



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:18 PM UTC

PDB ID : 1ORT / pdb_00001ort
Title : ORNITHINE TRANSCARBAMOYLASE FROM PSEUDOMONAS
AERUGINOSA
Authors : Villeret, V.; Dideberg, O.
Deposited on : 1995-08-24
Resolution : 3.00 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
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

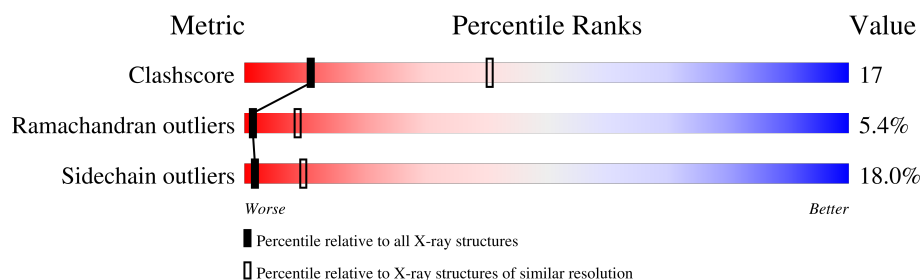
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	335	41% 38% 16% 5%
1	B	335	42% 36% 16% 5%
1	C	335	40% 38% 17% 5%
1	D	335	41% 38% 16% 5%
1	E	335	41% 38% 16% 5%
1	F	335	39% 39% 16% 5%
1	G	335	41% 39% 16% 5%
1	H	335	42% 37% 16% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	335	40% 38% 16% 5%
1	J	335	41% 38% 16% 5%
1	K	335	40% 38% 16% 6%
1	L	335	40% 38% 17% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31968 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 ORNITHINE TRANSCARBAMOYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	B	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	C	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	D	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	E	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	F	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	G	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	H	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	I	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	J	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	K	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			
1	L	335	Total	C	N	O	S	0	0	0
			2664	1682	466	500	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	GLY	GLU	engineered mutation	UNP P08308
B	105	GLY	GLU	engineered mutation	UNP P08308
C	105	GLY	GLU	engineered mutation	UNP P08308
D	105	GLY	GLU	engineered mutation	UNP P08308
E	105	GLY	GLU	engineered mutation	UNP P08308

Continued on next page...

Continued from previous page...

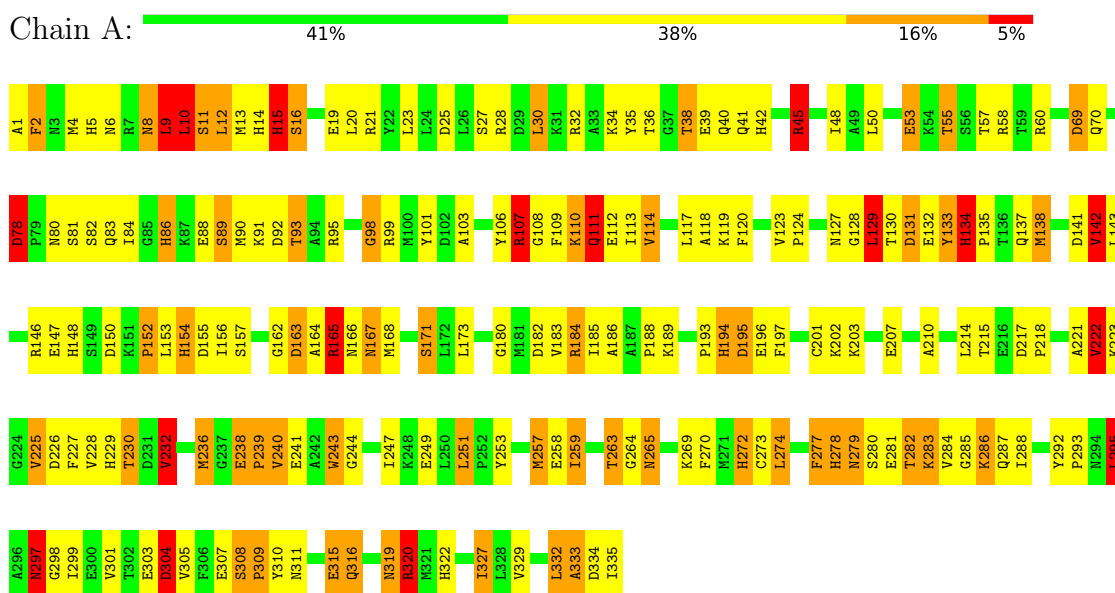
Chain	Residue	Modelled	Actual	Comment	Reference
F	105	GLY	GLU	engineered mutation	UNP P08308
G	105	GLY	GLU	engineered mutation	UNP P08308
H	105	GLY	GLU	engineered mutation	UNP P08308
I	105	GLY	GLU	engineered mutation	UNP P08308
J	105	GLY	GLU	engineered mutation	UNP P08308
K	105	GLY	GLU	engineered mutation	UNP P08308
L	105	GLY	GLU	engineered mutation	UNP P08308

3 Residue-property plots

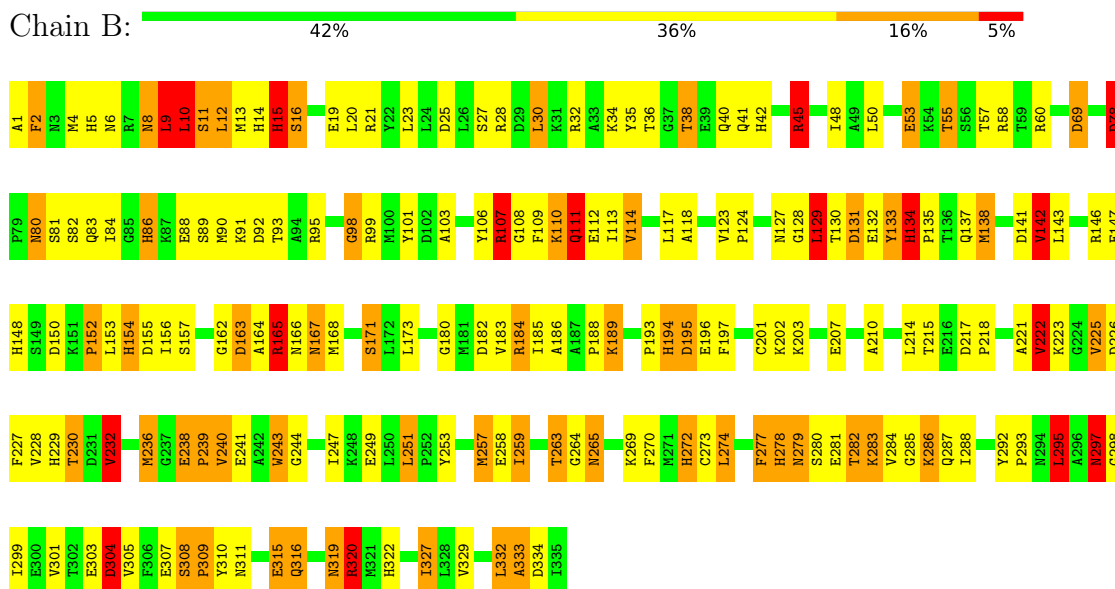
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

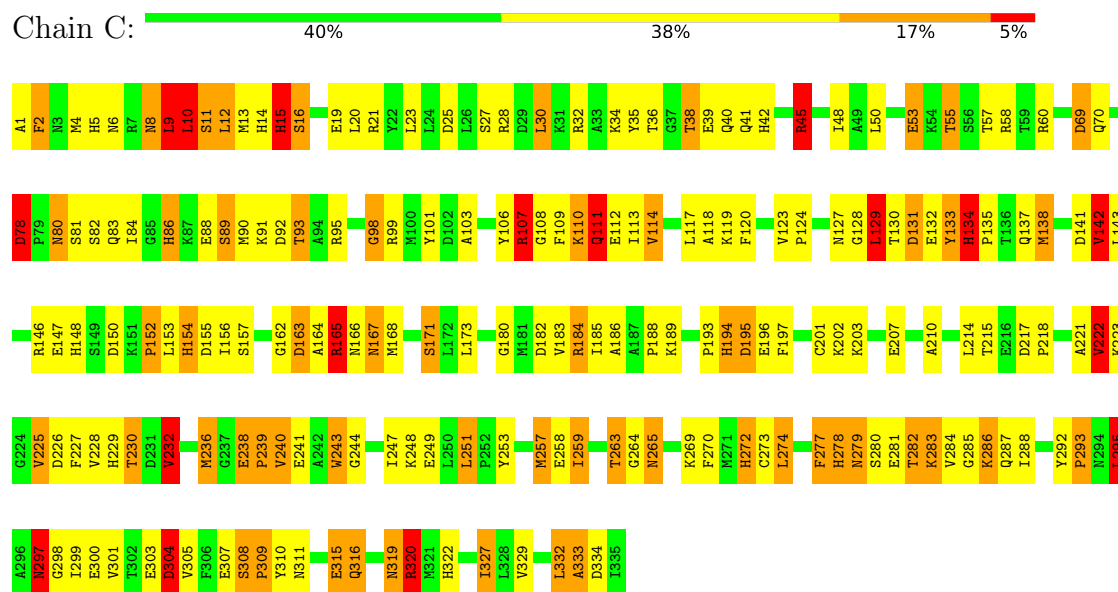
• Molecule 1: ORNITHINE TRANSCARBAMOYLASE



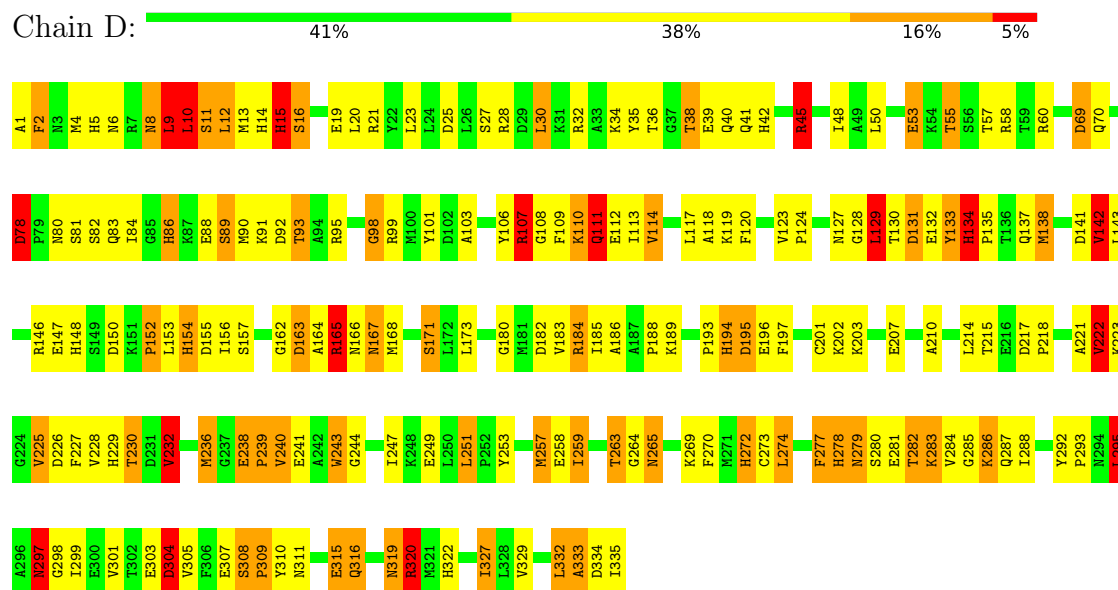
• Molecule 1: ORNITHINE TRANSCARBAMOYLASE



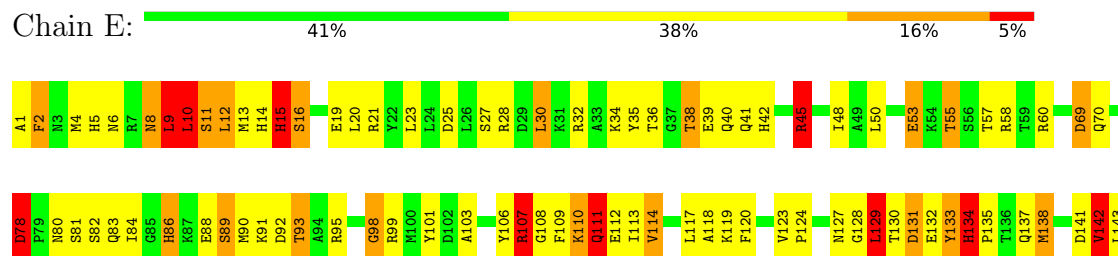
• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

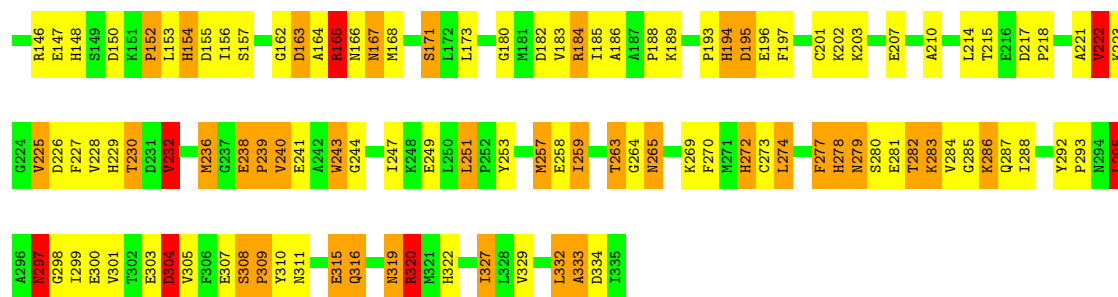


• Molecule 1: ORNITHINE TRANSCARBAMOYLASE



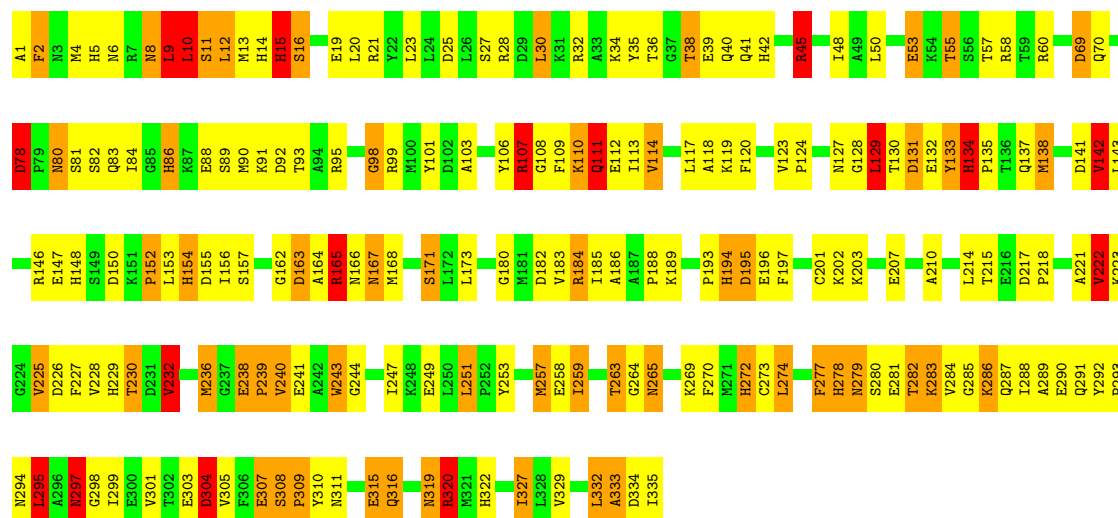
• Molecule 1: ORNITHINE TRANSCARBAMOYLASE





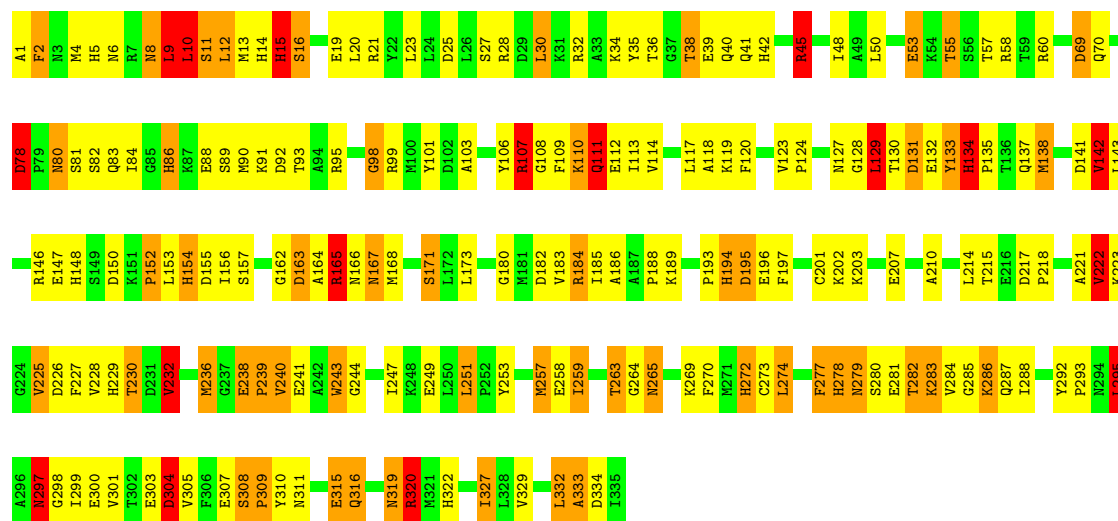
• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

Chain F: 39% 39% 16% 5%

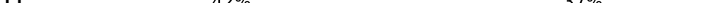


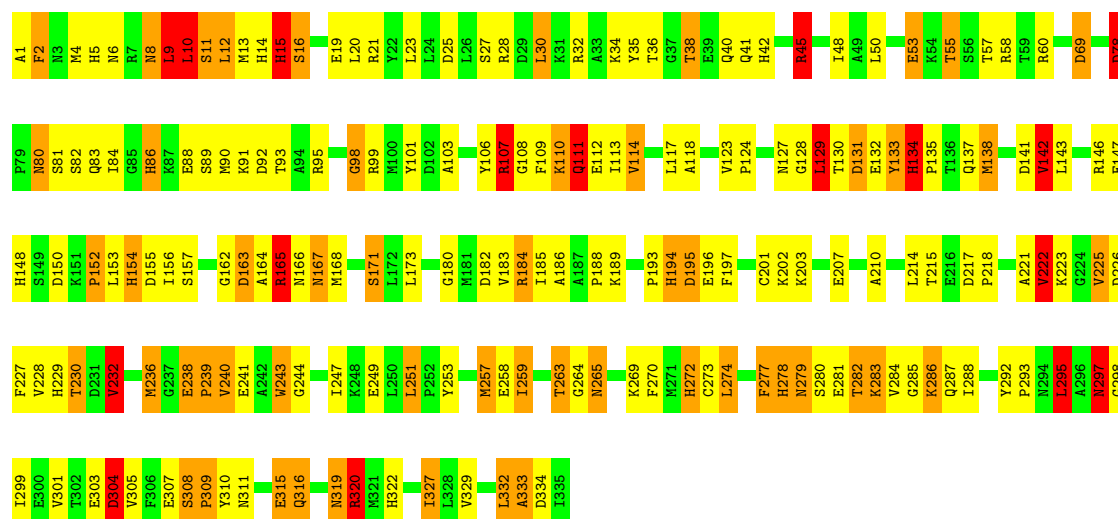
• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

Chain G: 41% 39% 16% 5%

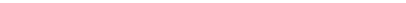


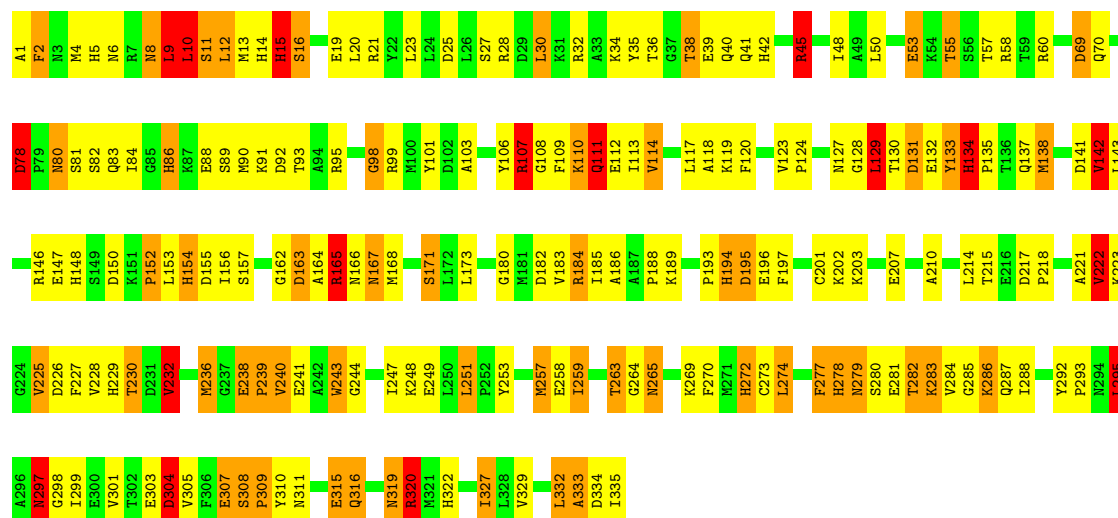
• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

Chain H:  42% 37% 16% 5%

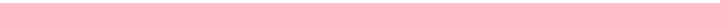


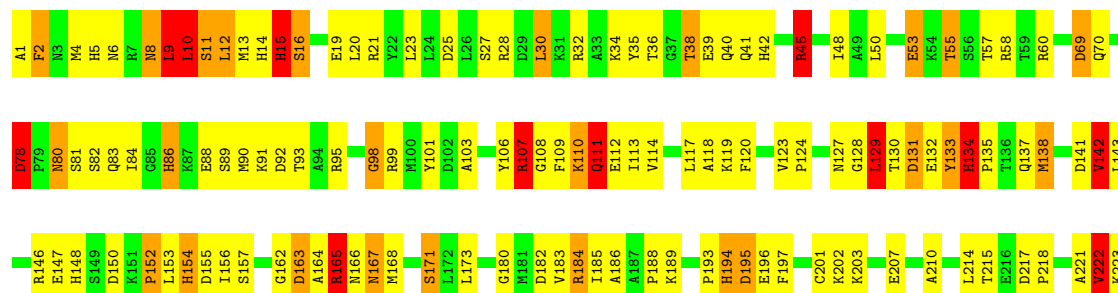
- Molecule 1: ORNITHINE TRANSCARBAMOYLASE

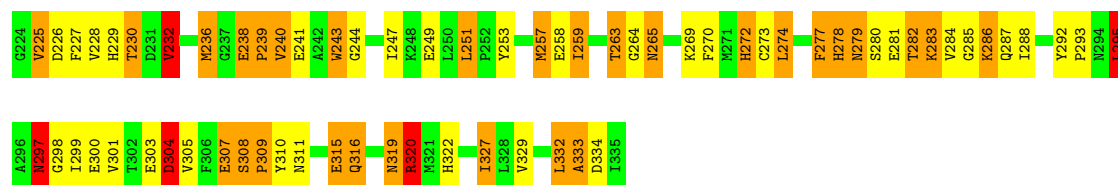
Chain I:  40% 38% 16% 5%



- Molecule 1: ORNITHINE TRANSCARBAMOYLASE

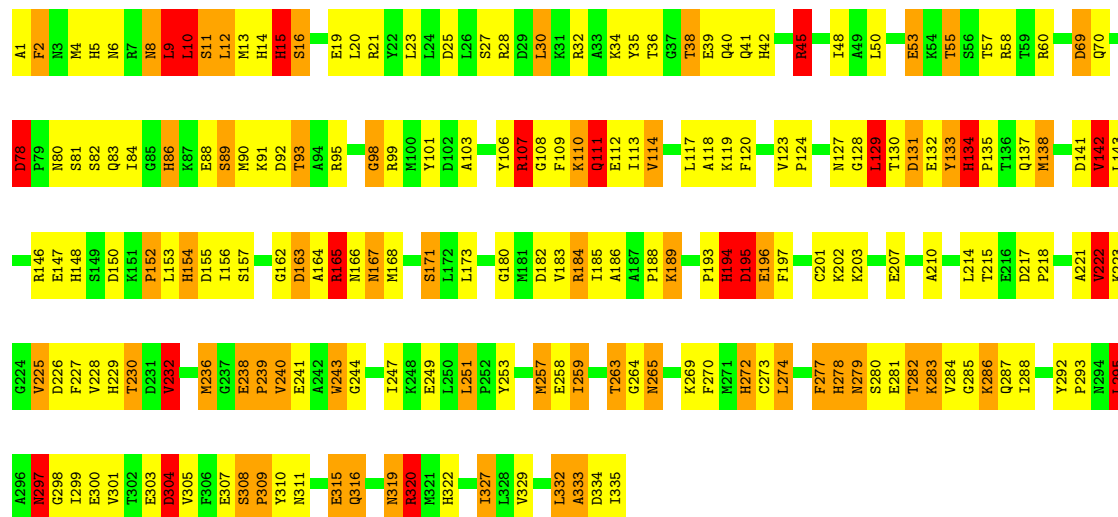
Chain J:  41% 38% 16% 5%





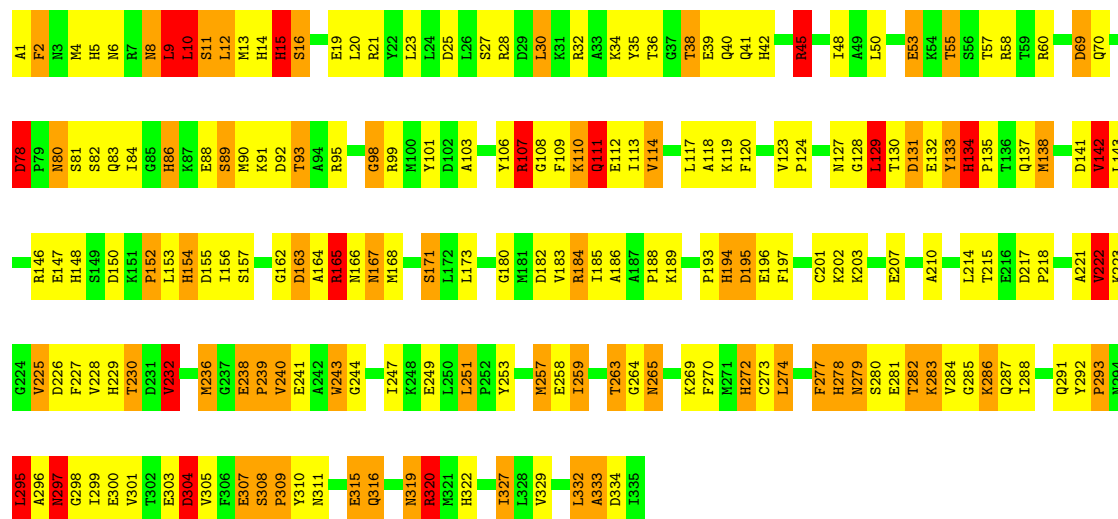
• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

Chain K: 40% 38% 16% 6%



• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

Chain L: 40% 38% 17% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	110.36Å 126.42Å 134.54Å 85.07° 59.24° 111.97°	Depositor
Resolution (Å)	5.50 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (5.50-3.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.216 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31968	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	B	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	C	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	D	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	E	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	F	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	G	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	H	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	I	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	J	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	K	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
1	L	1.21	20/2720 (0.7%)	2.37	156/3673 (4.2%)
All	All	1.21	240/32640 (0.7%)	2.37	1872/44076 (4.2%)

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	6
1	B	0	6
1	C	0	6
1	D	0	6
1	E	0	6
1	F	0	6
1	G	0	6
1	H	0	6
1	I	0	6
1	J	0	6
1	K	0	6
1	L	0	6
All	All	0	72

All (240) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	B	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	C	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	D	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	E	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	F	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	G	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	H	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	I	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	J	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	K	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	L	272	HIS	CD2-NE2	-7.77	1.29	1.37
1	A	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	B	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	C	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	D	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	E	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	F	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	G	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	H	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	I	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	J	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	K	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	L	134	HIS	CD2-NE2	-7.58	1.29	1.37
1	A	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	B	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	C	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	D	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	E	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	F	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	G	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	H	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	I	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	J	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	K	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	L	278	HIS	CD2-NE2	-7.26	1.29	1.37
1	A	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	B	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	C	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	D	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	E	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	F	148	HIS	CD2-NE2	-7.08	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	H	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	I	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	J	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	K	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	L	148	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	B	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	C	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	D	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	E	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	F	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	G	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	H	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	I	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	J	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	K	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	L	229	HIS	CD2-NE2	-7.02	1.30	1.37
1	A	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	B	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	C	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	D	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	E	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	F	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	G	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	H	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	I	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	J	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	K	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	L	5	HIS	CD2-NE2	-6.92	1.30	1.37
1	A	232	VAL	CA-CB	6.53	1.63	1.53
1	B	232	VAL	CA-CB	6.53	1.63	1.53
1	C	232	VAL	CA-CB	6.53	1.63	1.53
1	D	232	VAL	CA-CB	6.53	1.63	1.53
1	E	232	VAL	CA-CB	6.53	1.63	1.53
1	F	232	VAL	CA-CB	6.53	1.63	1.53
1	G	232	VAL	CA-CB	6.53	1.63	1.53
1	H	232	VAL	CA-CB	6.53	1.63	1.53
1	I	232	VAL	CA-CB	6.53	1.63	1.53
1	J	232	VAL	CA-CB	6.53	1.63	1.53
1	K	232	VAL	CA-CB	6.53	1.63	1.53
1	L	232	VAL	CA-CB	6.53	1.63	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	C	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	D	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	E	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	F	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	G	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	H	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	I	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	J	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	K	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	L	14	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	B	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	C	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	D	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	E	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	F	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	G	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	H	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	I	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	J	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	K	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	L	154	HIS	CD2-NE2	-6.46	1.30	1.37
1	A	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	C	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	D	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	E	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	F	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	G	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	H	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	I	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	J	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	K	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	L	322	HIS	CD2-NE2	-6.43	1.30	1.37
1	A	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	B	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	C	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	D	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	E	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	F	42	HIS	CD2-NE2	-6.40	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	H	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	I	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	J	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	K	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	L	42	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	272	HIS	CG-ND1	-6.28	1.31	1.38
1	B	272	HIS	CG-ND1	-6.28	1.31	1.38
1	C	272	HIS	CG-ND1	-6.28	1.31	1.38
1	D	272	HIS	CG-ND1	-6.28	1.31	1.38
1	E	272	HIS	CG-ND1	-6.28	1.31	1.38
1	F	272	HIS	CG-ND1	-6.28	1.31	1.38
1	G	272	HIS	CG-ND1	-6.28	1.31	1.38
1	H	272	HIS	CG-ND1	-6.28	1.31	1.38
1	I	272	HIS	CG-ND1	-6.28	1.31	1.38
1	J	272	HIS	CG-ND1	-6.28	1.31	1.38
1	K	272	HIS	CG-ND1	-6.28	1.31	1.38
1	L	272	HIS	CG-ND1	-6.28	1.31	1.38
1	A	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	C	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	D	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	E	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	F	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	G	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	H	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	I	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	J	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	K	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	L	15	HIS	CD2-NE2	-6.21	1.31	1.37
1	A	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	B	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	C	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	D	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	E	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	F	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	G	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	H	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	I	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	J	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	K	86	HIS	CD2-NE2	-6.00	1.31	1.37
1	L	86	HIS	CD2-NE2	-6.00	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	HIS	CG-ND1	-5.65	1.32	1.38
1	B	134	HIS	CG-ND1	-5.65	1.32	1.38
1	C	134	HIS	CG-ND1	-5.65	1.32	1.38
1	D	134	HIS	CG-ND1	-5.65	1.32	1.38
1	E	134	HIS	CG-ND1	-5.65	1.32	1.38
1	F	134	HIS	CG-ND1	-5.65	1.32	1.38
1	G	134	HIS	CG-ND1	-5.65	1.32	1.38
1	H	134	HIS	CG-ND1	-5.65	1.32	1.38
1	I	134	HIS	CG-ND1	-5.65	1.32	1.38
1	J	134	HIS	CG-ND1	-5.65	1.32	1.38
1	K	134	HIS	CG-ND1	-5.65	1.32	1.38
1	L	134	HIS	CG-ND1	-5.65	1.32	1.38
1	A	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	B	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	C	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	D	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	E	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	F	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	G	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	H	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	I	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	J	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	K	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	L	194	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	147	GLU	CA-CB	-5.57	1.44	1.53
1	B	147	GLU	CA-CB	-5.57	1.44	1.53
1	C	147	GLU	CA-CB	-5.57	1.44	1.53
1	D	147	GLU	CA-CB	-5.57	1.44	1.53
1	E	147	GLU	CA-CB	-5.57	1.44	1.53
1	F	147	GLU	CA-CB	-5.57	1.44	1.53
1	G	147	GLU	CA-CB	-5.57	1.44	1.53
1	H	147	GLU	CA-CB	-5.57	1.44	1.53
1	I	147	GLU	CA-CB	-5.57	1.44	1.53
1	J	147	GLU	CA-CB	-5.57	1.44	1.53
1	K	147	GLU	CA-CB	-5.57	1.44	1.53
1	L	147	GLU	CA-CB	-5.57	1.44	1.53
1	A	42	HIS	CG-ND1	-5.23	1.32	1.38
1	B	42	HIS	CG-ND1	-5.23	1.32	1.38
1	C	42	HIS	CG-ND1	-5.23	1.32	1.38
1	D	42	HIS	CG-ND1	-5.23	1.32	1.38
1	E	42	HIS	CG-ND1	-5.23	1.32	1.38
1	F	42	HIS	CG-ND1	-5.23	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	42	HIS	CG-ND1	-5.23	1.32	1.38
1	H	42	HIS	CG-ND1	-5.23	1.32	1.38
1	I	42	HIS	CG-ND1	-5.23	1.32	1.38
1	J	42	HIS	CG-ND1	-5.23	1.32	1.38
1	K	42	HIS	CG-ND1	-5.23	1.32	1.38
1	L	42	HIS	CG-ND1	-5.23	1.32	1.38
1	A	15	HIS	CG-ND1	-5.20	1.32	1.38
1	B	15	HIS	CG-ND1	-5.20	1.32	1.38
1	C	15	HIS	CG-ND1	-5.20	1.32	1.38
1	D	15	HIS	CG-ND1	-5.20	1.32	1.38
1	E	15	HIS	CG-ND1	-5.20	1.32	1.38
1	F	15	HIS	CG-ND1	-5.20	1.32	1.38
1	G	15	HIS	CG-ND1	-5.20	1.32	1.38
1	H	15	HIS	CG-ND1	-5.20	1.32	1.38
1	I	15	HIS	CG-ND1	-5.20	1.32	1.38
1	J	15	HIS	CG-ND1	-5.20	1.32	1.38
1	K	15	HIS	CG-ND1	-5.20	1.32	1.38
1	L	15	HIS	CG-ND1	-5.20	1.32	1.38
1	A	229	HIS	CG-ND1	-5.09	1.32	1.38
1	B	229	HIS	CG-ND1	-5.09	1.32	1.38
1	C	229	HIS	CG-ND1	-5.09	1.32	1.38
1	D	229	HIS	CG-ND1	-5.09	1.32	1.38
1	E	229	HIS	CG-ND1	-5.09	1.32	1.38
1	F	229	HIS	CG-ND1	-5.09	1.32	1.38
1	G	229	HIS	CG-ND1	-5.09	1.32	1.38
1	H	229	HIS	CG-ND1	-5.09	1.32	1.38
1	I	229	HIS	CG-ND1	-5.09	1.32	1.38
1	J	229	HIS	CG-ND1	-5.09	1.32	1.38
1	K	229	HIS	CG-ND1	-5.09	1.32	1.38
1	L	229	HIS	CG-ND1	-5.09	1.32	1.38

All (1872) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	B	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	C	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	D	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	E	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	F	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	G	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	H	6	ASN	CA-CB-CG	-15.31	97.29	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	J	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	K	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	L	6	ASN	CA-CB-CG	-15.31	97.29	112.60
1	A	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	B	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	C	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	D	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	E	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	F	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	G	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	H	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	I	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	J	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	K	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	L	297	ASN	CA-CB-CG	-13.23	99.37	112.60
1	A	12	LEU	N-CA-C	12.73	130.52	107.99
1	B	12	LEU	N-CA-C	12.73	130.52	107.99
1	C	12	LEU	N-CA-C	12.73	130.52	107.99
1	D	12	LEU	N-CA-C	12.73	130.52	107.99
1	E	12	LEU	N-CA-C	12.73	130.52	107.99
1	F	12	LEU	N-CA-C	12.73	130.52	107.99
1	G	12	LEU	N-CA-C	12.73	130.52	107.99
1	H	12	LEU	N-CA-C	12.73	130.52	107.99
1	I	12	LEU	N-CA-C	12.73	130.52	107.99
1	J	12	LEU	N-CA-C	12.73	130.52	107.99
1	K	12	LEU	N-CA-C	12.73	130.52	107.99
1	L	12	LEU	N-CA-C	12.73	130.52	107.99
1	A	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	B	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	C	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	D	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	E	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	F	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	G	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	H	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	I	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	J	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	K	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	L	21	ARG	CA-CB-CG	-11.40	91.30	114.10
1	A	134	HIS	N-CA-C	11.09	134.32	109.81
1	B	134	HIS	N-CA-C	11.09	134.32	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	134	HIS	N-CA-C	11.09	134.32	109.81
1	D	134	HIS	N-CA-C	11.09	134.32	109.81
1	E	134	HIS	N-CA-C	11.09	134.32	109.81
1	F	134	HIS	N-CA-C	11.09	134.32	109.81
1	G	134	HIS	N-CA-C	11.09	134.32	109.81
1	H	134	HIS	N-CA-C	11.09	134.32	109.81
1	I	134	HIS	N-CA-C	11.09	134.32	109.81
1	J	134	HIS	N-CA-C	11.09	134.32	109.81
1	K	134	HIS	N-CA-C	11.09	134.32	109.81
1	L	134	HIS	N-CA-C	11.09	134.32	109.81
1	A	35	TYR	N-CA-C	10.90	124.25	111.71
1	B	35	TYR	N-CA-C	10.90	124.25	111.71
1	C	35	TYR	N-CA-C	10.90	124.25	111.71
1	D	35	TYR	N-CA-C	10.90	124.25	111.71
1	E	35	TYR	N-CA-C	10.90	124.25	111.71
1	F	35	TYR	N-CA-C	10.90	124.25	111.71
1	G	35	TYR	N-CA-C	10.90	124.25	111.71
1	H	35	TYR	N-CA-C	10.90	124.25	111.71
1	I	35	TYR	N-CA-C	10.90	124.25	111.71
1	J	35	TYR	N-CA-C	10.90	124.25	111.71
1	K	35	TYR	N-CA-C	10.90	124.25	111.71
1	L	35	TYR	N-CA-C	10.90	124.25	111.71
1	A	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	B	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	C	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	D	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	E	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	F	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	G	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	H	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	I	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	J	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	K	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	L	304	ASP	CA-CB-CG	10.79	123.39	112.60
1	A	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	B	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	C	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	D	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	E	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	F	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	G	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	H	78	ASP	CA-CB-CG	-10.36	102.24	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	J	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	K	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	L	78	ASP	CA-CB-CG	-10.36	102.24	112.60
1	A	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	B	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	C	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	D	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	E	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	F	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	G	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	H	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	I	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	J	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	K	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	L	316	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	A	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	B	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	C	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	D	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	E	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	F	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	G	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	H	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	I	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	J	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	K	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	L	2	PHE	CA-CB-CG	-10.03	103.77	113.80
1	A	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	B	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	C	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	D	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	E	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	F	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	G	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	H	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	I	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	J	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	K	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	L	320	ARG	NE-CZ-NH2	-9.96	110.24	119.20
1	A	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	B	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	D	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	E	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	F	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	G	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	H	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	I	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	J	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	K	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	L	40	GLN	OE1-CD-NE2	-9.73	112.87	122.60
1	A	243	TRP	N-CA-C	-9.37	100.42	112.23
1	B	243	TRP	N-CA-C	-9.37	100.42	112.23
1	C	243	TRP	N-CA-C	-9.37	100.42	112.23
1	D	243	TRP	N-CA-C	-9.37	100.42	112.23
1	E	243	TRP	N-CA-C	-9.37	100.42	112.23
1	F	243	TRP	N-CA-C	-9.37	100.42	112.23
1	G	243	TRP	N-CA-C	-9.37	100.42	112.23
1	H	243	TRP	N-CA-C	-9.37	100.42	112.23
1	I	243	TRP	N-CA-C	-9.37	100.42	112.23
1	J	243	TRP	N-CA-C	-9.37	100.42	112.23
1	K	243	TRP	N-CA-C	-9.37	100.42	112.23
1	L	243	TRP	N-CA-C	-9.37	100.42	112.23
1	A	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	B	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	C	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	D	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	E	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	F	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	G	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	H	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	I	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	J	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	K	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	L	166	ASN	OD1-CG-ND2	-9.36	113.24	122.60
1	A	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	B	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	C	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	D	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	E	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	F	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	G	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	H	57	THR	CA-CB-OG1	-9.07	95.99	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	J	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	K	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	L	57	THR	CA-CB-OG1	-9.07	95.99	109.60
1	A	2	PHE	N-CA-C	-8.99	91.64	110.80
1	B	2	PHE	N-CA-C	-8.99	91.64	110.80
1	C	2	PHE	N-CA-C	-8.99	91.64	110.80
1	D	2	PHE	N-CA-C	-8.99	91.64	110.80
1	E	2	PHE	N-CA-C	-8.99	91.64	110.80
1	F	2	PHE	N-CA-C	-8.99	91.64	110.80
1	G	2	PHE	N-CA-C	-8.99	91.64	110.80
1	H	2	PHE	N-CA-C	-8.99	91.64	110.80
1	I	2	PHE	N-CA-C	-8.99	91.64	110.80
1	J	2	PHE	N-CA-C	-8.99	91.64	110.80
1	K	2	PHE	N-CA-C	-8.99	91.64	110.80
1	L	2	PHE	N-CA-C	-8.99	91.64	110.80
1	A	308	SER	CA-C-N	8.82	130.87	119.84
1	A	308	SER	C-N-CA	8.82	130.87	119.84
1	B	308	SER	CA-C-N	8.82	130.87	119.84
1	B	308	SER	C-N-CA	8.82	130.87	119.84
1	C	308	SER	CA-C-N	8.82	130.87	119.84
1	C	308	SER	C-N-CA	8.82	130.87	119.84
1	D	308	SER	CA-C-N	8.82	130.87	119.84
1	D	308	SER	C-N-CA	8.82	130.87	119.84
1	E	308	SER	CA-C-N	8.82	130.87	119.84
1	E	308	SER	C-N-CA	8.82	130.87	119.84
1	F	308	SER	CA-C-N	8.82	130.87	119.84
1	F	308	SER	C-N-CA	8.82	130.87	119.84
1	G	308	SER	CA-C-N	8.82	130.87	119.84
1	G	308	SER	C-N-CA	8.82	130.87	119.84
1	H	308	SER	CA-C-N	8.82	130.87	119.84
1	H	308	SER	C-N-CA	8.82	130.87	119.84
1	I	308	SER	CA-C-N	8.82	130.87	119.84
1	I	308	SER	C-N-CA	8.82	130.87	119.84
1	J	308	SER	CA-C-N	8.82	130.87	119.84
1	J	308	SER	C-N-CA	8.82	130.87	119.84
1	K	308	SER	CA-C-N	8.82	130.87	119.84
1	K	308	SER	C-N-CA	8.82	130.87	119.84
1	L	308	SER	CA-C-N	8.82	130.87	119.84
1	L	308	SER	C-N-CA	8.82	130.87	119.84
1	A	25	ASP	N-CA-C	-8.81	101.63	111.14
1	B	25	ASP	N-CA-C	-8.81	101.63	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	ASP	N-CA-C	-8.81	101.63	111.14
1	D	25	ASP	N-CA-C	-8.81	101.63	111.14
1	E	25	ASP	N-CA-C	-8.81	101.63	111.14
1	F	25	ASP	N-CA-C	-8.81	101.63	111.14
1	G	25	ASP	N-CA-C	-8.81	101.63	111.14
1	H	25	ASP	N-CA-C	-8.81	101.63	111.14
1	I	25	ASP	N-CA-C	-8.81	101.63	111.14
1	J	25	ASP	N-CA-C	-8.81	101.63	111.14
1	K	25	ASP	N-CA-C	-8.81	101.63	111.14
1	L	25	ASP	N-CA-C	-8.81	101.63	111.14
1	A	9	LEU	N-CA-C	-8.79	99.58	110.65
1	B	9	LEU	N-CA-C	-8.79	99.58	110.65
1	C	9	LEU	N-CA-C	-8.79	99.58	110.65
1	D	9	LEU	N-CA-C	-8.79	99.58	110.65
1	E	9	LEU	N-CA-C	-8.79	99.58	110.65
1	F	9	LEU	N-CA-C	-8.79	99.58	110.65
1	G	9	LEU	N-CA-C	-8.79	99.58	110.65
1	H	9	LEU	N-CA-C	-8.79	99.58	110.65
1	I	9	LEU	N-CA-C	-8.79	99.58	110.65
1	J	9	LEU	N-CA-C	-8.79	99.58	110.65
1	K	9	LEU	N-CA-C	-8.79	99.58	110.65
1	L	9	LEU	N-CA-C	-8.79	99.58	110.65
1	A	258	GLU	N-CA-C	-8.78	99.92	111.24
1	B	258	GLU	N-CA-C	-8.78	99.92	111.24
1	C	258	GLU	N-CA-C	-8.78	99.92	111.24
1	D	258	GLU	N-CA-C	-8.78	99.92	111.24
1	E	258	GLU	N-CA-C	-8.78	99.92	111.24
1	F	258	GLU	N-CA-C	-8.78	99.92	111.24
1	G	258	GLU	N-CA-C	-8.78	99.92	111.24
1	H	258	GLU	N-CA-C	-8.78	99.92	111.24
1	I	258	GLU	N-CA-C	-8.78	99.92	111.24
1	J	258	GLU	N-CA-C	-8.78	99.92	111.24
1	K	258	GLU	N-CA-C	-8.78	99.92	111.24
1	L	258	GLU	N-CA-C	-8.78	99.92	111.24
1	A	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	B	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	C	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	D	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	E	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	F	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	G	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	H	123	VAL	N-CA-CB	-8.75	98.96	111.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	J	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	K	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	L	123	VAL	N-CA-CB	-8.75	98.96	111.21
1	A	78	ASP	N-CA-C	8.65	128.93	109.81
1	B	78	ASP	N-CA-C	8.65	128.93	109.81
1	C	78	ASP	N-CA-C	8.65	128.93	109.81
1	D	78	ASP	N-CA-C	8.65	128.93	109.81
1	E	78	ASP	N-CA-C	8.65	128.93	109.81
1	F	78	ASP	N-CA-C	8.65	128.93	109.81
1	G	78	ASP	N-CA-C	8.65	128.93	109.81
1	H	78	ASP	N-CA-C	8.65	128.93	109.81
1	I	78	ASP	N-CA-C	8.65	128.93	109.81
1	J	78	ASP	N-CA-C	8.65	128.93	109.81
1	K	78	ASP	N-CA-C	8.65	128.93	109.81
1	L	78	ASP	N-CA-C	8.65	128.93	109.81
1	A	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	B	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	C	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	D	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	E	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	F	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	G	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	H	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	I	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	J	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	K	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	L	131	ASP	CA-CB-CG	8.60	121.20	112.60
1	A	2	PHE	N-CA-CB	8.45	124.77	110.49
1	B	2	PHE	N-CA-CB	8.45	124.77	110.49
1	C	2	PHE	N-CA-CB	8.45	124.77	110.49
1	D	2	PHE	N-CA-CB	8.45	124.77	110.49
1	E	2	PHE	N-CA-CB	8.45	124.77	110.49
1	F	2	PHE	N-CA-CB	8.45	124.77	110.49
1	G	2	PHE	N-CA-CB	8.45	124.77	110.49
1	H	2	PHE	N-CA-CB	8.45	124.77	110.49
1	I	2	PHE	N-CA-CB	8.45	124.77	110.49
1	J	2	PHE	N-CA-CB	8.45	124.77	110.49
1	K	2	PHE	N-CA-CB	8.45	124.77	110.49
1	L	2	PHE	N-CA-CB	8.45	124.77	110.49
1	A	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	B	40	GLN	CG-CD-NE2	8.37	128.96	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	D	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	E	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	F	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	G	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	H	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	I	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	J	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	K	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	L	40	GLN	CG-CD-NE2	8.37	128.96	116.40
1	A	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	B	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	C	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	D	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	E	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	F	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	G	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	H	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	I	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	J	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	K	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	L	195	ASP	CA-CB-CG	8.32	120.92	112.60
1	A	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	B	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	C	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	D	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	E	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	F	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	G	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	H	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	I	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	J	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	K	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	L	88	GLU	CA-CB-CG	-8.31	97.47	114.10
1	A	82	SER	N-CA-C	-8.24	94.89	108.49
1	B	82	SER	N-CA-C	-8.24	94.89	108.49
1	C	82	SER	N-CA-C	-8.24	94.89	108.49
1	D	82	SER	N-CA-C	-8.24	94.89	108.49
1	E	82	SER	N-CA-C	-8.24	94.89	108.49
1	F	82	SER	N-CA-C	-8.24	94.89	108.49
1	G	82	SER	N-CA-C	-8.24	94.89	108.49
1	H	82	SER	N-CA-C	-8.24	94.89	108.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	82	SER	N-CA-C	-8.24	94.89	108.49
1	J	82	SER	N-CA-C	-8.24	94.89	108.49
1	K	82	SER	N-CA-C	-8.24	94.89	108.49
1	L	82	SER	N-CA-C	-8.24	94.89	108.49
1	A	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	A	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	B	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	B	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	C	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	C	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	D	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	D	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	E	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	E	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	F	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	F	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	G	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	G	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	H	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	H	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	I	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	I	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	J	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	J	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	K	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	K	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	L	45	ARG	CA-CB-CG	8.22	130.54	114.10
1	L	165	ARG	CB-CG-CD	-8.22	92.39	111.30
1	A	137	GLN	N-CA-C	-8.10	102.43	111.82
1	B	137	GLN	N-CA-C	-8.10	102.43	111.82
1	C	137	GLN	N-CA-C	-8.10	102.43	111.82
1	D	137	GLN	N-CA-C	-8.10	102.43	111.82
1	E	137	GLN	N-CA-C	-8.10	102.43	111.82
1	F	137	GLN	N-CA-C	-8.10	102.43	111.82
1	G	137	GLN	N-CA-C	-8.10	102.43	111.82
1	H	137	GLN	N-CA-C	-8.10	102.43	111.82
1	I	137	GLN	N-CA-C	-8.10	102.43	111.82
1	J	137	GLN	N-CA-C	-8.10	102.43	111.82
1	K	137	GLN	N-CA-C	-8.10	102.43	111.82
1	L	137	GLN	N-CA-C	-8.10	102.43	111.82
1	A	226	ASP	CA-C-O	-7.68	112.00	120.38
1	B	226	ASP	CA-C-O	-7.68	112.00	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	ASP	CA-C-O	-7.68	112.00	120.38
1	D	226	ASP	CA-C-O	-7.68	112.00	120.38
1	E	226	ASP	CA-C-O	-7.68	112.00	120.38
1	F	226	ASP	CA-C-O	-7.68	112.00	120.38
1	G	226	ASP	CA-C-O	-7.68	112.00	120.38
1	H	226	ASP	CA-C-O	-7.68	112.00	120.38
1	I	226	ASP	CA-C-O	-7.68	112.00	120.38
1	J	226	ASP	CA-C-O	-7.68	112.00	120.38
1	K	226	ASP	CA-C-O	-7.68	112.00	120.38
1	L	226	ASP	CA-C-O	-7.68	112.00	120.38
1	A	333	ALA	N-CA-C	7.49	126.76	110.80
1	B	333	ALA	N-CA-C	7.49	126.76	110.80
1	C	333	ALA	N-CA-C	7.49	126.76	110.80
1	D	333	ALA	N-CA-C	7.49	126.76	110.80
1	E	333	ALA	N-CA-C	7.49	126.76	110.80
1	F	333	ALA	N-CA-C	7.49	126.76	110.80
1	G	333	ALA	N-CA-C	7.49	126.76	110.80
1	H	333	ALA	N-CA-C	7.49	126.76	110.80
1	I	333	ALA	N-CA-C	7.49	126.76	110.80
1	J	333	ALA	N-CA-C	7.49	126.76	110.80
1	K	333	ALA	N-CA-C	7.49	126.76	110.80
1	L	333	ALA	N-CA-C	7.49	126.76	110.80
1	A	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	B	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	C	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	D	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	E	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	F	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	G	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	H	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	I	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	J	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	K	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	L	278	HIS	CB-CG-CD2	-7.46	121.51	131.20
1	A	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	B	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	C	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	D	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	E	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	F	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	G	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	H	99	ARG	CA-CB-CG	-7.40	99.30	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	J	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	K	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	L	99	ARG	CA-CB-CG	-7.40	99.30	114.10
1	A	226	ASP	O-C-N	-7.34	114.63	123.29
1	B	226	ASP	O-C-N	-7.34	114.63	123.29
1	C	226	ASP	O-C-N	-7.34	114.63	123.29
1	D	226	ASP	O-C-N	-7.34	114.63	123.29
1	E	226	ASP	O-C-N	-7.34	114.63	123.29
1	F	226	ASP	O-C-N	-7.34	114.63	123.29
1	G	226	ASP	O-C-N	-7.34	114.63	123.29
1	H	226	ASP	O-C-N	-7.34	114.63	123.29
1	I	226	ASP	O-C-N	-7.34	114.63	123.29
1	J	226	ASP	O-C-N	-7.34	114.63	123.29
1	K	226	ASP	O-C-N	-7.34	114.63	123.29
1	L	226	ASP	O-C-N	-7.34	114.63	123.29
1	A	12	LEU	CA-C-O	7.18	128.14	120.46
1	B	12	LEU	CA-C-O	7.18	128.14	120.46
1	C	12	LEU	CA-C-O	7.18	128.14	120.46
1	D	12	LEU	CA-C-O	7.18	128.14	120.46
1	E	12	LEU	CA-C-O	7.18	128.14	120.46
1	F	12	LEU	CA-C-O	7.18	128.14	120.46
1	G	12	LEU	CA-C-O	7.18	128.14	120.46
1	H	12	LEU	CA-C-O	7.18	128.14	120.46
1	I	12	LEU	CA-C-O	7.18	128.14	120.46
1	J	12	LEU	CA-C-O	7.18	128.14	120.46
1	K	12	LEU	CA-C-O	7.18	128.14	120.46
1	L	12	LEU	CA-C-O	7.18	128.14	120.46
1	A	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	B	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	C	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	D	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	E	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	F	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	G	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	H	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	I	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	J	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	K	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	L	277	PHE	CA-CB-CG	-7.15	106.65	113.80
1	A	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	B	225	VAL	N-CA-CB	-7.13	99.47	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	D	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	E	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	F	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	G	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	H	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	I	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	J	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	K	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	L	225	VAL	N-CA-CB	-7.13	99.47	111.23
1	A	309	PRO	N-CA-C	7.09	127.08	112.47
1	B	309	PRO	N-CA-C	7.09	127.08	112.47
1	C	309	PRO	N-CA-C	7.09	127.08	112.47
1	D	309	PRO	N-CA-C	7.09	127.08	112.47
1	E	309	PRO	N-CA-C	7.09	127.08	112.47
1	F	309	PRO	N-CA-C	7.09	127.08	112.47
1	G	309	PRO	N-CA-C	7.09	127.08	112.47
1	H	309	PRO	N-CA-C	7.09	127.08	112.47
1	I	309	PRO	N-CA-C	7.09	127.08	112.47
1	J	309	PRO	N-CA-C	7.09	127.08	112.47
1	K	309	PRO	N-CA-C	7.09	127.08	112.47
1	L	309	PRO	N-CA-C	7.09	127.08	112.47
1	A	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	B	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	C	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	D	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	E	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	F	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	G	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	H	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	I	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	J	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	K	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	L	322	HIS	CB-CG-CD2	-7.08	121.99	131.20
1	A	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	B	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	C	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	D	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	E	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	F	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	G	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	H	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	J	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	K	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	L	80	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	A	38	THR	N-CA-CB	-7.04	99.41	110.46
1	B	38	THR	N-CA-CB	-7.04	99.41	110.46
1	C	38	THR	N-CA-CB	-7.04	99.41	110.46
1	D	38	THR	N-CA-CB	-7.04	99.41	110.46
1	E	38	THR	N-CA-CB	-7.04	99.41	110.46
1	F	38	THR	N-CA-CB	-7.04	99.41	110.46
1	G	38	THR	N-CA-CB	-7.04	99.41	110.46
1	H	38	THR	N-CA-CB	-7.04	99.41	110.46
1	I	38	THR	N-CA-CB	-7.04	99.41	110.46
1	J	38	THR	N-CA-CB	-7.04	99.41	110.46
1	K	38	THR	N-CA-CB	-7.04	99.41	110.46
1	L	38	THR	N-CA-CB	-7.04	99.41	110.46
1	A	329	VAL	CA-C-O	-7.03	113.40	120.85
1	B	329	VAL	CA-C-O	-7.03	113.40	120.85
1	C	329	VAL	CA-C-O	-7.03	113.40	120.85
1	D	329	VAL	CA-C-O	-7.03	113.40	120.85
1	E	329	VAL	CA-C-O	-7.03	113.40	120.85
1	F	329	VAL	CA-C-O	-7.03	113.40	120.85
1	G	329	VAL	CA-C-O	-7.03	113.40	120.85
1	H	329	VAL	CA-C-O	-7.03	113.40	120.85
1	I	329	VAL	CA-C-O	-7.03	113.40	120.85
1	J	329	VAL	CA-C-O	-7.03	113.40	120.85
1	K	329	VAL	CA-C-O	-7.03	113.40	120.85
1	L	329	VAL	CA-C-O	-7.03	113.40	120.85
1	A	193	PRO	CA-C-O	-7.03	113.41	121.56
1	B	193	PRO	CA-C-O	-7.03	113.41	121.56
1	C	193	PRO	CA-C-O	-7.03	113.41	121.56
1	D	193	PRO	CA-C-O	-7.03	113.41	121.56
1	E	193	PRO	CA-C-O	-7.03	113.41	121.56
1	F	193	PRO	CA-C-O	-7.03	113.41	121.56
1	G	193	PRO	CA-C-O	-7.03	113.41	121.56
1	H	193	PRO	CA-C-O	-7.03	113.41	121.56
1	I	193	PRO	CA-C-O	-7.03	113.41	121.56
1	J	193	PRO	CA-C-O	-7.03	113.41	121.56
1	K	193	PRO	CA-C-O	-7.03	113.41	121.56
1	L	193	PRO	CA-C-O	-7.03	113.41	121.56
1	A	272	HIS	CA-C-O	-7.02	111.42	119.98
1	B	272	HIS	CA-C-O	-7.02	111.42	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	HIS	CA-C-O	-7.02	111.42	119.98
1	D	272	HIS	CA-C-O	-7.02	111.42	119.98
1	E	272	HIS	CA-C-O	-7.02	111.42	119.98
1	F	272	HIS	CA-C-O	-7.02	111.42	119.98
1	G	272	HIS	CA-C-O	-7.02	111.42	119.98
1	H	272	HIS	CA-C-O	-7.02	111.42	119.98
1	I	272	HIS	CA-C-O	-7.02	111.42	119.98
1	J	272	HIS	CA-C-O	-7.02	111.42	119.98
1	K	272	HIS	CA-C-O	-7.02	111.42	119.98
1	L	272	HIS	CA-C-O	-7.02	111.42	119.98
1	A	128	GLY	N-CA-C	-7.01	104.36	112.50
1	B	128	GLY	N-CA-C	-7.01	104.36	112.50
1	C	128	GLY	N-CA-C	-7.01	104.36	112.50
1	D	128	GLY	N-CA-C	-7.01	104.36	112.50
1	E	128	GLY	N-CA-C	-7.01	104.36	112.50
1	F	128	GLY	N-CA-C	-7.01	104.36	112.50
1	G	128	GLY	N-CA-C	-7.01	104.36	112.50
1	H	128	GLY	N-CA-C	-7.01	104.36	112.50
1	I	128	GLY	N-CA-C	-7.01	104.36	112.50
1	J	128	GLY	N-CA-C	-7.01	104.36	112.50
1	K	128	GLY	N-CA-C	-7.01	104.36	112.50
1	L	128	GLY	N-CA-C	-7.01	104.36	112.50
1	A	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	B	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	C	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	D	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	E	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	F	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	G	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	H	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	I	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	J	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	K	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	L	319	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	A	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	B	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	C	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	D	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	E	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	F	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	G	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	H	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	J	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	K	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	L	146	ARG	NE-CZ-NH2	-6.98	112.92	119.20
1	A	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	B	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	C	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	D	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	E	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	F	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	G	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	H	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	I	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	J	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	K	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	L	141	ASP	CB-CA-C	-6.97	99.67	110.81
1	A	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	B	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	C	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	D	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	E	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	F	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	G	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	H	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	I	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	J	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	K	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	L	265	ASN	CA-CB-CG	6.93	119.53	112.60
1	A	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	B	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	C	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	D	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	E	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	F	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	G	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	H	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	I	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	J	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	K	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	L	137	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	A	226	ASP	N-CA-C	-6.88	98.00	109.07
1	B	226	ASP	N-CA-C	-6.88	98.00	109.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	ASP	N-CA-C	-6.88	98.00	109.07
1	D	226	ASP	N-CA-C	-6.88	98.00	109.07
1	E	226	ASP	N-CA-C	-6.88	98.00	109.07
1	F	226	ASP	N-CA-C	-6.88	98.00	109.07
1	G	226	ASP	N-CA-C	-6.88	98.00	109.07
1	H	226	ASP	N-CA-C	-6.88	98.00	109.07
1	I	226	ASP	N-CA-C	-6.88	98.00	109.07
1	J	226	ASP	N-CA-C	-6.88	98.00	109.07
1	K	226	ASP	N-CA-C	-6.88	98.00	109.07
1	L	226	ASP	N-CA-C	-6.88	98.00	109.07
1	A	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	B	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	C	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	D	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	E	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	F	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	G	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	H	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	I	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	J	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	K	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	L	167	ASN	CB-CG-ND2	6.87	126.71	116.40
1	A	207	GLU	N-CA-C	-6.85	103.74	111.14
1	B	207	GLU	N-CA-C	-6.85	103.74	111.14
1	C	207	GLU	N-CA-C	-6.85	103.74	111.14
1	D	207	GLU	N-CA-C	-6.85	103.74	111.14
1	E	207	GLU	N-CA-C	-6.85	103.74	111.14
1	F	207	GLU	N-CA-C	-6.85	103.74	111.14
1	G	207	GLU	N-CA-C	-6.85	103.74	111.14
1	H	207	GLU	N-CA-C	-6.85	103.74	111.14
1	I	207	GLU	N-CA-C	-6.85	103.74	111.14
1	J	207	GLU	N-CA-C	-6.85	103.74	111.14
1	K	207	GLU	N-CA-C	-6.85	103.74	111.14
1	L	207	GLU	N-CA-C	-6.85	103.74	111.14
1	A	16	SER	CA-C-O	-6.78	113.75	121.07
1	B	16	SER	CA-C-O	-6.78	113.75	121.07
1	C	16	SER	CA-C-O	-6.78	113.75	121.07
1	D	16	SER	CA-C-O	-6.78	113.75	121.07
1	E	16	SER	CA-C-O	-6.78	113.75	121.07
1	F	16	SER	CA-C-O	-6.78	113.75	121.07
1	G	16	SER	CA-C-O	-6.78	113.75	121.07
1	H	16	SER	CA-C-O	-6.78	113.75	121.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	16	SER	CA-C-O	-6.78	113.75	121.07
1	J	16	SER	CA-C-O	-6.78	113.75	121.07
1	K	16	SER	CA-C-O	-6.78	113.75	121.07
1	L	16	SER	CA-C-O	-6.78	113.75	121.07
1	A	166	ASN	N-CA-C	-6.74	96.45	110.80
1	B	166	ASN	N-CA-C	-6.74	96.45	110.80
1	C	166	ASN	N-CA-C	-6.74	96.45	110.80
1	D	166	ASN	N-CA-C	-6.74	96.45	110.80
1	E	166	ASN	N-CA-C	-6.74	96.45	110.80
1	F	166	ASN	N-CA-C	-6.74	96.45	110.80
1	G	166	ASN	N-CA-C	-6.74	96.45	110.80
1	H	166	ASN	N-CA-C	-6.74	96.45	110.80
1	I	166	ASN	N-CA-C	-6.74	96.45	110.80
1	J	166	ASN	N-CA-C	-6.74	96.45	110.80
1	K	166	ASN	N-CA-C	-6.74	96.45	110.80
1	L	166	ASN	N-CA-C	-6.74	96.45	110.80
1	A	12	LEU	O-C-N	6.70	131.57	123.13
1	B	12	LEU	O-C-N	6.70	131.57	123.13
1	C	12	LEU	O-C-N	6.70	131.57	123.13
1	D	12	LEU	O-C-N	6.70	131.57	123.13
1	E	12	LEU	O-C-N	6.70	131.57	123.13
1	F	12	LEU	O-C-N	6.70	131.57	123.13
1	G	12	LEU	O-C-N	6.70	131.57	123.13
1	H	12	LEU	O-C-N	6.70	131.57	123.13
1	I	12	LEU	O-C-N	6.70	131.57	123.13
1	J	12	LEU	O-C-N	6.70	131.57	123.13
1	K	12	LEU	O-C-N	6.70	131.57	123.13
1	L	12	LEU	O-C-N	6.70	131.57	123.13
1	A	310	TYR	N-CA-C	-6.70	105.10	113.20
1	B	310	TYR	N-CA-C	-6.70	105.10	113.20
1	C	310	TYR	N-CA-C	-6.70	105.10	113.20
1	D	310	TYR	N-CA-C	-6.70	105.10	113.20
1	E	310	TYR	N-CA-C	-6.70	105.10	113.20
1	F	310	TYR	N-CA-C	-6.70	105.10	113.20
1	G	310	TYR	N-CA-C	-6.70	105.10	113.20
1	H	310	TYR	N-CA-C	-6.70	105.10	113.20
1	I	310	TYR	N-CA-C	-6.70	105.10	113.20
1	J	310	TYR	N-CA-C	-6.70	105.10	113.20
1	K	310	TYR	N-CA-C	-6.70	105.10	113.20
1	L	310	TYR	N-CA-C	-6.70	105.10	113.20
1	A	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	B	279	ASN	CA-CB-CG	6.69	119.29	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	D	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	E	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	F	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	G	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	H	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	I	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	J	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	K	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	L	279	ASN	CA-CB-CG	6.69	119.29	112.60
1	A	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	B	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	C	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	D	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	E	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	F	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	G	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	H	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	I	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	J	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	K	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	L	311	ASN	OD1-CG-ND2	-6.67	115.93	122.60
1	A	11	SER	CA-C-N	-6.66	113.65	123.11
1	A	11	SER	C-N-CA	-6.66	113.65	123.11
1	B	11	SER	CA-C-N	-6.66	113.65	123.11
1	B	11	SER	C-N-CA	-6.66	113.65	123.11
1	C	11	SER	CA-C-N	-6.66	113.65	123.11
1	C	11	SER	C-N-CA	-6.66	113.65	123.11
1	D	11	SER	CA-C-N	-6.66	113.65	123.11
1	D	11	SER	C-N-CA	-6.66	113.65	123.11
1	E	11	SER	CA-C-N	-6.66	113.65	123.11
1	E	11	SER	C-N-CA	-6.66	113.65	123.11
1	F	11	SER	CA-C-N	-6.66	113.65	123.11
1	F	11	SER	C-N-CA	-6.66	113.65	123.11
1	G	11	SER	CA-C-N	-6.66	113.65	123.11
1	G	11	SER	C-N-CA	-6.66	113.65	123.11
1	H	11	SER	CA-C-N	-6.66	113.65	123.11
1	H	11	SER	C-N-CA	-6.66	113.65	123.11
1	I	11	SER	CA-C-N	-6.66	113.65	123.11
1	I	11	SER	C-N-CA	-6.66	113.65	123.11
1	J	11	SER	CA-C-N	-6.66	113.65	123.11
1	J	11	SER	C-N-CA	-6.66	113.65	123.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	11	SER	CA-C-N	-6.66	113.65	123.11
1	K	11	SER	C-N-CA	-6.66	113.65	123.11
1	L	11	SER	CA-C-N	-6.66	113.65	123.11
1	L	11	SER	C-N-CA	-6.66	113.65	123.11
1	A	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	B	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	C	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	D	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	E	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	F	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	G	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	H	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	I	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	J	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	K	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	L	42	HIS	CA-CB-CG	-6.62	107.18	113.80
1	A	57	THR	N-CA-C	6.55	118.97	111.11
1	B	57	THR	N-CA-C	6.55	118.97	111.11
1	C	57	THR	N-CA-C	6.55	118.97	111.11
1	D	57	THR	N-CA-C	6.55	118.97	111.11
1	E	57	THR	N-CA-C	6.55	118.97	111.11
1	F	57	THR	N-CA-C	6.55	118.97	111.11
1	G	57	THR	N-CA-C	6.55	118.97	111.11
1	H	57	THR	N-CA-C	6.55	118.97	111.11
1	I	57	THR	N-CA-C	6.55	118.97	111.11
1	J	57	THR	N-CA-C	6.55	118.97	111.11
1	K	57	THR	N-CA-C	6.55	118.97	111.11
1	L	57	THR	N-CA-C	6.55	118.97	111.11
1	A	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	B	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	C	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	D	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	E	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	F	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	G	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	H	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	I	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	J	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	K	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	L	8	ASN	CA-CB-CG	6.52	119.12	112.60
1	A	197	PHE	CA-C-O	-6.49	114.02	120.70
1	B	197	PHE	CA-C-O	-6.49	114.02	120.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	PHE	CA-C-O	-6.49	114.02	120.70
1	D	197	PHE	CA-C-O	-6.49	114.02	120.70
1	E	197	PHE	CA-C-O	-6.49	114.02	120.70
1	F	197	PHE	CA-C-O	-6.49	114.02	120.70
1	G	197	PHE	CA-C-O	-6.49	114.02	120.70
1	H	197	PHE	CA-C-O	-6.49	114.02	120.70
1	I	197	PHE	CA-C-O	-6.49	114.02	120.70
1	J	197	PHE	CA-C-O	-6.49	114.02	120.70
1	K	197	PHE	CA-C-O	-6.49	114.02	120.70
1	L	197	PHE	CA-C-O	-6.49	114.02	120.70
1	A	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	B	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	C	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	D	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	E	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	F	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	G	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	H	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	I	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	J	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	K	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	L	305	VAL	CA-CB-CG2	-6.49	99.38	110.40
1	A	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	B	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	C	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	D	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	E	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	F	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	G	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	H	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	I	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	J	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	K	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	L	167	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	A	155	ASP	N-CA-C	-6.44	102.79	111.87
1	B	155	ASP	N-CA-C	-6.44	102.79	111.87
1	C	155	ASP	N-CA-C	-6.44	102.79	111.87
1	D	155	ASP	N-CA-C	-6.44	102.79	111.87
1	E	155	ASP	N-CA-C	-6.44	102.79	111.87
1	F	155	ASP	N-CA-C	-6.44	102.79	111.87
1	G	155	ASP	N-CA-C	-6.44	102.79	111.87
1	H	155	ASP	N-CA-C	-6.44	102.79	111.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	155	ASP	N-CA-C	-6.44	102.79	111.87
1	J	155	ASP	N-CA-C	-6.44	102.79	111.87
1	K	155	ASP	N-CA-C	-6.44	102.79	111.87
1	L	155	ASP	N-CA-C	-6.44	102.79	111.87
1	A	194	HIS	N-CA-CB	6.39	119.37	109.97
1	B	194	HIS	N-CA-CB	6.39	119.37	109.97
1	C	194	HIS	N-CA-CB	6.39	119.37	109.97
1	D	194	HIS	N-CA-CB	6.39	119.37	109.97
1	E	194	HIS	N-CA-CB	6.39	119.37	109.97
1	F	194	HIS	N-CA-CB	6.39	119.37	109.97
1	G	194	HIS	N-CA-CB	6.39	119.37	109.97
1	H	194	HIS	N-CA-CB	6.39	119.37	109.97
1	I	194	HIS	N-CA-CB	6.39	119.37	109.97
1	J	194	HIS	N-CA-CB	6.39	119.37	109.97
1	K	194	HIS	N-CA-CB	6.39	119.37	109.97
1	L	194	HIS	N-CA-CB	6.39	119.37	109.97
1	A	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	B	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	C	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	D	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	E	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	F	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	G	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	H	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	I	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	J	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	K	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	L	60	ARG	CB-CG-CD	-6.38	96.62	111.30
1	A	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	B	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	C	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	D	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	E	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	F	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	G	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	H	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	I	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	J	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	K	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	L	171	SER	CA-CB-OG	-6.36	98.39	111.10
1	A	263	THR	N-CA-C	-6.35	102.15	110.53
1	B	263	THR	N-CA-C	-6.35	102.15	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	263	THR	N-CA-C	-6.35	102.15	110.53
1	D	263	THR	N-CA-C	-6.35	102.15	110.53
1	E	263	THR	N-CA-C	-6.35	102.15	110.53
1	F	263	THR	N-CA-C	-6.35	102.15	110.53
1	G	263	THR	N-CA-C	-6.35	102.15	110.53
1	H	263	THR	N-CA-C	-6.35	102.15	110.53
1	I	263	THR	N-CA-C	-6.35	102.15	110.53
1	J	263	THR	N-CA-C	-6.35	102.15	110.53
1	K	263	THR	N-CA-C	-6.35	102.15	110.53
1	L	263	THR	N-CA-C	-6.35	102.15	110.53
1	A	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	B	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	C	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	D	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	E	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	F	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	G	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	H	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	I	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	J	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	K	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	L	134	HIS	CA-CB-CG	6.30	120.10	113.80
1	A	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	B	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	C	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	D	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	E	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	F	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	G	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	H	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	I	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	J	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	K	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	L	57	THR	CA-CB-CG2	6.27	121.16	110.50
1	A	133	TYR	CA-C-N	6.25	137.04	121.80
1	A	133	TYR	C-N-CA	6.25	137.04	121.80
1	B	133	TYR	CA-C-N	6.25	137.04	121.80
1	B	133	TYR	C-N-CA	6.25	137.04	121.80
1	C	133	TYR	CA-C-N	6.25	137.04	121.80
1	C	133	TYR	C-N-CA	6.25	137.04	121.80
1	D	133	TYR	CA-C-N	6.25	137.04	121.80
1	D	133	TYR	C-N-CA	6.25	137.04	121.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	133	TYR	CA-C-N	6.25	137.04	121.80
1	E	133	TYR	C-N-CA	6.25	137.04	121.80
1	F	133	TYR	CA-C-N	6.25	137.04	121.80
1	F	133	TYR	C-N-CA	6.25	137.04	121.80
1	G	133	TYR	CA-C-N	6.25	137.04	121.80
1	G	133	TYR	C-N-CA	6.25	137.04	121.80
1	H	133	TYR	CA-C-N	6.25	137.04	121.80
1	H	133	TYR	C-N-CA	6.25	137.04	121.80
1	I	133	TYR	CA-C-N	6.25	137.04	121.80
1	I	133	TYR	C-N-CA	6.25	137.04	121.80
1	J	133	TYR	CA-C-N	6.25	137.04	121.80
1	J	133	TYR	C-N-CA	6.25	137.04	121.80
1	K	133	TYR	CA-C-N	6.25	137.04	121.80
1	K	133	TYR	C-N-CA	6.25	137.04	121.80
1	L	133	TYR	CA-C-N	6.25	137.04	121.80
1	L	133	TYR	C-N-CA	6.25	137.04	121.80
1	A	214	LEU	N-CA-C	-6.21	96.80	107.61
1	B	214	LEU	N-CA-C	-6.21	96.80	107.61
1	C	214	LEU	N-CA-C	-6.21	96.80	107.61
1	D	214	LEU	N-CA-C	-6.21	96.80	107.61
1	E	214	LEU	N-CA-C	-6.21	96.80	107.61
1	F	214	LEU	N-CA-C	-6.21	96.80	107.61
1	G	214	LEU	N-CA-C	-6.21	96.80	107.61
1	H	214	LEU	N-CA-C	-6.21	96.80	107.61
1	I	214	LEU	N-CA-C	-6.21	96.80	107.61
1	J	214	LEU	N-CA-C	-6.21	96.80	107.61
1	K	214	LEU	N-CA-C	-6.21	96.80	107.61
1	L	214	LEU	N-CA-C	-6.21	96.80	107.61
1	A	163	ASP	N-CA-CB	6.18	120.94	110.49
1	B	163	ASP	N-CA-CB	6.18	120.94	110.49
1	C	163	ASP	N-CA-CB	6.18	120.94	110.49
1	D	163	ASP	N-CA-CB	6.18	120.94	110.49
1	E	163	ASP	N-CA-CB	6.18	120.94	110.49
1	F	163	ASP	N-CA-CB	6.18	120.94	110.49
1	G	163	ASP	N-CA-CB	6.18	120.94	110.49
1	H	163	ASP	N-CA-CB	6.18	120.94	110.49
1	I	163	ASP	N-CA-CB	6.18	120.94	110.49
1	J	163	ASP	N-CA-CB	6.18	120.94	110.49
1	K	163	ASP	N-CA-CB	6.18	120.94	110.49
1	L	163	ASP	N-CA-CB	6.18	120.94	110.49
1	A	143	LEU	N-CA-C	-6.10	104.63	111.28
1	B	143	LEU	N-CA-C	-6.10	104.63	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	143	LEU	N-CA-C	-6.10	104.63	111.28
1	D	143	LEU	N-CA-C	-6.10	104.63	111.28
1	E	143	LEU	N-CA-C	-6.10	104.63	111.28
1	F	143	LEU	N-CA-C	-6.10	104.63	111.28
1	G	143	LEU	N-CA-C	-6.10	104.63	111.28
1	H	143	LEU	N-CA-C	-6.10	104.63	111.28
1	I	143	LEU	N-CA-C	-6.10	104.63	111.28
1	J	143	LEU	N-CA-C	-6.10	104.63	111.28
1	K	143	LEU	N-CA-C	-6.10	104.63	111.28
1	L	143	LEU	N-CA-C	-6.10	104.63	111.28
1	A	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	B	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	C	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	D	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	E	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	F	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	G	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	H	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	I	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	J	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	K	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	L	146	ARG	NH1-CZ-NH2	6.08	127.20	119.30
1	A	98	GLY	N-CA-C	-6.06	108.01	114.67
1	B	98	GLY	N-CA-C	-6.06	108.01	114.67
1	C	98	GLY	N-CA-C	-6.06	108.01	114.67
1	D	98	GLY	N-CA-C	-6.06	108.01	114.67
1	E	98	GLY	N-CA-C	-6.06	108.01	114.67
1	F	98	GLY	N-CA-C	-6.06	108.01	114.67
1	G	98	GLY	N-CA-C	-6.06	108.01	114.67
1	H	98	GLY	N-CA-C	-6.06	108.01	114.67
1	I	98	GLY	N-CA-C	-6.06	108.01	114.67
1	J	98	GLY	N-CA-C	-6.06	108.01	114.67
1	K	98	GLY	N-CA-C	-6.06	108.01	114.67
1	L	98	GLY	N-CA-C	-6.06	108.01	114.67
1	A	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	C	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	E	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	F	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	G	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	H	69	ASP	CA-CB-CG	6.01	118.61	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	J	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	K	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	L	69	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	88	GLU	CA-C-O	-5.99	111.95	120.51
1	B	88	GLU	CA-C-O	-5.99	111.95	120.51
1	C	88	GLU	CA-C-O	-5.99	111.95	120.51
1	D	88	GLU	CA-C-O	-5.99	111.95	120.51
1	E	88	GLU	CA-C-O	-5.99	111.95	120.51
1	F	88	GLU	CA-C-O	-5.99	111.95	120.51
1	G	88	GLU	CA-C-O	-5.99	111.95	120.51
1	H	88	GLU	CA-C-O	-5.99	111.95	120.51
1	I	88	GLU	CA-C-O	-5.99	111.95	120.51
1	J	88	GLU	CA-C-O	-5.99	111.95	120.51
1	K	88	GLU	CA-C-O	-5.99	111.95	120.51
1	L	88	GLU	CA-C-O	-5.99	111.95	120.51
1	A	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	B	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	C	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	D	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	E	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	F	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	G	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	H	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	I	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	J	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	K	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	L	163	ASP	CA-CB-CG	-5.97	106.63	112.60
1	A	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	A	238	GLU	N-CA-C	-5.91	97.72	109.60
1	B	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	B	238	GLU	N-CA-C	-5.91	97.72	109.60
1	C	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	C	238	GLU	N-CA-C	-5.91	97.72	109.60
1	D	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	D	238	GLU	N-CA-C	-5.91	97.72	109.60
1	E	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	E	238	GLU	N-CA-C	-5.91	97.72	109.60
1	F	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	F	238	GLU	N-CA-C	-5.91	97.72	109.60
1	G	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	G	238	GLU	N-CA-C	-5.91	97.72	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	H	238	GLU	N-CA-C	-5.91	97.72	109.60
1	I	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	I	238	GLU	N-CA-C	-5.91	97.72	109.60
1	J	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	J	238	GLU	N-CA-C	-5.91	97.72	109.60
1	K	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	K	238	GLU	N-CA-C	-5.91	97.72	109.60
1	L	83	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	L	238	GLU	N-CA-C	-5.91	97.72	109.60
1	A	163	ASP	N-CA-C	-5.90	98.24	110.80
1	B	163	ASP	N-CA-C	-5.90	98.24	110.80
1	C	163	ASP	N-CA-C	-5.90	98.24	110.80
1	D	163	ASP	N-CA-C	-5.90	98.24	110.80
1	E	163	ASP	N-CA-C	-5.90	98.24	110.80
1	F	163	ASP	N-CA-C	-5.90	98.24	110.80
1	G	163	ASP	N-CA-C	-5.90	98.24	110.80
1	H	163	ASP	N-CA-C	-5.90	98.24	110.80
1	I	163	ASP	N-CA-C	-5.90	98.24	110.80
1	J	163	ASP	N-CA-C	-5.90	98.24	110.80
1	K	163	ASP	N-CA-C	-5.90	98.24	110.80
1	L	163	ASP	N-CA-C	-5.90	98.24	110.80
1	A	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	B	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	C	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	D	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	E	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	F	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	G	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	H	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	I	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	J	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	K	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	L	249	GLU	CB-CA-C	-5.89	101.81	110.95
1	A	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	D	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	E	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	F	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	G	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	H	217	ASP	CA-CB-CG	5.87	118.47	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	J	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	K	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	L	217	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	167	ASN	N-CA-C	5.84	123.25	110.80
1	B	167	ASN	N-CA-C	5.84	123.25	110.80
1	C	167	ASN	N-CA-C	5.84	123.25	110.80
1	D	167	ASN	N-CA-C	5.84	123.25	110.80
1	E	167	ASN	N-CA-C	5.84	123.25	110.80
1	F	167	ASN	N-CA-C	5.84	123.25	110.80
1	G	167	ASN	N-CA-C	5.84	123.25	110.80
1	H	167	ASN	N-CA-C	5.84	123.25	110.80
1	I	167	ASN	N-CA-C	5.84	123.25	110.80
1	J	167	ASN	N-CA-C	5.84	123.25	110.80
1	K	167	ASN	N-CA-C	5.84	123.25	110.80
1	L	167	ASN	N-CA-C	5.84	123.25	110.80
1	A	272	HIS	O-C-N	-5.84	116.02	123.26
1	B	272	HIS	O-C-N	-5.84	116.02	123.26
1	C	272	HIS	O-C-N	-5.84	116.02	123.26
1	D	272	HIS	O-C-N	-5.84	116.02	123.26
1	E	272	HIS	O-C-N	-5.84	116.02	123.26
1	F	272	HIS	O-C-N	-5.84	116.02	123.26
1	G	272	HIS	O-C-N	-5.84	116.02	123.26
1	H	272	HIS	O-C-N	-5.84	116.02	123.26
1	I	272	HIS	O-C-N	-5.84	116.02	123.26
1	J	272	HIS	O-C-N	-5.84	116.02	123.26
1	K	272	HIS	O-C-N	-5.84	116.02	123.26
1	L	272	HIS	O-C-N	-5.84	116.02	123.26
1	A	133	TYR	O-C-N	5.82	130.33	122.59
1	B	133	TYR	O-C-N	5.82	130.33	122.59
1	C	133	TYR	O-C-N	5.82	130.33	122.59
1	D	133	TYR	O-C-N	5.82	130.33	122.59
1	E	133	TYR	O-C-N	5.82	130.33	122.59
1	F	133	TYR	O-C-N	5.82	130.33	122.59
1	G	133	TYR	O-C-N	5.82	130.33	122.59
1	H	133	TYR	O-C-N	5.82	130.33	122.59
1	I	133	TYR	O-C-N	5.82	130.33	122.59
1	J	133	TYR	O-C-N	5.82	130.33	122.59
1	K	133	TYR	O-C-N	5.82	130.33	122.59
1	L	133	TYR	O-C-N	5.82	130.33	122.59
1	A	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	B	230	THR	CA-CB-OG1	-5.81	100.88	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	D	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	E	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	F	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	G	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	H	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	I	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	J	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	K	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	L	230	THR	CA-CB-OG1	-5.81	100.88	109.60
1	A	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	B	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	C	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	D	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	E	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	F	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	G	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	H	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	I	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	J	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	K	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	L	155	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	228	VAL	N-CA-C	-5.73	100.09	108.11
1	B	228	VAL	N-CA-C	-5.73	100.09	108.11
1	C	228	VAL	N-CA-C	-5.73	100.09	108.11
1	D	228	VAL	N-CA-C	-5.73	100.09	108.11
1	E	228	VAL	N-CA-C	-5.73	100.09	108.11
1	F	228	VAL	N-CA-C	-5.73	100.09	108.11
1	G	228	VAL	N-CA-C	-5.73	100.09	108.11
1	H	228	VAL	N-CA-C	-5.73	100.09	108.11
1	I	228	VAL	N-CA-C	-5.73	100.09	108.11
1	J	228	VAL	N-CA-C	-5.73	100.09	108.11
1	K	228	VAL	N-CA-C	-5.73	100.09	108.11
1	L	228	VAL	N-CA-C	-5.73	100.09	108.11
1	A	110	LYS	CA-C-O	-5.69	115.52	122.41
1	B	110	LYS	CA-C-O	-5.69	115.52	122.41
1	C	110	LYS	CA-C-O	-5.69	115.52	122.41
1	D	110	LYS	CA-C-O	-5.69	115.52	122.41
1	E	110	LYS	CA-C-O	-5.69	115.52	122.41
1	F	110	LYS	CA-C-O	-5.69	115.52	122.41
1	G	110	LYS	CA-C-O	-5.69	115.52	122.41
1	H	110	LYS	CA-C-O	-5.69	115.52	122.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	110	LYS	CA-C-O	-5.69	115.52	122.41
1	J	110	LYS	CA-C-O	-5.69	115.52	122.41
1	K	110	LYS	CA-C-O	-5.69	115.52	122.41
1	L	110	LYS	CA-C-O	-5.69	115.52	122.41
1	A	38	THR	N-CA-C	-5.68	106.35	113.28
1	B	38	THR	N-CA-C	-5.68	106.35	113.28
1	C	38	THR	N-CA-C	-5.68	106.35	113.28
1	D	38	THR	N-CA-C	-5.68	106.35	113.28
1	E	38	THR	N-CA-C	-5.68	106.35	113.28
1	F	38	THR	N-CA-C	-5.68	106.35	113.28
1	G	38	THR	N-CA-C	-5.68	106.35	113.28
1	H	38	THR	N-CA-C	-5.68	106.35	113.28
1	I	38	THR	N-CA-C	-5.68	106.35	113.28
1	J	38	THR	N-CA-C	-5.68	106.35	113.28
1	K	38	THR	N-CA-C	-5.68	106.35	113.28
1	L	38	THR	N-CA-C	-5.68	106.35	113.28
1	A	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	B	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	C	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	D	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	E	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	F	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	G	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	H	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	I	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	J	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	K	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	L	114	VAL	CB-CA-C	-5.66	104.62	112.04
1	A	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	B	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	C	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	D	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	E	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	F	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	G	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	H	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	I	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	J	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	K	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	L	8	ASN	CB-CA-C	-5.65	99.51	109.62
1	A	301	VAL	N-CA-C	-5.64	100.90	108.35
1	B	301	VAL	N-CA-C	-5.64	100.90	108.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	VAL	N-CA-C	-5.64	100.90	108.35
1	D	301	VAL	N-CA-C	-5.64	100.90	108.35
1	E	301	VAL	N-CA-C	-5.64	100.90	108.35
1	F	301	VAL	N-CA-C	-5.64	100.90	108.35
1	G	301	VAL	N-CA-C	-5.64	100.90	108.35
1	H	301	VAL	N-CA-C	-5.64	100.90	108.35
1	I	301	VAL	N-CA-C	-5.64	100.90	108.35
1	J	301	VAL	N-CA-C	-5.64	100.90	108.35
1	K	301	VAL	N-CA-C	-5.64	100.90	108.35
1	L	301	VAL	N-CA-C	-5.64	100.90	108.35
1	A	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	B	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	C	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	D	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	E	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	F	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	G	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	H	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	I	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	J	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	K	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	L	14	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	A	193	PRO	O-C-N	-5.64	116.02	123.01
1	B	193	PRO	O-C-N	-5.64	116.02	123.01
1	C	193	PRO	O-C-N	-5.64	116.02	123.01
1	D	193	PRO	O-C-N	-5.64	116.02	123.01
1	E	193	PRO	O-C-N	-5.64	116.02	123.01
1	F	193	PRO	O-C-N	-5.64	116.02	123.01
1	G	193	PRO	O-C-N	-5.64	116.02	123.01
1	H	193	PRO	O-C-N	-5.64	116.02	123.01
1	I	193	PRO	O-C-N	-5.64	116.02	123.01
1	J	193	PRO	O-C-N	-5.64	116.02	123.01
1	K	193	PRO	O-C-N	-5.64	116.02	123.01
1	L	193	PRO	O-C-N	-5.64	116.02	123.01
1	A	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	B	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	C	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	D	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	E	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	F	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	G	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	H	83	GLN	CA-CB-CG	5.59	125.27	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	J	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	K	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	L	83	GLN	CA-CB-CG	5.59	125.27	114.10
1	A	20	LEU	N-CA-C	-5.58	105.10	111.07
1	B	20	LEU	N-CA-C	-5.58	105.10	111.07
1	C	20	LEU	N-CA-C	-5.58	105.10	111.07
1	D	20	LEU	N-CA-C	-5.58	105.10	111.07
1	E	20	LEU	N-CA-C	-5.58	105.10	111.07
1	F	20	LEU	N-CA-C	-5.58	105.10	111.07
1	G	20	LEU	N-CA-C	-5.58	105.10	111.07
1	H	20	LEU	N-CA-C	-5.58	105.10	111.07
1	I	20	LEU	N-CA-C	-5.58	105.10	111.07
1	J	20	LEU	N-CA-C	-5.58	105.10	111.07
1	K	20	LEU	N-CA-C	-5.58	105.10	111.07
1	L	20	LEU	N-CA-C	-5.58	105.10	111.07
1	A	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	B	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	C	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	D	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	E	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	F	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	G	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	H	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	I	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	J	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	K	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	L	107	ARG	CB-CG-CD	-5.58	98.47	111.30
1	A	327	ILE	CA-C-O	-5.57	114.94	120.85
1	B	327	ILE	CA-C-O	-5.57	114.94	120.85
1	C	327	ILE	CA-C-O	-5.57	114.94	120.85
1	D	327	ILE	CA-C-O	-5.57	114.94	120.85
1	E	327	ILE	CA-C-O	-5.57	114.94	120.85
1	F	327	ILE	CA-C-O	-5.57	114.94	120.85
1	G	327	ILE	CA-C-O	-5.57	114.94	120.85
1	H	327	ILE	CA-C-O	-5.57	114.94	120.85
1	I	327	ILE	CA-C-O	-5.57	114.94	120.85
1	J	327	ILE	CA-C-O	-5.57	114.94	120.85
1	K	327	ILE	CA-C-O	-5.57	114.94	120.85
1	L	327	ILE	CA-C-O	-5.57	114.94	120.85
1	A	152	PRO	CA-C-O	-5.57	114.99	121.95
1	A	183	VAL	N-CA-C	5.57	116.11	107.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	PRO	CA-C-O	-5.57	114.99	121.95
1	B	183	VAL	N-CA-C	5.57	116.11	107.99
1	C	152	PRO	CA-C-O	-5.57	114.99	121.95
1	C	183	VAL	N-CA-C	5.57	116.11	107.99
1	D	152	PRO	CA-C-O	-5.57	114.99	121.95
1	D	183	VAL	N-CA-C	5.57	116.11	107.99
1	E	152	PRO	CA-C-O	-5.57	114.99	121.95
1	E	183	VAL	N-CA-C	5.57	116.11	107.99
1	F	152	PRO	CA-C-O	-5.57	114.99	121.95
1	F	183	VAL	N-CA-C	5.57	116.11	107.99
1	G	152	PRO	CA-C-O	-5.57	114.99	121.95
1	G	183	VAL	N-CA-C	5.57	116.11	107.99
1	H	152	PRO	CA-C-O	-5.57	114.99	121.95
1	H	183	VAL	N-CA-C	5.57	116.11	107.99
1	I	152	PRO	CA-C-O	-5.57	114.99	121.95
1	I	183	VAL	N-CA-C	5.57	116.11	107.99
1	J	152	PRO	CA-C-O	-5.57	114.99	121.95
1	J	183	VAL	N-CA-C	5.57	116.11	107.99
1	K	152	PRO	CA-C-O	-5.57	114.99	121.95
1	K	183	VAL	N-CA-C	5.57	116.11	107.99
1	L	152	PRO	CA-C-O	-5.57	114.99	121.95
1	L	183	VAL	N-CA-C	5.57	116.11	107.99
1	A	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	B	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	C	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	D	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	E	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	F	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	G	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	H	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	I	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	J	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	K	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	L	147	GLU	CB-CG-CD	-5.54	103.18	112.60
1	A	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	B	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	C	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	D	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	E	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	F	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	G	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	H	309	PRO	CA-N-CD	-5.54	104.25	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	J	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	K	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	L	309	PRO	CA-N-CD	-5.54	104.25	112.00
1	A	295	LEU	N-CA-C	-5.50	99.08	110.80
1	B	295	LEU	N-CA-C	-5.50	99.08	110.80
1	C	295	LEU	N-CA-C	-5.50	99.08	110.80
1	D	295	LEU	N-CA-C	-5.50	99.08	110.80
1	E	295	LEU	N-CA-C	-5.50	99.08	110.80
1	F	295	LEU	N-CA-C	-5.50	99.08	110.80
1	G	295	LEU	N-CA-C	-5.50	99.08	110.80
1	H	295	LEU	N-CA-C	-5.50	99.08	110.80
1	I	295	LEU	N-CA-C	-5.50	99.08	110.80
1	J	295	LEU	N-CA-C	-5.50	99.08	110.80
1	K	295	LEU	N-CA-C	-5.50	99.08	110.80
1	L	295	LEU	N-CA-C	-5.50	99.08	110.80
1	A	60	ARG	CA-C-O	-5.50	115.23	121.00
1	B	60	ARG	CA-C-O	-5.50	115.23	121.00
1	C	60	ARG	CA-C-O	-5.50	115.23	121.00
1	D	60	ARG	CA-C-O	-5.50	115.23	121.00
1	E	60	ARG	CA-C-O	-5.50	115.23	121.00
1	F	60	ARG	CA-C-O	-5.50	115.23	121.00
1	G	60	ARG	CA-C-O	-5.50	115.23	121.00
1	H	60	ARG	CA-C-O	-5.50	115.23	121.00
1	I	60	ARG	CA-C-O	-5.50	115.23	121.00
1	J	60	ARG	CA-C-O	-5.50	115.23	121.00
1	K	60	ARG	CA-C-O	-5.50	115.23	121.00
1	L	60	ARG	CA-C-O	-5.50	115.23	121.00
1	A	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	B	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	C	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	D	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	E	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	F	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	G	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	H	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	I	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	J	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	K	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	L	229	HIS	CB-CA-C	-5.49	98.52	109.33
1	A	147	GLU	N-CA-C	5.48	119.68	112.89
1	A	332	LEU	CA-C-O	-5.48	112.68	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	GLU	N-CA-C	5.48	119.68	112.89
1	B	332	LEU	CA-C-O	-5.48	112.68	120.51
1	C	147	GLU	N-CA-C	5.48	119.68	112.89
1	C	332	LEU	CA-C-O	-5.48	112.68	120.51
1	D	147	GLU	N-CA-C	5.48	119.68	112.89
1	D	332	LEU	CA-C-O	-5.48	112.68	120.51
1	E	147	GLU	N-CA-C	5.48	119.68	112.89
1	E	332	LEU	CA-C-O	-5.48	112.68	120.51
1	F	147	GLU	N-CA-C	5.48	119.68	112.89
1	F	332	LEU	CA-C-O	-5.48	112.68	120.51
1	G	147	GLU	N-CA-C	5.48	119.68	112.89
1	G	332	LEU	CA-C-O	-5.48	112.68	120.51
1	H	147	GLU	N-CA-C	5.48	119.68	112.89
1	H	332	LEU	CA-C-O	-5.48	112.68	120.51
1	I	147	GLU	N-CA-C	5.48	119.68	112.89
1	I	332	LEU	CA-C-O	-5.48	112.68	120.51
1	J	147	GLU	N-CA-C	5.48	119.68	112.89
1	J	332	LEU	CA-C-O	-5.48	112.68	120.51
1	K	147	GLU	N-CA-C	5.48	119.68	112.89
1	K	332	LEU	CA-C-O	-5.48	112.68	120.51
1	L	147	GLU	N-CA-C	5.48	119.68	112.89
1	L	332	LEU	CA-C-O	-5.48	112.68	120.51
1	A	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	B	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	C	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	D	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	E	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	F	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	G	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	H	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	I	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	J	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	K	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	L	319	ASN	CA-CB-CG	-5.47	107.13	112.60
1	A	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	B	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	C	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	D	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	E	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	F	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	G	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	H	286	LYS	CA-CB-CG	-5.47	103.16	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	J	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	K	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	L	286	LYS	CA-CB-CG	-5.47	103.16	114.10
1	A	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	B	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	C	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	D	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	E	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	F	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	G	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	H	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	I	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	J	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	K	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	L	134	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	A	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	B	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	C	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	D	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	E	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	F	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	G	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	H	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	I	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	J	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	K	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	L	112	GLU	CB-CG-CD	5.44	121.84	112.60
1	A	110	LYS	N-CA-C	5.41	117.93	108.52
1	B	110	LYS	N-CA-C	5.41	117.93	108.52
1	C	110	LYS	N-CA-C	5.41	117.93	108.52
1	D	110	LYS	N-CA-C	5.41	117.93	108.52
1	E	110	LYS	N-CA-C	5.41	117.93	108.52
1	F	110	LYS	N-CA-C	5.41	117.93	108.52
1	G	110	LYS	N-CA-C	5.41	117.93	108.52
1	H	110	LYS	N-CA-C	5.41	117.93	108.52
1	I	110	LYS	N-CA-C	5.41	117.93	108.52
1	J	110	LYS	N-CA-C	5.41	117.93	108.52
1	K	110	LYS	N-CA-C	5.41	117.93	108.52
1	L	110	LYS	N-CA-C	5.41	117.93	108.52
1	A	274	LEU	O-C-N	-5.37	115.15	121.32
1	B	274	LEU	O-C-N	-5.37	115.15	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	274	LEU	O-C-N	-5.37	115.15	121.32
1	D	274	LEU	O-C-N	-5.37	115.15	121.32
1	E	274	LEU	O-C-N	-5.37	115.15	121.32
1	F	274	LEU	O-C-N	-5.37	115.15	121.32
1	G	274	LEU	O-C-N	-5.37	115.15	121.32
1	H	274	LEU	O-C-N	-5.37	115.15	121.32
1	I	274	LEU	O-C-N	-5.37	115.15	121.32
1	J	274	LEU	O-C-N	-5.37	115.15	121.32
1	K	274	LEU	O-C-N	-5.37	115.15	121.32
1	L	274	LEU	O-C-N	-5.37	115.15	121.32
1	A	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	B	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	C	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	D	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	E	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	F	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	G	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	H	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	I	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	J	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	K	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	L	301	VAL	CB-CA-C	-5.34	101.41	111.30
1	A	315	GLU	N-CA-C	-5.33	105.47	111.28
1	B	315	GLU	N-CA-C	-5.33	105.47	111.28
1	C	315	GLU	N-CA-C	-5.33	105.47	111.28
1	D	315	GLU	N-CA-C	-5.33	105.47	111.28
1	E	315	GLU	N-CA-C	-5.33	105.47	111.28
1	F	315	GLU	N-CA-C	-5.33	105.47	111.28
1	G	315	GLU	N-CA-C	-5.33	105.47	111.28
1	H	315	GLU	N-CA-C	-5.33	105.47	111.28
1	I	315	GLU	N-CA-C	-5.33	105.47	111.28
1	J	315	GLU	N-CA-C	-5.33	105.47	111.28
1	K	315	GLU	N-CA-C	-5.33	105.47	111.28
1	L	315	GLU	N-CA-C	-5.33	105.47	111.28
1	A	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	B	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	C	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	D	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	E	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	F	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	G	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	H	322	HIS	CB-CG-ND1	5.33	130.69	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	J	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	K	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	L	322	HIS	CB-CG-ND1	5.33	130.69	122.70
1	A	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	B	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	C	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	D	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	E	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	F	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	G	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	H	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	I	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	J	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	K	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	L	58	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	A	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	B	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	C	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	D	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	E	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	F	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	G	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	H	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	I	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	J	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	K	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	L	278	HIS	CB-CG-ND1	5.31	130.66	122.70
1	A	103	ALA	O-C-N	-5.29	117.70	123.26
1	B	103	ALA	O-C-N	-5.29	117.70	123.26
1	C	103	ALA	O-C-N	-5.29	117.70	123.26
1	D	103	ALA	O-C-N	-5.29	117.70	123.26
1	E	103	ALA	O-C-N	-5.29	117.70	123.26
1	F	103	ALA	O-C-N	-5.29	117.70	123.26
1	G	103	ALA	O-C-N	-5.29	117.70	123.26
1	H	103	ALA	O-C-N	-5.29	117.70	123.26
1	I	103	ALA	O-C-N	-5.29	117.70	123.26
1	J	103	ALA	O-C-N	-5.29	117.70	123.26
1	K	103	ALA	O-C-N	-5.29	117.70	123.26
1	L	103	ALA	O-C-N	-5.29	117.70	123.26
1	A	132	GLU	N-CA-C	-5.29	104.98	111.75
1	B	132	GLU	N-CA-C	-5.29	104.98	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	GLU	N-CA-C	-5.29	104.98	111.75
1	D	132	GLU	N-CA-C	-5.29	104.98	111.75
1	E	132	GLU	N-CA-C	-5.29	104.98	111.75
1	F	132	GLU	N-CA-C	-5.29	104.98	111.75
1	G	132	GLU	N-CA-C	-5.29	104.98	111.75
1	H	132	GLU	N-CA-C	-5.29	104.98	111.75
1	I	132	GLU	N-CA-C	-5.29	104.98	111.75
1	J	132	GLU	N-CA-C	-5.29	104.98	111.75
1	K	132	GLU	N-CA-C	-5.29	104.98	111.75
1	L	132	GLU	N-CA-C	-5.29	104.98	111.75
1	A	6	ASN	N-CA-C	5.28	121.74	113.72
1	A	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	B	6	ASN	N-CA-C	5.28	121.74	113.72
1	B	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	C	6	ASN	N-CA-C	5.28	121.74	113.72
1	C	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	D	6	ASN	N-CA-C	5.28	121.74	113.72
1	D	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	E	6	ASN	N-CA-C	5.28	121.74	113.72
1	E	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	F	6	ASN	N-CA-C	5.28	121.74	113.72
1	F	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	G	6	ASN	N-CA-C	5.28	121.74	113.72
1	G	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	H	6	ASN	N-CA-C	5.28	121.74	113.72
1	H	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	I	6	ASN	N-CA-C	5.28	121.74	113.72
1	I	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	J	6	ASN	N-CA-C	5.28	121.74	113.72
1	J	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	K	6	ASN	N-CA-C	5.28	121.74	113.72
1	K	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	L	6	ASN	N-CA-C	5.28	121.74	113.72
1	L	53	GLU	CB-CG-CD	5.28	121.57	112.60
1	A	265	ASN	N-CA-C	5.26	118.08	110.14
1	B	265	ASN	N-CA-C	5.26	118.08	110.14
1	C	265	ASN	N-CA-C	5.26	118.08	110.14
1	D	265	ASN	N-CA-C	5.26	118.08	110.14
1	E	265	ASN	N-CA-C	5.26	118.08	110.14
1	F	265	ASN	N-CA-C	5.26	118.08	110.14
1	G	265	ASN	N-CA-C	5.26	118.08	110.14
1	H	265	ASN	N-CA-C	5.26	118.08	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	265	ASN	N-CA-C	5.26	118.08	110.14
1	J	265	ASN	N-CA-C	5.26	118.08	110.14
1	K	265	ASN	N-CA-C	5.26	118.08	110.14
1	L	265	ASN	N-CA-C	5.26	118.08	110.14
1	A	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	B	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	C	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	D	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	E	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	F	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	G	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	H	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	I	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	J	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	K	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	L	112	GLU	CA-CB-CG	5.25	124.60	114.10
1	A	8	ASN	N-CA-CB	5.25	117.75	110.04
1	B	8	ASN	N-CA-CB	5.25	117.75	110.04
1	C	8	ASN	N-CA-CB	5.25	117.75	110.04
1	D	8	ASN	N-CA-CB	5.25	117.75	110.04
1	E	8	ASN	N-CA-CB	5.25	117.75	110.04
1	F	8	ASN	N-CA-CB	5.25	117.75	110.04
1	G	8	ASN	N-CA-CB	5.25	117.75	110.04
1	H	8	ASN	N-CA-CB	5.25	117.75	110.04
1	I	8	ASN	N-CA-CB	5.25	117.75	110.04
1	J	8	ASN	N-CA-CB	5.25	117.75	110.04
1	K	8	ASN	N-CA-CB	5.25	117.75	110.04
1	L	8	ASN	N-CA-CB	5.25	117.75	110.04
1	A	13	MET	N-CA-C	-5.24	106.14	112.54
1	B	13	MET	N-CA-C	-5.24	106.14	112.54
1	C	13	MET	N-CA-C	-5.24	106.14	112.54
1	D	13	MET	N-CA-C	-5.24	106.14	112.54
1	E	13	MET	N-CA-C	-5.24	106.14	112.54
1	F	13	MET	N-CA-C	-5.24	106.14	112.54
1	G	13	MET	N-CA-C	-5.24	106.14	112.54
1	H	13	MET	N-CA-C	-5.24	106.14	112.54
1	I	13	MET	N-CA-C	-5.24	106.14	112.54
1	J	13	MET	N-CA-C	-5.24	106.14	112.54
1	K	13	MET	N-CA-C	-5.24	106.14	112.54
1	L	13	MET	N-CA-C	-5.24	106.14	112.54
1	A	123	VAL	CA-C-O	-5.24	112.93	119.95
1	B	123	VAL	CA-C-O	-5.24	112.93	119.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	VAL	CA-C-O	-5.24	112.93	119.95
1	D	123	VAL	CA-C-O	-5.24	112.93	119.95
1	E	123	VAL	CA-C-O	-5.24	112.93	119.95
1	F	123	VAL	CA-C-O	-5.24	112.93	119.95
1	G	123	VAL	CA-C-O	-5.24	112.93	119.95
1	H	123	VAL	CA-C-O	-5.24	112.93	119.95
1	I	123	VAL	CA-C-O	-5.24	112.93	119.95
1	J	123	VAL	CA-C-O	-5.24	112.93	119.95
1	K	123	VAL	CA-C-O	-5.24	112.93	119.95
1	L	123	VAL	CA-C-O	-5.24	112.93	119.95
1	A	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	B	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	C	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	D	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	E	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	F	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	G	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	H	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	I	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	J	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	K	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	L	316	GLN	CG-CD-NE2	5.21	124.21	116.40
1	A	142	VAL	CA-C-O	-5.20	114.85	120.47
1	B	142	VAL	CA-C-O	-5.20	114.85	120.47
1	C	142	VAL	CA-C-O	-5.20	114.85	120.47
1	D	142	VAL	CA-C-O	-5.20	114.85	120.47
1	E	142	VAL	CA-C-O	-5.20	114.85	120.47
1	F	142	VAL	CA-C-O	-5.20	114.85	120.47
1	G	142	VAL	CA-C-O	-5.20	114.85	120.47
1	H	142	VAL	CA-C-O	-5.20	114.85	120.47
1	I	142	VAL	CA-C-O	-5.20	114.85	120.47
1	J	142	VAL	CA-C-O	-5.20	114.85	120.47
1	K	142	VAL	CA-C-O	-5.20	114.85	120.47
1	L	142	VAL	CA-C-O	-5.20	114.85	120.47
1	A	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	B	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	C	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	D	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	E	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	F	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	G	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	H	229	HIS	CB-CG-CD2	-5.20	124.44	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	J	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	K	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	L	229	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	9	LEU	CA-C-N	-5.20	114.36	122.05
1	A	9	LEU	C-N-CA	-5.20	114.36	122.05
1	B	9	LEU	CA-C-N	-5.20	114.36	122.05
1	B	9	LEU	C-N-CA	-5.20	114.36	122.05
1	C	9	LEU	CA-C-N	-5.20	114.36	122.05
1	C	9	LEU	C-N-CA	-5.20	114.36	122.05
1	D	9	LEU	CA-C-N	-5.20	114.36	122.05
1	D	9	LEU	C-N-CA	-5.20	114.36	122.05
1	E	9	LEU	CA-C-N	-5.20	114.36	122.05
1	E	9	LEU	C-N-CA	-5.20	114.36	122.05
1	F	9	LEU	CA-C-N	-5.20	114.36	122.05
1	F	9	LEU	C-N-CA	-5.20	114.36	122.05
1	G	9	LEU	CA-C-N	-5.20	114.36	122.05
1	G	9	LEU	C-N-CA	-5.20	114.36	122.05
1	H	9	LEU	CA-C-N	-5.20	114.36	122.05
1	H	9	LEU	C-N-CA	-5.20	114.36	122.05
1	I	9	LEU	CA-C-N	-5.20	114.36	122.05
1	I	9	LEU	C-N-CA	-5.20	114.36	122.05
1	J	9	LEU	CA-C-N	-5.20	114.36	122.05
1	J	9	LEU	C-N-CA	-5.20	114.36	122.05
1	K	9	LEU	CA-C-N	-5.20	114.36	122.05
1	K	9	LEU	C-N-CA	-5.20	114.36	122.05
1	L	9	LEU	CA-C-N	-5.20	114.36	122.05
1	L	9	LEU	C-N-CA	-5.20	114.36	122.05
1	A	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	B	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	C	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	D	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	E	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	F	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	G	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	H	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	I	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	J	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	K	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	L	34	LYS	CA-CB-CG	-5.19	103.72	114.10
1	A	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	B	222	VAL	N-CA-CB	-5.17	102.70	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	D	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	E	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	F	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	G	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	H	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	I	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	J	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	K	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	L	222	VAL	N-CA-CB	-5.17	102.70	111.23
1	A	195	ASP	CA-C-O	-5.16	113.13	120.51
1	B	195	ASP	CA-C-O	-5.16	113.13	120.51
1	C	195	ASP	CA-C-O	-5.16	113.13	120.51
1	D	195	ASP	CA-C-O	-5.16	113.13	120.51
1	E	195	ASP	CA-C-O	-5.16	113.13	120.51
1	F	195	ASP	CA-C-O	-5.16	113.13	120.51
1	G	195	ASP	CA-C-O	-5.16	113.13	120.51
1	H	195	ASP	CA-C-O	-5.16	113.13	120.51
1	I	195	ASP	CA-C-O	-5.16	113.13	120.51
1	J	195	ASP	CA-C-O	-5.16	113.13	120.51
1	K	195	ASP	CA-C-O	-5.16	113.13	120.51
1	L	195	ASP	CA-C-O	-5.16	113.13	120.51
1	A	164	ALA	N-CA-C	-5.11	104.45	111.81
1	B	164	ALA	N-CA-C	-5.11	104.45	111.81
1	C	164	ALA	N-CA-C	-5.11	104.45	111.81
1	D	164	ALA	N-CA-C	-5.11	104.45	111.81
1	E	164	ALA	N-CA-C	-5.11	104.45	111.81
1	F	164	ALA	N-CA-C	-5.11	104.45	111.81
1	G	164	ALA	N-CA-C	-5.11	104.45	111.81
1	H	164	ALA	N-CA-C	-5.11	104.45	111.81
1	I	164	ALA	N-CA-C	-5.11	104.45	111.81
1	J	164	ALA	N-CA-C	-5.11	104.45	111.81
1	K	164	ALA	N-CA-C	-5.11	104.45	111.81
1	L	164	ALA	N-CA-C	-5.11	104.45	111.81
1	A	203	LYS	N-CA-C	-5.11	104.78	111.02
1	B	203	LYS	N-CA-C	-5.11	104.78	111.02
1	C	203	LYS	N-CA-C	-5.11	104.78	111.02
1	D	203	LYS	N-CA-C	-5.11	104.78	111.02
1	E	203	LYS	N-CA-C	-5.11	104.78	111.02
1	F	203	LYS	N-CA-C	-5.11	104.78	111.02
1	G	203	LYS	N-CA-C	-5.11	104.78	111.02
1	H	203	LYS	N-CA-C	-5.11	104.78	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	203	LYS	N-CA-C	-5.11	104.78	111.02
1	J	203	LYS	N-CA-C	-5.11	104.78	111.02
1	K	203	LYS	N-CA-C	-5.11	104.78	111.02
1	L	203	LYS	N-CA-C	-5.11	104.78	111.02
1	A	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	B	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	C	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	D	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	E	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	F	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	G	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	H	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	I	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	J	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	K	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	L	101	TYR	CA-CB-CG	-5.09	104.74	113.90
1	A	274	LEU	N-CA-C	5.08	121.03	109.81
1	B	274	LEU	N-CA-C	5.08	121.03	109.81
1	C	274	LEU	N-CA-C	5.08	121.03	109.81
1	D	274	LEU	N-CA-C	5.08	121.03	109.81
1	E	274	LEU	N-CA-C	5.08	121.03	109.81
1	F	274	LEU	N-CA-C	5.08	121.03	109.81
1	G	274	LEU	N-CA-C	5.08	121.03	109.81
1	H	274	LEU	N-CA-C	5.08	121.03	109.81
1	I	274	LEU	N-CA-C	5.08	121.03	109.81
1	J	274	LEU	N-CA-C	5.08	121.03	109.81
1	K	274	LEU	N-CA-C	5.08	121.03	109.81
1	L	274	LEU	N-CA-C	5.08	121.03	109.81
1	A	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	A	241	GLU	O-C-N	5.07	129.34	122.59
1	B	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	B	241	GLU	O-C-N	5.07	129.34	122.59
1	C	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	C	241	GLU	O-C-N	5.07	129.34	122.59
1	D	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	D	241	GLU	O-C-N	5.07	129.34	122.59
1	E	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	E	241	GLU	O-C-N	5.07	129.34	122.59
1	F	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	F	241	GLU	O-C-N	5.07	129.34	122.59
1	G	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	G	241	GLU	O-C-N	5.07	129.34	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	H	241	GLU	O-C-N	5.07	129.34	122.59
1	I	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	I	241	GLU	O-C-N	5.07	129.34	122.59
1	J	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	J	241	GLU	O-C-N	5.07	129.34	122.59
1	K	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	K	241	GLU	O-C-N	5.07	129.34	122.59
1	L	137	GLN	CG-CD-NE2	5.07	124.01	116.40
1	L	241	GLU	O-C-N	5.07	129.34	122.59
1	A	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	B	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	C	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	D	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	E	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	F	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	G	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	H	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	I	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	J	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	K	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	L	184	ARG	CB-CG-CD	-5.07	99.64	111.30
1	A	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	B	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	C	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	D	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	E	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	F	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	G	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	H	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	I	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	J	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	K	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	L	129	LEU	CA-CB-CG	5.03	133.91	116.30
1	A	113	ILE	N-CA-C	5.02	115.74	110.62
1	B	113	ILE	N-CA-C	5.02	115.74	110.62
1	C	113	ILE	N-CA-C	5.02	115.74	110.62
1	D	113	ILE	N-CA-C	5.02	115.74	110.62
1	E	113	ILE	N-CA-C	5.02	115.74	110.62
1	F	113	ILE	N-CA-C	5.02	115.74	110.62
1	G	113	ILE	N-CA-C	5.02	115.74	110.62
1	H	113	ILE	N-CA-C	5.02	115.74	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	113	ILE	N-CA-C	5.02	115.74	110.62
1	J	113	ILE	N-CA-C	5.02	115.74	110.62
1	K	113	ILE	N-CA-C	5.02	115.74	110.62
1	L	113	ILE	N-CA-C	5.02	115.74	110.62
1	A	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	B	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	C	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	D	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	E	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	F	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	G	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	H	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	I	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	J	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	K	10	LEU	CA-CB-CG	5.00	133.82	116.30
1	L	10	LEU	CA-CB-CG	5.00	133.82	116.30

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	HIS	Peptide
1	A	238	GLU	Peptide
1	A	264	GLY	Peptide
1	A	308	SER	Peptide
1	A	45	ARG	Sidechain
1	A	78	ASP	Peptide
1	B	134	HIS	Peptide
1	B	238	GLU	Peptide
1	B	264	GLY	Peptide
1	B	308	SER	Peptide
1	B	45	ARG	Sidechain
1	B	78	ASP	Peptide
1	C	134	HIS	Peptide
1	C	238	GLU	Peptide
1	C	264	GLY	Peptide
1	C	308	SER	Peptide
1	C	45	ARG	Sidechain
1	C	78	ASP	Peptide
1	D	134	HIS	Peptide
1	D	238	GLU	Peptide
1	D	264	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	308	SER	Peptide
1	D	45	ARG	Sidechain
1	D	78	ASP	Peptide
1	E	134	HIS	Peptide
1	E	238	GLU	Peptide
1	E	264	GLY	Peptide
1	E	308	SER	Peptide
1	E	45	ARG	Sidechain
1	E	78	ASP	Peptide
1	F	134	HIS	Peptide
1	F	238	GLU	Peptide
1	F	264	GLY	Peptide
1	F	308	SER	Peptide
1	F	45	ARG	Sidechain
1	F	78	ASP	Peptide
1	G	134	HIS	Peptide
1	G	238	GLU	Peptide
1	G	264	GLY	Peptide
1	G	308	SER	Peptide
1	G	45	ARG	Sidechain
1	G	78	ASP	Peptide
1	H	134	HIS	Peptide
1	H	238	GLU	Peptide
1	H	264	GLY	Peptide
1	H	308	SER	Peptide
1	H	45	ARG	Sidechain
1	H	78	ASP	Peptide
1	I	134	HIS	Peptide
1	I	238	GLU	Peptide
1	I	264	GLY	Peptide
1	I	308	SER	Peptide
1	I	45	ARG	Sidechain
1	I	78	ASP	Peptide
1	J	134	HIS	Peptide
1	J	238	GLU	Peptide
1	J	264	GLY	Peptide
1	J	308	SER	Peptide
1	J	45	ARG	Sidechain
1	J	78	ASP	Peptide
1	K	134	HIS	Peptide
1	K	238	GLU	Peptide
1	K	264	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	K	308	SER	Peptide
1	K	45	ARG	Sidechain
1	K	78	ASP	Peptide
1	L	134	HIS	Peptide
1	L	238	GLU	Peptide
1	L	264	GLY	Peptide
1	L	308	SER	Peptide
1	L	45	ARG	Sidechain
1	L	78	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2664	0	2637	98	0
1	B	2664	0	2637	95	5
1	C	2664	0	2637	100	4
1	D	2664	0	2637	98	0
1	E	2664	0	2637	99	0
1	F	2664	0	2637	101	40
1	G	2664	0	2637	94	0
1	H	2664	0	2637	95	0
1	I	2664	0	2637	100	5
1	J	2664	0	2637	95	0
1	K	2664	0	2637	99	40
1	L	2664	0	2637	101	4
All	All	31968	0	31644	1051	49

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 17.

All (1051) 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:A:81:SER:HB2	1:E:55:THR:HG21	1.57	0.87
1:D:81:SER:HB2	1:K:55:THR:HG21	1.57	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:HG21	1:L:81:SER:HB2	1.57	0.87
1:C:81:SER:HB2	1:D:55:THR:HG21	1.57	0.87
1:F:81:SER:HB2	1:J:55:THR:HG21	1.57	0.86
1:G:55:THR:HG21	1:I:81:SER:HB2	1.57	0.86
1:F:107:ARG:HG3	1:F:129:LEU:HD13	1.58	0.86
1:I:107:ARG:HG3	1:I:129:LEU:HD13	1.58	0.86
1:D:107:ARG:HG3	1:D:129:LEU:HD13	1.58	0.86
1:A:107:ARG:HG3	1:A:129:LEU:HD13	1.58	0.86
1:C:107:ARG:HG3	1:C:129:LEU:HD13	1.58	0.85
1:E:107:ARG:HG3	1:E:129:LEU:HD13	1.58	0.85
1:H:81:SER:HB2	1:I:55:THR:HG21	1.57	0.85
1:B:81:SER:HB2	1:F:55:THR:HG21	1.57	0.85
1:K:107:ARG:HG3	1:K:129:LEU:HD13	1.58	0.85
1:L:107:ARG:HG3	1:L:129:LEU:HD13	1.58	0.85
1:G:81:SER:HB2	1:H:55:THR:HG21	1.57	0.84
1:B:55:THR:HG21	1:J:81:SER:HB2	1.57	0.84
1:C:55:THR:HG21	1:K:81:SER:HB2	1.57	0.84
1:E:81:SER:HB2	1:L:55:THR:HG21	1.57	0.84
1:B:107:ARG:HG3	1:B:129:LEU:HD13	1.58	0.83
1:H:107:ARG:HG3	1:H:129:LEU:HD13	1.58	0.83
1:C:127:ASN:HD21	1:C:129:LEU:HA	1.44	0.83
1:L:127:ASN:HD21	1:L:129:LEU:HA	1.44	0.83
1:E:127:ASN:HD21	1:E:129:LEU:HA	1.44	0.83
1:K:127:ASN:HD21	1:K:129:LEU:HA	1.44	0.83
1:D:127:ASN:HD21	1:D:129:LEU:HA	1.44	0.83
1:A:127:ASN:HD21	1:A:129:LEU:HA	1.44	0.82
1:B:127:ASN:HD21	1:B:129:LEU:HA	1.44	0.82
1:G:107:ARG:HG3	1:G:129:LEU:HD13	1.58	0.82
1:H:127:ASN:HD21	1:H:129:LEU:HA	1.44	0.82
1:J:107:ARG:HG3	1:J:129:LEU:HD13	1.58	0.82
1:F:127:ASN:HD21	1:F:129:LEU:HA	1.44	0.82
1:I:127:ASN:HD21	1:I:129:LEU:HA	1.44	0.82
1:G:127:ASN:HD21	1:G:129:LEU:HA	1.44	0.81
1:J:127:ASN:HD21	1:J:129:LEU:HA	1.44	0.81
1:I:218:PRO:HB2	1:I:259:ILE:HD11	1.66	0.78
1:F:218:PRO:HB2	1:F:259:ILE:HD11	1.66	0.78
1:B:240:VAL:HA	1:B:243:TRP:NE1	2.00	0.77
1:G:240:VAL:HA	1:G:243:TRP:NE1	2.00	0.77
1:H:240:VAL:HA	1:H:243:TRP:NE1	2.00	0.77
1:J:240:VAL:HA	1:J:243:TRP:NE1	2.00	0.77
1:C:240:VAL:HA	1:C:243:TRP:NE1	2.00	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:PRO:HB2	1:D:259:ILE:HD11	1.66	0.77
1:F:240:VAL:HA	1:F:243:TRP:NE1	2.00	0.77
1:I:240:VAL:HA	1:I:243:TRP:NE1	2.00	0.77
1:L:240:VAL:HA	1:L:243:TRP:NE1	2.00	0.77
1:A:218:PRO:HB2	1:A:259:ILE:HD11	1.66	0.77
1:A:240:VAL:HA	1:A:243:TRP:NE1	2.00	0.77
1:B:218:PRO:HB2	1:B:259:ILE:HD11	1.66	0.77
1:D:240:VAL:HA	1:D:243:TRP:NE1	2.00	0.77
1:J:218:PRO:HB2	1:J:259:ILE:HD11	1.66	0.77
1:H:218:PRO:HB2	1:H:259:ILE:HD11	1.66	0.76
1:C:218:PRO:HB2	1:C:259:ILE:HD11	1.66	0.76
1:G:218:PRO:HB2	1:G:259:ILE:HD11	1.66	0.76
1:L:218:PRO:HB2	1:L:259:ILE:HD11	1.66	0.76
1:E:218:PRO:HB2	1:E:259:ILE:HD11	1.66	0.75
1:K:218:PRO:HB2	1:K:259:ILE:HD11	1.66	0.75
1:E:240:VAL:HA	1:E:243:TRP:NE1	2.00	0.75
1:K:240:VAL:HA	1:K:243:TRP:NE1	2.00	0.75
1:C:133:TYR:CD2	1:C:134:HIS:HB2	2.23	0.73
1:H:133:TYR:CD2	1:H:134:HIS:HB2	2.23	0.73
1:L:133:TYR:CD2	1:L:134:HIS:HB2	2.23	0.73
1:B:133:TYR:CD2	1:B:134:HIS:HB2	2.23	0.73
1:A:133:TYR:CD2	1:A:134:HIS:HB2	2.23	0.73
1:D:133:TYR:CD2	1:D:134:HIS:HB2	2.23	0.73
1:G:133:TYR:CD2	1:G:134:HIS:HB2	2.23	0.72
1:J:133:TYR:CD2	1:J:134:HIS:HB2	2.23	0.72
1:F:133:TYR:CD2	1:F:134:HIS:HB2	2.23	0.72
1:I:133:TYR:CD2	1:I:134:HIS:HB2	2.23	0.72
1:E:133:TYR:CD2	1:E:134:HIS:HB2	2.23	0.72
1:K:133:TYR:CD2	1:K:134:HIS:HB2	2.23	0.72
1:C:127:ASN:ND2	1:C:129:LEU:HA	2.06	0.71
1:F:127:ASN:ND2	1:F:129:LEU:HA	2.06	0.71
1:I:127:ASN:ND2	1:I:129:LEU:HA	2.06	0.71
1:L:127:ASN:ND2	1:L:129:LEU:HA	2.06	0.71
1:E:127:ASN:ND2	1:E:129:LEU:HA	2.06	0.71
1:K:127:ASN:ND2	1:K:129:LEU:HA	2.06	0.71
1:H:127:ASN:ND2	1:H:129:LEU:HA	2.06	0.71
1:B:127:ASN:ND2	1:B:129:LEU:HA	2.06	0.70
1:G:127:ASN:ND2	1:G:129:LEU:HA	2.06	0.70
1:J:127:ASN:ND2	1:J:129:LEU:HA	2.06	0.70
1:A:127:ASN:ND2	1:A:129:LEU:HA	2.06	0.70
1:D:127:ASN:ND2	1:D:129:LEU:HA	2.06	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:HIS:CE1	1:E:320:ARG:HH22	2.11	0.69
1:K:134:HIS:CE1	1:K:320:ARG:HH22	2.11	0.69
1:L:134:HIS:CE1	1:L:320:ARG:HH22	2.11	0.69
1:C:134:HIS:CE1	1:C:320:ARG:HH22	2.11	0.69
1:H:134:HIS:CE1	1:H:320:ARG:HH22	2.11	0.69
1:B:134:HIS:CE1	1:B:320:ARG:HH22	2.11	0.69
1:G:134:HIS:CE1	1:G:320:ARG:HH22	2.11	0.69
1:J:134:HIS:CE1	1:J:320:ARG:HH22	2.11	0.69
1:F:134:HIS:CE1	1:F:320:ARG:HH22	2.11	0.68
1:I:134:HIS:CE1	1:I:320:ARG:HH22	2.11	0.68
1:E:134:HIS:HE1	1:E:320:ARG:HH22	1.42	0.68
1:K:134:HIS:HE1	1:K:320:ARG:HH22	1.42	0.68
1:F:134:HIS:HE1	1:F:320:ARG:HH22	1.42	0.68
1:F:247:ILE:O	1:F:251:LEU:HB2	1.94	0.68
1:I:134:HIS:HE1	1:I:320:ARG:HH22	1.42	0.68
1:I:247:ILE:O	1:I:251:LEU:HB2	1.94	0.68
1:A:134:HIS:CE1	1:A:320:ARG:HH22	2.11	0.68
1:A:236:MET:SD	1:A:284:VAL:HG11	2.34	0.68
1:C:134:HIS:HE1	1:C:320:ARG:HH22	1.42	0.68
1:D:236:MET:SD	1:D:284:VAL:HG11	2.34	0.68
1:E:247:ILE:O	1:E:251:LEU:HB2	1.94	0.68
1:K:247:ILE:O	1:K:251:LEU:HB2	1.94	0.68
1:B:236:MET:SD	1:B:284:VAL:HG11	2.34	0.67
1:C:236:MET:SD	1:C:284:VAL:HG11	2.34	0.67
1:D:134:HIS:CE1	1:D:320:ARG:HH22	2.11	0.67
1:H:236:MET:SD	1:H:284:VAL:HG11	2.34	0.67
1:L:134:HIS:HE1	1:L:320:ARG:HH22	1.42	0.67
1:G:247:ILE:O	1:G:251:LEU:HB2	1.94	0.67
1:J:247:ILE:O	1:J:251:LEU:HB2	1.94	0.67
1:L:236:MET:SD	1:L:284:VAL:HG11	2.34	0.67
1:K:236:MET:SD	1:K:284:VAL:HG11	2.34	0.67
1:E:236:MET:SD	1:E:284:VAL:HG11	2.34	0.67
1:F:236:MET:SD	1:F:284:VAL:HG11	2.34	0.67
1:I:236:MET:SD	1:I:284:VAL:HG11	2.34	0.67
1:B:134:HIS:HE1	1:B:320:ARG:HH22	1.42	0.67
1:H:134:HIS:HE1	1:H:320:ARG:HH22	1.42	0.67
1:D:134:HIS:HE1	1:D:320:ARG:HH22	1.42	0.66
1:B:91:LYS:O	1:B:95:ARG:HD3	1.96	0.66
1:C:247:ILE:O	1:C:251:LEU:HB2	1.94	0.66
1:D:247:ILE:O	1:D:251:LEU:HB2	1.94	0.66
1:L:247:ILE:O	1:L:251:LEU:HB2	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:HIS:HE1	1:A:320:ARG:HH22	1.42	0.66
1:H:91:LYS:O	1:H:95:ARG:HD3	1.96	0.66
1:A:247:ILE:O	1:A:251:LEU:HB2	1.94	0.66
1:H:247:ILE:O	1:H:251:LEU:HB2	1.94	0.66
1:J:236:MET:SD	1:J:284:VAL:HG11	2.34	0.66
1:B:247:ILE:O	1:B:251:LEU:HB2	1.94	0.66
1:F:91:LYS:O	1:F:95:ARG:HD3	1.96	0.66
1:G:236:MET:SD	1:G:284:VAL:HG11	2.34	0.65
1:E:91:LYS:O	1:E:95:ARG:HD3	1.96	0.65
1:I:91:LYS:O	1:I:95:ARG:HD3	1.96	0.65
1:K:91:LYS:O	1:K:95:ARG:HD3	1.96	0.65
1:J:91:LYS:O	1:J:95:ARG:HD3	1.96	0.65
1:G:91:LYS:O	1:G:95:ARG:HD3	1.96	0.65
1:L:91:LYS:O	1:L:95:ARG:HD3	1.96	0.65
1:D:91:LYS:O	1:D:95:ARG:HD3	1.96	0.65
1:A:91:LYS:O	1:A:95:ARG:HD3	1.96	0.65
1:C:91:LYS:O	1:C:95:ARG:HD3	1.96	0.65
1:J:134:HIS:HE1	1:J:320:ARG:HH22	1.42	0.65
1:G:134:HIS:HE1	1:G:320:ARG:HH22	1.42	0.64
1:C:227:PHE:HA	1:C:269:LYS:O	1.98	0.64
1:K:227:PHE:HA	1:K:269:LYS:O	1.98	0.64
1:E:227:PHE:HA	1:E:269:LYS:O	1.98	0.64
1:L:227:PHE:HA	1:L:269:LYS:O	1.98	0.64
1:B:227:PHE:HA	1:B:269:LYS:O	1.98	0.64
1:H:227:PHE:HA	1:H:269:LYS:O	1.98	0.64
1:F:227:PHE:HA	1:F:269:LYS:O	1.98	0.64
1:I:227:PHE:HA	1:I:269:LYS:O	1.98	0.64
1:E:188:PRO:HD3	1:E:253:TYR:CE2	2.33	0.64
1:K:188:PRO:HD3	1:K:253:TYR:CE2	2.33	0.64
1:L:188:PRO:HD3	1:L:253:TYR:CE2	2.33	0.64
1:A:188:PRO:HD3	1:A:253:TYR:CE2	2.33	0.64
1:A:227:PHE:HA	1:A:269:LYS:O	1.98	0.64
1:C:188:PRO:HD3	1:C:253:TYR:CE2	2.33	0.64
1:D:188:PRO:HD3	1:D:253:TYR:CE2	2.33	0.64
1:D:227:PHE:HA	1:D:269:LYS:O	1.98	0.64
1:G:188:PRO:HD3	1:G:253:TYR:CE2	2.33	0.64
1:J:188:PRO:HD3	1:J:253:TYR:CE2	2.33	0.64
1:J:227:PHE:HA	1:J:269:LYS:O	1.98	0.64
1:G:227:PHE:HA	1:G:269:LYS:O	1.98	0.63
1:F:188:PRO:HD3	1:F:253:TYR:CE2	2.33	0.63
1:I:188:PRO:HD3	1:I:253:TYR:CE2	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:MET:SD	1:F:171:SER:HB3	2.39	0.63
1:I:138:MET:SD	1:I:171:SER:HB3	2.39	0.63
1:D:138:MET:SD	1:D:171:SER:HB3	2.39	0.63
1:E:138:MET:SD	1:E:171:SER:HB3	2.39	0.63
1:K:138:MET:SD	1:K:171:SER:HB3	2.39	0.63
1:A:138:MET:SD	1:A:171:SER:HB3	2.39	0.62
1:G:86:HIS:CE1	1:H:283:LYS:HZ1	2.17	0.62
1:B:138:MET:SD	1:B:171:SER:HB3	2.39	0.62
1:B:283:LYS:HZ1	1:J:86:HIS:CE1	2.17	0.62
1:H:138:MET:SD	1:H:171:SER:HB3	2.39	0.62
1:C:138:MET:SD	1:C:171:SER:HB3	2.39	0.62
1:H:188:PRO:HD3	1:H:253:TYR:CE2	2.33	0.62
1:L:138:MET:SD	1:L:171:SER:HB3	2.39	0.62
1:B:188:PRO:HD3	1:B:253:TYR:CE2	2.33	0.62
1:G:138:MET:SD	1:G:171:SER:HB3	2.39	0.62
1:J:138:MET:SD	1:J:171:SER:HB3	2.39	0.62
1:C:283:LYS:HZ1	1:K:86:HIS:CE1	2.18	0.62
1:B:251:LEU:HD21	1:B:295:LEU:HD11	1.82	0.62
1:E:86:HIS:CE1	1:L:283:LYS:HZ1	2.18	0.62
1:H:251:LEU:HD21	1:H:295:LEU:HD11	1.82	0.62
1:C:86:HIS:CE1	1:D:283:LYS:HZ1	2.18	0.61
1:F:86:HIS:CE1	1:J:283:LYS:HZ1	2.18	0.61
1:D:86:HIS:CE1	1:K:283:LYS:HZ1	2.19	0.61
1:G:283:LYS:HZ1	1:I:86:HIS:CE1	2.19	0.60
1:B:86:HIS:CE1	1:F:283:LYS:HZ1	2.20	0.60
1:H:86:HIS:CE1	1:I:283:LYS:HZ1	2.20	0.60
1:A:86:HIS:CE1	1:E:283:LYS:HZ1	2.20	0.60
1:L:251:LEU:HD21	1:L:295:LEU:HD11	1.82	0.60
1:C:251:LEU:HD21	1:C:295:LEU:HD11	1.82	0.60
1:E:251:LEU:HD21	1:E:295:LEU:HD11	1.82	0.60
1:F:251:LEU:HD21	1:F:295:LEU:HD11	1.82	0.60
1:I:251:LEU:HD21	1:I:295:LEU:HD11	1.82	0.60
1:K:251:LEU:HD21	1:K:295:LEU:HD11	1.82	0.60
1:C:11:SER:HA	1:C:135:PRO:HG3	1.84	0.60
1:J:251:LEU:HD21	1:J:295:LEU:HD11	1.82	0.60
1:L:11:SER:HA	1:L:135:PRO:HG3	1.84	0.60
1:A:283:LYS:HZ1	1:L:86:HIS:CE1	2.20	0.60
1:K:11:SER:HA	1:K:135:PRO:HG3	1.84	0.60
1:E:11:SER:HA	1:E:135:PRO:HG3	1.84	0.59
1:G:251:LEU:HD21	1:G:295:LEU:HD11	1.82	0.59
1:H:98:GLY:O	1:K:1:ALA:HB3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:SER:HA	1:B:135:PRO:HG3	1.84	0.59
1:B:98:GLY:O	1:E:1:ALA:HB3	2.02	0.59
1:A:251:LEU:HD21	1:A:295:LEU:HD11	1.82	0.59
1:H:1:ALA:HB3	1:K:98:GLY:O	2.02	0.59
1:H:11:SER:HA	1:H:135:PRO:HG3	1.84	0.59
1:B:1:ALA:HB3	1:E:98:GLY:O	2.02	0.59
1:D:251:LEU:HD21	1:D:295:LEU:HD11	1.82	0.59
1:C:1:ALA:HB3	1:F:98:GLY:O	2.02	0.59
1:D:36:THR:HG23	1:F:30:LEU:HD13	1.85	0.59
1:F:11:SER:HA	1:F:135:PRO:HG3	1.84	0.59
1:I:11:SER:HA	1:I:135:PRO:HG3	1.84	0.59
1:A:36:THR:HG23	1:I:30:LEU:HD13	1.85	0.59
1:B:30:LEU:HD13	1:L:36:THR:HG23	1.85	0.59
1:C:36:THR:HG23	1:H:30:LEU:HD13	1.85	0.59
1:F:282:THR:HG23	1:F:285:GLY:HA3	1.85	0.59
1:I:98:GLY:O	1:L:1:ALA:HB3	2.02	0.59
1:I:282:THR:HG23	1:I:285:GLY:HA3	1.85	0.59
1:E:107:ARG:NH1	1:E:129:LEU:HD11	2.18	0.59
1:K:107:ARG:NH1	1:K:129:LEU:HD11	2.18	0.59
1:G:1:ALA:HB3	1:J:98:GLY:O	2.02	0.58
1:J:11:SER:HA	1:J:135:PRO:HG3	1.84	0.58
1:D:107:ARG:NH1	1:D:129:LEU:HD11	2.18	0.58
1:G:11:SER:HA	1:G:135:PRO:HG3	1.84	0.58
1:G:107:ARG:NH1	1:G:129:LEU:HD11	2.18	0.58
1:G:282:THR:HG23	1:G:285:GLY:HA3	1.85	0.58
1:J:107:ARG:NH1	1:J:129:LEU:HD11	2.18	0.58
1:A:107:ARG:NH1	1:A:129:LEU:HD11	2.18	0.58
1:B:282:THR:HG23	1:B:285:GLY:HA3	1.85	0.58
1:G:98:GLY:O	1:J:1:ALA:HB3	2.02	0.58
1:J:282:THR:HG23	1:J:285:GLY:HA3	1.85	0.58
1:A:1:ALA:HB3	1:D:98:GLY:O	2.02	0.58
1:A:282:THR:HG23	1:A:285:GLY:HA3	1.85	0.58
1:C:107:ARG:NH1	1:C:129:LEU:HD11	2.18	0.58
1:F:107:ARG:NH1	1:F:129:LEU:HD11	2.18	0.58
1:G:36:THR:HG23	1:L:30:LEU:HD13	1.85	0.58
1:A:98:GLY:O	1:D:1:ALA:HB3	2.02	0.58
1:B:36:THR:HG23	1:G:30:LEU:HD13	1.85	0.58
1:D:282:THR:HG23	1:D:285:GLY:HA3	1.85	0.58
1:H:282:THR:HG23	1:H:285:GLY:HA3	1.85	0.58
1:I:107:ARG:NH1	1:I:129:LEU:HD11	2.18	0.58
1:L:107:ARG:NH1	1:L:129:LEU:HD11	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LEU:HD13	1:J:36:THR:HG23	1.85	0.58
1:I:1:ALA:HB3	1:L:98:GLY:O	2.02	0.58
1:C:98:GLY:O	1:F:1:ALA:HB3	2.02	0.58
1:H:36:THR:HG23	1:J:30:LEU:HD13	1.85	0.58
1:E:30:LEU:HD13	1:F:36:THR:HG23	1.85	0.58
1:I:36:THR:HG23	1:K:30:LEU:HD13	1.85	0.58
1:H:138:MET:HE3	1:H:138:MET:HA	1.86	0.58
1:A:11:SER:HA	1:A:135:PRO:HG3	1.84	0.58
1:B:138:MET:HE3	1:B:138:MET:HA	1.86	0.58
1:K:282:THR:HG23	1:K:285:GLY:HA3	1.85	0.58
1:A:30:LEU:HD13	1:K:36:THR:HG23	1.85	0.57
1:D:11:SER:HA	1:D:135:PRO:HG3	1.84	0.57
1:D:81:SER:HB2	1:K:55:THR:CG2	2.33	0.57
1:E:282:THR:HG23	1:E:285:GLY:HA3	1.85	0.57
1:L:138:MET:HE3	1:L:138:MET:HA	1.86	0.57
1:A:81:SER:HB2	1:E:55:THR:CG2	2.33	0.57
1:C:138:MET:HE3	1:C:138:MET:HA	1.86	0.57
1:C:282:THR:HG23	1:C:285:GLY:HA3	1.85	0.57
1:D:30:LEU:HD13	1:E:36:THR:HG23	1.85	0.57
1:E:138:MET:HE3	1:E:138:MET:HA	1.86	0.57
1:K:138:MET:HE3	1:K:138:MET:HA	1.86	0.57
1:L:282:THR:HG23	1:L:285:GLY:HA3	1.85	0.57
1:B:107:ARG:NH1	1:B:129:LEU:HD11	2.18	0.57
1:I:138:MET:HE3	1:I:138:MET:HA	1.86	0.57
1:F:138:MET:HE3	1:F:138:MET:HA	1.86	0.57
1:H:107:ARG:NH1	1:H:129:LEU:HD11	2.18	0.57
1:A:138:MET:HA	1:A:138:MET:HE3	1.86	0.57
1:F:138:MET:O	1:F:142:VAL:HG12	2.05	0.57
1:I:138:MET:O	1:I:142:VAL:HG12	2.05	0.57
1:D:138:MET:HE3	1:D:138:MET:HA	1.86	0.57
1:C:81:SER:HB2	1:D:55:THR:CG2	2.33	0.57
1:C:138:MET:O	1:C:142:VAL:HG12	2.05	0.57
1:F:107:ARG:HH11	1:F:129:LEU:HD11	1.70	0.56
1:G:138:MET:HE3	1:G:138:MET:HA	1.86	0.56
1:I:107:ARG:HH11	1:I:129:LEU:HD11	1.70	0.56
1:J:138:MET:HE3	1:J:138:MET:HA	1.86	0.56
1:L:138:MET:O	1:L:142:VAL:HG12	2.05	0.56
1:A:55:THR:CG2	1:L:81:SER:HB2	2.33	0.56
1:G:107:ARG:HH11	1:G:129:LEU:HD11	1.70	0.56
1:J:107:ARG:HH11	1:J:129:LEU:HD11	1.70	0.56
1:F:81:SER:HB2	1:J:55:THR:CG2	2.33	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:THR:CG2	1:I:81:SER:HB2	2.33	0.56
1:L:107:ARG:HH11	1:L:129:LEU:HD11	1.70	0.56
1:C:107:ARG:HH11	1:C:129:LEU:HD11	1.70	0.56
1:D:138:MET:O	1:D:142:VAL:HG12	2.05	0.56
1:B:138:MET:O	1:B:142:VAL:HG12	2.05	0.56
1:A:138:MET:O	1:A:142:VAL:HG12	2.05	0.56
1:H:138:MET:O	1:H:142:VAL:HG12	2.05	0.56
1:K:107:ARG:HH11	1:K:129:LEU:HD11	1.70	0.56
1:E:107:ARG:HH11	1:E:129:LEU:HD11	1.70	0.56
1:F:138:MET:HA	1:F:138:MET:CE	2.36	0.56
1:I:138:MET:HA	1:I:138:MET:CE	2.36	0.56
1:J:138:MET:O	1:J:142:VAL:HG12	2.05	0.56
1:E:138:MET:O	1:E:142:VAL:HG12	2.05	0.56
1:B:81:SER:HB2	1:F:55:THR:CG2	2.33	0.55
1:G:138:MET:O	1:G:142:VAL:HG12	2.05	0.55
1:H:81:SER:HB2	1:I:55:THR:CG2	2.33	0.55
1:D:138:MET:HA	1:D:138:MET:CE	2.36	0.55
1:K:138:MET:O	1:K:142:VAL:HG12	2.05	0.55
1:A:138:MET:HA	1:A:138:MET:CE	2.36	0.55
1:B:107:ARG:HH11	1:B:129:LEU:HD11	1.70	0.55
1:E:138:MET:HA	1:E:138:MET:CE	2.36	0.55
1:H:107:ARG:HH11	1:H:129:LEU:HD11	1.70	0.55
1:K:138:MET:HA	1:K:138:MET:CE	2.36	0.55
1:G:186:ALA:HB2	1:G:221:ALA:CB	2.37	0.55
1:J:186:ALA:HB2	1:J:221:ALA:CB	2.37	0.55
1:D:107:ARG:HH11	1:D:129:LEU:HD11	1.70	0.55
1:A:107:ARG:HH11	1:A:129:LEU:HD11	1.70	0.54
1:B:186:ALA:HB2	1:B:221:ALA:CB	2.37	0.54
1:F:157:SER:HB3	1:F:182:ASP:HB3	1.90	0.54
1:H:186:ALA:HB2	1:H:221:ALA:CB	2.37	0.54
1:K:186:ALA:HB2	1:K:221:ALA:CB	2.37	0.54
1:C:186:ALA:HB2	1:C:221:ALA:CB	2.37	0.54
1:E:186:ALA:HB2	1:E:221:ALA:CB	2.37	0.54
1:I:157:SER:HB3	1:I:182:ASP:HB3	1.90	0.54
1:L:186:ALA:HB2	1:L:221:ALA:CB	2.37	0.54
1:A:186:ALA:HB2	1:A:221:ALA:CB	2.37	0.54
1:B:133:TYR:CE2	1:B:134:HIS:HB2	2.43	0.54
1:D:157:SER:HB3	1:D:182:ASP:HB3	1.90	0.54
1:J:133:TYR:CE2	1:J:134:HIS:HB2	2.43	0.54
1:A:157:SER:HB3	1:A:182:ASP:HB3	1.90	0.54
1:D:186:ALA:HB2	1:D:221:ALA:CB	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:TYR:CE2	1:G:134:HIS:HB2	2.43	0.54
1:H:133:TYR:CE2	1:H:134:HIS:HB2	2.43	0.54
1:L:157:SER:HB3	1:L:182:ASP:HB3	1.90	0.54
1:C:55:THR:CG2	1:K:81:SER:HB2	2.33	0.54
1:C:157:SER:HB3	1:C:182:ASP:HB3	1.90	0.54
1:E:81:SER:HB2	1:L:55:THR:CG2	2.33	0.54
1:E:133:TYR:CE2	1:E:134:HIS:HB2	2.43	0.54
1:I:186:ALA:HB2	1:I:221:ALA:CB	2.37	0.54
1:B:150:ASP:O	1:G:152:PRO:HG3	2.08	0.53
1:F:186:ALA:HB2	1:F:221:ALA:CB	2.37	0.53
1:H:150:ASP:O	1:J:152:PRO:HG3	2.08	0.53
1:I:133:TYR:CE2	1:I:134:HIS:HB2	2.43	0.53
1:K:133:TYR:CE2	1:K:134:HIS:HB2	2.43	0.53
1:A:45:ARG:NH1	1:A:45:ARG:HB2	2.24	0.53
1:E:152:PRO:HG3	1:F:150:ASP:O	2.08	0.53
1:F:45:ARG:NH1	1:F:45:ARG:HB2	2.24	0.53
1:F:133:TYR:CE2	1:F:134:HIS:HB2	2.43	0.53
1:I:45:ARG:HB2	1:I:45:ARG:NH1	2.24	0.53
1:I:150:ASP:O	1:K:152:PRO:HG3	2.08	0.53
1:B:152:PRO:HG3	1:L:150:ASP:O	2.08	0.53
1:D:45:ARG:HB2	1:D:45:ARG:NH1	2.24	0.53
1:G:157:SER:HB3	1:G:182:ASP:HB3	1.90	0.53
1:H:108:GLY:O	1:H:130:THR:HA	2.09	0.53
1:B:108:GLY:O	1:B:130:THR:HA	2.09	0.53
1:C:138:MET:HA	1:C:138:MET:CE	2.36	0.53
1:C:150:ASP:O	1:H:152:PRO:HG3	2.08	0.53
1:J:157:SER:HB3	1:J:182:ASP:HB3	1.90	0.53
1:L:133:TYR:CE2	1:L:134:HIS:HB2	2.43	0.53
1:L:138:MET:HA	1:L:138:MET:CE	2.36	0.53
1:A:152:PRO:HG3	1:K:150:ASP:O	2.08	0.53
1:G:108:GLY:O	1:G:130:THR:HA	2.09	0.53
1:B:157:SER:HB3	1:B:182:ASP:HB3	1.90	0.53
1:C:133:TYR:CE2	1:C:134:HIS:HB2	2.43	0.53
1:D:152:PRO:HG3	1:E:150:ASP:O	2.08	0.53
1:H:157:SER:HB3	1:H:182:ASP:HB3	1.90	0.53
1:J:45:ARG:NH1	1:J:45:ARG:HB2	2.24	0.53
1:J:108:GLY:O	1:J:130:THR:HA	2.09	0.53
1:A:150:ASP:O	1:I:152:PRO:HG3	2.08	0.53
1:C:152:PRO:HG3	1:J:150:ASP:O	2.08	0.53
1:F:108:GLY:O	1:F:130:THR:HA	2.09	0.53
1:G:45:ARG:HB2	1:G:45:ARG:NH1	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ARG:NH1	1:C:45:ARG:HB2	2.24	0.53
1:D:150:ASP:O	1:F:152:PRO:HG3	2.08	0.53
1:G:150:ASP:O	1:L:152:PRO:HG3	2.08	0.53
1:I:108:GLY:O	1:I:130:THR:HA	2.09	0.53
1:K:157:SER:HB3	1:K:182:ASP:HB3	1.90	0.53
1:D:133:TYR:CE2	1:D:134:HIS:HB2	2.43	0.53
1:E:45:ARG:NH1	1:E:45:ARG:HB2	2.24	0.53
1:E:157:SER:HB3	1:E:182:ASP:HB3	1.90	0.53
1:A:133:TYR:CE2	1:A:134:HIS:HB2	2.43	0.52
1:C:108:GLY:O	1:C:130:THR:HA	2.09	0.52
1:K:45:ARG:NH1	1:K:45:ARG:HB2	2.24	0.52
1:L:45:ARG:HB2	1:L:45:ARG:NH1	2.24	0.52
1:L:108:GLY:O	1:L:130:THR:HA	2.09	0.52
1:J:153:LEU:HA	1:J:156:ILE:HD12	1.92	0.52
1:A:153:LEU:HA	1:A:156:ILE:HD12	1.92	0.52
1:D:153:LEU:HA	1:D:156:ILE:HD12	1.92	0.52
1:G:153:LEU:HA	1:G:156:ILE:HD12	1.92	0.52
1:L:153:LEU:HA	1:L:156:ILE:HD12	1.92	0.52
1:C:153:LEU:HA	1:C:156:ILE:HD12	1.92	0.52
1:G:138:MET:HA	1:G:138:MET:CE	2.36	0.52
1:E:108:GLY:O	1:E:130:THR:HA	2.09	0.52
1:F:153:LEU:HA	1:F:156:ILE:HD12	1.92	0.52
1:H:45:ARG:NH1	1:H:45:ARG:HB2	2.24	0.52
1:I:153:LEU:HA	1:I:156:ILE:HD12	1.92	0.52
1:J:138:MET:HA	1:J:138:MET:CE	2.36	0.52
1:K:108:GLY:O	1:K:130:THR:HA	2.09	0.52
1:B:45:ARG:HB2	1:B:45:ARG:NH1	2.24	0.52
1:B:109:PHE:CD2	1:B:110:LYS:HG3	2.45	0.52
1:E:109:PHE:CD2	1:E:110:LYS:HG3	2.45	0.52
1:H:109:PHE:CD2	1:H:110:LYS:HG3	2.45	0.52
1:H:138:MET:HA	1:H:138:MET:CE	2.36	0.52
1:K:109:PHE:CD2	1:K:110:LYS:HG3	2.45	0.52
1:E:153:LEU:HA	1:E:156:ILE:HD12	1.92	0.51
1:G:109:PHE:CD2	1:G:110:LYS:HG3	2.45	0.51
1:K:153:LEU:HA	1:K:156:ILE:HD12	1.92	0.51
1:D:108:GLY:O	1:D:130:THR:HA	2.09	0.51
1:D:109:PHE:CD2	1:D:110:LYS:HG3	2.45	0.51
1:J:109:PHE:CD2	1:J:110:LYS:HG3	2.45	0.51
1:A:108:GLY:O	1:A:130:THR:HA	2.09	0.51
1:A:109:PHE:CD2	1:A:110:LYS:HG3	2.45	0.51
1:B:138:MET:HA	1:B:138:MET:CE	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:PHE:CD2	1:C:110:LYS:HG3	2.45	0.51
1:L:109:PHE:CD2	1:L:110:LYS:HG3	2.45	0.51
1:B:8:ASN:ND2	1:B:118:ALA:HB1	2.26	0.51
1:H:8:ASN:ND2	1:H:118:ALA:HB1	2.26	0.51
1:C:8:ASN:ND2	1:C:118:ALA:HB1	2.26	0.51
1:K:8:ASN:ND2	1:K:118:ALA:HB1	2.26	0.51
1:L:8:ASN:ND2	1:L:118:ALA:HB1	2.26	0.51
1:B:153:LEU:HA	1:B:156:ILE:HD12	1.92	0.51
1:E:8:ASN:ND2	1:E:118:ALA:HB1	2.26	0.51
1:H:153:LEU:HA	1:H:156:ILE:HD12	1.92	0.51
1:G:81:SER:HB2	1:H:55:THR:CG2	2.33	0.50
1:I:109:PHE:CD2	1:I:110:LYS:HG3	2.45	0.50
1:E:9:LEU:O	1:E:9:LEU:HD13	2.12	0.50
1:F:109:PHE:CD2	1:F:110:LYS:HG3	2.45	0.50
1:K:9:LEU:HD13	1:K:9:LEU:O	2.12	0.50
1:J:9:LEU:HD13	1:J:9:LEU:O	2.12	0.50
1:B:55:THR:CG2	1:J:81:SER:HB2	2.33	0.50
1:D:8:ASN:ND2	1:D:118:ALA:HB1	2.26	0.50
1:F:8:ASN:ND2	1:F:118:ALA:HB1	2.26	0.50
1:G:9:LEU:HD13	1:G:9:LEU:O	2.12	0.50
1:H:9:LEU:HD13	1:H:9:LEU:O	2.12	0.50
1:I:8:ASN:ND2	1:I:118:ALA:HB1	2.26	0.50
1:A:8:ASN:ND2	1:A:118:ALA:HB1	2.26	0.50
1:B:9:LEU:HD13	1:B:9:LEU:O	2.12	0.50
1:C:9:LEU:HD13	1:C:9:LEU:O	2.12	0.50
1:D:9:LEU:HD13	1:D:9:LEU:O	2.12	0.50
1:L:9:LEU:O	1:L:9:LEU:HD13	2.12	0.50
1:A:9:LEU:HD13	1:A:9:LEU:O	2.12	0.50
1:G:8:ASN:ND2	1:G:118:ALA:HB1	2.26	0.50
1:J:8:ASN:ND2	1:J:118:ALA:HB1	2.26	0.50
1:B:278:HIS:HE1	1:J:92:ASP:OD2	1.95	0.50
1:G:92:ASP:OD2	1:H:278:HIS:HE1	1.95	0.50
1:A:53:GLU:HG3	1:A:106:TYR:OH	2.12	0.49
1:D:53:GLU:HG3	1:D:106:TYR:OH	2.12	0.49
1:E:53:GLU:HG3	1:E:106:TYR:OH	2.12	0.49
1:K:53:GLU:HG3	1:K:106:TYR:OH	2.12	0.49
1:G:53:GLU:HG3	1:G:106:TYR:OH	2.12	0.49
1:J:53:GLU:HG3	1:J:106:TYR:OH	2.12	0.49
1:I:9:LEU:HD13	1:I:9:LEU:O	2.12	0.49
1:F:9:LEU:HD13	1:F:9:LEU:O	2.12	0.49
1:F:280:SER:O	1:F:286:LYS:HG3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:280:SER:O	1:I:286:LYS:HG3	2.13	0.49
1:C:92:ASP:OD2	1:D:278:HIS:HE1	1.95	0.49
1:G:278:HIS:HE1	1:I:92:ASP:OD2	1.95	0.49
1:H:53:GLU:HG3	1:H:106:TYR:OH	2.12	0.49
1:H:150:ASP:HB3	1:J:152:PRO:HB3	1.95	0.49
1:A:278:HIS:HE1	1:L:92:ASP:OD2	1.95	0.49
1:B:53:GLU:HG3	1:B:106:TYR:OH	2.12	0.49
1:B:150:ASP:HB3	1:G:152:PRO:HB3	1.95	0.49
1:B:152:PRO:HB3	1:L:150:ASP:HB3	1.95	0.49
1:G:280:SER:O	1:G:286:LYS:HG3	2.13	0.49
1:C:150:ASP:HB3	1:H:152:PRO:HB3	1.95	0.49
1:F:92:ASP:OD2	1:J:278:HIS:HE1	1.95	0.49
1:J:280:SER:O	1:J:286:LYS:HG3	2.13	0.49
1:C:152:PRO:HB3	1:J:150:ASP:HB3	1.95	0.49
1:D:92:ASP:OD2	1:K:278:HIS:HE1	1.95	0.49
1:E:152:PRO:HB3	1:F:150:ASP:HB3	1.95	0.49
1:G:150:ASP:HB3	1:L:152:PRO:HB3	1.95	0.49
1:J:278:HIS:HA	1:J:298:GLY:HA2	1.95	0.49
1:L:278:HIS:HA	1:L:298:GLY:HA2	1.95	0.49
1:B:280:SER:O	1:B:286:LYS:HG3	2.13	0.48
1:C:278:HIS:HA	1:C:298:GLY:HA2	1.95	0.48
1:G:278:HIS:HA	1:G:298:GLY:HA2	1.95	0.48
1:I:150:ASP:HB3	1:K:152:PRO:HB3	1.95	0.48
1:J:230:THR:HG22	1:J:270:PHE:CE1	2.49	0.48
1:L:53:GLU:HG3	1:L:106:TYR:OH	2.12	0.48
1:A:92:ASP:OD2	1:E:278:HIS:HE1	1.95	0.48
1:F:278:HIS:HA	1:F:298:GLY:HA2	1.95	0.48
1:G:230:THR:HG22	1:G:270:PHE:CE1	2.49	0.48
1:I:278:HIS:HA	1:I:298:GLY:HA2	1.95	0.48
1:C:53:GLU:HG3	1:C:106:TYR:OH	2.12	0.48
1:H:280:SER:O	1:H:286:LYS:HG3	2.13	0.48
1:A:280:SER:O	1:A:286:LYS:HG3	2.13	0.48
1:C:278:HIS:HE1	1:K:92:ASP:OD2	1.95	0.48
1:E:92:ASP:OD2	1:L:278:HIS:HE1	1.95	0.48
1:E:230:THR:HG22	1:E:270:PHE:CE1	2.49	0.48
1:F:53:GLU:HG3	1:F:106:TYR:OH	2.12	0.48
1:K:230:THR:HG22	1:K:270:PHE:CE1	2.49	0.48
1:B:92:ASP:OD2	1:F:278:HIS:HE1	1.95	0.48
1:C:280:SER:O	1:C:286:LYS:HG3	2.13	0.48
1:D:280:SER:O	1:D:286:LYS:HG3	2.13	0.48
1:H:230:THR:HG22	1:H:270:PHE:CE1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:THR:HG22	1:B:270:PHE:CE1	2.49	0.48
1:B:278:HIS:HA	1:B:298:GLY:HA2	1.95	0.48
1:H:278:HIS:HA	1:H:298:GLY:HA2	1.95	0.48
1:I:53:GLU:HG3	1:I:106:TYR:OH	2.12	0.48
1:L:280:SER:O	1:L:286:LYS:HG3	2.13	0.48
1:D:150:ASP:HB3	1:F:152:PRO:HB3	1.95	0.48
1:D:230:THR:HG22	1:D:270:PHE:CE1	2.49	0.48
1:H:92:ASP:OD2	1:I:278:HIS:HE1	1.95	0.48
1:A:150:ASP:HB3	1:I:152:PRO:HB3	1.95	0.48
1:A:230:THR:HG22	1:A:270:PHE:CE1	2.49	0.48
1:E:280:SER:O	1:E:286:LYS:HG3	2.13	0.48
1:L:230:THR:HG22	1:L:270:PHE:CE1	2.49	0.48
1:A:90:MET:HE3	1:A:117:LEU:HD22	1.96	0.48
1:A:273:CYS:O	1:A:273:CYS:SG	2.72	0.48
1:C:230:THR:HG22	1:C:270:PHE:CE1	2.49	0.48
1:D:90:MET:HE3	1:D:117:LEU:HD22	1.96	0.48
1:D:273:CYS:SG	1:D:273:CYS:O	2.72	0.48
1:K:280:SER:O	1:K:286:LYS:HG3	2.13	0.48
1:G:90:MET:HE3	1:G:117:LEU:HD22	1.96	0.47
1:J:90:MET:HE3	1:J:117:LEU:HD22	1.96	0.47
1:F:90:MET:HE3	1:F:117:LEU:HD22	1.96	0.47
1:I:90:MET:HE3	1:I:117:LEU:HD22	1.96	0.47
1:A:152:PRO:HB3	1:K:150:ASP:HB3	1.95	0.47
1:D:152:PRO:HB3	1:E:150:ASP:HB3	1.95	0.47
1:F:230:THR:HG22	1:F:270:PHE:CE1	2.49	0.47
1:B:90:MET:HE3	1:B:117:LEU:HD22	1.96	0.47
1:H:90:MET:HE3	1:H:117:LEU:HD22	1.96	0.47
1:I:230:THR:HG22	1:I:270:PHE:CE1	2.49	0.47
1:K:278:HIS:HA	1:K:298:GLY:HA2	1.95	0.47
1:E:273:CYS:O	1:E:273:CYS:SG	2.72	0.47
1:E:278:HIS:HA	1:E:298:GLY:HA2	1.95	0.47
1:I:273:CYS:SG	1:I:273:CYS:O	2.72	0.47
1:K:273:CYS:SG	1:K:273:CYS:O	2.72	0.47
1:L:273:CYS:O	1:L:273:CYS:SG	2.72	0.47
1:A:278:HIS:HA	1:A:298:GLY:HA2	1.95	0.47
1:B:273:CYS:SG	1:B:273:CYS:O	2.72	0.47
1:C:90:MET:HE3	1:C:117:LEU:HD22	1.96	0.47
1:C:273:CYS:O	1:C:273:CYS:SG	2.72	0.47
1:D:278:HIS:HA	1:D:298:GLY:HA2	1.95	0.47
1:F:273:CYS:O	1:F:273:CYS:SG	2.72	0.47
1:L:90:MET:HE3	1:L:117:LEU:HD22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273:CYS:O	1:H:273:CYS:SG	2.72	0.47
1:E:90:MET:HE3	1:E:117:LEU:HD22	1.96	0.47
1:B:243:TRP:HB2	1:B:247:ILE:HD11	1.97	0.47
1:F:243:TRP:HB2	1:F:247:ILE:HD11	1.97	0.47
1:G:273:CYS:SG	1:G:273:CYS:O	2.72	0.47
1:I:243:TRP:HB2	1:I:247:ILE:HD11	1.97	0.47
1:K:90:MET:HE3	1:K:117:LEU:HD22	1.96	0.47
1:H:243:TRP:HB2	1:H:247:ILE:HD11	1.97	0.46
1:J:273:CYS:O	1:J:273:CYS:SG	2.72	0.46
1:A:230:THR:HG22	1:A:270:PHE:HE1	1.81	0.46
1:A:243:TRP:HB2	1:A:247:ILE:HD11	1.97	0.46
1:B:247:ILE:HD12	1:B:292:TYR:CE2	2.51	0.46
1:D:230:THR:HG22	1:D:270:PHE:HE1	1.81	0.46
1:D:243:TRP:HB2	1:D:247:ILE:HD11	1.97	0.46
1:F:247:ILE:HD12	1:F:292:TYR:CE2	2.51	0.46
1:H:247:ILE:HD12	1:H:292:TYR:CE2	2.51	0.46
1:I:247:ILE:HD12	1:I:292:TYR:CE2	2.51	0.46
1:G:247:ILE:HD12	1:G:292:TYR:CE2	2.51	0.46
1:J:247:ILE:HD12	1:J:292:TYR:CE2	2.51	0.46
1:E:283:LYS:NZ	1:E:283:LYS:HB3	2.31	0.46
1:I:36:THR:CG2	1:K:30:LEU:HD13	2.46	0.46
1:K:247:ILE:HD12	1:K:292:TYR:CE2	2.51	0.46
1:L:247:ILE:HD12	1:L:292:TYR:CE2	2.51	0.46
1:A:283:LYS:NZ	1:A:283:LYS:HB3	2.31	0.46
1:B:283:LYS:NZ	1:B:283:LYS:HB3	2.31	0.46
1:C:247:ILE:HD12	1:C:292:TYR:CE2	2.51	0.46
1:E:30:LEU:HD13	1:F:36:THR:CG2	2.46	0.46
1:E:247:ILE:HD12	1:E:292:TYR:CE2	2.51	0.46
1:H:283:LYS:NZ	1:H:283:LYS:HB3	2.31	0.46
1:K:283:LYS:HB3	1:K:283:LYS:NZ	2.31	0.46
1:D:283:LYS:NZ	1:D:283:LYS:HB3	2.31	0.46
1:E:243:TRP:HB2	1:E:247:ILE:HD11	1.97	0.46
1:K:230:THR:HG22	1:K:270:PHE:HE1	1.81	0.46
1:K:243:TRP:HB2	1:K:247:ILE:HD11	1.97	0.46
1:E:230:THR:HG22	1:E:270:PHE:HE1	1.81	0.46
1:L:283:LYS:NZ	1:L:283:LYS:HB3	2.31	0.46
1:C:243:TRP:HB2	1:C:247:ILE:HD11	1.97	0.46
1:H:180:GLY:HA2	1:H:210:ALA:HB2	1.98	0.46
1:I:134:HIS:HA	1:I:135:PRO:HD2	1.58	0.46
1:L:243:TRP:HB2	1:L:247:ILE:HD11	1.97	0.46
1:A:30:LEU:HD13	1:K:36:THR:CG2	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLY:HA2	1:B:210:ALA:HB2	1.98	0.46
1:C:283:LYS:NZ	1:C:283:LYS:HB3	2.31	0.46
1:F:180:GLY:HA2	1:F:210:ALA:HB2	1.98	0.46
1:F:230:THR:HG22	1:F:270:PHE:HE1	1.81	0.46
1:I:180:GLY:HA2	1:I:210:ALA:HB2	1.98	0.46
1:J:230:THR:HG22	1:J:270:PHE:HE1	1.81	0.46
1:J:232:VAL:HB	1:J:277:PHE:HD2	1.81	0.46
1:L:232:VAL:HB	1:L:277:PHE:HD2	1.81	0.46
1:C:232:VAL:HB	1:C:277:PHE:HD2	1.81	0.46
1:E:232:VAL:HB	1:E:277:PHE:HD2	1.81	0.46
1:I:230:THR:HG22	1:I:270:PHE:HE1	1.81	0.46
1:C:230:THR:HG22	1:C:270:PHE:HE1	1.81	0.45
1:G:230:THR:HG22	1:G:270:PHE:HE1	1.81	0.45
1:G:232:VAL:HB	1:G:277:PHE:HD2	1.81	0.45
1:K:232:VAL:HB	1:K:277:PHE:HD2	1.81	0.45
1:B:230:THR:HG22	1:B:270:PHE:HE1	1.81	0.45
1:A:180:GLY:HA2	1:A:210:ALA:HB2	1.98	0.45
1:C:36:THR:CG2	1:H:30:LEU:HD13	2.46	0.45
1:D:180:GLY:HA2	1:D:210:ALA:HB2	1.98	0.45
1:F:134:HIS:HA	1:F:135:PRO:HD2	1.58	0.45
1:G:243:TRP:HB2	1:G:247:ILE:HD11	1.97	0.45
1:L:230:THR:HG22	1:L:270:PHE:HE1	1.81	0.45
1:A:247:ILE:HD12	1:A:292:TYR:CE2	2.51	0.45
1:B:30:LEU:HD13	1:L:36:THR:CG2	2.46	0.45
1:D:247:ILE:HD12	1:D:292:TYR:CE2	2.51	0.45
1:J:243:TRP:HB2	1:J:247:ILE:HD11	1.97	0.45
1:J:283:LYS:NZ	1:J:283:LYS:HB3	2.31	0.45
1:L:180:GLY:HA2	1:L:210:ALA:HB2	1.98	0.45
1:C:133:TYR:CE2	1:C:168:MET:SD	3.10	0.45
1:C:180:GLY:HA2	1:C:210:ALA:HB2	1.98	0.45
1:D:232:VAL:HB	1:D:277:PHE:HD2	1.81	0.45
1:E:133:TYR:CE2	1:E:168:MET:SD	3.10	0.45
1:G:283:LYS:NZ	1:G:283:LYS:HB3	2.31	0.45
1:K:133:TYR:CE2	1:K:168:MET:SD	3.10	0.45
1:L:133:TYR:CE2	1:L:168:MET:SD	3.10	0.45
1:A:232:VAL:HB	1:A:277:PHE:HD2	1.81	0.45
1:B:133:TYR:CE2	1:B:168:MET:SD	3.10	0.45
1:H:133:TYR:CE2	1:H:168:MET:SD	3.10	0.45
1:A:222:VAL:HG22	1:A:263:THR:HG22	1.99	0.45
1:B:36:THR:CG2	1:G:30:LEU:HD13	2.46	0.45
1:C:30:LEU:HD13	1:J:36:THR:CG2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:VAL:HG22	1:D:263:THR:HG22	1.99	0.45
1:G:36:THR:CG2	1:L:30:LEU:HD13	2.46	0.45
1:H:36:THR:CG2	1:J:30:LEU:HD13	2.46	0.45
1:H:222:VAL:HG22	1:H:263:THR:HG22	1.99	0.45
1:B:222:VAL:HG22	1:B:263:THR:HG22	1.99	0.45
1:G:12:LEU:HD13	1:G:15:HIS:CE1	2.52	0.45
1:I:232:VAL:HB	1:I:277:PHE:HD2	1.81	0.45
1:J:12:LEU:HD13	1:J:15:HIS:CE1	2.52	0.45
1:L:12:LEU:HD13	1:L:15:HIS:CE1	2.52	0.45
1:A:133:TYR:CE2	1:A:168:MET:SD	3.10	0.45
1:A:283:LYS:HD2	1:A:287:GLN:OE1	2.17	0.45
1:C:12:LEU:HD13	1:C:15:HIS:CE1	2.52	0.45
1:D:133:TYR:CE2	1:D:168:MET:SD	3.10	0.45
1:D:283:LYS:HD2	1:D:287:GLN:OE1	2.17	0.45
1:E:173:LEU:HG	1:E:201:CYS:SG	2.57	0.45
1:E:180:GLY:HA2	1:E:210:ALA:HB2	1.98	0.45
1:F:283:LYS:HD2	1:F:287:GLN:OE1	2.17	0.45
1:H:230:THR:HG22	1:H:270:PHE:HE1	1.81	0.45
1:I:283:LYS:NZ	1:I:283:LYS:HB3	2.31	0.45
1:K:173:LEU:HG	1:K:201:CYS:SG	2.57	0.45
1:A:28:ARG:O	1:A:32:ARG:HG3	2.17	0.45
1:A:173:LEU:HG	1:A:201:CYS:SG	2.57	0.45
1:D:28:ARG:O	1:D:32:ARG:HG3	2.17	0.45
1:D:173:LEU:HG	1:D:201:CYS:SG	2.57	0.45
1:F:232:VAL:HB	1:F:277:PHE:HD2	1.81	0.45
1:G:180:GLY:HA2	1:G:210:ALA:HB2	1.98	0.45
1:G:222:VAL:HG22	1:G:263:THR:HG22	1.99	0.45
1:I:222:VAL:HG22	1:I:263:THR:HG22	1.99	0.45
1:I:283:LYS:HD2	1:I:287:GLN:OE1	2.17	0.45
1:J:180:GLY:HA2	1:J:210:ALA:HB2	1.98	0.45
1:K:180:GLY:HA2	1:K:210:ALA:HB2	1.98	0.45
1:L:173:LEU:HG	1:L:201:CYS:SG	2.57	0.45
1:A:257:MET:HB2	1:A:304:ASP:OD1	2.18	0.44
1:B:11:SER:HA	1:B:135:PRO:CG	2.47	0.44
1:C:173:LEU:HG	1:C:201:CYS:SG	2.57	0.44
1:C:257:MET:HB2	1:C:304:ASP:OD1	2.18	0.44
1:D:12:LEU:HD13	1:D:15:HIS:CE1	2.52	0.44
1:F:222:VAL:HG22	1:F:263:THR:HG22	1.99	0.44
1:F:283:LYS:NZ	1:F:283:LYS:HB3	2.31	0.44
1:J:222:VAL:HG22	1:J:263:THR:HG22	1.99	0.44
1:J:283:LYS:HD2	1:J:287:GLN:OE1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:257:MET:HB2	1:L:304:ASP:OD1	2.18	0.44
1:A:12:LEU:HD13	1:A:15:HIS:CE1	2.52	0.44
1:A:109:PHE:CE1	1:A:131:ASP:HB3	2.53	0.44
1:B:28:ARG:O	1:B:32:ARG:HG3	2.17	0.44
1:C:11:SER:HA	1:C:135:PRO:CG	2.47	0.44
1:D:109:PHE:CE1	1:D:131:ASP:HB3	2.53	0.44
1:D:257:MET:HB2	1:D:304:ASP:OD1	2.18	0.44
1:F:129:LEU:HB3	1:F:134:HIS:CD2	2.53	0.44
1:F:133:TYR:CE2	1:F:168:MET:SD	3.10	0.44
1:G:133:TYR:CE2	1:G:168:MET:SD	3.10	0.44
1:G:283:LYS:HD2	1:G:287:GLN:OE1	2.17	0.44
1:H:11:SER:HA	1:H:135:PRO:CG	2.47	0.44
1:I:129:LEU:HB3	1:I:134:HIS:CD2	2.53	0.44
1:J:133:TYR:CE2	1:J:168:MET:SD	3.10	0.44
1:L:222:VAL:HG22	1:L:263:THR:HG22	1.99	0.44
1:B:232:VAL:HB	1:B:277:PHE:HD2	1.81	0.44
1:C:222:VAL:HG22	1:C:263:THR:HG22	1.99	0.44
1:C:283:LYS:HD2	1:C:287:GLN:OE1	2.17	0.44
1:F:173:LEU:HG	1:F:201:CYS:SG	2.57	0.44
1:H:28:ARG:O	1:H:32:ARG:HG3	2.17	0.44
1:I:173:LEU:HG	1:I:201:CYS:SG	2.57	0.44
1:L:11:SER:HA	1:L:135:PRO:CG	2.47	0.44
1:L:283:LYS:HD2	1:L:287:GLN:OE1	2.17	0.44
1:B:12:LEU:HD13	1:B:15:HIS:CE1	2.52	0.44
1:D:129:LEU:HB3	1:D:134:HIS:CD2	2.53	0.44
1:H:12:LEU:HD13	1:H:15:HIS:CE1	2.52	0.44
1:H:257:MET:HB2	1:H:304:ASP:OD1	2.18	0.44
1:A:129:LEU:HB3	1:A:134:HIS:CD2	2.53	0.44
1:B:257:MET:HB2	1:B:304:ASP:OD1	2.18	0.44
1:E:12:LEU:HD13	1:E:15:HIS:CE1	2.52	0.44
1:F:257:MET:HB2	1:F:304:ASP:OD1	2.18	0.44
1:H:232:VAL:HB	1:H:277:PHE:HD2	1.81	0.44
1:I:12:LEU:HD13	1:I:15:HIS:CE1	2.52	0.44
1:I:133:TYR:CE2	1:I:168:MET:SD	3.10	0.44
1:I:257:MET:HB2	1:I:304:ASP:OD1	2.18	0.44
1:K:12:LEU:HD13	1:K:15:HIS:CE1	2.52	0.44
1:K:283:LYS:HD2	1:K:287:GLN:OE1	2.17	0.44
1:L:129:LEU:HB3	1:L:134:HIS:CD2	2.53	0.44
1:C:129:LEU:HB3	1:C:134:HIS:CD2	2.53	0.44
1:E:109:PHE:CE1	1:E:131:ASP:HB3	2.53	0.44
1:E:257:MET:HB2	1:E:304:ASP:OD1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:173:LEU:HG	1:H:201:CYS:SG	2.57	0.44
1:K:109:PHE:CE1	1:K:131:ASP:HB3	2.53	0.44
1:K:257:MET:HB2	1:K:304:ASP:OD1	2.18	0.44
1:L:28:ARG:O	1:L:32:ARG:HG3	2.17	0.44
1:L:109:PHE:CE1	1:L:131:ASP:HB3	2.53	0.44
1:B:109:PHE:CE1	1:B:131:ASP:HB3	2.53	0.44
1:C:28:ARG:O	1:C:32:ARG:HG3	2.17	0.44
1:C:109:PHE:CE1	1:C:131:ASP:HB3	2.53	0.44
1:E:129:LEU:HB3	1:E:134:HIS:CD2	2.53	0.44
1:E:283:LYS:HD2	1:E:287:GLN:OE1	2.17	0.44
1:F:12:LEU:HD13	1:F:15:HIS:CE1	2.52	0.44
1:G:173:LEU:HG	1:G:201:CYS:SG	2.57	0.44
1:I:109:PHE:CE1	1:I:131:ASP:HB3	2.53	0.44
1:J:41:GLN:HG2	1:J:69:ASP:O	2.18	0.44
1:J:173:LEU:HG	1:J:201:CYS:SG	2.57	0.44
1:B:173:LEU:HG	1:B:201:CYS:SG	2.57	0.44
1:B:283:LYS:HD2	1:B:287:GLN:OE1	2.17	0.44
1:D:36:THR:CG2	1:F:30:LEU:HD13	2.46	0.44
1:F:45:ARG:HB2	1:F:45:ARG:CZ	2.48	0.44
1:F:109:PHE:CE1	1:F:131:ASP:HB3	2.53	0.44
1:G:41:GLN:HG2	1:G:69:ASP:O	2.18	0.44
1:G:109:PHE:CE1	1:G:131:ASP:HB3	2.53	0.44
1:H:109:PHE:CE1	1:H:131:ASP:HB3	2.53	0.44
1:I:45:ARG:HB2	1:I:45:ARG:CZ	2.48	0.44
1:J:109:PHE:CE1	1:J:131:ASP:HB3	2.53	0.44
1:J:129:LEU:HB3	1:J:134:HIS:CD2	2.53	0.44
1:K:129:LEU:HB3	1:K:134:HIS:CD2	2.53	0.44
1:A:36:THR:CG2	1:I:30:LEU:HD13	2.46	0.44
1:B:53:GLU:HB2	1:B:108:GLY:HA2	2.00	0.44
1:G:45:ARG:HB2	1:G:45:ARG:CZ	2.48	0.44
1:G:129:LEU:HB3	1:G:134:HIS:CD2	2.53	0.44
1:H:53:GLU:HB2	1:H:108:GLY:HA2	2.00	0.44
1:H:283:LYS:HD2	1:H:287:GLN:OE1	2.17	0.44
1:J:11:SER:HA	1:J:135:PRO:CG	2.47	0.44
1:J:45:ARG:HB2	1:J:45:ARG:CZ	2.48	0.44
1:K:28:ARG:O	1:K:32:ARG:HG3	2.17	0.44
1:K:222:VAL:HG22	1:K:263:THR:HG22	1.99	0.44
1:A:236:MET:SD	1:A:284:VAL:CG1	3.05	0.43
1:C:236:MET:SD	1:C:284:VAL:CG1	3.05	0.43
1:D:11:SER:HA	1:D:135:PRO:CG	2.47	0.43
1:E:28:ARG:O	1:E:32:ARG:HG3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:VAL:HG22	1:E:263:THR:HG22	1.99	0.43
1:G:11:SER:HA	1:G:135:PRO:CG	2.47	0.43
1:H:41:GLN:HG2	1:H:69:ASP:O	2.18	0.43
1:L:236:MET:SD	1:L:284:VAL:CG1	3.05	0.43
1:A:11:SER:HA	1:A:135:PRO:CG	2.47	0.43
1:A:45:ARG:HB2	1:A:45:ARG:CZ	2.48	0.43
1:B:41:GLN:HG2	1:B:69:ASP:O	2.18	0.43
1:B:45:ARG:NH2	1:E:334:ASP:O	2.52	0.43
1:D:45:ARG:HB2	1:D:45:ARG:CZ	2.48	0.43
1:D:53:GLU:HB2	1:D:108:GLY:HA2	2.00	0.43
1:D:236:MET:SD	1:D:284:VAL:CG1	3.05	0.43
1:E:236:MET:SD	1:E:284:VAL:CG1	3.05	0.43
1:H:45:ARG:NH2	1:K:334:ASP:O	2.52	0.43
1:I:11:SER:HA	1:I:135:PRO:CG	2.47	0.43
1:J:28:ARG:O	1:J:32:ARG:HG3	2.17	0.43
1:A:53:GLU:HB2	1:A:108:GLY:HA2	2.00	0.43
1:B:45:ARG:HB2	1:B:45:ARG:CZ	2.48	0.43
1:B:91:LYS:HG2	1:B:95:ARG:HH11	1.84	0.43
1:B:129:LEU:HB3	1:B:134:HIS:CD2	2.53	0.43
1:C:334:ASP:O	1:F:45:ARG:NH2	2.52	0.43
1:F:11:SER:HA	1:F:135:PRO:CG	2.47	0.43
1:G:28:ARG:O	1:G:32:ARG:HG3	2.17	0.43
1:H:91:LYS:HG2	1:H:95:ARG:HH11	1.84	0.43
1:I:45:ARG:NH2	1:L:334:ASP:O	2.52	0.43
1:E:45:ARG:HB2	1:E:45:ARG:CZ	2.48	0.43
1:H:45:ARG:HB2	1:H:45:ARG:CZ	2.48	0.43
1:H:129:LEU:HB3	1:H:134:HIS:CD2	2.53	0.43
1:I:41:GLN:HG2	1:I:69:ASP:O	2.18	0.43
1:K:45:ARG:HB2	1:K:45:ARG:CZ	2.48	0.43
1:A:45:ARG:NH2	1:D:334:ASP:O	2.52	0.43
1:K:11:SER:HA	1:K:135:PRO:CG	2.47	0.43
1:K:236:MET:SD	1:K:284:VAL:CG1	3.05	0.43
1:A:334:ASP:O	1:D:45:ARG:NH2	2.52	0.43
1:C:41:GLN:HG2	1:C:69:ASP:O	2.18	0.43
1:C:45:ARG:HB2	1:C:45:ARG:CZ	2.48	0.43
1:E:11:SER:HA	1:E:135:PRO:CG	2.47	0.43
1:F:28:ARG:O	1:F:32:ARG:HG3	2.17	0.43
1:F:41:GLN:HG2	1:F:69:ASP:O	2.18	0.43
1:I:53:GLU:HB2	1:I:108:GLY:HA2	2.00	0.43
1:I:90:MET:HE3	1:I:117:LEU:HB2	2.01	0.43
1:F:53:GLU:HB2	1:F:108:GLY:HA2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:MET:HE3	1:F:117:LEU:HB2	2.01	0.43
1:F:335:ILE:HG21	1:F:335:ILE:HD13	1.80	0.43
1:G:91:LYS:HG2	1:G:95:ARG:HH11	1.84	0.43
1:G:334:ASP:O	1:J:45:ARG:NH2	2.52	0.43
1:J:91:LYS:HG2	1:J:95:ARG:HH11	1.84	0.43
1:L:41:GLN:HG2	1:L:69:ASP:O	2.18	0.43
1:L:45:ARG:HB2	1:L:45:ARG:CZ	2.48	0.43
1:A:91:LYS:HG2	1:A:95:ARG:HH11	1.84	0.43
1:C:53:GLU:HB2	1:C:108:GLY:HA2	2.00	0.43
1:C:91:LYS:HG2	1:C:95:ARG:HH11	1.84	0.43
1:E:41:GLN:HG2	1:E:69:ASP:O	2.18	0.43
1:G:45:ARG:NH2	1:J:334:ASP:O	2.52	0.43
1:I:28:ARG:O	1:I:32:ARG:HG3	2.17	0.43
1:J:257:MET:HB2	1:J:304:ASP:OD1	2.18	0.43
1:A:41:GLN:HG2	1:A:69:ASP:O	2.18	0.43
1:D:41:GLN:HG2	1:D:69:ASP:O	2.18	0.43
1:D:91:LYS:HG2	1:D:95:ARG:HH11	1.84	0.43
1:G:257:MET:HB2	1:G:304:ASP:OD1	2.18	0.43
1:I:335:ILE:HD13	1:I:335:ILE:HG21	1.80	0.43
1:L:53:GLU:HB2	1:L:108:GLY:HA2	2.00	0.43
1:L:91:LYS:HG2	1:L:95:ARG:HH11	1.84	0.43
1:A:272:HIS:H	1:A:316:GLN:HE22	1.67	0.43
1:D:272:HIS:H	1:D:316:GLN:HE22	1.67	0.43
1:G:53:GLU:HB2	1:G:108:GLY:HA2	2.00	0.43
1:I:334:ASP:O	1:L:45:ARG:NH2	2.52	0.43
1:J:53:GLU:HB2	1:J:108:GLY:HA2	2.00	0.43
1:K:41:GLN:HG2	1:K:69:ASP:O	2.18	0.43
1:K:134:HIS:HA	1:K:135:PRO:HD2	1.58	0.43
1:K:272:HIS:H	1:K:316:GLN:HE22	1.67	0.43
1:C:90:MET:HE3	1:C:117:LEU:HB2	2.01	0.42
1:E:53:GLU:HB2	1:E:108:GLY:HA2	2.00	0.42
1:E:272:HIS:H	1:E:316:GLN:HE22	1.67	0.42
1:K:53:GLU:HB2	1:K:108:GLY:HA2	2.00	0.42
1:L:90:MET:HE3	1:L:117:LEU:HB2	2.01	0.42
1:A:288:ILE:HD13	1:A:299:ILE:HD11	2.02	0.42
1:C:45:ARG:NH2	1:F:334:ASP:O	2.52	0.42
1:D:30:LEU:HD13	1:E:36:THR:CG2	2.46	0.42
1:D:288:ILE:HD13	1:D:299:ILE:HD11	2.02	0.42
1:E:90:MET:HE3	1:E:117:LEU:HB2	2.01	0.42
1:F:288:ILE:HD13	1:F:299:ILE:HD11	2.02	0.42
1:G:133:TYR:HE2	1:G:168:MET:HE1	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133:TYR:HE2	1:H:168:MET:HE1	1.85	0.42
1:I:288:ILE:HD13	1:I:299:ILE:HD11	2.02	0.42
1:J:133:TYR:HE2	1:J:168:MET:HE1	1.85	0.42
1:B:133:TYR:HE2	1:B:168:MET:HE1	1.85	0.42
1:B:334:ASP:O	1:E:45:ARG:NH2	2.52	0.42
1:C:288:ILE:HD13	1:C:299:ILE:HD11	2.02	0.42
1:E:91:LYS:HG2	1:E:95:ARG:HH11	1.84	0.42
1:G:90:MET:HE3	1:G:117:LEU:HB2	2.01	0.42
1:H:334:ASP:O	1:K:45:ARG:NH2	2.52	0.42
1:I:272:HIS:H	1:I:316:GLN:HE22	1.67	0.42
1:K:90:MET:HE3	1:K:117:LEU:HB2	2.01	0.42
1:L:288:ILE:HD13	1:L:299:ILE:HD11	2.02	0.42
1:B:134:HIS:CE1	1:B:320:ARG:NH2	2.85	0.42
1:B:240:VAL:HA	1:B:243:TRP:CD1	2.55	0.42
1:F:272:HIS:H	1:F:316:GLN:HE22	1.67	0.42
1:H:240:VAL:HA	1:H:243:TRP:CD1	2.55	0.42
1:H:259:ILE:HD13	1:H:259:ILE:HA	1.88	0.42
1:K:91:LYS:HG2	1:K:95:ARG:HH11	1.84	0.42
1:C:240:VAL:HA	1:C:243:TRP:CD1	2.55	0.42
1:F:111:GLN:HA	1:F:130:THR:HG21	2.02	0.42
1:G:134:HIS:HA	1:G:135:PRO:HD2	1.58	0.42
1:H:90:MET:HE3	1:H:117:LEU:HB2	2.01	0.42
1:I:111:GLN:HA	1:I:130:THR:HG21	2.02	0.42
1:J:90:MET:HE3	1:J:117:LEU:HB2	2.01	0.42
1:L:240:VAL:HA	1:L:243:TRP:CD1	2.55	0.42
1:A:90:MET:HE3	1:A:117:LEU:HB2	2.01	0.42
1:B:90:MET:HE3	1:B:117:LEU:HB2	2.01	0.42
1:F:133:TYR:HE2	1:F:168:MET:HE1	1.85	0.42
1:H:272:HIS:H	1:H:316:GLN:HE22	1.67	0.42
1:J:134:HIS:HA	1:J:135:PRO:HD2	1.58	0.42
1:B:218:PRO:HD3	1:B:253:TYR:CE1	2.55	0.42
1:B:259:ILE:HD13	1:B:259:ILE:HA	1.88	0.42
1:B:272:HIS:H	1:B:316:GLN:HE22	1.67	0.42
1:D:90:MET:HE3	1:D:117:LEU:HB2	2.01	0.42
1:H:218:PRO:HD3	1:H:253:TYR:CE1	2.55	0.42
1:H:288:ILE:HD13	1:H:299:ILE:HD11	2.02	0.42
1:I:133:TYR:HE2	1:I:168:MET:HE1	1.85	0.42
1:A:10:LEU:HD22	1:A:10:LEU:O	2.20	0.42
1:A:133:TYR:HE2	1:A:168:MET:HE1	1.85	0.42
1:B:288:ILE:HD13	1:B:299:ILE:HD11	2.02	0.42
1:F:218:PRO:HD3	1:F:253:TYR:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:218:PRO:HD3	1:I:253:TYR:CE1	2.55	0.42
1:A:259:ILE:HD13	1:A:259:ILE:HA	1.88	0.42
1:B:4:MET:SD	1:B:19:GLU:OE1	2.78	0.42
1:C:4:MET:SD	1:C:19:GLU:OE1	2.78	0.42
1:C:133:TYR:HE2	1:C:168:MET:HE1	1.85	0.42
1:C:218:PRO:HD3	1:C:253:TYR:CE1	2.55	0.42
1:D:10:LEU:HD22	1:D:10:LEU:O	2.20	0.42
1:D:133:TYR:HE2	1:D:168:MET:HE1	1.85	0.42
1:E:134:HIS:HA	1:E:135:PRO:HD2	1.58	0.42
1:E:165:ARG:HG2	1:E:165:ARG:HH11	1.85	0.42
1:F:91:LYS:HG2	1:F:95:ARG:HH11	1.84	0.42
1:G:4:MET:SD	1:G:19:GLU:OE1	2.78	0.42
1:G:10:LEU:HD22	1:G:10:LEU:O	2.20	0.42
1:H:4:MET:SD	1:H:19:GLU:OE1	2.78	0.42
1:J:4:MET:SD	1:J:19:GLU:OE1	2.78	0.42
1:J:10:LEU:HD22	1:J:10:LEU:O	2.20	0.42
1:K:10:LEU:O	1:K:10:LEU:HD22	2.20	0.42
1:K:133:TYR:HE2	1:K:168:MET:HE1	1.85	0.42
1:L:4:MET:SD	1:L:19:GLU:OE1	2.78	0.42
1:L:133:TYR:HE2	1:L:168:MET:HE1	1.85	0.42
1:L:218:PRO:HD3	1:L:253:TYR:CE1	2.55	0.42
1:A:335:ILE:HG21	1:A:335:ILE:HD13	1.80	0.42
1:B:165:ARG:HG2	1:B:165:ARG:HH11	1.85	0.42
1:D:259:ILE:HD13	1:D:259:ILE:HA	1.88	0.42
1:E:10:LEU:HD22	1:E:10:LEU:O	2.20	0.42
1:E:133:TYR:HE2	1:E:168:MET:HE1	1.85	0.42
1:G:278:HIS:O	1:G:279:ASN:HB3	2.20	0.42
1:H:165:ARG:HG2	1:H:165:ARG:HH11	1.85	0.42
1:I:91:LYS:HG2	1:I:95:ARG:HH11	1.84	0.42
1:K:165:ARG:HG2	1:K:165:ARG:HH11	1.85	0.42
1:A:134:HIS:HA	1:A:135:PRO:HD2	1.58	0.41
1:C:272:HIS:H	1:C:316:GLN:HE22	1.67	0.41
1:F:278:HIS:O	1:F:279:ASN:HB3	2.20	0.41
1:I:134:HIS:CE1	1:I:320:ARG:NH2	2.85	0.41
1:I:278:HIS:O	1:I:279:ASN:HB3	2.20	0.41
1:J:278:HIS:O	1:J:279:ASN:HB3	2.20	0.41
1:L:272:HIS:H	1:L:316:GLN:HE22	1.67	0.41
1:A:278:HIS:O	1:A:279:ASN:HB3	2.20	0.41
1:B:236:MET:SD	1:B:284:VAL:CG1	3.05	0.41
1:D:278:HIS:O	1:D:279:ASN:HB3	2.20	0.41
1:E:4:MET:SD	1:E:19:GLU:OE1	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:GLN:HA	1:G:130:THR:HG21	2.02	0.41
1:G:218:PRO:HD3	1:G:253:TYR:CE1	2.55	0.41
1:H:236:MET:SD	1:H:284:VAL:CG1	3.05	0.41
1:J:165:ARG:HH11	1:J:165:ARG:HG2	1.85	0.41
1:J:218:PRO:HD3	1:J:253:TYR:CE1	2.55	0.41
1:K:4:MET:SD	1:K:19:GLU:OE1	2.78	0.41
1:A:4:MET:SD	1:A:19:GLU:OE1	2.78	0.41
1:D:4:MET:SD	1:D:19:GLU:OE1	2.78	0.41
1:E:111:GLN:HA	1:E:114:VAL:HG23	2.02	0.41
1:F:134:HIS:CE1	1:F:320:ARG:NH2	2.85	0.41
1:G:165:ARG:HG2	1:G:165:ARG:HH11	1.85	0.41
1:J:111:GLN:HA	1:J:130:THR:HG21	2.02	0.41
1:K:111:GLN:HA	1:K:114:VAL:HG23	2.02	0.41
1:B:10:LEU:HD22	1:B:10:LEU:O	2.20	0.41
1:E:218:PRO:HD3	1:E:253:TYR:CE1	2.55	0.41
1:F:165:ARG:HG2	1:F:165:ARG:HH11	1.85	0.41
1:G:119:LYS:HD2	1:G:120:PHE:CE1	2.56	0.41
1:G:272:HIS:H	1:G:316:GLN:HE22	1.67	0.41
1:H:10:LEU:HD22	1:H:10:LEU:O	2.20	0.41
1:J:272:HIS:H	1:J:316:GLN:HE22	1.67	0.41
1:K:218:PRO:HD3	1:K:253:TYR:CE1	2.55	0.41
1:G:4:MET:SD	1:G:19:GLU:HG2	2.61	0.41
1:I:10:LEU:O	1:I:10:LEU:HD22	2.20	0.41
1:I:165:ARG:HG2	1:I:165:ARG:HH11	1.85	0.41
1:J:119:LYS:HD2	1:J:120:PHE:CE1	2.56	0.41
1:K:288:ILE:HD13	1:K:299:ILE:HD11	2.02	0.41
1:B:95:ARG:NH2	1:F:307:GLU:OE2	2.54	0.41
1:C:10:LEU:HD22	1:C:10:LEU:O	2.20	0.41
1:C:111:GLN:HA	1:C:114:VAL:HG23	2.02	0.41
1:C:165:ARG:HG2	1:C:165:ARG:HH11	1.85	0.41
1:C:278:HIS:O	1:C:279:ASN:HB3	2.20	0.41
1:D:335:ILE:HG21	1:D:335:ILE:HD13	1.80	0.41
1:E:39:GLU:OE2	1:E:70:GLN:NE2	2.54	0.41
1:E:288:ILE:HD13	1:E:299:ILE:HD11	2.02	0.41
1:F:10:LEU:O	1:F:10:LEU:HD22	2.20	0.41
1:F:95:ARG:NH2	1:J:307:GLU:OE2	2.54	0.41
1:F:111:GLN:HA	1:F:114:VAL:HG23	2.02	0.41
1:H:95:ARG:NH2	1:I:307:GLU:OE2	2.54	0.41
1:I:111:GLN:HA	1:I:114:VAL:HG23	2.02	0.41
1:J:4:MET:SD	1:J:19:GLU:HG2	2.61	0.41
1:K:39:GLU:OE2	1:K:70:GLN:NE2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:LEU:HD22	1:L:10:LEU:O	2.20	0.41
1:L:278:HIS:O	1:L:279:ASN:HB3	2.20	0.41
1:C:4:MET:SD	1:C:19:GLU:HG2	2.61	0.41
1:F:4:MET:SD	1:F:19:GLU:OE1	2.78	0.41
1:F:236:MET:SD	1:F:284:VAL:CG1	3.05	0.41
1:J:39:GLU:OE2	1:J:70:GLN:NE2	2.54	0.41
1:K:134:HIS:CE1	1:K:320:ARG:NH2	2.85	0.41
1:L:4:MET:SD	1:L:19:GLU:HG2	2.61	0.41
1:L:111:GLN:HA	1:L:114:VAL:HG23	2.02	0.41
1:L:165:ARG:HH11	1:L:165:ARG:HG2	1.85	0.41
1:L:259:ILE:HA	1:L:259:ILE:HD13	1.88	0.41
1:A:111:GLN:HA	1:A:130:THR:HG21	2.02	0.41
1:B:4:MET:SD	1:B:19:GLU:HG2	2.61	0.41
1:C:111:GLN:HA	1:C:130:THR:HG21	2.02	0.41
1:E:278:HIS:O	1:E:279:ASN:HB3	2.20	0.41
1:F:78:ASP:HB3	1:F:80:ASN:N	2.36	0.41
1:G:39:GLU:OE2	1:G:70:GLN:NE2	2.54	0.41
1:G:288:ILE:HD13	1:G:299:ILE:HD11	2.02	0.41
1:H:4:MET:SD	1:H:19:GLU:HG2	2.61	0.41
1:I:4:MET:SD	1:I:19:GLU:HG2	2.61	0.41
1:I:39:GLU:OE2	1:I:70:GLN:NE2	2.54	0.41
1:I:78:ASP:HB3	1:I:80:ASN:N	2.36	0.41
1:K:119:LYS:HD2	1:K:120:PHE:CE1	2.56	0.41
1:L:111:GLN:HA	1:L:130:THR:HG21	2.02	0.41
1:A:240:VAL:HA	1:A:243:TRP:CD1	2.55	0.41
1:B:111:GLN:HA	1:B:114:VAL:HG23	2.02	0.41
1:B:270:PHE:CZ	1:B:272:HIS:HB2	2.56	0.41
1:C:39:GLU:OE2	1:C:70:GLN:NE2	2.54	0.41
1:C:119:LYS:HD2	1:C:120:PHE:CE1	2.56	0.41
1:C:134:HIS:CE1	1:C:320:ARG:NH2	2.85	0.41
1:C:270:PHE:CZ	1:C:272:HIS:HB2	2.56	0.41
1:D:111:GLN:HA	1:D:130:THR:HG21	2.02	0.41
1:D:134:HIS:HA	1:D:135:PRO:HD2	1.58	0.41
1:E:119:LYS:HD2	1:E:120:PHE:CE1	2.56	0.41
1:E:134:HIS:CE1	1:E:320:ARG:NH2	2.85	0.41
1:F:4:MET:SD	1:F:19:GLU:HG2	2.61	0.41
1:F:39:GLU:OE2	1:F:70:GLN:NE2	2.54	0.41
1:F:119:LYS:HD2	1:F:120:PHE:CE1	2.56	0.41
1:H:111:GLN:HA	1:H:114:VAL:HG23	2.02	0.41
1:H:270:PHE:CZ	1:H:272:HIS:HB2	2.56	0.41
1:I:4:MET:SD	1:I:19:GLU:OE1	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:LYS:HD2	1:I:120:PHE:CE1	2.56	0.41
1:J:236:MET:SD	1:J:284:VAL:CG1	3.05	0.41
1:J:288:ILE:HD13	1:J:299:ILE:HD11	2.02	0.41
1:K:278:HIS:O	1:K:279:ASN:HB3	2.20	0.41
1:K:335:ILE:HD13	1:K:335:ILE:HG21	1.80	0.41
1:L:39:GLU:OE2	1:L:70:GLN:NE2	2.54	0.41
1:L:119:LYS:HD2	1:L:120:PHE:CE1	2.56	0.41
1:L:134:HIS:CE1	1:L:320:ARG:NH2	2.85	0.41
1:L:270:PHE:CZ	1:L:272:HIS:HB2	2.56	0.41
1:B:278:HIS:O	1:B:279:ASN:HB3	2.20	0.41
1:C:78:ASP:HB3	1:C:80:ASN:N	2.36	0.41
1:G:236:MET:SD	1:G:284:VAL:CG1	3.05	0.41
1:I:236:MET:SD	1:I:284:VAL:CG1	3.05	0.41
1:I:240:VAL:HA	1:I:243:TRP:CD1	2.55	0.41
1:I:270:PHE:CZ	1:I:272:HIS:HB2	2.56	0.41
1:K:4:MET:SD	1:K:19:GLU:HG2	2.61	0.41
1:L:78:ASP:HB3	1:L:80:ASN:N	2.36	0.41
1:A:4:MET:SD	1:A:19:GLU:HG2	2.61	0.40
1:A:39:GLU:OE2	1:A:70:GLN:NE2	2.54	0.40
1:A:218:PRO:HD3	1:A:253:TYR:CE1	2.55	0.40
1:B:78:ASP:HB3	1:B:80:ASN:N	2.36	0.40
1:C:259:ILE:HA	1:C:259:ILE:HD13	1.88	0.40
1:D:240:VAL:HA	1:D:243:TRP:CD1	2.55	0.40
1:E:4:MET:SD	1:E:19:GLU:HG2	2.61	0.40
1:F:270:PHE:CZ	1:F:272:HIS:HB2	2.56	0.40
1:G:78:ASP:HB3	1:G:80:ASN:N	2.36	0.40
1:H:78:ASP:HB3	1:H:80:ASN:N	2.36	0.40
1:H:134:HIS:CE1	1:H:320:ARG:NH2	2.85	0.40
1:K:111:GLN:HA	1:K:130:THR:HG21	2.02	0.40
1:A:111:GLN:HA	1:A:114:VAL:HG23	2.02	0.40
1:A:134:HIS:CE1	1:A:320:ARG:NH2	2.85	0.40
1:D:39:GLU:OE2	1:D:70:GLN:NE2	2.54	0.40
1:D:119:LYS:HD2	1:D:120:PHE:CE1	2.56	0.40
1:D:218:PRO:HD3	1:D:253:TYR:CE1	2.55	0.40
1:E:111:GLN:HA	1:E:130:THR:HG21	2.02	0.40
1:F:240:VAL:HA	1:F:243:TRP:CD1	2.55	0.40
1:H:278:HIS:O	1:H:279:ASN:HB3	2.20	0.40
1:J:78:ASP:HB3	1:J:80:ASN:N	2.36	0.40
1:K:272:HIS:HE1	1:K:300:GLU:OE2	2.05	0.40
1:A:119:LYS:HD2	1:A:120:PHE:CE1	2.56	0.40
1:A:165:ARG:HG2	1:A:165:ARG:HH11	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:SER:O	1:C:93:THR:HG23	2.22	0.40
1:C:272:HIS:HE1	1:C:300:GLU:OE2	2.05	0.40
1:D:4:MET:SD	1:D:19:GLU:HG2	2.61	0.40
1:D:89:SER:O	1:D:93:THR:HG23	2.22	0.40
1:E:89:SER:O	1:E:93:THR:HG23	2.22	0.40
1:E:243:TRP:CZ3	1:E:288:ILE:HG12	2.57	0.40
1:E:272:HIS:HE1	1:E:300:GLU:OE2	2.05	0.40
1:J:272:HIS:HE1	1:J:300:GLU:OE2	2.05	0.40
1:K:89:SER:O	1:K:93:THR:HG23	2.22	0.40
1:K:243:TRP:CZ3	1:K:288:ILE:HG12	2.57	0.40
1:L:89:SER:O	1:L:93:THR:HG23	2.22	0.40
1:A:89:SER:O	1:A:93:THR:HG23	2.22	0.40
1:C:243:TRP:CZ3	1:C:288:ILE:HG12	2.57	0.40
1:D:111:GLN:HA	1:D:114:VAL:HG23	2.02	0.40
1:D:134:HIS:CE1	1:D:320:ARG:NH2	2.85	0.40
1:D:165:ARG:HG2	1:D:165:ARG:HH11	1.85	0.40
1:F:243:TRP:CZ3	1:F:288:ILE:HG12	2.57	0.40
1:G:272:HIS:HE1	1:G:300:GLU:OE2	2.05	0.40
1:I:243:TRP:CZ3	1:I:288:ILE:HG12	2.57	0.40
1:K:270:PHE:CZ	1:K:272:HIS:HB2	2.56	0.40
1:L:243:TRP:CZ3	1:L:288:ILE:HG12	2.57	0.40
1:L:272:HIS:HE1	1:L:300:GLU:OE2	2.05	0.40
1:E:95:ARG:NH2	1:L:307:GLU:OE2	2.54	0.40
1:E:270:PHE:CZ	1:E:272:HIS:HB2	2.56	0.40

All (49) 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:B:189:LYS:NZ	1:I:248:LYS:CE[1_654]	0.62	1.58
1:F:291:GLN:O	1:K:194:HIS:NE2[1_654]	0.69	1.51
1:F:289:ALA:O	1:K:195:ASP:OD2[1_654]	0.88	1.32
1:F:291:GLN:O	1:K:194:HIS:CE1[1_654]	0.90	1.30
1:F:291:GLN:C	1:K:194:HIS:NE2[1_654]	1.10	1.10
1:F:289:ALA:O	1:K:195:ASP:CG[1_654]	1.32	0.88
1:F:291:GLN:O	1:K:194:HIS:CD2[1_654]	1.33	0.87
1:F:291:GLN:C	1:K:194:HIS:CE1[1_654]	1.37	0.83
1:F:290:GLU:OE1	1:K:196:GLU:OE2[1_654]	1.39	0.81
1:F:289:ALA:C	1:K:195:ASP:OD2[1_654]	1.46	0.74
1:F:290:GLU:CD	1:K:196:GLU:OE1[1_654]	1.46	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:GLU:O	1:K:195:ASP:OD1[1_654]	1.48	0.72
1:B:189:LYS:NZ	1:I:248:LYS:NZ[1_654]	1.49	0.71
1:F:291:GLN:O	1:K:194:HIS:ND1[1_654]	1.49	0.71
1:F:290:GLU:O	1:K:195:ASP:N[1_654]	1.55	0.65
1:F:291:GLN:C	1:K:194:HIS:CD2[1_654]	1.59	0.61
1:F:290:GLU:CA	1:K:195:ASP:CB[1_654]	1.60	0.60
1:F:290:GLU:C	1:K:195:ASP:OD1[1_654]	1.60	0.60
1:F:292:TYR:N	1:K:195:ASP:OD1[1_654]	1.64	0.56
1:F:292:TYR:N	1:K:194:HIS:CE1[1_654]	1.72	0.48
1:F:291:GLN:O	1:K:194:HIS:CG[1_654]	1.73	0.47
1:C:293:PRO:CG	1:L:291:GLN:NE2[1_446]	1.75	0.45
1:F:290:GLU:OE1	1:K:196:GLU:CD[1_654]	1.76	0.44
1:F:291:GLN:CA	1:K:194:HIS:CD2[1_654]	1.76	0.44
1:F:290:GLU:OE1	1:K:196:GLU:OE1[1_654]	1.78	0.42
1:F:289:ALA:O	1:K:195:ASP:CB[1_654]	1.79	0.41
1:F:289:ALA:C	1:K:195:ASP:CG[1_654]	1.83	0.37
1:F:292:TYR:CA	1:K:194:HIS:CE1[1_654]	1.83	0.37
1:F:291:GLN:C	1:K:194:HIS:ND1[1_654]	1.90	0.30
1:B:189:LYS:NZ	1:I:248:LYS:CD[1_654]	1.91	0.29
1:F:290:GLU:O	1:K:195:ASP:CA[1_654]	1.93	0.27
1:F:290:GLU:C	1:K:195:ASP:CG[1_654]	1.94	0.26
1:F:290:GLU:O	1:K:195:ASP:CG[1_654]	1.95	0.25
1:F:290:GLU:CG	1:K:196:GLU:OE1[1_654]	2.04	0.16
1:F:291:GLN:CA	1:K:194:HIS:NE2[1_654]	2.04	0.16
1:F:294:ASN:CB	1:K:189:LYS:O[1_654]	2.04	0.16
1:F:290:GLU:C	1:K:195:ASP:CB[1_654]	2.05	0.15
1:F:291:GLN:C	1:K:194:HIS:CG[1_654]	2.05	0.15
1:F:290:GLU:O	1:K:195:ASP:CB[1_654]	2.06	0.14
1:C:248:LYS:NZ	1:L:296:ALA:CB[1_446]	2.07	0.13
1:B:189:LYS:CE	1:I:248:LYS:CE[1_654]	2.08	0.12
1:F:291:GLN:N	1:K:195:ASP:OD1[1_654]	2.08	0.12
1:F:290:GLU:OE2	1:K:196:GLU:OE1[1_654]	2.09	0.11
1:F:291:GLN:CG	1:K:194:HIS:CD2[1_654]	2.13	0.07
1:C:248:LYS:NZ	1:L:293:PRO:O[1_446]	2.15	0.05
1:B:189:LYS:CE	1:I:248:LYS:NZ[1_654]	2.18	0.02
1:C:293:PRO:CB	1:L:291:GLN:NE2[1_446]	2.19	0.01
1:F:291:GLN:C	1:K:195:ASP:OD1[1_654]	2.19	0.01
1:F:292:TYR:N	1:K:194:HIS:NE2[1_654]	2.19	0.01

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	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	B	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	C	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	D	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	E	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	F	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	G	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	H	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	I	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	J	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	K	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
1	L	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	1	9
All	All	3996/4020 (99%)	3240 (81%)	540 (14%)	216 (5%)	1	9

All (216) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	ASP
1	A	240	VAL
1	A	244	GLY
1	A	274	LEU
1	A	297	ASN
1	A	333	ALA
1	B	163	ASP
1	B	240	VAL
1	B	244	GLY
1	B	274	LEU
1	B	297	ASN
1	B	333	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	163	ASP
1	C	240	VAL
1	C	244	GLY
1	C	274	LEU
1	C	297	ASN
1	C	333	ALA
1	D	163	ASP
1	D	240	VAL
1	D	244	GLY
1	D	274	LEU
1	D	297	ASN
1	D	333	ALA
1	E	163	ASP
1	E	240	VAL
1	E	244	GLY
1	E	274	LEU
1	E	297	ASN
1	E	333	ALA
1	F	163	ASP
1	F	240	VAL
1	F	244	GLY
1	F	274	LEU
1	F	297	ASN
1	F	333	ALA
1	G	163	ASP
1	G	240	VAL
1	G	244	GLY
1	G	274	LEU
1	G	297	ASN
1	G	333	ALA
1	H	163	ASP
1	H	240	VAL
1	H	244	GLY
1	H	274	LEU
1	H	297	ASN
1	H	333	ALA
1	I	163	ASP
1	I	240	VAL
1	I	244	GLY
1	I	274	LEU
1	I	297	ASN
1	I	333	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	163	ASP
1	J	240	VAL
1	J	244	GLY
1	J	274	LEU
1	J	297	ASN
1	J	333	ALA
1	K	163	ASP
1	K	240	VAL
1	K	244	GLY
1	K	274	LEU
1	K	297	ASN
1	K	333	ALA
1	L	163	ASP
1	L	240	VAL
1	L	244	GLY
1	L	274	LEU
1	L	297	ASN
1	L	333	ALA
1	A	89	SER
1	A	154	HIS
1	A	309	PRO
1	B	89	SER
1	B	154	HIS
1	B	309	PRO
1	C	89	SER
1	C	154	HIS
1	C	309	PRO
1	D	89	SER
1	D	154	HIS
1	D	309	PRO
1	E	89	SER
1	E	154	HIS
1	E	309	PRO
1	F	89	SER
1	F	154	HIS
1	F	309	PRO
1	G	89	SER
1	G	154	HIS
1	G	309	PRO
1	H	89	SER
1	H	154	HIS
1	H	309	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	89	SER
1	I	154	HIS
1	I	309	PRO
1	J	89	SER
1	J	154	HIS
1	J	309	PRO
1	K	89	SER
1	K	154	HIS
1	K	309	PRO
1	L	89	SER
1	L	154	HIS
1	L	309	PRO
1	A	111	GLN
1	A	162	GLY
1	A	239	PRO
1	A	319	ASN
1	B	111	GLN
1	B	162	GLY
1	B	239	PRO
1	B	319	ASN
1	C	111	GLN
1	C	162	GLY
1	C	239	PRO
1	C	319	ASN
1	D	111	GLN
1	D	162	GLY
1	D	239	PRO
1	D	319	ASN
1	E	111	GLN
1	E	162	GLY
1	E	239	PRO
1	E	319	ASN
1	F	111	GLN
1	F	162	GLY
1	F	239	PRO
1	F	319	ASN
1	G	111	GLN
1	G	162	GLY
1	G	239	PRO
1	G	319	ASN
1	H	111	GLN
1	H	162	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	239	PRO
1	H	319	ASN
1	I	111	GLN
1	I	162	GLY
1	I	239	PRO
1	I	319	ASN
1	J	111	GLN
1	J	162	GLY
1	J	239	PRO
1	J	319	ASN
1	K	111	GLN
1	K	162	GLY
1	K	239	PRO
1	K	319	ASN
1	L	111	GLN
1	L	162	GLY
1	L	239	PRO
1	L	319	ASN
1	A	2	PHE
1	A	15	HIS
1	B	2	PHE
1	B	15	HIS
1	C	2	PHE
1	C	15	HIS
1	D	2	PHE
1	D	15	HIS
1	E	2	PHE
1	E	15	HIS
1	F	2	PHE
1	F	15	HIS
1	G	2	PHE
1	G	15	HIS
1	H	2	PHE
1	H	15	HIS
1	I	2	PHE
1	I	15	HIS
1	J	2	PHE
1	J	15	HIS
1	K	2	PHE
1	K	15	HIS
1	L	2	PHE
1	L	15	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	78	ASP
1	A	167	ASN
1	B	78	ASP
1	B	167	ASN
1	C	78	ASP
1	C	167	ASN
1	D	78	ASP
1	D	167	ASN
1	E	78	ASP
1	E	167	ASN
1	F	78	ASP
1	F	167	ASN
1	G	78	ASP
1	G	167	ASN
1	H	78	ASP
1	H	167	ASN
1	I	78	ASP
1	I	167	ASN
1	J	78	ASP
1	J	167	ASN
1	K	78	ASP
1	K	167	ASN
1	L	78	ASP
1	L	167	ASN
1	A	134	HIS
1	B	134	HIS
1	C	134	HIS
1	D	134	HIS
1	E	134	HIS
1	F	134	HIS
1	G	134	HIS
1	H	134	HIS
1	I	134	HIS
1	J	134	HIS
1	K	134	HIS
1	L	134	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	B	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	C	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	D	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	E	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	F	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	G	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	H	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	I	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	J	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	K	284/284 (100%)	233 (82%)	51 (18%)	2	10
1	L	284/284 (100%)	233 (82%)	51 (18%)	2	10
All	All	3408/3408 (100%)	2796 (82%)	612 (18%)	2	10

All (612) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	10	LEU
1	A	16	SER
1	A	23	LEU
1	A	27	SER
1	A	30	LEU
1	A	38	THR
1	A	45	ARG
1	A	48	ILE
1	A	50	LEU
1	A	55	THR
1	A	84	ILE
1	A	93	THR
1	A	107	ARG
1	A	111	GLN
1	A	124	PRO
1	A	129	LEU
1	A	138	MET
1	A	142	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	165	ARG
1	A	184	ARG
1	A	185	ILE
1	A	189	LYS
1	A	194	HIS
1	A	195	ASP
1	A	196	GLU
1	A	202	LYS
1	A	215	THR
1	A	222	VAL
1	A	223	LYS
1	A	225	VAL
1	A	232	VAL
1	A	236	MET
1	A	239	PRO
1	A	251	LEU
1	A	257	MET
1	A	259	ILE
1	A	265	ASN
1	A	281	GLU
1	A	282	THR
1	A	283	LYS
1	A	293	PRO
1	A	295	LEU
1	A	297	ASN
1	A	303	GLU
1	A	304	ASP
1	A	307	GLU
1	A	315	GLU
1	A	320	ARG
1	A	327	ILE
1	A	332	LEU
1	B	9	LEU
1	B	10	LEU
1	B	16	SER
1	B	23	LEU
1	B	27	SER
1	B	30	LEU
1	B	38	THR
1	B	45	ARG
1	B	48	ILE
1	B	50	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	55	THR
1	B	84	ILE
1	B	93	THR
1	B	107	ARG
1	B	111	GLN
1	B	124	PRO
1	B	129	LEU
1	B	138	MET
1	B	142	VAL
1	B	165	ARG
1	B	184	ARG
1	B	185	ILE
1	B	189	LYS
1	B	194	HIS
1	B	195	ASP
1	B	196	GLU
1	B	202	LYS
1	B	215	THR
1	B	222	VAL
1	B	223	LYS
1	B	225	VAL
1	B	232	VAL
1	B	236	MET
1	B	239	PRO
1	B	251	LEU
1	B	257	MET
1	B	259	ILE
1	B	265	ASN
1	B	281	GLU
1	B	282	THR
1	B	283	LYS
1	B	293	PRO
1	B	295	LEU
1	B	297	ASN
1	B	303	GLU
1	B	304	ASP
1	B	307	GLU
1	B	315	GLU
1	B	320	ARG
1	B	327	ILE
1	B	332	LEU
1	C	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	10	LEU
1	C	16	SER
1	C	23	LEU
1	C	27	SER
1	C	30	LEU
1	C	38	THR
1	C	45	ARG
1	C	48	ILE
1	C	50	LEU
1	C	55	THR
1	C	84	ILE
1	C	93	THR
1	C	107	ARG
1	C	111	GLN
1	C	124	PRO
1	C	129	LEU
1	C	138	MET
1	C	142	VAL
1	C	165	ARG
1	C	184	ARG
1	C	185	ILE
1	C	189	LYS
1	C	194	HIS
1	C	195	ASP
1	C	196	GLU
1	C	202	LYS
1	C	215	THR
1	C	222	VAL
1	C	223	LYS
1	C	225	VAL
1	C	232	VAL
1	C	236	MET
1	C	239	PRO
1	C	251	LEU
1	C	257	MET
1	C	259	ILE
1	C	265	ASN
1	C	281	GLU
1	C	282	THR
1	C	283	LYS
1	C	293	PRO
1	C	295	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	297	ASN
1	C	303	GLU
1	C	304	ASP
1	C	307	GLU
1	C	315	GLU
1	C	320	ARG
1	C	327	ILE
1	C	332	LEU
1	D	9	LEU
1	D	10	LEU
1	D	16	SER
1	D	23	LEU
1	D	27	SER
1	D	30	LEU
1	D	38	THR
1	D	45	ARG
1	D	48	ILE
1	D	50	LEU
1	D	55	THR
1	D	84	ILE
1	D	93	THR
1	D	107	ARG
1	D	111	GLN
1	D	124	PRO
1	D	129	LEU
1	D	138	MET
1	D	142	VAL
1	D	165	ARG
1	D	184	ARG
1	D	185	ILE
1	D	189	LYS
1	D	194	HIS
1	D	195	ASP
1	D	196	GLU
1	D	202	LYS
1	D	215	THR
1	D	222	VAL
1	D	223	LYS
1	D	225	VAL
1	D	232	VAL
1	D	236	MET
1	D	239	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	251	LEU
1	D	257	MET
1	D	259	ILE
1	D	265	ASN
1	D	281	GLU
1	D	282	THR
1	D	283	LYS
1	D	293	PRO
1	D	295	LEU
1	D	297	ASN
1	D	303	GLU
1	D	304	ASP
1	D	307	GLU
1	D	315	GLU
1	D	320	ARG
1	D	327	ILE
1	D	332	LEU
1	E	9	LEU
1	E	10	LEU
1	E	16	SER
1	E	23	LEU
1	E	27	SER
1	E	30	LEU
1	E	38	THR
1	E	45	ARG
1	E	48	ILE
1	E	50	LEU
1	E	55	THR
1	E	84	ILE
1	E	93	THR
1	E	107	ARG
1	E	111	GLN
1	E	124	PRO
1	E	129	LEU
1	E	138	MET
1	E	142	VAL
1	E	165	ARG
1	E	184	ARG
1	E	185	ILE
1	E	189	LYS
1	E	194	HIS
1	E	195	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	196	GLU
1	E	202	LYS
1	E	215	THR
1	E	222	VAL
1	E	223	LYS
1	E	225	VAL
1	E	232	VAL
1	E	236	MET
1	E	239	PRO
1	E	251	LEU
1	E	257	MET
1	E	259	ILE
1	E	265	ASN
1	E	281	GLU
1	E	282	THR
1	E	283	LYS
1	E	293	PRO
1	E	295	LEU
1	E	297	ASN
1	E	303	GLU
1	E	304	ASP
1	E	307	GLU
1	E	315	GLU
1	E	320	ARG
1	E	327	ILE
1	E	332	LEU
1	F	9	LEU
1	F	10	LEU
1	F	16	SER
1	F	23	LEU
1	F	27	SER
1	F	30	LEU
1	F	38	THR
1	F	45	ARG
1	F	48	ILE
1	F	50	LEU
1	F	55	THR
1	F	84	ILE
1	F	93	THR
1	F	107	ARG
1	F	111	GLN
1	F	124	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	129	LEU
1	F	138	MET
1	F	142	VAL
1	F	165	ARG
1	F	184	ARG
1	F	185	ILE
1	F	189	LYS
1	F	194	HIS
1	F	195	ASP
1	F	196	GLU
1	F	202	LYS
1	F	215	THR
1	F	222	VAL
1	F	223	LYS
1	F	225	VAL
1	F	232	VAL
1	F	236	MET
1	F	239	PRO
1	F	251	LEU
1	F	257	MET
1	F	259	ILE
1	F	265	ASN
1	F	281	GLU
1	F	282	THR
1	F	283	LYS
1	F	293	PRO
1	F	295	LEU
1	F	297	ASN
1	F	303	GLU
1	F	304	ASP
1	F	307	GLU
1	F	315	GLU
1	F	320	ARG
1	F	327	ILE
1	F	332	LEU
1	G	9	LEU
1	G	10	LEU
1	G	16	SER
1	G	23	LEU
1	G	27	SER
1	G	30	LEU
1	G	38	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	45	ARG
1	G	48	ILE
1	G	50	LEU
1	G	55	THR
1	G	84	ILE
1	G	93	THR
1	G	107	ARG
1	G	111	GLN
1	G	124	PRO
1	G	129	LEU
1	G	138	MET
1	G	142	VAL
1	G	165	ARG
1	G	184	ARG
1	G	185	ILE
1	G	189	LYS
1	G	194	HIS
1	G	195	ASP
1	G	196	GLU
1	G	202	LYS
1	G	215	THR
1	G	222	VAL
1	G	223	LYS
1	G	225	VAL
1	G	232	VAL
1	G	236	MET
1	G	239	PRO
1	G	251	LEU
1	G	257	MET
1	G	259	ILE
1	G	265	ASN
1	G	281	GLU
1	G	282	THR
1	G	283	LYS
1	G	293	PRO
1	G	295	LEU
1	G	297	ASN
1	G	303	GLU
1	G	304	ASP
1	G	307	GLU
1	G	315	GLU
1	G	320	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	327	ILE
1	G	332	LEU
1	H	9	LEU
1	H	10	LEU
1	H	16	SER
1	H	23	LEU
1	H	27	SER
1	H	30	LEU
1	H	38	THR
1	H	45	ARG
1	H	48	ILE
1	H	50	LEU
1	H	55	THR
1	H	84	ILE
1	H	93	THR
1	H	107	ARG
1	H	111	GLN
1	H	124	PRO
1	H	129	LEU
1	H	138	MET
1	H	142	VAL
1	H	165	ARG
1	H	184	ARG
1	H	185	ILE
1	H	189	LYS
1	H	194	HIS
1	H	195	ASP
1	H	196	GLU
1	H	202	LYS
1	H	215	THR
1	H	222	VAL
1	H	223	LYS
1	H	225	VAL
1	H	232	VAL
1	H	236	MET
1	H	239	PRO
1	H	251	LEU
1	H	257	MET
1	H	259	ILE
1	H	265	ASN
1	H	281	GLU
1	H	282	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	283	LYS
1	H	293	PRO
1	H	295	LEU
1	H	297	ASN
1	H	303	GLU
1	H	304	ASP
1	H	307	GLU
1	H	315	GLU
1	H	320	ARG
1	H	327	ILE
1	H	332	LEU
1	I	9	LEU
1	I	10	LEU
1	I	16	SER
1	I	23	LEU
1	I	27	SER
1	I	30	LEU
1	I	38	THR
1	I	45	ARG
1	I	48	ILE
1	I	50	LEU
1	I	55	THR
1	I	84	ILE
1	I	93	THR
1	I	107	ARG
1	I	111	GLN
1	I	124	PRO
1	I	129	LEU
1	I	138	MET
1	I	142	VAL
1	I	165	ARG
1	I	184	ARG
1	I	185	ILE
1	I	189	LYS
1	I	194	HIS
1	I	195	ASP
1	I	196	GLU
1	I	202	LYS
1	I	215	THR
1	I	222	VAL
1	I	223	LYS
1	I	225	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	232	VAL
1	I	236	MET
1	I	239	PRO
1	I	251	LEU
1	I	257	MET
1	I	259	ILE
1	I	265	ASN
1	I	281	GLU
1	I	282	THR
1	I	283	LYS
1	I	293	PRO
1	I	295	LEU
1	I	297	ASN
1	I	303	GLU
1	I	304	ASP
1	I	307	GLU
1	I	315	GLU
1	I	320	ARG
1	I	327	ILE
1	I	332	LEU
1	J	9	LEU
1	J	10	LEU
1	J	16	SER
1	J	23	LEU
1	J	27	SER
1	J	30	LEU
1	J	38	THR
1	J	45	ARG
1	J	48	ILE
1	J	50	LEU
1	J	55	THR
1	J	84	ILE
1	J	93	THR
1	J	107	ARG
1	J	111	GLN
1	J	124	PRO
1	J	129	LEU
1	J	138	MET
1	J	142	VAL
1	J	165	ARG
1	J	184	ARG
1	J	185	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	189	LYS
1	J	194	HIS
1	J	195	ASP
1	J	196	GLU
1	J	202	LYS
1	J	215	THR
1	J	222	VAL
1	J	223	LYS
1	J	225	VAL
1	J	232	VAL
1	J	236	MET
1	J	239	PRO
1	J	251	LEU
1	J	257	MET
1	J	259	ILE
1	J	265	ASN
1	J	281	GLU
1	J	282	THR
1	J	283	LYS
1	J	293	PRO
1	J	295	LEU
1	J	297	ASN
1	J	303	GLU
1	J	304	ASP
1	J	307	GLU
1	J	315	GLU
1	J	320	ARG
1	J	327	ILE
1	J	332	LEU
1	K	9	LEU
1	K	10	LEU
1	K	16	SER
1	K	23	LEU
1	K	27	SER
1	K	30	LEU
1	K	38	THR
1	K	45	ARG
1	K	48	ILE
1	K	50	LEU
1	K	55	THR
1	K	84	ILE
1	K	93	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	107	ARG
1	K	111	GLN
1	K	124	PRO
1	K	129	LEU
1	K	138	MET
1	K	142	VAL
1	K	165	ARG
1	K	184	ARG
1	K	185	ILE
1	K	189	LYS
1	K	194	HIS
1	K	195	ASP
1	K	196	GLU
1	K	202	LYS
1	K	215	THR
1	K	222	VAL
1	K	223	LYS
1	K	225	VAL
1	K	232	VAL
1	K	236	MET
1	K	239	PRO
1	K	251	LEU
1	K	257	MET
1	K	259	ILE
1	K	265	ASN
1	K	281	GLU
1	K	282	THR
1	K	283	LYS
1	K	293	PRO
1	K	295	LEU
1	K	297	ASN
1	K	303	GLU
1	K	304	ASP
1	K	307	GLU
1	K	315	GLU
1	K	320	ARG
1	K	327	ILE
1	K	332	LEU
1	L	9	LEU
1	L	10	LEU
1	L	16	SER
1	L	23	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	27	SER
1	L	30	LEU
1	L	38	THR
1	L	45	ARG
1	L	48	ILE
1	L	50	LEU
1	L	55	THR
1	L	84	ILE
1	L	93	THR
1	L	107	ARG
1	L	111	GLN
1	L	124	PRO
1	L	129	LEU
1	L	138	MET
1	L	142	VAL
1	L	165	ARG
1	L	184	ARG
1	L	185	ILE
1	L	189	LYS
1	L	194	HIS
1	L	195	ASP
1	L	196	GLU
1	L	202	LYS
1	L	215	THR
1	L	222	VAL
1	L	223	LYS
1	L	225	VAL
1	L	232	VAL
1	L	236	MET
1	L	239	PRO
1	L	251	LEU
1	L	257	MET
1	L	259	ILE
1	L	265	ASN
1	L	281	GLU
1	L	282	THR
1	L	283	LYS
1	L	293	PRO
1	L	295	LEU
1	L	297	ASN
1	L	303	GLU
1	L	304	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	307	GLU
1	L	315	GLU
1	L	320	ARG
1	L	327	ILE
1	L	332	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	6	ASN
1	A	80	ASN
1	A	86	HIS
1	A	127	ASN
1	A	134	HIS
1	A	137	GLN
1	A	229	HIS
1	A	272	HIS
1	A	311	ASN
1	A	316	GLN
1	B	5	HIS
1	B	6	ASN
1	B	80	ASN
1	B	86	HIS
1	B	127	ASN
1	B	134	HIS
1	B	137	GLN
1	B	229	HIS
1	B	272	HIS
1	B	278	HIS
1	B	311	ASN
1	B	316	GLN
1	C	5	HIS
1	C	6	ASN
1	C	80	ASN
1	C	86	HIS
1	C	127	ASN
1	C	134	HIS
1	C	137	GLN
1	C	229	HIS
1	C	272	HIS
1	C	278	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	311	ASN
1	C	316	GLN
1	D	5	HIS
1	D	6	ASN
1	D	80	ASN
1	D	86	HIS
1	D	127	ASN
1	D	134	HIS
1	D	137	GLN
1	D	229	HIS
1	D	272	HIS
1	D	311	ASN
1	D	316	GLN
1	E	6	ASN
1	E	80	ASN
1	E	86	HIS
1	E	127	ASN
1	E	137	GLN
1	E	229	HIS
1	E	272	HIS
1	E	278	HIS
1	E	291	GLN
1	E	311	ASN
1	E	316	GLN
1	F	6	ASN
1	F	80	ASN
1	F	86	HIS
1	F	127	ASN
1	F	137	GLN
1	F	229	HIS
1	F	272	HIS
1	F	311	ASN
1	F	316	GLN
1	G	6	ASN
1	G	80	ASN
1	G	86	HIS
1	G	127	ASN
1	G	137	GLN
1	G	229	HIS
1	G	272	HIS
1	G	278	HIS
1	G	311	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	316	GLN
1	H	5	HIS
1	H	6	ASN
1	H	80	ASN
1	H	86	HIS
1	H	127	ASN
1	H	134	HIS
1	H	137	GLN
1	H	229	HIS
1	H	272	HIS
1	H	278	HIS
1	H	311	ASN
1	H	316	GLN
1	I	6	ASN
1	I	80	ASN
1	I	86	HIS
1	I	127	ASN
1	I	137	GLN
1	I	229	HIS
1	I	272	HIS
1	I	311	ASN
1	I	316	GLN
1	J	6	ASN
1	J	80	ASN
1	J	86	HIS
1	J	127	ASN
1	J	137	GLN
1	J	229	HIS
1	J	272	HIS
1	J	278	HIS
1	J	311	ASN
1	J	316	GLN
1	K	6	ASN
1	K	80	ASN
1	K	86	HIS
1	K	127	ASN
1	K	137	GLN
1	K	229	HIS
1	K	272	HIS
1	K	278	HIS
1	K	291	GLN
1	K	311	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	316	GLN
1	L	6	ASN
1	L	80	ASN
1	L	86	HIS
1	L	127	ASN
1	L	134	HIS
1	L	137	GLN
1	L	229	HIS
1	L	272	HIS
1	L	278	HIS
1	L	311	ASN
1	L	316	GLN

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](#)

There are no ligands in this entry.

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.