	1.30	1.37
1	J	12	HIS	CD2-NE2	-6.25	1.30	1.37
1	L	209	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	209	HIS	CD2-NE2	-6.25	1.30	1.37
1	E	12	HIS	CD2-NE2	-6.25	1.30	1.37
1	L	36	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	36	HIS	CD2-NE2	-6.23	1.30	1.37
1	G	12	HIS	CD2-NE2	-6.23	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	12	HIS	CD2-NE2	-6.23	1.31	1.37
1	J	209	HIS	CD2-NE2	-6.22	1.31	1.37
1	D	36	HIS	CD2-NE2	-6.22	1.31	1.37
1	K	36	HIS	CD2-NE2	-6.22	1.31	1.37
1	I	12	HIS	CD2-NE2	-6.22	1.31	1.37
1	H	209	HIS	CD2-NE2	-6.21	1.31	1.37
1	H	36	HIS	CD2-NE2	-6.20	1.31	1.37
1	J	36	HIS	CD2-NE2	-6.20	1.31	1.37
1	B	247	HIS	CD2-NE2	-6.19	1.31	1.37
1	C	247	HIS	CD2-NE2	-6.18	1.31	1.37
1	G	209	HIS	CD2-NE2	-6.18	1.31	1.37
1	K	209	HIS	CD2-NE2	-6.17	1.31	1.37
1	E	36	HIS	CD2-NE2	-6.17	1.31	1.37
1	F	12	HIS	CD2-NE2	-6.16	1.31	1.37
1	G	247	HIS	CD2-NE2	-6.15	1.31	1.37
1	F	247	HIS	CD2-NE2	-6.15	1.31	1.37
1	K	247	HIS	CD2-NE2	-6.14	1.31	1.37
1	I	247	HIS	CD2-NE2	-6.13	1.31	1.37
1	J	247	HIS	CD2-NE2	-6.13	1.31	1.37
1	H	247	HIS	CD2-NE2	-6.13	1.31	1.37
1	A	247	HIS	CD2-NE2	-6.12	1.31	1.37
1	L	247	HIS	CD2-NE2	-6.12	1.31	1.37
1	E	247	HIS	CD2-NE2	-6.10	1.31	1.37
1	D	247	HIS	CD2-NE2	-6.10	1.31	1.37
1	E	271	HIS	CD2-NE2	-6.09	1.31	1.37
1	L	271	HIS	CD2-NE2	-6.07	1.31	1.37
1	D	271	HIS	CD2-NE2	-6.07	1.31	1.37
1	C	271	HIS	CD2-NE2	-6.06	1.31	1.37
1	A	271	HIS	CD2-NE2	-6.05	1.31	1.37
1	K	148	HIS	CD2-NE2	-6.05	1.31	1.37
1	F	271	HIS	CD2-NE2	-6.04	1.31	1.37
1	B	271	HIS	CD2-NE2	-6.04	1.31	1.37
1	G	387	HIS	CD2-NE2	-6.03	1.31	1.37
1	H	271	HIS	CD2-NE2	-6.03	1.31	1.37
1	K	271	HIS	CD2-NE2	-6.03	1.31	1.37
1	B	148	HIS	CD2-NE2	-6.02	1.31	1.37
1	G	271	HIS	CD2-NE2	-6.02	1.31	1.37
1	F	148	HIS	CD2-NE2	-6.02	1.31	1.37
1	I	148	HIS	CD2-NE2	-6.02	1.31	1.37
1	J	271	HIS	CD2-NE2	-6.02	1.31	1.37
1	I	271	HIS	CD2-NE2	-6.02	1.31	1.37
1	G	148	HIS	CD2-NE2	-6.00	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	148	HIS	CD2-NE2	-6.00	1.31	1.37
1	J	148	HIS	CD2-NE2	-6.00	1.31	1.37
1	A	148	HIS	CD2-NE2	-6.00	1.31	1.37
1	D	148	HIS	CD2-NE2	-5.99	1.31	1.37
1	F	387	HIS	CD2-NE2	-5.99	1.31	1.37
1	C	387	HIS	CD2-NE2	-5.98	1.31	1.37
1	B	387	HIS	CD2-NE2	-5.98	1.31	1.37
1	H	387	HIS	CD2-NE2	-5.96	1.31	1.37
1	C	148	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	387	HIS	CD2-NE2	-5.95	1.31	1.37
1	I	387	HIS	CD2-NE2	-5.95	1.31	1.37
1	L	148	HIS	CD2-NE2	-5.94	1.31	1.37
1	K	387	HIS	CD2-NE2	-5.94	1.31	1.37
1	E	387	HIS	CD2-NE2	-5.93	1.31	1.37
1	H	148	HIS	CD2-NE2	-5.92	1.31	1.37
1	D	387	HIS	CD2-NE2	-5.92	1.31	1.37
1	J	387	HIS	CD2-NE2	-5.91	1.31	1.37
1	L	387	HIS	CD2-NE2	-5.89	1.31	1.37
1	H	210	HIS	CG-ND1	-5.53	1.32	1.38
1	I	210	HIS	CG-ND1	-5.51	1.32	1.38
1	J	271	HIS	CG-ND1	-5.51	1.32	1.38
1	G	210	HIS	CG-ND1	-5.49	1.32	1.38
1	C	210	HIS	CG-ND1	-5.48	1.32	1.38
1	L	271	HIS	CG-ND1	-5.46	1.32	1.38
1	L	210	HIS	CG-ND1	-5.45	1.32	1.38
1	E	271	HIS	CA-CB	-5.45	1.45	1.53
1	A	210	HIS	CG-ND1	-5.44	1.32	1.38
1	A	271	HIS	CG-ND1	-5.43	1.32	1.38
1	F	210	HIS	CG-ND1	-5.43	1.32	1.38
1	C	271	HIS	CA-CB	-5.42	1.45	1.53
1	B	271	HIS	CG-ND1	-5.42	1.32	1.38
1	G	271	HIS	CG-ND1	-5.42	1.32	1.38
1	D	210	HIS	CG-ND1	-5.41	1.32	1.38
1	F	271	HIS	CA-CB	-5.41	1.45	1.53
1	H	271	HIS	CA-CB	-5.41	1.45	1.53
1	J	271	HIS	CA-CB	-5.41	1.45	1.53
1	L	271	HIS	CA-CB	-5.41	1.45	1.53
1	E	271	HIS	CG-ND1	-5.41	1.32	1.38
1	H	271	HIS	CG-ND1	-5.41	1.32	1.38
1	K	271	HIS	CG-ND1	-5.41	1.32	1.38
1	K	271	HIS	CA-CB	-5.41	1.45	1.53
1	B	210	HIS	CG-ND1	-5.40	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	271	HIS	CA-CB	-5.40	1.45	1.53
1	E	210	HIS	CG-ND1	-5.40	1.32	1.38
1	A	271	HIS	CA-CB	-5.40	1.45	1.53
1	I	271	HIS	CG-ND1	-5.40	1.32	1.38
1	D	271	HIS	CG-ND1	-5.39	1.32	1.38
1	K	210	HIS	CG-ND1	-5.39	1.32	1.38
1	C	271	HIS	CG-ND1	-5.39	1.32	1.38
1	J	210	HIS	CG-ND1	-5.38	1.32	1.38
1	D	271	HIS	CA-CB	-5.37	1.45	1.53
1	G	271	HIS	CA-CB	-5.37	1.45	1.53
1	F	271	HIS	CG-ND1	-5.35	1.32	1.38
1	B	271	HIS	CA-CB	-5.33	1.45	1.53
1	F	30	HIS	CG-ND1	-5.01	1.32	1.38
1	K	30	HIS	CG-ND1	-5.00	1.32	1.38

All (1202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	39	ASN	OD1-CG-ND2	-10.50	112.10	122.60
1	K	39	ASN	OD1-CG-ND2	-10.50	112.10	122.60
1	B	39	ASN	OD1-CG-ND2	-10.50	112.10	122.60
1	E	39	ASN	OD1-CG-ND2	-10.48	112.12	122.60
1	C	39	ASN	OD1-CG-ND2	-10.47	112.13	122.60
1	I	39	ASN	OD1-CG-ND2	-10.47	112.13	122.60
1	A	39	ASN	OD1-CG-ND2	-10.47	112.13	122.60
1	F	39	ASN	OD1-CG-ND2	-10.46	112.14	122.60
1	G	39	ASN	OD1-CG-ND2	-10.43	112.17	122.60
1	L	39	ASN	OD1-CG-ND2	-10.42	112.18	122.60
1	J	39	ASN	OD1-CG-ND2	-10.42	112.18	122.60
1	D	39	ASN	OD1-CG-ND2	-10.40	112.20	122.60
1	G	98	GLN	OE1-CD-NE2	-9.86	112.74	122.60
1	L	98	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	C	98	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	F	98	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	K	98	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	A	98	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	H	98	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	I	98	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	B	98	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	D	98	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	E	98	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	J	98	GLN	OE1-CD-NE2	-9.80	112.80	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	189	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	C	189	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	K	189	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	H	189	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	F	189	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	B	189	GLN	OE1-CD-NE2	-9.74	112.86	122.60
1	A	189	GLN	OE1-CD-NE2	-9.73	112.86	122.60
1	D	189	GLN	OE1-CD-NE2	-9.72	112.88	122.60
1	G	189	GLN	OE1-CD-NE2	-9.72	112.88	122.60
1	I	189	GLN	OE1-CD-NE2	-9.71	112.89	122.60
1	J	189	GLN	OE1-CD-NE2	-9.70	112.90	122.60
1	L	189	GLN	OE1-CD-NE2	-9.70	112.91	122.60
1	J	159	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	F	159	ASN	OD1-CG-ND2	-9.34	113.26	122.60
1	D	159	ASN	OD1-CG-ND2	-9.34	113.26	122.60
1	H	159	ASN	OD1-CG-ND2	-9.34	113.27	122.60
1	B	159	ASN	OD1-CG-ND2	-9.33	113.27	122.60
1	L	159	ASN	OD1-CG-ND2	-9.32	113.28	122.60
1	A	159	ASN	OD1-CG-ND2	-9.31	113.29	122.60
1	E	159	ASN	OD1-CG-ND2	-9.31	113.29	122.60
1	I	159	ASN	OD1-CG-ND2	-9.30	113.30	122.60
1	K	159	ASN	OD1-CG-ND2	-9.30	113.30	122.60
1	G	159	ASN	OD1-CG-ND2	-9.29	113.31	122.60
1	C	159	ASN	OD1-CG-ND2	-9.28	113.32	122.60
1	L	97	LEU	N-CA-C	8.94	123.72	111.39
1	K	97	LEU	N-CA-C	8.93	123.71	111.39
1	F	97	LEU	N-CA-C	8.92	123.70	111.39
1	H	97	LEU	N-CA-C	8.92	123.70	111.39
1	J	97	LEU	N-CA-C	8.92	123.70	111.39
1	A	97	LEU	N-CA-C	8.91	123.69	111.39
1	D	97	LEU	N-CA-C	8.90	123.67	111.39
1	E	97	LEU	N-CA-C	8.90	123.67	111.39
1	C	97	LEU	N-CA-C	8.89	123.66	111.39
1	G	97	LEU	N-CA-C	8.89	123.66	111.39
1	B	97	LEU	N-CA-C	8.88	123.65	111.39
1	I	97	LEU	N-CA-C	8.88	123.64	111.39
1	J	180	PHE	N-CA-C	8.77	129.20	109.81
1	L	180	PHE	N-CA-C	8.77	129.20	109.81
1	B	180	PHE	N-CA-C	8.77	129.19	109.81
1	K	180	PHE	N-CA-C	8.77	129.19	109.81
1	C	180	PHE	N-CA-C	8.76	129.18	109.81
1	A	180	PHE	N-CA-C	8.76	129.18	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	180	PHE	N-CA-C	8.76	129.17	109.81
1	F	180	PHE	N-CA-C	8.76	129.17	109.81
1	I	180	PHE	N-CA-C	8.76	129.18	109.81
1	E	180	PHE	N-CA-C	8.76	129.16	109.81
1	G	180	PHE	N-CA-C	8.75	129.15	109.81
1	H	180	PHE	N-CA-C	8.75	129.14	109.81
1	F	426	GLU	N-CA-C	8.33	119.98	111.07
1	D	426	GLU	N-CA-C	8.32	119.98	111.07
1	H	426	GLU	N-CA-C	8.32	119.97	111.07
1	K	426	GLU	N-CA-C	8.32	119.97	111.07
1	G	426	GLU	N-CA-C	8.30	119.96	111.07
1	B	426	GLU	N-CA-C	8.30	119.95	111.07
1	A	426	GLU	N-CA-C	8.29	119.95	111.07
1	J	426	GLU	N-CA-C	8.29	119.94	111.07
1	C	426	GLU	N-CA-C	8.28	119.93	111.07
1	L	426	GLU	N-CA-C	8.28	119.93	111.07
1	E	426	GLU	N-CA-C	8.27	119.92	111.07
1	I	426	GLU	N-CA-C	8.26	119.91	111.07
1	F	124	VAL	CB-CA-C	-8.20	99.69	110.84
1	H	124	VAL	CB-CA-C	-8.20	99.69	110.84
1	D	124	VAL	CB-CA-C	-8.19	99.70	110.84
1	E	124	VAL	CB-CA-C	-8.19	99.70	110.84
1	J	124	VAL	CB-CA-C	-8.18	99.72	110.84
1	G	124	VAL	CB-CA-C	-8.17	99.73	110.84
1	A	124	VAL	CB-CA-C	-8.17	99.73	110.84
1	L	124	VAL	CB-CA-C	-8.16	99.74	110.84
1	K	124	VAL	CB-CA-C	-8.16	99.74	110.84
1	C	124	VAL	CB-CA-C	-8.16	99.75	110.84
1	B	124	VAL	CB-CA-C	-8.15	99.75	110.84
1	I	124	VAL	CB-CA-C	-8.15	99.76	110.84
1	K	277	ASN	OD1-CG-ND2	-8.12	114.48	122.60
1	G	188	ALA	N-CA-C	8.11	121.97	112.72
1	H	277	ASN	OD1-CG-ND2	-8.11	114.49	122.60
1	I	277	ASN	OD1-CG-ND2	-8.10	114.50	122.60
1	E	277	ASN	OD1-CG-ND2	-8.10	114.50	122.60
1	C	277	ASN	OD1-CG-ND2	-8.09	114.51	122.60
1	E	188	ALA	N-CA-C	8.09	121.95	112.72
1	A	277	ASN	OD1-CG-ND2	-8.09	114.51	122.60
1	J	188	ALA	N-CA-C	8.09	121.94	112.72
1	L	277	ASN	OD1-CG-ND2	-8.09	114.52	122.60
1	B	277	ASN	OD1-CG-ND2	-8.08	114.52	122.60
1	H	188	ALA	N-CA-C	8.08	121.94	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	ALA	N-CA-C	8.07	121.92	112.72
1	G	277	ASN	OD1-CG-ND2	-8.07	114.53	122.60
1	B	188	ALA	N-CA-C	8.07	121.92	112.72
1	I	188	ALA	N-CA-C	8.07	121.92	112.72
1	A	188	ALA	N-CA-C	8.07	121.92	112.72
1	F	188	ALA	N-CA-C	8.06	121.91	112.72
1	F	277	ASN	OD1-CG-ND2	-8.06	114.54	122.60
1	D	188	ALA	N-CA-C	8.06	121.91	112.72
1	D	277	ASN	OD1-CG-ND2	-8.05	114.55	122.60
1	J	277	ASN	OD1-CG-ND2	-8.04	114.56	122.60
1	D	219	ASN	OD1-CG-ND2	-8.03	114.57	122.60
1	K	188	ALA	N-CA-C	8.03	121.87	112.72
1	G	219	ASN	OD1-CG-ND2	-8.03	114.57	122.60
1	I	219	ASN	OD1-CG-ND2	-8.01	114.59	122.60
1	L	188	ALA	N-CA-C	8.01	121.85	112.72
1	E	219	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	J	219	ASN	OD1-CG-ND2	-7.99	114.61	122.60
1	H	219	ASN	OD1-CG-ND2	-7.99	114.61	122.60
1	A	219	ASN	OD1-CG-ND2	-7.98	114.62	122.60
1	C	219	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	F	219	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	K	219	ASN	OD1-CG-ND2	-7.96	114.64	122.60
1	L	219	ASN	OD1-CG-ND2	-7.95	114.65	122.60
1	B	219	ASN	OD1-CG-ND2	-7.94	114.66	122.60
1	D	236	GLN	OE1-CD-NE2	-7.88	114.72	122.60
1	B	236	GLN	OE1-CD-NE2	-7.86	114.74	122.60
1	G	236	GLN	OE1-CD-NE2	-7.85	114.75	122.60
1	L	236	GLN	OE1-CD-NE2	-7.85	114.75	122.60
1	H	236	GLN	OE1-CD-NE2	-7.84	114.76	122.60
1	J	236	GLN	OE1-CD-NE2	-7.84	114.76	122.60
1	K	236	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	A	236	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	I	236	GLN	OE1-CD-NE2	-7.80	114.80	122.60
1	C	236	GLN	OE1-CD-NE2	-7.78	114.83	122.60
1	F	236	GLN	OE1-CD-NE2	-7.77	114.83	122.60
1	E	236	GLN	OE1-CD-NE2	-7.76	114.84	122.60
1	I	409	GLN	OE1-CD-NE2	-7.68	114.92	122.60
1	D	409	GLN	OE1-CD-NE2	-7.67	114.93	122.60
1	K	409	GLN	OE1-CD-NE2	-7.67	114.93	122.60
1	F	409	GLN	OE1-CD-NE2	-7.66	114.94	122.60
1	B	409	GLN	OE1-CD-NE2	-7.63	114.97	122.60
1	H	409	GLN	OE1-CD-NE2	-7.63	114.97	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	GLN	OE1-CD-NE2	-7.62	114.97	122.60
1	L	409	GLN	OE1-CD-NE2	-7.62	114.98	122.60
1	C	409	GLN	OE1-CD-NE2	-7.60	115.00	122.60
1	G	409	GLN	OE1-CD-NE2	-7.60	115.00	122.60
1	H	293	GLN	OE1-CD-NE2	-7.58	115.02	122.60
1	J	409	GLN	OE1-CD-NE2	-7.58	115.03	122.60
1	B	293	GLN	OE1-CD-NE2	-7.57	115.03	122.60
1	E	409	GLN	OE1-CD-NE2	-7.57	115.03	122.60
1	E	293	GLN	OE1-CD-NE2	-7.57	115.03	122.60
1	K	293	GLN	OE1-CD-NE2	-7.57	115.03	122.60
1	L	293	GLN	OE1-CD-NE2	-7.55	115.05	122.60
1	G	293	GLN	OE1-CD-NE2	-7.54	115.06	122.60
1	A	293	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	I	293	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	F	293	GLN	OE1-CD-NE2	-7.51	115.09	122.60
1	J	293	GLN	OE1-CD-NE2	-7.51	115.09	122.60
1	D	293	GLN	OE1-CD-NE2	-7.48	115.12	122.60
1	C	293	GLN	OE1-CD-NE2	-7.48	115.12	122.60
1	K	168	ASN	OD1-CG-ND2	-7.31	115.29	122.60
1	H	168	ASN	OD1-CG-ND2	-7.31	115.29	122.60
1	D	168	ASN	OD1-CG-ND2	-7.30	115.30	122.60
1	L	168	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	G	168	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	I	168	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	A	168	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	F	168	ASN	OD1-CG-ND2	-7.28	115.32	122.60
1	C	168	ASN	OD1-CG-ND2	-7.27	115.33	122.60
1	B	168	ASN	OD1-CG-ND2	-7.26	115.34	122.60
1	J	168	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	E	168	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	D	338	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	E	338	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	I	338	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	F	338	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	K	338	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	K	39	ASN	CB-CG-ND2	7.01	126.92	116.40
1	L	39	ASN	CB-CG-ND2	7.01	126.92	116.40
1	L	338	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	C	338	ASN	OD1-CG-ND2	-7.01	115.59	122.60
1	H	39	ASN	CB-CG-ND2	7.01	126.91	116.40
1	H	338	ASN	OD1-CG-ND2	-7.00	115.59	122.60
1	B	39	ASN	CB-CG-ND2	7.00	126.90	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	189	GLN	CG-CD-NE2	7.00	126.90	116.40
1	I	39	ASN	CB-CG-ND2	7.00	126.90	116.40
1	A	39	ASN	CB-CG-ND2	7.00	126.90	116.40
1	A	338	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	J	338	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	E	39	ASN	CB-CG-ND2	7.00	126.89	116.40
1	K	189	GLN	CG-CD-NE2	7.00	126.89	116.40
1	C	39	ASN	CB-CG-ND2	6.99	126.89	116.40
1	F	39	ASN	CB-CG-ND2	6.99	126.89	116.40
1	D	39	ASN	CB-CG-ND2	6.99	126.88	116.40
1	G	39	ASN	CB-CG-ND2	6.98	126.87	116.40
1	H	189	GLN	CG-CD-NE2	6.98	126.87	116.40
1	C	189	GLN	CG-CD-NE2	6.98	126.87	116.40
1	A	189	GLN	CG-CD-NE2	6.98	126.86	116.40
1	E	189	GLN	CG-CD-NE2	6.98	126.86	116.40
1	J	39	ASN	CB-CG-ND2	6.98	126.86	116.40
1	B	338	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	G	338	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	L	189	GLN	CG-CD-NE2	6.97	126.85	116.40
1	B	189	GLN	CG-CD-NE2	6.96	126.85	116.40
1	J	189	GLN	CG-CD-NE2	6.96	126.84	116.40
1	D	189	GLN	CG-CD-NE2	6.95	126.83	116.40
1	G	189	GLN	CG-CD-NE2	6.95	126.83	116.40
1	I	189	GLN	CG-CD-NE2	6.95	126.82	116.40
1	L	285	ASP	CA-CB-CG	6.85	119.45	112.60
1	H	285	ASP	CA-CB-CG	6.85	119.45	112.60
1	K	285	ASP	CA-CB-CG	6.84	119.44	112.60
1	G	285	ASP	CA-CB-CG	6.83	119.44	112.60
1	C	285	ASP	CA-CB-CG	6.83	119.43	112.60
1	F	285	ASP	CA-CB-CG	6.82	119.42	112.60
1	I	285	ASP	CA-CB-CG	6.82	119.42	112.60
1	J	285	ASP	CA-CB-CG	6.82	119.42	112.60
1	B	285	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	285	ASP	CA-CB-CG	6.81	119.41	112.60
1	E	285	ASP	CA-CB-CG	6.81	119.41	112.60
1	D	285	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	211	HIS	CB-CG-CD2	-6.75	122.42	131.20
1	K	211	HIS	CB-CG-CD2	-6.74	122.44	131.20
1	D	211	HIS	CB-CG-CD2	-6.74	122.44	131.20
1	L	264	ASN	N-CA-C	6.74	119.00	110.24
1	H	211	HIS	CB-CG-CD2	-6.73	122.44	131.20
1	E	211	HIS	CB-CG-CD2	-6.73	122.45	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	211	HIS	CB-CG-CD2	-6.73	122.45	131.20
1	F	264	ASN	N-CA-C	6.73	118.98	110.24
1	J	201	GLN	OE1-CD-NE2	-6.73	115.87	122.60
1	D	264	ASN	N-CA-C	6.72	118.98	110.24
1	L	201	GLN	OE1-CD-NE2	-6.72	115.88	122.60
1	B	309	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	C	201	GLN	OE1-CD-NE2	-6.72	115.88	122.60
1	J	211	HIS	CB-CG-CD2	-6.72	122.47	131.20
1	A	211	HIS	CB-CG-CD2	-6.71	122.47	131.20
1	F	201	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	G	201	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	E	201	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	I	211	HIS	CB-CG-CD2	-6.71	122.47	131.20
1	J	264	ASN	N-CA-C	6.71	118.96	110.24
1	H	201	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	H	264	ASN	N-CA-C	6.70	118.95	110.24
1	K	264	ASN	N-CA-C	6.70	118.95	110.24
1	A	201	GLN	OE1-CD-NE2	-6.70	115.90	122.60
1	A	264	ASN	N-CA-C	6.70	118.95	110.24
1	C	211	HIS	CB-CG-CD2	-6.70	122.49	131.20
1	G	211	HIS	CB-CG-CD2	-6.70	122.49	131.20
1	E	264	ASN	N-CA-C	6.70	118.94	110.24
1	I	264	ASN	N-CA-C	6.70	118.94	110.24
1	D	309	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	L	211	HIS	CB-CG-CD2	-6.69	122.50	131.20
1	D	201	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	I	201	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	D	213	VAL	N-CA-C	6.69	117.44	110.62
1	K	201	GLN	OE1-CD-NE2	-6.69	115.91	122.60
1	A	309	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	I	309	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	C	264	ASN	N-CA-C	6.69	118.93	110.24
1	G	309	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	G	264	ASN	N-CA-C	6.68	118.93	110.24
1	B	264	ASN	N-CA-C	6.68	118.92	110.24
1	L	309	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	K	309	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	C	309	ASN	OD1-CG-ND2	-6.67	115.94	122.60
1	J	309	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	F	213	VAL	N-CA-C	6.65	117.41	110.62
1	E	213	VAL	N-CA-C	6.65	117.40	110.62
1	E	309	ASN	OD1-CG-ND2	-6.64	115.95	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	F	309	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	H	309	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	I	213	VAL	N-CA-C	6.64	117.39	110.62
1	A	213	VAL	N-CA-C	6.63	117.38	110.62
1	J	213	VAL	N-CA-C	6.63	117.38	110.62
1	B	213	VAL	N-CA-C	6.63	117.38	110.62
1	K	213	VAL	N-CA-C	6.63	117.38	110.62
1	G	213	VAL	N-CA-C	6.62	117.38	110.62
1	H	175	VAL	CA-C-O	-6.62	114.15	121.17
1	D	175	VAL	CA-C-O	-6.62	114.16	121.17
1	G	223	THR	N-CA-CB	-6.61	99.04	111.00
1	C	179	TYR	O-C-N	6.61	131.53	122.41
1	J	179	TYR	O-C-N	6.61	131.53	122.41
1	I	175	VAL	CA-C-O	-6.60	114.17	121.17
1	J	214	ALA	N-CA-C	6.60	120.05	110.28
1	G	179	TYR	O-C-N	6.60	131.52	122.41
1	L	213	VAL	N-CA-C	6.60	117.35	110.62
1	E	223	THR	N-CA-CB	-6.60	99.06	111.00
1	A	223	THR	N-CA-CB	-6.60	99.06	111.00
1	B	214	ALA	N-CA-C	6.60	120.04	110.28
1	I	223	THR	N-CA-CB	-6.60	99.06	111.00
1	B	175	VAL	CA-C-O	-6.59	114.18	121.17
1	C	223	THR	N-CA-CB	-6.59	99.07	111.00
1	A	175	VAL	CA-C-O	-6.59	114.18	121.17
1	H	213	VAL	N-CA-C	6.59	117.34	110.62
1	D	33	ILE	N-CA-CB	-6.59	101.99	111.21
1	F	223	THR	N-CA-CB	-6.59	99.08	111.00
1	K	175	VAL	CA-C-O	-6.58	114.19	121.17
1	K	223	THR	N-CA-CB	-6.58	99.08	111.00
1	C	213	VAL	N-CA-C	6.58	117.33	110.62
1	F	33	ILE	N-CA-CB	-6.58	101.99	111.21
1	A	214	ALA	N-CA-C	6.58	120.02	110.28
1	C	175	VAL	CA-C-O	-6.58	114.19	121.17
1	C	214	ALA	N-CA-C	6.58	120.02	110.28
1	F	179	TYR	O-C-N	6.58	131.49	122.41
1	G	214	ALA	N-CA-C	6.58	120.02	110.28
1	H	214	ALA	N-CA-C	6.58	120.02	110.28
1	H	223	THR	N-CA-CB	-6.58	99.09	111.00
1	D	214	ALA	N-CA-C	6.58	120.02	110.28
1	E	175	VAL	CA-C-O	-6.58	114.20	121.17
1	L	223	THR	N-CA-CB	-6.58	99.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ILE	N-CA-CB	-6.58	102.00	111.21
1	D	223	THR	N-CA-CB	-6.57	99.10	111.00
1	I	33	ILE	N-CA-CB	-6.57	102.01	111.21
1	K	179	TYR	O-C-N	6.57	131.48	122.41
1	B	223	THR	N-CA-CB	-6.57	99.10	111.00
1	A	179	TYR	O-C-N	6.57	131.48	122.41
1	J	223	THR	N-CA-CB	-6.57	99.11	111.00
1	K	33	ILE	N-CA-CB	-6.57	102.01	111.21
1	B	66	VAL	N-CA-C	6.57	117.31	108.11
1	F	175	VAL	CA-C-O	-6.57	114.21	121.17
1	J	66	VAL	N-CA-C	6.57	117.30	108.11
1	K	214	ALA	N-CA-C	6.57	120.00	110.28
1	L	214	ALA	N-CA-C	6.57	120.00	110.28
1	F	66	VAL	N-CA-C	6.56	117.30	108.11
1	G	175	VAL	CA-C-O	-6.56	114.21	121.17
1	J	33	ILE	N-CA-CB	-6.56	102.02	111.21
1	L	175	VAL	CA-C-O	-6.56	114.21	121.17
1	E	214	ALA	N-CA-C	6.56	119.99	110.28
1	H	33	ILE	N-CA-CB	-6.56	102.02	111.21
1	H	179	TYR	O-C-N	6.56	131.46	122.41
1	J	175	VAL	CA-C-O	-6.56	114.22	121.17
1	A	33	ILE	N-CA-CB	-6.56	102.03	111.21
1	E	179	TYR	O-C-N	6.56	131.46	122.41
1	I	214	ALA	N-CA-C	6.56	119.99	110.28
1	C	33	ILE	N-CA-CB	-6.56	102.03	111.21
1	D	179	TYR	O-C-N	6.55	131.46	122.41
1	F	214	ALA	N-CA-C	6.55	119.98	110.28
1	G	164	TYR	O-C-N	-6.55	114.29	122.35
1	I	179	TYR	O-C-N	6.55	131.45	122.41
1	D	66	VAL	N-CA-C	6.55	117.28	108.11
1	E	33	ILE	N-CA-CB	-6.55	102.04	111.21
1	L	66	VAL	N-CA-C	6.55	117.28	108.11
1	A	66	VAL	N-CA-C	6.55	117.28	108.11
1	H	66	VAL	N-CA-C	6.55	117.28	108.11
1	L	33	ILE	N-CA-CB	-6.54	102.05	111.21
1	B	179	TYR	O-C-N	6.54	131.44	122.41
1	C	66	VAL	N-CA-C	6.54	117.27	108.11
1	H	164	TYR	O-C-N	-6.54	114.30	122.35
1	L	164	TYR	O-C-N	-6.54	114.30	122.35
1	J	164	TYR	O-C-N	-6.54	114.31	122.35
1	E	164	TYR	O-C-N	-6.53	114.32	122.35
1	G	33	ILE	N-CA-CB	-6.53	102.07	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	66	VAL	N-CA-C	6.53	117.25	108.11
1	L	179	TYR	O-C-N	6.53	131.42	122.41
1	B	164	TYR	O-C-N	-6.53	114.32	122.35
1	E	66	VAL	N-CA-C	6.52	117.24	108.11
1	A	164	TYR	O-C-N	-6.52	114.33	122.35
1	K	66	VAL	N-CA-C	6.52	117.24	108.11
1	D	164	TYR	O-C-N	-6.52	114.33	122.35
1	K	164	TYR	O-C-N	-6.51	114.34	122.35
1	I	66	VAL	N-CA-C	6.51	117.23	108.11
1	D	236	GLN	CG-CD-NE2	6.50	126.15	116.40
1	C	164	TYR	O-C-N	-6.50	114.36	122.35
1	F	164	TYR	O-C-N	-6.50	114.36	122.35
1	B	236	GLN	CG-CD-NE2	6.49	126.13	116.40
1	G	236	GLN	CG-CD-NE2	6.49	126.13	116.40
1	L	236	GLN	CG-CD-NE2	6.49	126.13	116.40
1	E	236	GLN	CG-CD-NE2	6.48	126.12	116.40
1	K	236	GLN	CG-CD-NE2	6.48	126.12	116.40
1	I	164	TYR	O-C-N	-6.47	114.39	122.35
1	A	236	GLN	CG-CD-NE2	6.47	126.10	116.40
1	F	236	GLN	CG-CD-NE2	6.46	126.09	116.40
1	L	124	VAL	N-CA-CB	6.46	118.74	110.99
1	H	236	GLN	CG-CD-NE2	6.46	126.08	116.40
1	I	30	HIS	CB-CG-CD2	-6.46	122.81	131.20
1	J	236	GLN	CG-CD-NE2	6.46	126.08	116.40
1	C	236	GLN	CG-CD-NE2	6.45	126.07	116.40
1	D	124	VAL	N-CA-CB	6.45	118.73	110.99
1	G	30	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	J	124	VAL	N-CA-CB	6.45	118.72	110.99
1	B	30	HIS	CB-CG-CD2	-6.44	122.82	131.20
1	I	236	GLN	CG-CD-NE2	6.44	126.06	116.40
1	I	124	VAL	N-CA-CB	6.44	118.72	110.99
1	F	30	HIS	CB-CG-CD2	-6.44	122.83	131.20
1	A	124	VAL	N-CA-CB	6.43	118.71	110.99
1	G	124	VAL	N-CA-CB	6.43	118.71	110.99
1	E	124	VAL	N-CA-CB	6.43	118.70	110.99
1	F	124	VAL	N-CA-CB	6.43	118.70	110.99
1	A	30	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	H	30	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	K	30	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	C	30	HIS	CB-CG-CD2	-6.42	122.86	131.20
1	C	124	VAL	N-CA-CB	6.42	118.69	110.99
1	J	30	HIS	CB-CG-CD2	-6.42	122.86	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	VAL	N-CA-CB	6.42	118.69	110.99
1	H	124	VAL	N-CA-CB	6.41	118.69	110.99
1	D	30	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	E	30	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	K	124	VAL	N-CA-CB	6.41	118.68	110.99
1	L	30	HIS	CB-CG-CD2	-6.40	122.88	131.20
1	F	10	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	C	10	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	H	10	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	K	10	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	K	172	ARG	O-C-N	-6.37	116.87	121.84
1	G	288	ALA	N-CA-C	6.36	120.17	111.39
1	B	172	ARG	O-C-N	-6.35	116.89	121.84
1	D	172	ARG	O-C-N	-6.35	116.89	121.84
1	C	172	ARG	O-C-N	-6.35	116.89	121.84
1	C	288	ALA	N-CA-C	6.35	120.15	111.39
1	F	288	ALA	N-CA-C	6.34	120.14	111.39
1	G	10	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	I	288	ALA	N-CA-C	6.34	120.14	111.39
1	B	288	ALA	N-CA-C	6.34	120.14	111.39
1	I	172	ARG	O-C-N	-6.34	116.89	121.84
1	A	10	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	B	10	ASN	OD1-CG-ND2	-6.34	116.26	122.60
1	J	288	ALA	N-CA-C	6.33	120.13	111.39
1	H	148	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	D	288	ALA	N-CA-C	6.33	120.13	111.39
1	H	288	ALA	N-CA-C	6.33	120.13	111.39
1	A	288	ALA	N-CA-C	6.33	120.12	111.39
1	L	10	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	L	172	ARG	O-C-N	-6.33	116.91	121.84
1	E	148	HIS	CB-CG-CD2	-6.32	122.98	131.20
1	B	148	HIS	CB-CG-CD2	-6.32	122.98	131.20
1	L	288	ALA	N-CA-C	6.32	120.11	111.39
1	E	288	ALA	N-CA-C	6.31	120.10	111.39
1	A	172	ARG	O-C-N	-6.31	116.92	121.84
1	K	288	ALA	N-CA-C	6.31	120.10	111.39
1	D	10	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	J	148	HIS	CB-CG-CD2	-6.31	123.00	131.20
1	A	148	HIS	CB-CG-CD2	-6.31	123.00	131.20
1	I	10	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	H	172	ARG	O-C-N	-6.31	116.92	121.84
1	G	148	HIS	CB-CG-CD2	-6.30	123.01	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	172	ARG	O-C-N	-6.30	116.92	121.84
1	L	148	HIS	CB-CG-CD2	-6.30	123.01	131.20
1	C	148	HIS	CB-CG-CD2	-6.30	123.01	131.20
1	F	148	HIS	CB-CG-CD2	-6.30	123.01	131.20
1	J	10	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	F	172	ARG	O-C-N	-6.28	116.94	121.84
1	I	148	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	D	148	HIS	CB-CG-CD2	-6.28	123.03	131.20
1	E	162	THR	N-CA-C	6.28	119.38	109.96
1	I	162	THR	N-CA-C	6.28	119.38	109.96
1	K	162	THR	N-CA-C	6.28	119.38	109.96
1	E	172	ARG	O-C-N	-6.28	116.94	121.84
1	J	162	THR	N-CA-C	6.28	119.37	109.96
1	F	162	THR	N-CA-C	6.27	119.37	109.96
1	L	162	THR	N-CA-C	6.27	119.37	109.96
1	E	10	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	G	172	ARG	O-C-N	-6.27	116.95	121.84
1	A	162	THR	N-CA-C	6.27	119.36	109.96
1	L	304	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	G	162	THR	N-CA-C	6.27	119.36	109.96
1	K	148	HIS	CB-CG-CD2	-6.27	123.05	131.20
1	B	162	THR	N-CA-C	6.26	119.36	109.96
1	D	162	THR	N-CA-C	6.26	119.36	109.96
1	C	162	THR	N-CA-C	6.26	119.34	109.96
1	H	162	THR	N-CA-C	6.26	119.34	109.96
1	I	304	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	C	304	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	B	304	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	A	304	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	E	304	HIS	CB-CG-CD2	-6.24	123.08	131.20
1	G	304	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	G	350	SER	O-C-N	-6.24	114.15	121.32
1	H	304	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	J	304	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	K	304	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	F	304	HIS	CB-CG-CD2	-6.23	123.11	131.20
1	L	350	SER	O-C-N	-6.22	114.17	121.32
1	E	350	SER	O-C-N	-6.21	114.17	121.32
1	E	384	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	D	304	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	I	350	SER	O-C-N	-6.20	114.19	121.32
1	H	419	ASN	OD1-CG-ND2	-6.20	116.41	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	384	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	B	103	ASP	CA-CB-CG	6.19	118.79	112.60
1	D	384	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	J	103	ASP	CA-CB-CG	6.19	118.79	112.60
1	F	350	SER	O-C-N	-6.19	114.21	121.32
1	E	419	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	K	103	ASP	CA-CB-CG	6.18	118.78	112.60
1	C	350	SER	O-C-N	-6.18	114.22	121.32
1	J	350	SER	O-C-N	-6.18	114.22	121.32
1	C	103	ASP	CA-CB-CG	6.17	118.78	112.60
1	A	350	SER	O-C-N	-6.17	114.22	121.32
1	D	103	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	419	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	B	350	SER	O-C-N	-6.17	114.23	121.32
1	K	350	SER	O-C-N	-6.17	114.23	121.32
1	A	384	ASN	OD1-CG-ND2	-6.17	116.44	122.60
1	G	103	ASP	CA-CB-CG	6.16	118.76	112.60
1	D	350	SER	O-C-N	-6.16	114.23	121.32
1	A	103	ASP	CA-CB-CG	6.16	118.76	112.60
1	K	419	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	I	384	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	L	313	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	B	313	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	F	384	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	J	419	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	F	103	ASP	CA-CB-CG	6.15	118.75	112.60
1	H	350	SER	O-C-N	-6.15	114.25	121.32
1	J	384	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	C	384	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	G	419	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	C	419	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	E	103	ASP	CA-CB-CG	6.14	118.74	112.60
1	K	313	ASN	OD1-CG-ND2	-6.14	116.46	122.60
1	B	384	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	H	103	ASP	CA-CB-CG	6.13	118.73	112.60
1	H	313	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	I	103	ASP	CA-CB-CG	6.13	118.73	112.60
1	I	419	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	K	384	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	H	384	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	L	384	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	A	313	ASN	OD1-CG-ND2	-6.12	116.48	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	J	313	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	L	419	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	E	313	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	D	419	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	L	103	ASP	CA-CB-CG	6.11	118.71	112.60
1	F	419	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	J	462	PHE	CA-CB-CG	-6.09	107.71	113.80
1	D	313	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	G	313	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	C	313	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	I	313	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	E	360	PHE	N-CA-C	6.08	123.23	109.81
1	F	313	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	C	462	PHE	CA-CB-CG	-6.07	107.73	113.80
1	F	462	PHE	CA-CB-CG	-6.07	107.73	113.80
1	H	360	PHE	N-CA-C	6.07	123.22	109.81
1	I	360	PHE	N-CA-C	6.06	123.21	109.81
1	E	462	PHE	CA-CB-CG	-6.06	107.74	113.80
1	K	360	PHE	N-CA-C	6.06	123.21	109.81
1	D	462	PHE	CA-CB-CG	-6.06	107.74	113.80
1	F	360	PHE	N-CA-C	6.06	123.20	109.81
1	A	360	PHE	N-CA-C	6.06	123.19	109.81
1	J	331	MET	N-CA-C	6.05	117.87	109.15
1	A	462	PHE	CA-CB-CG	-6.05	107.75	113.80
1	C	360	PHE	N-CA-C	6.05	123.18	109.81
1	E	331	MET	N-CA-C	6.05	117.86	109.15
1	G	360	PHE	N-CA-C	6.05	123.18	109.81
1	I	462	PHE	CA-CB-CG	-6.05	107.75	113.80
1	J	360	PHE	N-CA-C	6.05	123.18	109.81
1	J	52	SER	N-CA-C	6.05	118.65	111.33
1	K	462	PHE	CA-CB-CG	-6.05	107.75	113.80
1	L	360	PHE	N-CA-C	6.05	123.17	109.81
1	L	462	PHE	CA-CB-CG	-6.05	107.75	113.80
1	B	360	PHE	N-CA-C	6.04	123.17	109.81
1	D	331	MET	N-CA-C	6.04	117.85	109.15
1	C	331	MET	N-CA-C	6.04	117.84	109.15
1	D	360	PHE	N-CA-C	6.04	123.15	109.81
1	H	462	PHE	CA-CB-CG	-6.04	107.76	113.80
1	F	52	SER	N-CA-C	6.03	118.63	111.33
1	I	52	SER	N-CA-C	6.03	118.63	111.33
1	G	462	PHE	CA-CB-CG	-6.03	107.77	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	331	MET	N-CA-C	6.03	117.83	109.15
1	G	331	MET	N-CA-C	6.03	117.83	109.15
1	B	52	SER	N-CA-C	6.02	118.61	111.33
1	B	331	MET	N-CA-C	6.02	117.82	109.15
1	B	462	PHE	CA-CB-CG	-6.02	107.78	113.80
1	K	52	SER	N-CA-C	6.02	118.61	111.33
1	A	331	MET	N-CA-C	6.01	117.81	109.15
1	E	52	SER	N-CA-C	6.01	118.61	111.33
1	F	331	MET	N-CA-C	6.01	117.81	109.15
1	L	52	SER	N-CA-C	6.01	118.60	111.33
1	I	331	MET	N-CA-C	6.01	117.80	109.15
1	L	4	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	A	52	SER	N-CA-C	6.00	118.59	111.33
1	G	52	SER	N-CA-C	6.00	118.59	111.33
1	H	331	MET	N-CA-C	6.00	117.79	109.15
1	E	4	HIS	CB-CG-CD2	-6.00	123.41	131.20
1	D	52	SER	N-CA-C	5.99	118.58	111.33
1	L	331	MET	N-CA-C	5.99	117.78	109.15
1	H	4	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	H	52	SER	N-CA-C	5.99	118.58	111.33
1	B	247	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	D	247	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	C	52	SER	N-CA-C	5.98	118.57	111.33
1	H	247	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	A	247	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	D	4	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	F	4	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	K	247	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	F	247	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	G	4	HIS	CB-CG-CD2	-5.97	123.43	131.20
1	A	4	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	E	247	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	I	4	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	G	247	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	I	247	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	L	247	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	K	4	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	J	247	HIS	CB-CG-CD2	-5.96	123.46	131.20
1	C	247	HIS	CB-CG-CD2	-5.95	123.46	131.20
1	B	4	HIS	CB-CG-CD2	-5.95	123.47	131.20
1	C	4	HIS	CB-CG-CD2	-5.93	123.49	131.20
1	J	4	HIS	CB-CG-CD2	-5.93	123.49	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	317	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	D	179	TYR	CA-C-O	5.91	128.57	121.66
1	B	179	TYR	CA-C-O	5.91	128.57	121.66
1	I	15	LYS	CA-CB-CG	-5.90	102.29	114.10
1	D	317	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	I	433	VAL	O-C-N	-5.90	116.35	122.66
1	G	433	VAL	O-C-N	-5.89	116.35	122.66
1	D	15	LYS	CA-CB-CG	-5.89	102.32	114.10
1	L	179	TYR	CA-C-O	5.89	128.55	121.66
1	G	15	LYS	CA-CB-CG	-5.89	102.32	114.10
1	B	15	LYS	CA-CB-CG	-5.89	102.33	114.10
1	E	179	TYR	CA-C-O	5.89	128.55	121.66
1	I	179	TYR	CA-C-O	5.89	128.55	121.66
1	L	15	LYS	CA-CB-CG	-5.89	102.33	114.10
1	C	433	VAL	O-C-N	-5.88	116.36	122.66
1	H	317	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	B	317	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	K	15	LYS	CA-CB-CG	-5.88	102.34	114.10
1	C	15	LYS	CA-CB-CG	-5.88	102.34	114.10
1	G	179	TYR	CA-C-O	5.88	128.54	121.66
1	A	15	LYS	CA-CB-CG	-5.88	102.34	114.10
1	L	433	VAL	O-C-N	-5.88	116.37	122.66
1	E	15	LYS	CA-CB-CG	-5.88	102.35	114.10
1	F	15	LYS	CA-CB-CG	-5.88	102.35	114.10
1	J	15	LYS	CA-CB-CG	-5.87	102.36	114.10
1	H	179	TYR	CA-C-O	5.87	128.53	121.66
1	L	317	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	A	179	TYR	CA-C-O	5.87	128.53	121.66
1	G	317	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	I	317	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	K	179	TYR	CA-C-O	5.87	128.53	121.66
1	F	179	TYR	CA-C-O	5.86	128.52	121.66
1	F	433	VAL	O-C-N	-5.86	116.39	122.66
1	A	433	VAL	O-C-N	-5.86	116.39	122.66
1	H	15	LYS	CA-CB-CG	-5.86	102.38	114.10
1	A	317	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	B	433	VAL	O-C-N	-5.86	116.39	122.66
1	E	433	VAL	O-C-N	-5.86	116.39	122.66
1	K	433	VAL	O-C-N	-5.85	116.40	122.66
1	J	317	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	E	317	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	F	317	ASN	OD1-CG-ND2	-5.84	116.76	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	123	THR	N-CA-C	5.83	118.98	109.24
1	K	123	THR	N-CA-C	5.83	118.98	109.24
1	J	179	TYR	CA-C-O	5.83	128.48	121.66
1	D	433	VAL	O-C-N	-5.83	116.42	122.66
1	E	123	THR	N-CA-C	5.82	118.97	109.24
1	C	179	TYR	CA-C-O	5.82	128.47	121.66
1	J	433	VAL	O-C-N	-5.82	116.43	122.66
1	F	123	THR	N-CA-C	5.82	118.96	109.24
1	G	123	THR	N-CA-C	5.82	118.96	109.24
1	H	433	VAL	O-C-N	-5.82	116.43	122.66
1	A	123	THR	N-CA-C	5.81	118.95	109.24
1	J	123	THR	N-CA-C	5.81	118.94	109.24
1	K	317	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	L	123	THR	N-CA-C	5.81	118.94	109.24
1	D	123	THR	N-CA-C	5.80	118.93	109.24
1	B	123	THR	N-CA-C	5.80	118.93	109.24
1	I	244	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	C	123	THR	N-CA-C	5.80	118.93	109.24
1	H	123	THR	N-CA-C	5.80	118.92	109.24
1	F	244	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	G	447	ARG	CA-CB-CG	-5.79	102.52	114.10
1	E	244	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	B	447	ARG	CA-CB-CG	-5.79	102.52	114.10
1	C	447	ARG	CA-CB-CG	-5.79	102.53	114.10
1	J	271	HIS	CB-CG-CD2	-5.79	123.68	131.20
1	L	244	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	E	447	ARG	CA-CB-CG	-5.78	102.53	114.10
1	K	447	ARG	CA-CB-CG	-5.77	102.56	114.10
1	A	447	ARG	CA-CB-CG	-5.77	102.56	114.10
1	D	447	ARG	CA-CB-CG	-5.77	102.56	114.10
1	L	447	ARG	CA-CB-CG	-5.77	102.56	114.10
1	F	447	ARG	CA-CB-CG	-5.77	102.56	114.10
1	H	447	ARG	CA-CB-CG	-5.77	102.57	114.10
1	J	447	ARG	CA-CB-CG	-5.77	102.57	114.10
1	C	98	GLN	CG-CD-NE2	5.76	125.04	116.40
1	B	271	HIS	CB-CG-CD2	-5.76	123.72	131.20
1	G	271	HIS	CB-CG-CD2	-5.76	123.72	131.20
1	A	244	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	C	244	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	L	271	HIS	CB-CG-CD2	-5.75	123.73	131.20
1	I	447	ARG	CA-CB-CG	-5.75	102.61	114.10
1	K	244	ASN	OD1-CG-ND2	-5.75	116.85	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	98	GLN	CG-CD-NE2	5.74	125.02	116.40
1	B	98	GLN	CG-CD-NE2	5.74	125.01	116.40
1	E	36	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	E	233	ASP	CA-CB-CG	5.74	118.34	112.60
1	H	233	ASP	CA-CB-CG	5.74	118.34	112.60
1	H	271	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	C	233	ASP	CA-CB-CG	5.74	118.34	112.60
1	K	98	GLN	CG-CD-NE2	5.74	125.01	116.40
1	L	98	GLN	CG-CD-NE2	5.74	125.00	116.40
1	E	271	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	H	98	GLN	CG-CD-NE2	5.74	125.00	116.40
1	A	271	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	A	98	GLN	CG-CD-NE2	5.73	125.00	116.40
1	C	36	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	K	271	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	K	36	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	D	98	GLN	CG-CD-NE2	5.73	124.99	116.40
1	G	233	ASP	CA-CB-CG	5.73	118.33	112.60
1	J	98	GLN	CG-CD-NE2	5.73	124.99	116.40
1	A	233	ASP	CA-CB-CG	5.72	118.32	112.60
1	G	36	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	I	271	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	E	98	GLN	CG-CD-NE2	5.72	124.98	116.40
1	G	209	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	J	36	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	K	233	ASP	CA-CB-CG	5.72	118.32	112.60
1	F	98	GLN	CG-CD-NE2	5.71	124.97	116.40
1	F	233	ASP	CA-CB-CG	5.71	118.31	112.60
1	H	244	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	C	271	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	I	98	GLN	CG-CD-NE2	5.71	124.97	116.40
1	A	36	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	F	271	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	G	244	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	D	233	ASP	CA-CB-CG	5.71	118.31	112.60
1	B	36	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	D	271	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	H	36	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	J	244	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	I	226	ASN	CA-CB-CG	-5.71	106.89	112.60
1	B	233	ASP	CA-CB-CG	5.71	118.31	112.60
1	D	244	ASN	OD1-CG-ND2	-5.70	116.90	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	226	ASN	CA-CB-CG	-5.70	106.90	112.60
1	F	226	ASN	CA-CB-CG	-5.70	106.90	112.60
1	I	36	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	K	226	ASN	CA-CB-CG	-5.70	106.90	112.60
1	D	226	ASN	CA-CB-CG	-5.70	106.90	112.60
1	B	244	ASN	OD1-CG-ND2	-5.70	116.91	122.60
1	I	233	ASP	CA-CB-CG	5.70	118.30	112.60
1	L	233	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	226	ASN	CA-CB-CG	-5.69	106.91	112.60
1	F	36	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	B	226	ASN	CA-CB-CG	-5.69	106.91	112.60
1	D	36	HIS	CB-CG-CD2	-5.69	123.81	131.20
1	J	226	ASN	CA-CB-CG	-5.69	106.91	112.60
1	J	233	ASP	CA-CB-CG	5.68	118.28	112.60
1	K	209	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	L	36	HIS	CB-CG-CD2	-5.68	123.82	131.20
1	D	280	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	G	226	ASN	CA-CB-CG	-5.67	106.93	112.60
1	A	209	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	F	209	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	I	209	HIS	CB-CG-CD2	-5.66	123.84	131.20
1	G	280	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	J	209	HIS	CB-CG-CD2	-5.66	123.85	131.20
1	L	209	HIS	CB-CG-CD2	-5.65	123.85	131.20
1	H	209	HIS	CB-CG-CD2	-5.65	123.85	131.20
1	C	226	ASN	CA-CB-CG	-5.65	106.95	112.60
1	H	226	ASN	CA-CB-CG	-5.65	106.95	112.60
1	F	280	ASN	OD1-CG-ND2	-5.64	116.95	122.60
1	L	226	ASN	CA-CB-CG	-5.64	106.95	112.60
1	E	280	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	C	209	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	I	280	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	L	280	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	B	209	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	K	280	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	D	209	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	E	209	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	A	280	ASN	OD1-CG-ND2	-5.62	116.98	122.60
1	B	280	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	B	45	GLU	N-CA-C	5.59	119.10	112.72
1	C	280	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	J	280	ASN	OD1-CG-ND2	-5.59	117.01	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	280	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	K	45	GLU	N-CA-C	5.58	119.08	112.72
1	I	45	GLU	N-CA-C	5.58	119.08	112.72
1	D	45	GLU	N-CA-C	5.57	119.08	112.72
1	K	29	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	F	127	GLY	CA-C-N	5.56	125.32	119.76
1	F	127	GLY	C-N-CA	5.56	125.32	119.76
1	A	45	GLU	N-CA-C	5.56	119.06	112.72
1	B	29	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	G	45	GLU	N-CA-C	5.56	119.06	112.72
1	J	45	GLU	N-CA-C	5.56	119.06	112.72
1	K	127	GLY	CA-C-N	5.56	125.32	119.76
1	K	127	GLY	C-N-CA	5.56	125.32	119.76
1	F	45	GLU	N-CA-C	5.55	119.05	112.72
1	L	45	GLU	N-CA-C	5.55	119.05	112.72
1	C	45	GLU	N-CA-C	5.55	119.05	112.72
1	H	45	GLU	N-CA-C	5.55	119.04	112.72
1	H	29	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	C	127	GLY	CA-C-N	5.53	125.28	119.76
1	C	127	GLY	C-N-CA	5.53	125.28	119.76
1	D	29	GLN	OE1-CD-NE2	-5.53	117.08	122.60
1	E	45	GLU	N-CA-C	5.53	119.02	112.72
1	D	216	ALA	N-CA-C	5.52	119.19	111.74
1	G	29	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	E	127	GLY	CA-C-N	5.52	125.28	119.76
1	E	127	GLY	C-N-CA	5.52	125.28	119.76
1	K	275	ALA	N-CA-C	5.51	118.45	108.69
1	K	216	ALA	N-CA-C	5.51	119.18	111.74
1	G	275	ALA	N-CA-C	5.51	118.44	108.69
1	D	127	GLY	CA-C-N	5.51	125.27	119.76
1	D	127	GLY	C-N-CA	5.51	125.27	119.76
1	I	216	ALA	N-CA-C	5.51	119.17	111.74
1	H	127	GLY	CA-C-N	5.50	125.27	119.76
1	H	127	GLY	C-N-CA	5.50	125.27	119.76
1	A	127	GLY	CA-C-N	5.50	125.26	119.76
1	A	127	GLY	C-N-CA	5.50	125.26	119.76
1	B	216	ALA	N-CA-C	5.50	119.17	111.74
1	F	275	ALA	N-CA-C	5.50	118.42	108.69
1	H	244	ASN	CA-CB-CG	-5.50	107.10	112.60
1	J	275	ALA	N-CA-C	5.50	118.42	108.69
1	L	127	GLY	CA-C-N	5.50	125.26	119.76
1	L	127	GLY	C-N-CA	5.50	125.26	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	216	ALA	N-CA-C	5.49	119.16	111.74
1	J	29	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	J	127	GLY	CA-C-N	5.49	125.25	119.76
1	J	127	GLY	C-N-CA	5.49	125.25	119.76
1	A	29	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	A	216	ALA	N-CA-C	5.49	119.15	111.74
1	H	216	ALA	N-CA-C	5.49	119.15	111.74
1	L	29	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	B	127	GLY	CA-C-N	5.49	125.25	119.76
1	B	127	GLY	C-N-CA	5.49	125.25	119.76
1	J	216	ALA	N-CA-C	5.49	119.15	111.74
1	A	275	ALA	N-CA-C	5.48	118.40	108.69
1	E	29	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	E	216	ALA	N-CA-C	5.48	119.14	111.74
1	H	275	ALA	N-CA-C	5.48	118.39	108.69
1	C	29	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	C	275	ALA	N-CA-C	5.48	118.39	108.69
1	E	275	ALA	N-CA-C	5.48	118.39	108.69
1	L	216	ALA	N-CA-C	5.48	119.13	111.74
1	F	29	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	G	127	GLY	CA-C-N	5.48	125.24	119.76
1	G	127	GLY	C-N-CA	5.48	125.24	119.76
1	I	29	GLN	OE1-CD-NE2	-5.47	117.12	122.60
1	I	275	ALA	N-CA-C	5.47	118.38	108.69
1	K	244	ASN	CA-CB-CG	-5.47	107.12	112.60
1	B	275	ALA	N-CA-C	5.47	118.37	108.69
1	I	127	GLY	CA-C-N	5.47	125.23	119.76
1	I	127	GLY	C-N-CA	5.47	125.23	119.76
1	C	244	ASN	CA-CB-CG	-5.47	107.13	112.60
1	D	244	ASN	CA-CB-CG	-5.47	107.13	112.60
1	G	216	ALA	N-CA-C	5.47	119.12	111.74
1	C	216	ALA	N-CA-C	5.46	119.12	111.74
1	L	275	ALA	N-CA-C	5.46	118.36	108.69
1	I	244	ASN	CA-CB-CG	-5.46	107.14	112.60
1	A	244	ASN	CA-CB-CG	-5.46	107.14	112.60
1	B	244	ASN	CA-CB-CG	-5.45	107.15	112.60
1	D	275	ALA	N-CA-C	5.45	118.34	108.69
1	J	244	ASN	CA-CB-CG	-5.45	107.15	112.60
1	B	102	ARG	N-CA-CB	-5.44	103.37	110.88
1	E	244	ASN	CA-CB-CG	-5.44	107.16	112.60
1	G	360	PHE	CA-CB-CG	5.44	119.24	113.80
1	G	244	ASN	CA-CB-CG	-5.43	107.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	244	ASN	CA-CB-CG	-5.42	107.18	112.60
1	H	36	HIS	CA-CB-CG	5.42	119.22	113.80
1	I	102	ARG	N-CA-CB	-5.42	103.41	110.88
1	D	36	HIS	CA-CB-CG	5.42	119.22	113.80
1	E	159	ASN	CA-CB-CG	-5.41	107.19	112.60
1	K	168	ASN	CB-CG-ND2	5.41	124.52	116.40
1	B	360	PHE	CA-CB-CG	5.41	119.21	113.80
1	C	159	ASN	CA-CB-CG	-5.41	107.19	112.60
1	L	244	ASN	CA-CB-CG	-5.41	107.19	112.60
1	B	171	HIS	CA-CB-CG	-5.41	108.39	113.80
1	F	102	ARG	N-CA-CB	-5.41	103.42	110.88
1	J	360	PHE	CA-CB-CG	5.41	119.21	113.80
1	B	159	ASN	CA-CB-CG	-5.41	107.19	112.60
1	D	168	ASN	CB-CG-ND2	5.40	124.50	116.40
1	G	102	ARG	N-CA-CB	-5.40	103.42	110.88
1	G	168	ASN	CB-CG-ND2	5.40	124.50	116.40
1	H	171	HIS	CA-CB-CG	-5.40	108.40	113.80
1	I	168	ASN	CB-CG-ND2	5.40	124.50	116.40
1	A	102	ARG	N-CA-CB	-5.40	103.43	110.88
1	A	168	ASN	CB-CG-ND2	5.40	124.50	116.40
1	C	102	ARG	N-CA-CB	-5.40	103.43	110.88
1	H	168	ASN	CB-CG-ND2	5.40	124.50	116.40
1	A	360	PHE	CA-CB-CG	5.40	119.20	113.80
1	C	168	ASN	CB-CG-ND2	5.40	124.50	116.40
1	E	360	PHE	CA-CB-CG	5.40	119.20	113.80
1	F	360	PHE	CA-CB-CG	5.39	119.19	113.80
1	H	102	ARG	N-CA-CB	-5.39	103.44	110.88
1	C	366	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	D	102	ARG	N-CA-CB	-5.39	103.44	110.88
1	D	360	PHE	CA-CB-CG	5.39	119.19	113.80
1	L	168	ASN	CB-CG-ND2	5.39	124.49	116.40
1	C	360	PHE	CA-CB-CG	5.39	119.19	113.80
1	I	36	HIS	CA-CB-CG	5.39	119.19	113.80
1	J	102	ARG	N-CA-CB	-5.39	103.44	110.88
1	K	23	ASP	CA-CB-CG	5.39	117.99	112.60
1	L	159	ASN	CA-CB-CG	-5.39	107.21	112.60
1	B	168	ASN	CB-CG-ND2	5.39	124.48	116.40
1	K	102	ARG	N-CA-CB	-5.39	103.45	110.88
1	F	168	ASN	CB-CG-ND2	5.38	124.48	116.40
1	J	351	PRO	N-CA-C	5.38	123.56	112.47
1	G	23	ASP	CA-CB-CG	5.38	117.98	112.60
1	J	36	HIS	CA-CB-CG	5.38	119.18	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	102	ARG	N-CA-CB	-5.38	103.45	110.88
1	F	23	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	175	VAL	O-C-N	-5.38	116.64	121.91
1	C	351	PRO	N-CA-C	5.38	123.55	112.47
1	E	168	ASN	CB-CG-ND2	5.38	124.47	116.40
1	I	23	ASP	CA-CB-CG	5.38	117.98	112.60
1	J	366	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	K	351	PRO	N-CA-C	5.38	123.55	112.47
1	L	23	ASP	CA-CB-CG	5.38	117.98	112.60
1	E	102	ARG	N-CA-CB	-5.38	103.46	110.88
1	K	159	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	36	HIS	CA-CB-CG	5.37	119.17	113.80
1	D	351	PRO	N-CA-C	5.37	123.54	112.47
1	F	366	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	L	36	HIS	CA-CB-CG	5.37	119.17	113.80
1	L	360	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	159	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	171	HIS	CA-CB-CG	-5.37	108.43	113.80
1	J	168	ASN	CB-CG-ND2	5.37	124.46	116.40
1	A	351	PRO	N-CA-C	5.37	123.53	112.47
1	F	36	HIS	CA-CB-CG	5.37	119.17	113.80
1	G	36	HIS	CA-CB-CG	5.37	119.17	113.80
1	B	351	PRO	N-CA-C	5.37	123.53	112.47
1	L	351	PRO	N-CA-C	5.37	123.53	112.47
1	A	23	ASP	CA-CB-CG	5.37	117.97	112.60
1	F	159	ASN	CA-CB-CG	-5.37	107.23	112.60
1	I	159	ASN	CA-CB-CG	-5.37	107.23	112.60
1	F	171	HIS	CA-CB-CG	-5.36	108.44	113.80
1	H	351	PRO	N-CA-C	5.36	123.52	112.47
1	J	171	HIS	CA-CB-CG	-5.36	108.44	113.80
1	K	171	HIS	CA-CB-CG	-5.36	108.44	113.80
1	L	366	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	J	175	VAL	O-C-N	-5.36	116.66	121.91
1	L	171	HIS	CA-CB-CG	-5.36	108.44	113.80
1	D	171	HIS	CA-CB-CG	-5.36	108.44	113.80
1	E	175	VAL	O-C-N	-5.36	116.66	121.91
1	C	36	HIS	CA-CB-CG	5.36	119.16	113.80
1	G	175	VAL	O-C-N	-5.36	116.66	121.91
1	G	159	ASN	CA-CB-CG	-5.36	107.24	112.60
1	H	360	PHE	CA-CB-CG	5.36	119.16	113.80
1	K	36	HIS	CA-CB-CG	5.36	119.16	113.80
1	C	23	ASP	CA-CB-CG	5.35	117.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	HIS	CA-CB-CG	-5.35	108.45	113.80
1	E	351	PRO	N-CA-C	5.35	123.50	112.47
1	F	175	VAL	O-C-N	-5.35	116.66	121.91
1	G	171	HIS	CA-CB-CG	-5.35	108.45	113.80
1	H	159	ASN	CA-CB-CG	-5.35	107.25	112.60
1	I	351	PRO	N-CA-C	5.35	123.50	112.47
1	K	360	PHE	CA-CB-CG	5.35	119.15	113.80
1	D	159	ASN	CA-CB-CG	-5.35	107.25	112.60
1	L	175	VAL	O-C-N	-5.35	116.66	121.91
1	A	175	VAL	O-C-N	-5.35	116.67	121.91
1	E	23	ASP	CA-CB-CG	5.35	117.95	112.60
1	F	351	PRO	N-CA-C	5.35	123.48	112.47
1	B	36	HIS	CA-CB-CG	5.34	119.14	113.80
1	B	175	VAL	O-C-N	-5.34	116.67	121.91
1	C	179	TYR	N-CA-C	5.34	118.06	108.17
1	G	351	PRO	N-CA-C	5.34	123.48	112.47
1	E	366	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	F	179	TYR	N-CA-C	5.34	118.05	108.17
1	I	171	HIS	CA-CB-CG	-5.34	108.46	113.80
1	I	360	PHE	CA-CB-CG	5.34	119.14	113.80
1	L	179	TYR	N-CA-C	5.34	118.05	108.17
1	A	366	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	I	366	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	J	23	ASP	CA-CB-CG	5.34	117.94	112.60
1	J	159	ASN	CA-CB-CG	-5.34	107.26	112.60
1	H	179	TYR	N-CA-C	5.34	118.04	108.17
1	K	175	VAL	O-C-N	-5.34	116.68	121.91
1	D	23	ASP	CA-CB-CG	5.33	117.93	112.60
1	I	175	VAL	O-C-N	-5.33	116.68	121.91
1	E	36	HIS	CA-CB-CG	5.33	119.13	113.80
1	E	171	HIS	CA-CB-CG	-5.33	108.47	113.80
1	J	179	TYR	N-CA-C	5.33	118.03	108.17
1	K	179	TYR	N-CA-C	5.33	118.03	108.17
1	B	23	ASP	CA-CB-CG	5.33	117.92	112.60
1	H	366	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	D	175	VAL	O-C-N	-5.32	116.69	121.91
1	G	366	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	179	TYR	N-CA-C	5.32	118.01	108.17
1	H	23	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	366	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	B	179	TYR	N-CA-C	5.31	118.00	108.17
1	G	179	TYR	N-CA-C	5.31	118.00	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	179	TYR	N-CA-C	5.31	117.99	108.17
1	E	179	TYR	N-CA-C	5.30	117.98	108.17
1	E	81	ALA	N-CA-C	5.30	117.06	111.28
1	K	366	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	D	179	TYR	N-CA-C	5.29	117.96	108.17
1	L	81	ALA	N-CA-C	5.29	117.04	111.28
1	I	81	ALA	N-CA-C	5.28	117.04	111.28
1	B	366	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	F	81	ALA	N-CA-C	5.28	117.03	111.28
1	J	81	ALA	N-CA-C	5.28	117.03	111.28
1	H	211	HIS	CB-CG-ND1	5.28	130.61	122.70
1	A	81	ALA	N-CA-C	5.27	117.03	111.28
1	B	211	HIS	CB-CG-ND1	5.27	130.61	122.70
1	H	175	VAL	O-C-N	-5.27	116.75	121.91
1	C	81	ALA	N-CA-C	5.27	117.02	111.28
1	D	81	ALA	N-CA-C	5.27	117.02	111.28
1	J	211	HIS	CB-CG-ND1	5.26	130.60	122.70
1	I	122	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	81	ALA	N-CA-C	5.25	117.01	111.28
1	F	211	HIS	CB-CG-ND1	5.25	130.58	122.70
1	D	211	HIS	CB-CG-ND1	5.25	130.57	122.70
1	K	122	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	122	ASP	CA-CB-CG	5.25	117.84	112.60
1	H	122	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	122	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	211	HIS	CB-CG-ND1	5.24	130.56	122.70
1	J	122	ASP	CA-CB-CG	5.24	117.84	112.60
1	L	122	ASP	CA-CB-CG	5.24	117.84	112.60
1	I	211	HIS	CB-CG-ND1	5.24	130.56	122.70
1	F	122	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	211	HIS	CB-CG-ND1	5.24	130.55	122.70
1	C	210	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	E	211	HIS	CB-CG-ND1	5.23	130.55	122.70
1	H	81	ALA	N-CA-C	5.23	116.98	111.28
1	L	210	HIS	CB-CG-CD2	-5.23	124.41	131.20
1	L	211	HIS	CB-CG-ND1	5.23	130.54	122.70
1	K	211	HIS	CB-CG-ND1	5.23	130.54	122.70
1	F	210	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	E	122	ASP	CA-CB-CG	5.22	117.82	112.60
1	G	211	HIS	CB-CG-ND1	5.22	130.53	122.70
1	H	210	HIS	CB-CG-CD2	-5.22	124.41	131.20
1	I	210	HIS	CB-CG-CD2	-5.22	124.42	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	122	ASP	CA-CB-CG	5.21	117.81	112.60
1	K	164	TYR	N-CA-C	5.21	120.50	113.72
1	C	122	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	210	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	K	210	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	G	122	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	210	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	J	433	VAL	N-CA-C	-5.20	101.91	108.93
1	D	175	VAL	N-CA-C	5.20	115.41	110.42
1	E	175	VAL	N-CA-C	5.20	115.41	110.42
1	G	210	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	K	433	VAL	N-CA-C	-5.20	101.91	108.93
1	H	164	TYR	N-CA-C	5.19	120.47	113.72
1	D	210	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	E	210	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	E	433	VAL	N-CA-C	-5.19	101.93	108.93
1	D	226	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	A	433	VAL	N-CA-C	-5.18	101.93	108.93
1	I	433	VAL	N-CA-C	-5.18	101.93	108.93
1	F	433	VAL	N-CA-C	-5.18	101.94	108.93
1	G	175	VAL	N-CA-C	5.18	115.39	110.42
1	C	433	VAL	N-CA-C	-5.18	101.94	108.93
1	G	433	VAL	N-CA-C	-5.18	101.94	108.93
1	L	433	VAL	N-CA-C	-5.18	101.94	108.93
1	F	164	TYR	N-CA-C	5.18	120.45	113.72
1	F	175	VAL	N-CA-C	5.18	115.39	110.42
1	K	175	VAL	N-CA-C	5.18	115.39	110.42
1	E	164	TYR	N-CA-C	5.17	120.45	113.72
1	H	226	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	J	210	HIS	CB-CG-CD2	-5.17	124.47	131.20
1	L	164	TYR	N-CA-C	5.17	120.45	113.72
1	C	175	VAL	N-CA-C	5.17	115.39	110.42
1	I	226	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	164	TYR	N-CA-C	5.17	120.44	113.72
1	L	175	VAL	N-CA-C	5.17	115.38	110.42
1	K	226	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	B	433	VAL	N-CA-C	-5.17	101.95	108.93
1	H	433	VAL	N-CA-C	-5.17	101.96	108.93
1	C	164	TYR	N-CA-C	5.16	120.43	113.72
1	J	164	TYR	N-CA-C	5.16	120.43	113.72
1	D	433	VAL	N-CA-C	-5.16	101.96	108.93
1	F	226	ASN	OD1-CG-ND2	-5.16	117.44	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	VAL	N-CA-C	5.16	115.38	110.42
1	I	30	HIS	CB-CG-ND1	5.16	130.44	122.70
1	A	226	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	G	164	TYR	N-CA-C	5.15	120.42	113.72
1	J	175	VAL	N-CA-C	5.15	115.37	110.42
1	E	226	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	G	226	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	I	175	VAL	N-CA-C	5.15	115.36	110.42
1	H	175	VAL	N-CA-C	5.15	115.36	110.42
1	B	226	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	D	164	TYR	N-CA-C	5.14	120.41	113.72
1	I	164	TYR	N-CA-C	5.14	120.41	113.72
1	L	226	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	F	30	HIS	CB-CG-ND1	5.14	130.41	122.70
1	G	101	ASP	CA-CB-CG	5.14	117.74	112.60
1	K	30	HIS	CB-CG-ND1	5.14	130.41	122.70
1	B	175	VAL	N-CA-C	5.14	115.36	110.42
1	B	164	TYR	N-CA-C	5.14	120.40	113.72
1	C	226	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	E	101	ASP	CA-CB-CG	5.13	117.73	112.60
1	H	30	HIS	CB-CG-ND1	5.13	130.40	122.70
1	H	101	ASP	CA-CB-CG	5.13	117.73	112.60
1	G	30	HIS	CB-CG-ND1	5.12	130.39	122.70
1	C	30	HIS	CB-CG-ND1	5.12	130.39	122.70
1	D	101	ASP	CA-CB-CG	5.12	117.72	112.60
1	I	101	ASP	CA-CB-CG	5.12	117.72	112.60
1	D	30	HIS	CB-CG-ND1	5.12	130.38	122.70
1	E	30	HIS	CB-CG-ND1	5.12	130.38	122.70
1	H	172	ARG	N-CA-CB	-5.12	101.12	110.65
1	A	30	HIS	CB-CG-ND1	5.12	130.38	122.70
1	E	172	ARG	N-CA-CB	-5.12	101.13	110.65
1	D	338	ASN	N-CA-C	5.12	121.70	110.80
1	B	30	HIS	CB-CG-ND1	5.12	130.37	122.70
1	B	172	ARG	N-CA-CB	-5.12	101.13	110.65
1	J	172	ARG	N-CA-CB	-5.12	101.13	110.65
1	C	338	ASN	N-CA-C	5.11	121.69	110.80
1	H	338	ASN	N-CA-C	5.11	121.69	110.80
1	K	172	ARG	N-CA-CB	-5.11	101.14	110.65
1	B	338	ASN	N-CA-C	5.11	121.68	110.80
1	C	172	ARG	N-CA-CB	-5.11	101.15	110.65
1	F	338	ASN	N-CA-C	5.11	121.67	110.80
1	J	226	ASN	OD1-CG-ND2	-5.11	117.50	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	30	HIS	CB-CG-ND1	5.11	130.36	122.70
1	L	338	ASN	N-CA-C	5.11	121.68	110.80
1	A	338	ASN	N-CA-C	5.10	121.67	110.80
1	A	172	ARG	N-CA-CB	-5.10	101.16	110.65
1	D	172	ARG	N-CA-CB	-5.10	101.16	110.65
1	F	172	ARG	N-CA-CB	-5.10	101.16	110.65
1	K	338	ASN	N-CA-C	5.10	121.67	110.80
1	A	101	ASP	CA-CB-CG	5.10	117.70	112.60
1	E	338	ASN	N-CA-C	5.10	121.66	110.80
1	I	338	ASN	N-CA-C	5.10	121.66	110.80
1	C	256	MET	CA-C-N	5.10	124.71	119.05
1	C	256	MET	C-N-CA	5.10	124.71	119.05
1	G	338	ASN	N-CA-C	5.10	121.66	110.80
1	C	101	ASP	CA-CB-CG	5.10	117.70	112.60
1	K	101	ASP	CA-CB-CG	5.10	117.70	112.60
1	E	338	ASN	CB-CG-ND2	5.09	124.04	116.40
1	J	30	HIS	CB-CG-ND1	5.09	130.34	122.70
1	B	256	MET	CA-C-N	5.09	124.70	119.05
1	B	256	MET	C-N-CA	5.09	124.70	119.05
1	H	256	MET	CA-C-N	5.09	124.70	119.05
1	H	256	MET	C-N-CA	5.09	124.70	119.05
1	B	101	ASP	CA-CB-CG	5.09	117.69	112.60
1	H	338	ASN	CB-CG-ND2	5.09	124.03	116.40
1	J	338	ASN	N-CA-C	5.09	121.63	110.80
1	L	172	ARG	N-CA-CB	-5.08	101.19	110.65
1	G	172	ARG	N-CA-CB	-5.08	101.19	110.65
1	I	172	ARG	N-CA-CB	-5.08	101.20	110.65
1	J	101	ASP	CA-CB-CG	5.08	117.68	112.60
1	K	338	ASN	CB-CG-ND2	5.08	124.03	116.40
1	F	338	ASN	CB-CG-ND2	5.08	124.02	116.40
1	D	338	ASN	CB-CG-ND2	5.08	124.02	116.40
1	E	256	MET	CA-C-N	5.08	124.69	119.05
1	E	256	MET	C-N-CA	5.08	124.69	119.05
1	D	256	MET	CA-C-N	5.08	124.68	119.05
1	D	256	MET	C-N-CA	5.08	124.68	119.05
1	G	37	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	H	37	GLN	OE1-CD-NE2	-5.08	117.53	122.60
1	J	170	GLY	O-C-N	-5.08	116.10	122.70
1	K	256	MET	CA-C-N	5.08	124.68	119.05
1	K	256	MET	C-N-CA	5.08	124.68	119.05
1	I	37	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	I	338	ASN	CB-CG-ND2	5.07	124.01	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	338	ASN	CB-CG-ND2	5.07	124.01	116.40
1	B	338	ASN	CB-CG-ND2	5.07	124.01	116.40
1	L	101	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	338	ASN	CB-CG-ND2	5.07	124.00	116.40
1	A	256	MET	CA-C-N	5.07	124.67	119.05
1	A	256	MET	C-N-CA	5.07	124.67	119.05
1	A	338	ASN	CB-CG-ND2	5.07	124.00	116.40
1	E	37	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	A	37	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	L	338	ASN	CB-CG-ND2	5.06	123.99	116.40
1	F	37	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	F	101	ASP	CA-CB-CG	5.06	117.66	112.60
1	L	256	MET	CA-C-N	5.06	124.66	119.05
1	L	256	MET	C-N-CA	5.06	124.66	119.05
1	D	170	GLY	O-C-N	-5.06	116.13	122.70
1	G	256	MET	CA-C-N	5.05	124.66	119.05
1	G	256	MET	C-N-CA	5.05	124.66	119.05
1	J	256	MET	CA-C-N	5.05	124.66	119.05
1	J	256	MET	C-N-CA	5.05	124.66	119.05
1	K	37	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	C	37	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	C	170	GLY	O-C-N	-5.05	116.13	122.70
1	F	256	MET	CA-C-N	5.05	124.66	119.05
1	F	256	MET	C-N-CA	5.05	124.66	119.05
1	I	256	MET	CA-C-N	5.05	124.66	119.05
1	I	256	MET	C-N-CA	5.05	124.66	119.05
1	G	338	ASN	CB-CG-ND2	5.05	123.98	116.40
1	B	170	GLY	O-C-N	-5.05	116.14	122.70
1	A	170	GLY	O-C-N	-5.05	116.14	122.70
1	G	170	GLY	O-C-N	-5.04	116.14	122.70
1	E	170	GLY	O-C-N	-5.04	116.15	122.70
1	K	337	ARG	O-C-N	-5.04	116.94	122.38
1	B	337	ARG	O-C-N	-5.03	116.94	122.38
1	K	170	GLY	O-C-N	-5.03	116.16	122.70
1	I	170	GLY	O-C-N	-5.03	116.16	122.70
1	L	37	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	37	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	E	391	PRO	N-CA-C	5.03	118.39	110.50
1	L	170	GLY	O-C-N	-5.03	116.17	122.70
1	I	391	PRO	N-CA-C	5.02	118.39	110.50
1	D	37	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	D	337	ARG	O-C-N	-5.02	116.96	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	37	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	L	337	ARG	O-C-N	-5.00	116.98	122.38

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	352	LYS	Peptide
1	B	224	ARG	Sidechain
1	B	352	LYS	Peptide
1	C	224	ARG	Sidechain
1	C	352	LYS	Peptide
1	D	224	ARG	Sidechain
1	D	352	LYS	Peptide
1	E	224	ARG	Sidechain
1	E	352	LYS	Peptide
1	F	224	ARG	Sidechain
1	F	352	LYS	Peptide
1	G	224	ARG	Sidechain
1	G	352	LYS	Peptide
1	H	224	ARG	Sidechain
1	H	352	LYS	Peptide
1	I	224	ARG	Sidechain
1	I	352	LYS	Peptide
1	J	224	ARG	Sidechain
1	J	352	LYS	Peptide
1	K	224	ARG	Sidechain
1	K	352	LYS	Peptide
1	L	224	ARG	Sidechain
1	L	352	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3455	0	3371	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3455	0	3371	55	0
1	C	3455	0	3371	61	2
1	D	3455	0	3371	56	0
1	E	3455	0	3371	54	0
1	F	3455	0	3371	54	2
1	G	3455	0	3371	53	0
1	H	3455	0	3371	58	0
1	I	3455	0	3371	56	0
1	J	3455	0	3371	59	0
1	K	3455	0	3371	63	0
1	L	3455	0	3371	57	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	10	0	5	1	0
3	B	10	0	5	1	0
3	C	10	0	5	1	0
3	D	10	0	5	1	0
3	E	10	0	5	1	0
3	F	10	0	5	1	0
3	G	10	0	5	1	0
3	H	10	0	5	1	0
3	I	10	0	5	1	0
3	J	10	0	5	1	0
3	K	10	0	5	1	0
3	L	10	0	5	1	0
All	All	41604	0	40512	622	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (622) 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:K:258:LYS:HG2	1:K:320:LYS:HB3	1.79	0.65
1:C:258:LYS:HG2	1:C:320:LYS:HB3	1.79	0.65
1:E:258:LYS:HG2	1:E:320:LYS:HB3	1.79	0.65
1:G:258:LYS:HG2	1:G:320:LYS:HB3	1.79	0.65
1:F:258:LYS:HG2	1:F:320:LYS:HB3	1.79	0.65
1:I:258:LYS:HG2	1:I:320:LYS:HB3	1.79	0.65
1:B:258:LYS:HG2	1:B:320:LYS:HB3	1.79	0.65
1:L:258:LYS:HG2	1:L:320:LYS:HB3	1.79	0.64
1:A:258:LYS:HG2	1:A:320:LYS:HB3	1.79	0.63
1:J:258:LYS:HG2	1:J:320:LYS:HB3	1.79	0.63
1:H:258:LYS:HG2	1:H:320:LYS:HB3	1.79	0.63
1:D:258:LYS:HG2	1:D:320:LYS:HB3	1.79	0.63
1:D:192:ARG:HD3	1:D:219:ASN:HD22	1.64	0.63
1:C:261:PHE:HB2	1:K:457:PRO:HD2	1.79	0.63
1:J:192:ARG:HD3	1:J:219:ASN:HD22	1.64	0.63
1:F:192:ARG:HD3	1:F:219:ASN:HD22	1.64	0.62
1:G:192:ARG:HD3	1:G:219:ASN:HD22	1.64	0.62
1:A:192:ARG:HD3	1:A:219:ASN:HD22	1.64	0.62
1:I:192:ARG:HD3	1:I:219:ASN:HD22	1.64	0.62
1:H:192:ARG:HD3	1:H:219:ASN:HD22	1.64	0.62
1:L:192:ARG:HD3	1:L:219:ASN:HD22	1.64	0.62
1:B:192:ARG:HD3	1:B:219:ASN:HD22	1.64	0.62
1:E:192:ARG:HD3	1:E:219:ASN:HD22	1.64	0.61
1:C:192:ARG:HD3	1:C:219:ASN:HD22	1.64	0.61
1:K:192:ARG:HD3	1:K:219:ASN:HD22	1.64	0.61
1:C:92:LEU:HA	1:C:99:GLY:HA2	1.83	0.61
1:A:92:LEU:HA	1:A:99:GLY:HA2	1.83	0.61
1:D:456:THR:O	1:J:458:HIS:HE1	1.84	0.61
1:E:92:LEU:HA	1:E:99:GLY:HA2	1.83	0.61
1:C:383:LYS:NZ	1:C:383:LYS:HB3	2.16	0.61
1:I:92:LEU:HA	1:I:99:GLY:HA2	1.83	0.61
1:A:383:LYS:NZ	1:A:383:LYS:HB3	2.16	0.61
1:J:92:LEU:HA	1:J:99:GLY:HA2	1.83	0.60
1:L:92:LEU:HA	1:L:99:GLY:HA2	1.83	0.60
1:D:383:LYS:NZ	1:D:383:LYS:HB3	2.16	0.60
1:G:92:LEU:HA	1:G:99:GLY:HA2	1.83	0.60
1:H:92:LEU:HA	1:H:99:GLY:HA2	1.83	0.60
1:H:383:LYS:NZ	1:H:383:LYS:HB3	2.16	0.60
1:K:92:LEU:HA	1:K:99:GLY:HA2	1.83	0.60
1:L:383:LYS:NZ	1:L:383:LYS:HB3	2.16	0.60
1:D:92:LEU:HA	1:D:99:GLY:HA2	1.83	0.60
1:J:383:LYS:HB3	1:J:383:LYS:NZ	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:LYS:NZ	1:E:383:LYS:HB3	2.16	0.60
1:H:214:ALA:HB3	1:H:218:GLN:HB2	1.84	0.60
1:F:214:ALA:HB3	1:F:218:GLN:HB2	1.84	0.60
1:F:92:LEU:HA	1:F:99:GLY:HA2	1.83	0.60
1:C:214:ALA:HB3	1:C:218:GLN:HB2	1.84	0.59
1:B:92:LEU:HA	1:B:99:GLY:HA2	1.83	0.59
1:B:383:LYS:HB3	1:B:383:LYS:NZ	2.16	0.59
1:F:383:LYS:NZ	1:F:383:LYS:HB3	2.16	0.59
1:I:383:LYS:NZ	1:I:383:LYS:HB3	2.16	0.59
1:J:214:ALA:HB3	1:J:218:GLN:HB2	1.84	0.59
1:K:383:LYS:NZ	1:K:383:LYS:HB3	2.16	0.59
1:A:214:ALA:HB3	1:A:218:GLN:HB2	1.84	0.59
1:C:457:PRO:HD2	1:K:261:PHE:HB2	1.84	0.59
1:D:214:ALA:HB3	1:D:218:GLN:HB2	1.84	0.59
1:I:214:ALA:HB3	1:I:218:GLN:HB2	1.84	0.59
1:K:214:ALA:HB3	1:K:218:GLN:HB2	1.84	0.59
1:B:457:PRO:HD2	1:L:261:PHE:HB2	1.84	0.59
1:L:214:ALA:HB3	1:L:218:GLN:HB2	1.84	0.59
1:E:214:ALA:HB3	1:E:218:GLN:HB2	1.84	0.59
1:A:269:HIS:HE1	1:A:359:ARG:NH1	2.01	0.59
1:G:383:LYS:NZ	1:G:383:LYS:HB3	2.16	0.59
1:F:269:HIS:HE1	1:F:359:ARG:NH1	2.01	0.59
1:B:214:ALA:HB3	1:B:218:GLN:HB2	1.84	0.59
1:G:214:ALA:HB3	1:G:218:GLN:HB2	1.84	0.59
1:G:269:HIS:HE1	1:G:359:ARG:NH1	2.01	0.59
1:H:425:ARG:HG2	1:H:429:LYS:HD2	1.85	0.59
1:J:180:PHE:HB3	1:K:29:GLN:HB3	1.82	0.59
1:J:269:HIS:HE1	1:J:359:ARG:NH1	2.01	0.59
1:C:269:HIS:HE1	1:C:359:ARG:NH1	2.01	0.58
1:A:425:ARG:HG2	1:A:429:LYS:HD2	1.85	0.58
1:D:269:HIS:HE1	1:D:359:ARG:NH1	2.01	0.58
1:D:180:PHE:HB3	1:E:29:GLN:HB3	1.84	0.58
1:E:457:PRO:HD2	1:I:261:PHE:HB2	1.86	0.58
1:B:76:ILE:HD12	1:B:85:LEU:HD23	1.86	0.58
1:D:458:HIS:HE1	1:J:456:THR:O	1.86	0.58
1:E:425:ARG:HG2	1:E:429:LYS:HD2	1.85	0.58
1:G:76:ILE:HD12	1:G:85:LEU:HD23	1.86	0.58
1:G:425:ARG:HG2	1:G:429:LYS:HD2	1.85	0.58
1:I:269:HIS:HE1	1:I:359:ARG:NH1	2.01	0.58
1:K:425:ARG:HG2	1:K:429:LYS:HD2	1.85	0.58
1:D:425:ARG:HG2	1:D:429:LYS:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:ILE:HD12	1:E:85:LEU:HD23	1.86	0.58
1:J:76:ILE:HD12	1:J:85:LEU:HD23	1.86	0.58
1:D:76:ILE:HD12	1:D:85:LEU:HD23	1.86	0.58
1:E:269:HIS:HE1	1:E:359:ARG:NH1	2.01	0.58
1:F:76:ILE:HD12	1:F:85:LEU:HD23	1.86	0.58
1:B:19:LEU:HD11	1:B:42:PHE:HZ	1.69	0.58
1:I:76:ILE:HD12	1:I:85:LEU:HD23	1.86	0.58
1:J:425:ARG:HG2	1:J:429:LYS:HD2	1.84	0.58
1:L:76:ILE:HD12	1:L:85:LEU:HD23	1.86	0.58
1:F:456:THR:O	1:H:458:HIS:HE1	1.85	0.58
1:H:19:LEU:HD11	1:H:42:PHE:HZ	1.69	0.58
1:B:425:ARG:HG2	1:B:429:LYS:HD2	1.85	0.58
1:F:19:LEU:HD11	1:F:42:PHE:HZ	1.69	0.58
1:F:458:HIS:HE1	1:H:456:THR:O	1.86	0.58
1:J:19:LEU:HD11	1:J:42:PHE:HZ	1.69	0.58
1:L:269:HIS:HE1	1:L:359:ARG:NH1	2.01	0.58
1:L:425:ARG:HG2	1:L:429:LYS:HD2	1.85	0.58
1:A:76:ILE:HD12	1:A:85:LEU:HD23	1.86	0.57
1:C:76:ILE:HD12	1:C:85:LEU:HD23	1.86	0.57
1:K:269:HIS:HE1	1:K:359:ARG:NH1	2.01	0.57
1:H:269:HIS:HE1	1:H:359:ARG:NH1	2.01	0.57
1:F:425:ARG:HG2	1:F:429:LYS:HD2	1.85	0.57
1:I:425:ARG:HG2	1:I:429:LYS:HD2	1.85	0.57
1:C:425:ARG:HG2	1:C:429:LYS:HD2	1.85	0.57
1:E:456:THR:O	1:I:458:HIS:HE1	1.87	0.57
1:G:19:LEU:HD11	1:G:42:PHE:HZ	1.69	0.57
1:L:314:PRO:HB2	1:L:446:ARG:NH1	2.20	0.57
1:E:19:LEU:HD11	1:E:42:PHE:HZ	1.69	0.57
1:E:314:PRO:HB2	1:E:446:ARG:NH1	2.20	0.57
1:K:19:LEU:HD11	1:K:42:PHE:HZ	1.69	0.57
1:H:66:VAL:HG13	1:H:92:LEU:HB2	1.87	0.57
1:K:66:VAL:HG13	1:K:92:LEU:HB2	1.87	0.57
1:B:269:HIS:HE1	1:B:359:ARG:NH1	2.01	0.57
1:E:66:VAL:HG13	1:E:92:LEU:HB2	1.87	0.57
1:L:19:LEU:HD11	1:L:42:PHE:HZ	1.69	0.57
1:L:66:VAL:HG13	1:L:92:LEU:HB2	1.87	0.57
1:B:261:PHE:HB2	1:L:457:PRO:HD2	1.86	0.57
1:H:76:ILE:HD12	1:H:85:LEU:HD23	1.86	0.57
1:I:66:VAL:HG13	1:I:92:LEU:HB2	1.87	0.57
1:K:76:ILE:HD12	1:K:85:LEU:HD23	1.86	0.57
1:B:66:VAL:HG13	1:B:92:LEU:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:THR:O	1:G:458:HIS:HE1	1.88	0.56
1:D:19:LEU:HD11	1:D:42:PHE:HZ	1.69	0.56
1:A:66:VAL:HG13	1:A:92:LEU:HB2	1.87	0.56
1:A:314:PRO:HB2	1:A:446:ARG:NH1	2.20	0.56
1:A:457:PRO:HD2	1:G:261:PHE:HB2	1.87	0.56
1:C:19:LEU:HD11	1:C:42:PHE:HZ	1.69	0.56
1:D:66:VAL:HG13	1:D:92:LEU:HB2	1.87	0.56
1:D:314:PRO:HB2	1:D:446:ARG:NH1	2.20	0.56
1:H:314:PRO:HB2	1:H:446:ARG:NH1	2.20	0.56
1:I:314:PRO:HB2	1:I:446:ARG:NH1	2.20	0.56
1:J:314:PRO:HB2	1:J:446:ARG:NH1	2.20	0.56
1:A:19:LEU:HD11	1:A:42:PHE:HZ	1.69	0.56
1:B:351:PRO:HB2	1:B:352:LYS:HG3	1.88	0.56
1:C:66:VAL:HG13	1:C:92:LEU:HB2	1.87	0.56
1:I:19:LEU:HD11	1:I:42:PHE:HZ	1.69	0.56
1:J:351:PRO:HB2	1:J:352:LYS:HG3	1.88	0.56
1:K:314:PRO:HB2	1:K:446:ARG:NH1	2.20	0.56
1:A:261:PHE:HB2	1:G:457:PRO:HD2	1.88	0.56
1:C:314:PRO:HB2	1:C:446:ARG:NH1	2.20	0.56
1:F:66:VAL:HG13	1:F:92:LEU:HB2	1.87	0.56
1:G:314:PRO:HB2	1:G:446:ARG:NH1	2.20	0.56
1:L:351:PRO:HB2	1:L:352:LYS:HG3	1.88	0.56
1:C:351:PRO:HB2	1:C:352:LYS:HG3	1.88	0.56
1:E:351:PRO:HB2	1:E:352:LYS:HG3	1.88	0.56
1:B:314:PRO:HB2	1:B:446:ARG:NH1	2.20	0.56
1:E:261:PHE:HB2	1:I:457:PRO:HD2	1.88	0.56
1:G:66:VAL:HG13	1:G:92:LEU:HB2	1.87	0.56
1:K:351:PRO:HB2	1:K:352:LYS:HG3	1.88	0.56
1:F:314:PRO:HB2	1:F:446:ARG:NH1	2.20	0.55
1:J:66:VAL:HG13	1:J:92:LEU:HB2	1.87	0.55
1:F:351:PRO:HB2	1:F:352:LYS:HG3	1.88	0.55
1:G:351:PRO:HB2	1:G:352:LYS:HG3	1.88	0.55
1:A:93:GLU:HB3	1:A:98:GLN:OE1	2.07	0.55
1:A:458:HIS:HE1	1:G:456:THR:O	1.89	0.55
1:C:93:GLU:HB3	1:C:98:GLN:OE1	2.07	0.55
1:I:351:PRO:HB2	1:I:352:LYS:HG3	1.88	0.55
1:G:65:MET:HE2	1:G:94:PRO:HD3	1.89	0.55
1:B:65:MET:HE2	1:B:94:PRO:HD3	1.89	0.55
1:D:93:GLU:HB3	1:D:98:GLN:OE1	2.07	0.55
1:K:65:MET:HE2	1:K:94:PRO:HD3	1.89	0.55
1:H:65:MET:HE2	1:H:94:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:351:PRO:HB2	1:H:352:LYS:HG3	1.88	0.55
1:K:93:GLU:HB3	1:K:98:GLN:OE1	2.07	0.55
1:C:65:MET:HE2	1:C:94:PRO:HD3	1.89	0.55
1:E:65:MET:HE2	1:E:94:PRO:HD3	1.89	0.55
1:J:65:MET:HE2	1:J:94:PRO:HD3	1.89	0.55
1:L:458:HIS:HD2	1:L:460:VAL:H	1.55	0.55
1:A:458:HIS:HD2	1:A:460:VAL:H	1.55	0.55
1:B:93:GLU:HB3	1:B:98:GLN:OE1	2.07	0.54
1:D:351:PRO:HB2	1:D:352:LYS:HG3	1.88	0.54
1:F:65:MET:HE2	1:F:94:PRO:HD3	1.89	0.54
1:H:93:GLU:HB3	1:H:98:GLN:OE1	2.07	0.54
1:J:93:GLU:HB3	1:J:98:GLN:OE1	2.07	0.54
1:A:351:PRO:HB2	1:A:352:LYS:HG3	1.88	0.54
1:I:93:GLU:HB3	1:I:98:GLN:OE1	2.07	0.54
1:E:458:HIS:HE1	1:I:456:THR:O	1.89	0.54
1:G:93:GLU:HB3	1:G:98:GLN:OE1	2.07	0.54
1:I:458:HIS:HD2	1:I:460:VAL:H	1.55	0.54
1:E:458:HIS:HD2	1:E:460:VAL:H	1.55	0.54
1:D:65:MET:HE2	1:D:94:PRO:HD3	1.89	0.54
1:I:65:MET:HE2	1:I:94:PRO:HD3	1.89	0.54
1:F:93:GLU:HB3	1:F:98:GLN:OE1	2.07	0.54
1:H:458:HIS:HD2	1:H:460:VAL:H	1.55	0.54
1:A:65:MET:HE2	1:A:94:PRO:HD3	1.89	0.54
1:C:180:PHE:HB3	1:D:29:GLN:HB3	1.90	0.54
1:G:458:HIS:HD2	1:G:460:VAL:H	1.55	0.54
1:H:180:PHE:HB3	1:I:29:GLN:HB3	1.89	0.54
1:J:458:HIS:HD2	1:J:460:VAL:H	1.55	0.54
1:L:93:GLU:HB3	1:L:98:GLN:OE1	2.07	0.54
1:F:458:HIS:HD2	1:F:460:VAL:H	1.55	0.54
1:C:192:ARG:HD3	1:C:219:ASN:ND2	2.23	0.53
1:C:458:HIS:HD2	1:C:460:VAL:H	1.55	0.53
1:D:458:HIS:HD2	1:D:460:VAL:H	1.55	0.53
1:I:192:ARG:HD3	1:I:219:ASN:ND2	2.23	0.53
1:L:65:MET:HE2	1:L:94:PRO:HD3	1.89	0.53
1:B:458:HIS:HE1	1:L:456:THR:O	1.91	0.53
1:E:93:GLU:HB3	1:E:98:GLN:OE1	2.07	0.53
1:G:192:ARG:HD3	1:G:219:ASN:ND2	2.23	0.53
1:A:192:ARG:HD3	1:A:219:ASN:ND2	2.23	0.53
1:B:456:THR:O	1:L:458:HIS:HE1	1.90	0.53
1:D:457:PRO:HD2	1:J:261:PHE:HB2	1.89	0.53
1:H:286:LYS:HB2	1:H:290:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:286:LYS:HB2	1:L:290:LEU:O	2.09	0.53
1:K:192:ARG:HD3	1:K:219:ASN:ND2	2.23	0.53
1:F:286:LYS:HB2	1:F:290:LEU:O	2.09	0.53
1:D:261:PHE:HB2	1:J:457:PRO:HD2	1.89	0.53
1:D:286:LYS:HB2	1:D:290:LEU:O	2.09	0.53
1:F:192:ARG:HD3	1:F:219:ASN:ND2	2.23	0.53
1:G:286:LYS:HB2	1:G:290:LEU:O	2.09	0.53
1:J:192:ARG:HD3	1:J:219:ASN:ND2	2.24	0.53
1:B:458:HIS:HD2	1:B:460:VAL:H	1.55	0.53
1:F:457:PRO:HD2	1:H:261:PHE:HB2	1.90	0.53
1:H:192:ARG:HD3	1:H:219:ASN:ND2	2.23	0.53
1:E:286:LYS:HB2	1:E:290:LEU:O	2.09	0.53
1:B:180:PHE:HB3	1:C:29:GLN:HB3	1.91	0.53
1:D:192:ARG:HD3	1:D:219:ASN:ND2	2.23	0.53
1:J:286:LYS:HB2	1:J:290:LEU:O	2.09	0.53
1:B:286:LYS:HB2	1:B:290:LEU:O	2.09	0.52
1:C:286:LYS:HB2	1:C:290:LEU:O	2.09	0.52
1:K:458:HIS:HD2	1:K:460:VAL:H	1.55	0.52
1:E:192:ARG:HD3	1:E:219:ASN:ND2	2.23	0.52
1:I:286:LYS:HB2	1:I:290:LEU:O	2.09	0.52
1:D:348:VAL:HG21	1:D:353:ALA:HB3	1.92	0.52
1:G:348:VAL:HG21	1:G:353:ALA:HB3	1.92	0.52
1:L:192:ARG:HD3	1:L:219:ASN:ND2	2.23	0.52
1:A:29:GLN:HB3	1:F:180:PHE:HB3	1.90	0.52
1:A:286:LYS:HB2	1:A:290:LEU:O	2.09	0.52
1:B:192:ARG:HD3	1:B:219:ASN:ND2	2.23	0.52
1:G:5:VAL:HG11	1:G:43:PHE:HZ	1.75	0.52
1:K:348:VAL:HG21	1:K:353:ALA:HB3	1.92	0.52
1:I:348:VAL:HG21	1:I:353:ALA:HB3	1.92	0.52
1:A:348:VAL:HG21	1:A:353:ALA:HB3	1.92	0.52
1:D:5:VAL:HG11	1:D:43:PHE:HZ	1.75	0.52
1:F:348:VAL:HG21	1:F:353:ALA:HB3	1.92	0.52
1:K:286:LYS:HB2	1:K:290:LEU:O	2.09	0.52
1:A:180:PHE:HB3	1:B:29:GLN:HB3	1.90	0.52
1:C:5:VAL:HG11	1:C:43:PHE:HZ	1.75	0.52
1:C:348:VAL:HG21	1:C:353:ALA:HB3	1.92	0.52
1:K:5:VAL:HG11	1:K:43:PHE:HZ	1.75	0.51
1:E:5:VAL:HG11	1:E:43:PHE:HZ	1.75	0.51
1:K:180:PHE:HB3	1:L:29:GLN:HB3	1.92	0.51
1:L:348:VAL:HG21	1:L:353:ALA:HB3	1.92	0.51
1:B:5:VAL:HG11	1:B:43:PHE:HZ	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:VAL:HG11	1:I:43:PHE:HZ	1.75	0.51
1:K:169:LYS:HA	1:L:252:THR:HB	1.91	0.51
1:H:5:VAL:HG11	1:H:43:PHE:HZ	1.75	0.51
1:I:180:PHE:HB3	1:J:29:GLN:HB3	1.93	0.51
1:B:348:VAL:HG21	1:B:353:ALA:HB3	1.92	0.51
1:F:5:VAL:HG11	1:F:43:PHE:HZ	1.75	0.51
1:E:348:VAL:HG21	1:E:353:ALA:HB3	1.92	0.51
1:E:467:SER:OG	1:H:171:HIS:ND1	2.35	0.51
1:F:261:PHE:HB2	1:H:457:PRO:HD2	1.92	0.51
1:B:169:LYS:HA	1:C:252:THR:HB	1.92	0.50
1:J:348:VAL:HG21	1:J:353:ALA:HB3	1.92	0.50
1:D:169:LYS:HA	1:E:252:THR:HB	1.92	0.50
1:E:333:ALA:O	1:E:341:ALA:HB1	2.12	0.50
1:G:29:GLN:HB3	1:L:180:PHE:HB3	1.93	0.50
1:K:101:ASP:HB3	1:K:110:ARG:HH22	1.76	0.50
1:B:334:TYR:CE2	1:B:391:PRO:HG3	2.47	0.50
1:C:458:HIS:HE1	1:K:456:THR:O	1.93	0.50
1:J:5:VAL:HG11	1:J:43:PHE:HZ	1.75	0.50
1:J:339:ARG:NH2	1:K:50:ASP:CG	2.69	0.50
1:K:333:ALA:O	1:K:341:ALA:HB1	2.12	0.50
1:L:5:VAL:HG11	1:L:43:PHE:HZ	1.75	0.50
1:L:334:TYR:CE2	1:L:391:PRO:HG3	2.47	0.50
1:A:334:TYR:CE2	1:A:391:PRO:HG3	2.47	0.50
1:B:333:ALA:O	1:B:341:ALA:HB1	2.12	0.50
1:C:101:ASP:HB3	1:C:110:ARG:HH22	1.77	0.50
1:G:333:ALA:O	1:G:341:ALA:HB1	2.12	0.50
1:H:348:VAL:HG21	1:H:353:ALA:HB3	1.92	0.50
1:D:101:ASP:HB3	1:D:110:ARG:HH22	1.77	0.50
1:D:334:TYR:CE2	1:D:391:PRO:HG3	2.47	0.50
1:E:101:ASP:HB3	1:E:110:ARG:HH22	1.76	0.50
1:G:296:TYR:CZ	1:G:385:LYS:HG2	2.47	0.50
1:H:333:ALA:O	1:H:341:ALA:HB1	2.12	0.50
1:H:359:ARG:NH1	3:H:471:GLU:OE1	2.44	0.50
1:E:296:TYR:CZ	1:E:385:LYS:HG2	2.47	0.49
1:F:101:ASP:HB3	1:F:110:ARG:HH22	1.77	0.49
1:F:333:ALA:O	1:F:341:ALA:HB1	2.12	0.49
1:H:101:ASP:HB3	1:H:110:ARG:HH22	1.77	0.49
1:B:296:TYR:CZ	1:B:385:LYS:HG2	2.47	0.49
1:I:296:TYR:CZ	1:I:385:LYS:HG2	2.47	0.49
1:I:333:ALA:O	1:I:341:ALA:HB1	2.12	0.49
1:K:296:TYR:CZ	1:K:385:LYS:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:TYR:CE2	1:E:391:PRO:HG3	2.47	0.49
1:F:296:TYR:CZ	1:F:385:LYS:HG2	2.47	0.49
1:H:334:TYR:CE2	1:H:391:PRO:HG3	2.47	0.49
1:A:5:VAL:HG11	1:A:43:PHE:HZ	1.75	0.49
1:D:296:TYR:CZ	1:D:385:LYS:HG2	2.47	0.49
1:C:333:ALA:O	1:C:341:ALA:HB1	2.12	0.49
1:I:101:ASP:HB3	1:I:110:ARG:HH22	1.77	0.49
1:I:334:TYR:CE2	1:I:391:PRO:HG3	2.47	0.49
1:J:101:ASP:HB3	1:J:110:ARG:HH22	1.77	0.49
1:J:296:TYR:CZ	1:J:385:LYS:HG2	2.47	0.49
1:J:333:ALA:O	1:J:341:ALA:HB1	2.12	0.49
1:K:359:ARG:NH1	3:K:471:GLU:OE1	2.45	0.49
1:B:101:ASP:HB3	1:B:110:ARG:HH22	1.76	0.49
1:J:383:LYS:HB3	1:J:383:LYS:HZ3	1.77	0.49
1:D:333:ALA:O	1:D:341:ALA:HB1	2.12	0.49
1:E:359:ARG:NH1	3:E:471:GLU:OE1	2.45	0.49
1:F:334:TYR:CE1	1:F:388:PRO:HB2	2.48	0.49
1:G:334:TYR:CE1	1:G:388:PRO:HB2	2.48	0.49
1:H:383:LYS:HB3	1:H:383:LYS:HZ3	1.77	0.49
1:L:333:ALA:O	1:L:341:ALA:HB1	2.12	0.49
1:A:17:VAL:HG21	1:A:38:VAL:HG21	1.95	0.49
1:A:101:ASP:HB3	1:A:110:ARG:HH22	1.76	0.49
1:H:334:TYR:CE1	1:H:388:PRO:HB2	2.48	0.49
1:I:334:TYR:CE1	1:I:388:PRO:HB2	2.48	0.49
1:G:334:TYR:CE2	1:G:391:PRO:HG3	2.47	0.49
1:H:111:ALA:HB3	1:H:228:MET:HE1	1.95	0.49
1:L:296:TYR:CZ	1:L:385:LYS:HG2	2.47	0.49
1:C:296:TYR:CZ	1:C:385:LYS:HG2	2.47	0.49
1:C:359:ARG:NH1	3:C:471:GLU:OE1	2.45	0.49
1:G:101:ASP:HB3	1:G:110:ARG:HH22	1.76	0.49
1:A:296:TYR:CZ	1:A:385:LYS:HG2	2.47	0.48
1:B:111:ALA:HB3	1:B:228:MET:HE1	1.95	0.48
1:B:334:TYR:CE1	1:B:388:PRO:HB2	2.48	0.48
1:C:334:TYR:CE2	1:C:391:PRO:HG3	2.47	0.48
1:J:111:ALA:HB3	1:J:228:MET:HE1	1.95	0.48
1:J:334:TYR:CE1	1:J:388:PRO:HB2	2.48	0.48
1:D:111:ALA:HB3	1:D:228:MET:HE1	1.95	0.48
1:D:334:TYR:CE1	1:D:388:PRO:HB2	2.48	0.48
1:G:180:PHE:HB3	1:H:29:GLN:HB3	1.94	0.48
1:J:334:TYR:CE2	1:J:391:PRO:HG3	2.47	0.48
1:K:334:TYR:CE1	1:K:388:PRO:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:ASP:HB3	1:L:110:ARG:HH22	1.76	0.48
1:L:111:ALA:HB3	1:L:228:MET:HE1	1.95	0.48
1:A:169:LYS:HA	1:B:252:THR:HB	1.96	0.48
1:I:17:VAL:HG21	1:I:38:VAL:HG21	1.95	0.48
1:L:17:VAL:HG21	1:L:38:VAL:HG21	1.95	0.48
1:F:111:ALA:HB3	1:F:228:MET:HE1	1.95	0.48
1:F:334:TYR:CE2	1:F:391:PRO:HG3	2.47	0.48
1:C:334:TYR:CE1	1:C:388:PRO:HB2	2.48	0.48
1:E:111:ALA:HB3	1:E:228:MET:HE1	1.95	0.48
1:K:334:TYR:CE2	1:K:391:PRO:HG3	2.47	0.48
1:C:17:VAL:HG21	1:C:38:VAL:HG21	1.95	0.48
1:C:111:ALA:HB3	1:C:228:MET:HE1	1.95	0.48
1:C:456:THR:O	1:K:458:HIS:HE1	1.95	0.48
1:E:334:TYR:CE1	1:E:388:PRO:HB2	2.48	0.48
1:L:231:LYS:HA	1:L:231:LYS:HD2	1.66	0.48
1:L:334:TYR:CE1	1:L:388:PRO:HB2	2.48	0.48
1:E:17:VAL:HG21	1:E:38:VAL:HG21	1.95	0.48
1:H:17:VAL:HG21	1:H:38:VAL:HG21	1.95	0.48
1:H:296:TYR:CZ	1:H:385:LYS:HG2	2.47	0.48
1:J:17:VAL:HG21	1:J:38:VAL:HG21	1.95	0.48
1:A:111:ALA:HB3	1:A:228:MET:HE1	1.95	0.48
1:A:334:TYR:CE1	1:A:388:PRO:HB2	2.48	0.48
1:D:17:VAL:HG21	1:D:38:VAL:HG21	1.95	0.48
1:D:120:ILE:O	1:D:281:LEU:HD21	2.14	0.48
1:A:333:ALA:O	1:A:341:ALA:HB1	2.12	0.48
1:B:17:VAL:HG21	1:B:38:VAL:HG21	1.95	0.48
1:G:111:ALA:HB3	1:G:228:MET:HE1	1.95	0.48
1:G:120:ILE:O	1:G:281:LEU:HD21	2.14	0.48
1:H:120:ILE:O	1:H:281:LEU:HD21	2.14	0.48
1:B:458:HIS:CD2	1:B:460:VAL:H	2.32	0.48
1:C:120:ILE:O	1:C:281:LEU:HD21	2.14	0.48
1:F:120:ILE:O	1:F:281:LEU:HD21	2.14	0.48
1:K:120:ILE:O	1:K:281:LEU:HD21	2.14	0.48
1:A:120:ILE:O	1:A:281:LEU:HD21	2.14	0.47
1:B:120:ILE:O	1:B:281:LEU:HD21	2.14	0.47
1:B:359:ARG:NH1	3:B:473:GLU:OE1	2.45	0.47
1:G:231:LYS:HD2	1:G:231:LYS:HA	1.66	0.47
1:J:120:ILE:O	1:J:281:LEU:HD21	2.14	0.47
1:C:169:LYS:HA	1:D:252:THR:HB	1.96	0.47
1:E:458:HIS:CD2	1:E:460:VAL:H	2.32	0.47
1:G:17:VAL:HG21	1:G:38:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:169:LYS:HA	1:I:252:THR:HB	1.96	0.47
1:K:458:HIS:CD2	1:K:460:VAL:H	2.32	0.47
1:I:111:ALA:HB3	1:I:228:MET:HE1	1.95	0.47
1:F:339:ARG:CZ	1:F:359:ARG:NH2	2.78	0.47
1:J:458:HIS:CD2	1:J:460:VAL:H	2.32	0.47
1:K:17:VAL:HG21	1:K:38:VAL:HG21	1.95	0.47
1:D:339:ARG:CZ	1:D:359:ARG:NH2	2.78	0.47
1:G:339:ARG:CZ	1:G:359:ARG:NH2	2.78	0.47
1:K:111:ALA:HB3	1:K:228:MET:HE1	1.95	0.47
1:L:120:ILE:O	1:L:281:LEU:HD21	2.14	0.47
1:A:339:ARG:CZ	1:A:359:ARG:NH2	2.78	0.47
1:B:339:ARG:CZ	1:B:359:ARG:NH2	2.78	0.47
1:D:359:ARG:NH1	3:D:471:GLU:OE1	2.45	0.47
1:E:120:ILE:O	1:E:281:LEU:HD21	2.14	0.47
1:F:17:VAL:HG21	1:F:38:VAL:HG21	1.95	0.47
1:G:458:HIS:CD2	1:G:460:VAL:H	2.32	0.47
1:H:339:ARG:CZ	1:H:359:ARG:NH2	2.78	0.47
1:H:458:HIS:CD2	1:H:460:VAL:H	2.32	0.47
1:I:359:ARG:NH1	3:I:471:GLU:OE1	2.45	0.47
1:E:231:LYS:HD2	1:E:231:LYS:HA	1.66	0.47
1:E:339:ARG:CZ	1:E:359:ARG:NH2	2.78	0.47
1:E:180:PHE:HB3	1:F:29:GLN:HB3	1.96	0.47
1:F:359:ARG:NH1	3:F:471:GLU:OE1	2.44	0.47
1:G:252:THR:HB	1:L:169:LYS:HA	1.96	0.47
1:L:339:ARG:CZ	1:L:359:ARG:NH2	2.78	0.47
1:I:169:LYS:HA	1:J:252:THR:HB	1.96	0.47
1:K:339:ARG:CZ	1:K:359:ARG:NH2	2.78	0.46
1:A:458:HIS:CD2	1:A:460:VAL:H	2.32	0.46
1:F:255:PHE:HB3	1:F:363:PRO:HB2	1.98	0.46
1:I:383:LYS:HB3	1:I:383:LYS:HZ3	1.79	0.46
1:I:458:HIS:CD2	1:I:460:VAL:H	2.32	0.46
1:B:171:HIS:ND1	1:K:467:SER:OG	2.40	0.46
1:I:339:ARG:CZ	1:I:359:ARG:NH2	2.78	0.46
1:J:339:ARG:CZ	1:J:359:ARG:NH2	2.78	0.46
1:B:255:PHE:HB3	1:B:363:PRO:HB2	1.98	0.46
1:L:458:HIS:CD2	1:L:460:VAL:H	2.32	0.46
1:D:272:MET:HE3	1:D:272:MET:HB2	1.84	0.46
1:G:255:PHE:HB3	1:G:363:PRO:HB2	1.98	0.46
1:L:359:ARG:NH1	3:L:471:GLU:OE1	2.45	0.46
1:D:458:HIS:CD2	1:D:460:VAL:H	2.32	0.46
1:J:255:PHE:HB3	1:J:363:PRO:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:255:PHE:HB3	1:L:363:PRO:HB2	1.98	0.46
1:A:359:ARG:NH1	3:A:471:GLU:OE1	2.45	0.46
1:C:339:ARG:CZ	1:C:359:ARG:NH2	2.78	0.46
1:D:255:PHE:HB3	1:D:363:PRO:HB2	1.98	0.46
1:E:169:LYS:HA	1:F:252:THR:HB	1.98	0.46
1:H:255:PHE:HB3	1:H:363:PRO:HB2	1.98	0.46
1:C:458:HIS:CD2	1:C:460:VAL:H	2.32	0.46
1:B:231:LYS:HA	1:B:231:LYS:HD2	1.66	0.45
1:B:272:MET:HE3	1:B:272:MET:HB2	1.84	0.45
1:H:168:ASN:HB3	1:I:138:ILE:O	2.16	0.45
1:I:255:PHE:HB3	1:I:363:PRO:HB2	1.98	0.45
1:J:359:ARG:NH1	3:J:471:GLU:OE1	2.45	0.45
1:F:458:HIS:CD2	1:F:460:VAL:H	2.32	0.45
1:I:196:CYS:SG	1:I:206:VAL:HG11	2.57	0.45
1:J:169:LYS:HA	1:K:252:THR:HB	1.98	0.45
1:B:196:CYS:SG	1:B:206:VAL:HG11	2.57	0.45
1:I:120:ILE:O	1:I:281:LEU:HD21	2.14	0.45
1:A:196:CYS:SG	1:A:206:VAL:HG11	2.57	0.45
1:A:255:PHE:HB3	1:A:363:PRO:HB2	1.98	0.45
1:C:255:PHE:HB3	1:C:363:PRO:HB2	1.98	0.45
1:K:255:PHE:HB3	1:K:363:PRO:HB2	1.98	0.45
1:C:196:CYS:SG	1:C:206:VAL:HG11	2.57	0.45
1:E:255:PHE:HB3	1:E:363:PRO:HB2	1.98	0.45
1:D:196:CYS:SG	1:D:206:VAL:HG11	2.57	0.45
1:A:231:LYS:HD2	1:A:231:LYS:HA	1.66	0.45
1:G:196:CYS:SG	1:G:206:VAL:HG11	2.57	0.45
1:G:359:ARG:NH1	3:G:471:GLU:OE1	2.45	0.45
1:J:196:CYS:SG	1:J:206:VAL:HG11	2.57	0.45
1:J:231:LYS:HD2	1:J:231:LYS:HA	1.66	0.45
1:G:269:HIS:HE1	1:G:359:ARG:CZ	2.31	0.45
1:H:196:CYS:SG	1:H:206:VAL:HG11	2.57	0.45
1:E:196:CYS:SG	1:E:206:VAL:HG11	2.57	0.44
1:E:269:HIS:HE1	1:E:359:ARG:CZ	2.31	0.44
1:K:191:ILE:HG12	1:K:249:PHE:CD2	2.53	0.44
1:B:191:ILE:HG12	1:B:249:PHE:CD2	2.53	0.44
1:C:269:HIS:HE1	1:C:359:ARG:CZ	2.31	0.44
1:E:191:ILE:HG12	1:E:249:PHE:CD2	2.53	0.44
1:L:191:ILE:HG12	1:L:249:PHE:CD2	2.53	0.44
1:D:191:ILE:HG12	1:D:249:PHE:CD2	2.53	0.44
1:J:269:HIS:HE1	1:J:359:ARG:CZ	2.31	0.44
1:K:196:CYS:SG	1:K:206:VAL:HG11	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:HG12	1:A:249:PHE:CD2	2.53	0.44
1:K:383:LYS:HB3	1:K:383:LYS:HZ3	1.81	0.44
1:F:196:CYS:SG	1:F:206:VAL:HG11	2.57	0.44
1:I:191:ILE:HG12	1:I:249:PHE:CD2	2.53	0.44
1:L:269:HIS:HE1	1:L:359:ARG:CZ	2.31	0.44
1:B:269:HIS:HE1	1:B:359:ARG:CZ	2.31	0.44
1:C:191:ILE:HG12	1:C:249:PHE:CD2	2.53	0.44
1:C:114:TYR:CD1	1:C:431:GLY:HA3	2.53	0.44
1:C:295:LEU:O	1:C:388:PRO:HD3	2.18	0.44
1:H:191:ILE:HG12	1:H:249:PHE:CD2	2.53	0.44
1:I:269:HIS:HE1	1:I:359:ARG:CZ	2.31	0.44
1:J:114:TYR:CD1	1:J:431:GLY:HA3	2.53	0.44
1:L:196:CYS:SG	1:L:206:VAL:HG11	2.57	0.44
1:A:114:TYR:CD1	1:A:431:GLY:HA3	2.53	0.43
1:A:295:LEU:O	1:A:388:PRO:HD3	2.18	0.43
1:D:383:LYS:HB3	1:D:383:LYS:HZ3	1.83	0.43
1:D:192:ARG:HH11	1:D:219:ASN:ND2	2.16	0.43
1:G:114:TYR:CD1	1:G:431:GLY:HA3	2.53	0.43
1:E:114:TYR:CD1	1:E:431:GLY:HA3	2.53	0.43
1:F:114:TYR:CD1	1:F:431:GLY:HA3	2.53	0.43
1:F:192:ARG:HH11	1:F:219:ASN:ND2	2.17	0.43
1:F:269:HIS:HE1	1:F:359:ARG:CZ	2.31	0.43
1:H:114:TYR:CD1	1:H:431:GLY:HA3	2.53	0.43
1:J:191:ILE:HG12	1:J:249:PHE:CD2	2.53	0.43
1:A:192:ARG:HH11	1:A:219:ASN:ND2	2.17	0.43
1:C:272:MET:HE3	1:C:272:MET:HB2	1.83	0.43
1:D:269:HIS:HE1	1:D:359:ARG:CZ	2.31	0.43
1:E:192:ARG:HH11	1:E:219:ASN:ND2	2.17	0.43
1:G:191:ILE:HG12	1:G:249:PHE:CD2	2.53	0.43
1:I:231:LYS:HD2	1:I:231:LYS:HA	1.66	0.43
1:K:231:LYS:HA	1:K:231:LYS:HD2	1.66	0.43
1:B:295:LEU:O	1:B:388:PRO:HD3	2.18	0.43
1:H:269:HIS:HE1	1:H:359:ARG:CZ	2.31	0.43
1:I:114:TYR:CD1	1:I:431:GLY:HA3	2.53	0.43
1:J:295:LEU:O	1:J:388:PRO:HD3	2.18	0.43
1:L:295:LEU:O	1:L:388:PRO:HD3	2.18	0.43
1:B:192:ARG:HH11	1:B:219:ASN:ND2	2.17	0.43
1:B:235:ILE:HD13	1:B:235:ILE:HA	1.86	0.43
1:D:114:TYR:CD1	1:D:431:GLY:HA3	2.53	0.43
1:K:269:HIS:HE1	1:K:359:ARG:CZ	2.31	0.43
1:A:269:HIS:HE1	1:A:359:ARG:CZ	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:TYR:CE2	1:G:102:ARG:HB3	2.54	0.43
1:H:295:LEU:O	1:H:388:PRO:HD3	2.18	0.43
1:L:192:ARG:HH11	1:L:219:ASN:ND2	2.17	0.43
1:A:100:TYR:CE2	1:A:102:ARG:HB3	2.54	0.43
1:B:114:TYR:CD1	1:B:431:GLY:HA3	2.53	0.43
1:I:272:MET:HE3	1:I:272:MET:HB2	1.83	0.43
1:L:114:TYR:CD1	1:L:431:GLY:HA3	2.53	0.43
1:C:231:LYS:HD2	1:C:231:LYS:HA	1.66	0.43
1:D:100:TYR:CE2	1:D:102:ARG:HB3	2.54	0.43
1:E:383:LYS:HB3	1:E:383:LYS:HZ3	1.83	0.43
1:F:191:ILE:HG12	1:F:249:PHE:CD2	2.53	0.43
1:F:295:LEU:O	1:F:388:PRO:HD3	2.18	0.43
1:I:295:LEU:O	1:I:388:PRO:HD3	2.18	0.43
1:C:100:TYR:CE2	1:C:102:ARG:HB3	2.54	0.43
1:D:231:LYS:HA	1:D:231:LYS:HD2	1.66	0.43
1:J:100:TYR:CE2	1:J:102:ARG:HB3	2.54	0.43
1:K:100:TYR:CE2	1:K:102:ARG:HB3	2.54	0.43
1:K:114:TYR:CD1	1:K:431:GLY:HA3	2.53	0.43
1:L:100:TYR:CE2	1:L:102:ARG:HB3	2.54	0.43
1:C:383:LYS:HB3	1:C:383:LYS:HZ3	1.84	0.42
1:G:295:LEU:O	1:G:388:PRO:HD3	2.18	0.42
1:B:100:TYR:CE2	1:B:102:ARG:HB3	2.54	0.42
1:B:191:ILE:O	1:B:195:MET:HG3	2.19	0.42
1:C:149:VAL:HG21	1:K:462:PHE:CD1	2.54	0.42
1:E:100:TYR:CE2	1:E:102:ARG:HB3	2.54	0.42
1:G:192:ARG:HH11	1:G:219:ASN:ND2	2.17	0.42
1:I:100:TYR:CE2	1:I:102:ARG:HB3	2.54	0.42
1:C:192:ARG:HH11	1:C:219:ASN:ND2	2.17	0.42
1:D:295:LEU:O	1:D:388:PRO:HD3	2.18	0.42
1:E:191:ILE:O	1:E:195:MET:HG3	2.20	0.42
1:E:295:LEU:O	1:E:388:PRO:HD3	2.18	0.42
1:H:191:ILE:O	1:H:195:MET:HG3	2.20	0.42
1:H:192:ARG:HH11	1:H:219:ASN:ND2	2.17	0.42
1:K:191:ILE:O	1:K:195:MET:HG3	2.20	0.42
1:L:272:MET:HE3	1:L:272:MET:HB2	1.84	0.42
1:C:191:ILE:O	1:C:195:MET:HG3	2.20	0.42
1:C:315:THR:HB	1:K:465:TYR:CE2	2.53	0.42
1:J:191:ILE:O	1:J:195:MET:HG3	2.20	0.42
1:K:192:ARG:HH11	1:K:219:ASN:ND2	2.17	0.42
1:K:295:LEU:O	1:K:388:PRO:HD3	2.18	0.42
1:G:191:ILE:O	1:G:195:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:192:ARG:HH11	1:I:219:ASN:ND2	2.17	0.42
1:J:235:ILE:HD13	1:J:235:ILE:HA	1.86	0.42
1:A:252:THR:HB	1:F:169:LYS:HA	2.01	0.42
1:F:100:TYR:CE2	1:F:102:ARG:HB3	2.54	0.42
1:L:191:ILE:O	1:L:195:MET:HG3	2.20	0.42
1:F:191:ILE:O	1:F:195:MET:HG3	2.20	0.42
1:G:169:LYS:HA	1:H:252:THR:HB	2.02	0.42
1:H:100:TYR:CE2	1:H:102:ARG:HB3	2.54	0.42
1:H:231:LYS:HA	1:H:231:LYS:HD2	1.66	0.42
1:J:192:ARG:HH11	1:J:219:ASN:ND2	2.17	0.42
1:K:272:MET:HB2	1:K:272:MET:HE3	1.83	0.42
1:D:466:TYR:CZ	1:J:138:ILE:HG21	2.55	0.42
1:F:296:TYR:O	1:F:381:GLY:HA3	2.20	0.42
1:G:296:TYR:O	1:G:381:GLY:HA3	2.20	0.42
1:H:296:TYR:O	1:H:381:GLY:HA3	2.20	0.42
1:L:383:LYS:HB3	1:L:383:LYS:HZ3	1.84	0.42
1:E:296:TYR:O	1:E:381:GLY:HA3	2.20	0.42
1:F:57:TRP:CH2	1:F:91:ILE:HG13	2.55	0.42
1:G:272:MET:HB2	1:G:272:MET:HE3	1.83	0.42
1:I:312:ALA:HB1	1:I:361:PRO:HB3	2.02	0.42
1:J:296:TYR:O	1:J:381:GLY:HA3	2.20	0.42
1:L:57:TRP:CH2	1:L:91:ILE:HG13	2.55	0.42
1:C:138:ILE:HG21	1:K:466:TYR:CZ	2.55	0.41
1:C:312:ALA:HB1	1:C:361:PRO:HB3	2.02	0.41
1:D:296:TYR:O	1:D:381:GLY:HA3	2.20	0.41
1:K:296:TYR:O	1:K:381:GLY:HA3	2.20	0.41
1:E:57:TRP:CH2	1:E:91:ILE:HG13	2.55	0.41
1:G:312:ALA:HB1	1:G:361:PRO:HB3	2.02	0.41
1:B:296:TYR:O	1:B:381:GLY:HA3	2.20	0.41
1:C:296:TYR:O	1:C:381:GLY:HA3	2.20	0.41
1:G:57:TRP:CH2	1:G:91:ILE:HG13	2.55	0.41
1:I:191:ILE:O	1:I:195:MET:HG3	2.20	0.41
1:K:312:ALA:HB1	1:K:361:PRO:HB3	2.02	0.41
1:L:235:ILE:HD13	1:L:235:ILE:HA	1.86	0.41
1:D:57:TRP:CH2	1:D:91:ILE:HG13	2.55	0.41
1:F:418:LEU:HD11	1:F:446:ARG:HB3	2.02	0.41
1:I:57:TRP:CH2	1:I:91:ILE:HG13	2.55	0.41
1:A:235:ILE:HD13	1:A:235:ILE:HA	1.86	0.41
1:A:296:TYR:O	1:A:381:GLY:HA3	2.20	0.41
1:A:312:ALA:HB1	1:A:361:PRO:HB3	2.02	0.41
1:C:57:TRP:CH2	1:C:91:ILE:HG13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:HD11	1:C:446:ARG:HB3	2.02	0.41
1:H:57:TRP:CH2	1:H:91:ILE:HG13	2.55	0.41
1:E:312:ALA:HB1	1:E:361:PRO:HB3	2.02	0.41
1:G:418:LEU:HD11	1:G:446:ARG:HB3	2.02	0.41
1:J:312:ALA:HB1	1:J:361:PRO:HB3	2.02	0.41
1:K:418:LEU:HD11	1:K:446:ARG:HB3	2.02	0.41
1:A:191:ILE:O	1:A:195:MET:HG3	2.20	0.41
1:F:272:MET:HE3	1:F:272:MET:HB2	1.83	0.41
1:B:312:ALA:HB1	1:B:361:PRO:HB3	2.02	0.41
1:F:312:ALA:HB1	1:F:361:PRO:HB3	2.02	0.41
1:D:191:ILE:O	1:D:195:MET:HG3	2.19	0.41
1:F:231:LYS:HA	1:F:231:LYS:HD2	1.66	0.41
1:J:272:MET:HE3	1:J:272:MET:HB2	1.83	0.41
1:J:418:LEU:HD11	1:J:446:ARG:HB3	2.02	0.41
1:K:191:ILE:HG22	1:K:195:MET:HE3	2.03	0.41
1:L:296:TYR:O	1:L:381:GLY:HA3	2.20	0.41
1:L:312:ALA:HB1	1:L:361:PRO:HB3	2.02	0.41
1:B:57:TRP:CH2	1:B:91:ILE:HG13	2.55	0.41
1:B:191:ILE:HG22	1:B:195:MET:HE3	2.03	0.41
1:D:312:ALA:HB1	1:D:361:PRO:HB3	2.02	0.41
1:F:334:TYR:HA	1:F:343:ILE:HB	2.04	0.41
1:H:334:TYR:HA	1:H:343:ILE:HB	2.04	0.41
1:H:418:LEU:HD11	1:H:446:ARG:HB3	2.02	0.41
1:L:334:TYR:HA	1:L:343:ILE:HB	2.03	0.41
1:C:191:ILE:HG22	1:C:195:MET:HE3	2.03	0.40
1:C:466:TYR:CZ	1:K:138:ILE:HG21	2.56	0.40
1:E:191:ILE:HG22	1:E:195:MET:HE3	2.03	0.40
1:H:312:ALA:HB1	1:H:361:PRO:HB3	2.02	0.40
1:I:191:ILE:HG22	1:I:195:MET:HE3	2.03	0.40
1:J:191:ILE:HG22	1:J:195:MET:HE3	2.03	0.40
1:J:390:GLU:HA	1:J:391:PRO:HD3	1.92	0.40
1:C:235:ILE:HD13	1:C:235:ILE:HA	1.86	0.40
1:C:465:TYR:CE2	1:K:315:THR:HB	2.56	0.40
1:D:334:TYR:HA	1:D:343:ILE:HB	2.03	0.40
1:I:418:LEU:HD11	1:I:446:ARG:HB3	2.02	0.40
1:J:57:TRP:CH2	1:J:91:ILE:HG13	2.55	0.40
1:K:57:TRP:CH2	1:K:91:ILE:HG13	2.55	0.40
1:H:68:MET:HA	1:H:69:PRO:HD2	1.94	0.40
1:H:390:GLU:HA	1:H:391:PRO:HD3	1.92	0.40
1:A:191:ILE:HG22	1:A:195:MET:HE3	2.03	0.40
1:D:235:ILE:HD13	1:D:235:ILE:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TRP:CH2	1:A:91:ILE:HG13	2.55	0.40
1:A:334:TYR:HA	1:A:343:ILE:HB	2.03	0.40
1:I:296:TYR:O	1:I:381:GLY:HA3	2.20	0.40
1:K:334:TYR:HA	1:K:343:ILE:HB	2.04	0.40
1:L:100:TYR:C	1:L:102:ARG:H	2.30	0.40
1:L:191:ILE:HG22	1:L:195:MET:HE3	2.03	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]	1.12	1.08
1:C:1:SER:OG	1:F:13:GLU:CD[4_454]	2.07	0.13

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%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	B	437/468 (93%)	393 (90%)	29 (7%)	15 (3%)	3	11
1	C	437/468 (93%)	393 (90%)	29 (7%)	15 (3%)	3	11
1	D	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	E	437/468 (93%)	392 (90%)	30 (7%)	15 (3%)	3	11
1	F	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	G	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	H	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	I	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	J	437/468 (93%)	393 (90%)	29 (7%)	15 (3%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
1	L	437/468 (93%)	394 (90%)	28 (6%)	15 (3%)	3	11
All	All	5244/5616 (93%)	4723 (90%)	341 (6%)	180 (3%)	3	11

All (180) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	F	338	ASN
1	F	340	SER
1	G	40	ALA
1	G	286	LYS
1	G	338	ASN
1	G	340	SER
1	H	40	ALA
1	H	286	LYS
1	H	338	ASN
1	H	340	SER
1	I	40	ALA
1	I	286	LYS
1	I	338	ASN
1	I	340	SER
1	J	40	ALA
1	J	286	LYS
1	J	338	ASN
1	J	340	SER
1	K	40	ALA
1	K	286	LYS
1	K	338	ASN
1	K	340	SER
1	L	40	ALA
1	L	286	LYS
1	L	338	ASN
1	L	340	SER
1	A	285	ASP
1	A	350	SER
1	B	285	ASP
1	B	350	SER
1	C	285	ASP
1	C	350	SER
1	D	285	ASP
1	D	350	SER
1	E	285	ASP
1	E	350	SER
1	F	285	ASP
1	F	350	SER
1	G	285	ASP
1	G	350	SER
1	H	285	ASP
1	H	350	SER

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Mol	Chain	Res	Type
1	I	285	ASP
1	I	350	SER
1	J	285	ASP
1	J	350	SER
1	K	285	ASP
1	K	350	SER
1	L	285	ASP
1	L	350	SER
1	A	36	HIS
1	A	170	GLY
1	A	351	PRO
1	A	353	ALA
1	B	36	HIS
1	B	170	GLY
1	B	351	PRO
1	B	353	ALA
1	C	36	HIS
1	C	170	GLY
1	C	351	PRO
1	C	353	ALA
1	D	36	HIS
1	D	170	GLY
1	D	351	PRO
1	D	353	ALA
1	E	36	HIS
1	E	170	GLY
1	E	351	PRO
1	E	353	ALA
1	F	36	HIS
1	F	170	GLY
1	F	351	PRO
1	F	353	ALA
1	G	36	HIS
1	G	170	GLY
1	G	351	PRO
1	G	353	ALA
1	H	36	HIS
1	H	170	GLY
1	H	351	PRO
1	H	353	ALA
1	I	36	HIS
1	I	170	GLY

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Mol	Chain	Res	Type
1	I	351	PRO
1	I	353	ALA
1	J	36	HIS
1	J	170	GLY
1	J	351	PRO
1	J	353	ALA
1	K	36	HIS
1	K	170	GLY
1	K	351	PRO
1	K	353	ALA
1	L	36	HIS
1	L	170	GLY
1	L	351	PRO
1	L	353	ALA
1	A	228	MET
1	A	277	ASN
1	A	352	LYS
1	B	228	MET
1	B	277	ASN
1	B	352	LYS
1	C	228	MET
1	C	277	ASN
1	C	352	LYS
1	D	228	MET
1	D	277	ASN
1	D	352	LYS
1	E	228	MET
1	E	277	ASN
1	E	352	LYS
1	F	228	MET
1	F	277	ASN
1	F	352	LYS
1	G	228	MET
1	G	277	ASN
1	G	352	LYS
1	H	228	MET
1	H	277	ASN
1	H	352	LYS
1	I	228	MET
1	I	277	ASN
1	I	352	LYS
1	J	228	MET

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Mol	Chain	Res	Type
1	J	277	ASN
1	J	352	LYS
1	K	228	MET
1	K	277	ASN
1	K	352	LYS
1	L	228	MET
1	L	277	ASN
1	L	352	LYS
1	A	386	ILE
1	B	386	ILE
1	C	386	ILE
1	D	386	ILE
1	E	386	ILE
1	F	386	ILE
1	G	386	ILE
1	H	386	ILE
1	I	386	ILE
1	J	386	ILE
1	K	386	ILE
1	L	386	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLU	C	471	-	8,9,9	1.28	2 (25%)	8,11,11	1.09	0
3	GLU	F	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	G	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	K	471	-	8,9,9	1.28	2 (25%)	8,11,11	1.08	0
3	GLU	E	471	-	8,9,9	1.30	2 (25%)	8,11,11	1.09	0
3	GLU	A	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	B	473	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	H	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	J	471	-	8,9,9	1.28	2 (25%)	8,11,11	1.08	0
3	GLU	D	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0
3	GLU	I	471	-	8,9,9	1.30	2 (25%)	8,11,11	1.09	0
3	GLU	L	471	-	8,9,9	1.29	2 (25%)	8,11,11	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLU	C	471	-	-	6/9/9/9	-
3	GLU	F	471	-	-	6/9/9/9	-
3	GLU	G	471	-	-	6/9/9/9	-
3	GLU	K	471	-	-	6/9/9/9	-
3	GLU	E	471	-	-	6/9/9/9	-
3	GLU	A	471	-	-	6/9/9/9	-
3	GLU	B	473	-	-	6/9/9/9	-
3	GLU	H	471	-	-	6/9/9/9	-
3	GLU	J	471	-	-	6/9/9/9	-
3	GLU	D	471	-	-	6/9/9/9	-
3	GLU	I	471	-	-	6/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLU	L	471	-	-	6/9/9/9	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	471	GLU	OE2-CD	-2.29	1.23	1.30
3	I	471	GLU	OE2-CD	-2.29	1.23	1.30
3	J	471	GLU	OE2-CD	-2.27	1.23	1.30
3	E	471	GLU	OE2-CD	-2.27	1.23	1.30
3	A	471	GLU	OE2-CD	-2.27	1.23	1.30
3	F	471	GLU	OE2-CD	-2.27	1.23	1.30
3	K	471	GLU	OE2-CD	-2.27	1.23	1.30
3	H	471	GLU	OE2-CD	-2.27	1.23	1.30
3	C	471	GLU	OE2-CD	-2.27	1.23	1.30
3	D	471	GLU	OE2-CD	-2.26	1.23	1.30
3	L	471	GLU	OE2-CD	-2.26	1.23	1.30
3	B	473	GLU	OE2-CD	-2.24	1.23	1.30
3	I	471	GLU	OXT-C	-2.11	1.23	1.30
3	E	471	GLU	OXT-C	-2.10	1.23	1.30
3	B	473	GLU	OXT-C	-2.10	1.24	1.30
3	F	471	GLU	OXT-C	-2.09	1.24	1.30
3	D	471	GLU	OXT-C	-2.09	1.24	1.30
3	A	471	GLU	OXT-C	-2.08	1.24	1.30
3	G	471	GLU	OXT-C	-2.08	1.24	1.30
3	L	471	GLU	OXT-C	-2.08	1.24	1.30
3	J	471	GLU	OXT-C	-2.07	1.24	1.30
3	K	471	GLU	OXT-C	-2.07	1.24	1.30
3	C	471	GLU	OXT-C	-2.07	1.24	1.30
3	H	471	GLU	OXT-C	-2.06	1.24	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	471	GLU	OXT-C-CA-CB
3	B	473	GLU	OXT-C-CA-CB
3	C	471	GLU	OXT-C-CA-CB
3	D	471	GLU	OXT-C-CA-CB
3	E	471	GLU	OXT-C-CA-CB
3	F	471	GLU	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
3	G	471	GLU	OXT-C-CA-CB
3	H	471	GLU	OXT-C-CA-CB
3	I	471	GLU	OXT-C-CA-CB
3	J	471	GLU	OXT-C-CA-CB
3	K	471	GLU	OXT-C-CA-CB
3	L	471	GLU	OXT-C-CA-CB
3	A	471	GLU	OXT-C-CA-N
3	B	473	GLU	OXT-C-CA-N
3	C	471	GLU	OXT-C-CA-N
3	D	471	GLU	OXT-C-CA-N
3	E	471	GLU	OXT-C-CA-N
3	F	471	GLU	OXT-C-CA-N
3	G	471	GLU	OXT-C-CA-N
3	H	471	GLU	OXT-C-CA-N
3	I	471	GLU	OXT-C-CA-N
3	J	471	GLU	OXT-C-CA-N
3	K	471	GLU	OXT-C-CA-N
3	L	471	GLU	OXT-C-CA-N
3	A	471	GLU	O-C-CA-CB
3	B	473	GLU	O-C-CA-CB
3	C	471	GLU	O-C-CA-CB
3	D	471	GLU	O-C-CA-CB
3	E	471	GLU	O-C-CA-CB
3	F	471	GLU	O-C-CA-CB
3	G	471	GLU	O-C-CA-CB
3	H	471	GLU	O-C-CA-CB
3	I	471	GLU	O-C-CA-CB
3	J	471	GLU	O-C-CA-CB
3	K	471	GLU	O-C-CA-CB
3	L	471	GLU	O-C-CA-CB
3	A	471	GLU	O-C-CA-N
3	B	473	GLU	O-C-CA-N
3	C	471	GLU	O-C-CA-N
3	D	471	GLU	O-C-CA-N
3	E	471	GLU	O-C-CA-N
3	F	471	GLU	O-C-CA-N
3	G	471	GLU	O-C-CA-N
3	H	471	GLU	O-C-CA-N
3	I	471	GLU	O-C-CA-N
3	J	471	GLU	O-C-CA-N
3	K	471	GLU	O-C-CA-N
3	L	471	GLU	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
3	C	471	GLU	OE2-CD-CG-CB
3	E	471	GLU	OE2-CD-CG-CB
3	F	471	GLU	OE2-CD-CG-CB
3	G	471	GLU	OE2-CD-CG-CB
3	H	471	GLU	OE2-CD-CG-CB
3	J	471	GLU	OE1-CD-CG-CB
3	L	471	GLU	OE2-CD-CG-CB
3	A	471	GLU	OE1-CD-CG-CB
3	A	471	GLU	OE2-CD-CG-CB
3	B	473	GLU	OE1-CD-CG-CB
3	B	473	GLU	OE2-CD-CG-CB
3	C	471	GLU	OE1-CD-CG-CB
3	D	471	GLU	OE1-CD-CG-CB
3	D	471	GLU	OE2-CD-CG-CB
3	E	471	GLU	OE1-CD-CG-CB
3	F	471	GLU	OE1-CD-CG-CB
3	G	471	GLU	OE1-CD-CG-CB
3	H	471	GLU	OE1-CD-CG-CB
3	I	471	GLU	OE1-CD-CG-CB
3	I	471	GLU	OE2-CD-CG-CB
3	J	471	GLU	OE2-CD-CG-CB
3	K	471	GLU	OE1-CD-CG-CB
3	K	471	GLU	OE2-CD-CG-CB
3	L	471	GLU	OE1-CD-CG-CB

There are no ring outliers.

12 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	471	GLU	1	0
3	F	471	GLU	1	0
3	G	471	GLU	1	0
3	K	471	GLU	1	0
3	E	471	GLU	1	0
3	A	471	GLU	1	0
3	B	473	GLU	1	0
3	H	471	GLU	1	0
3	J	471	GLU	1	0
3	D	471	GLU	1	0
3	I	471	GLU	1	0
3	L	471	GLU	1	0

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.