



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 12:37 PM EDT

PDB ID : 1ORT  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

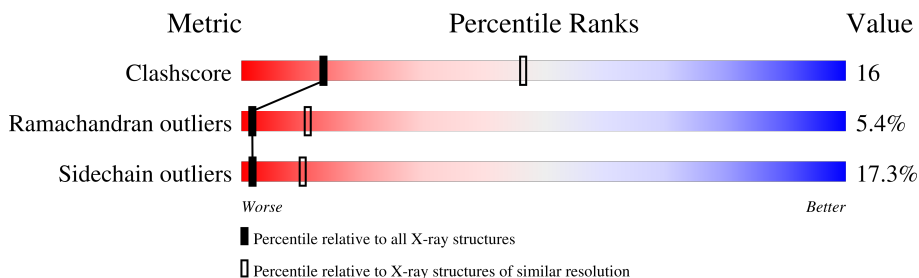
# 1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)




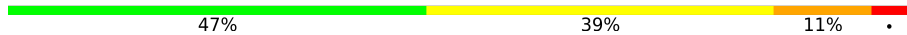
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	
1	B	335	
1	C	335	
1	D	335	
1	E	335	
1	F	335	
1	G	335	
1	H	335	

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Mol	Chain	Length	Quality of chain
1	I	335	 47% 39% 11% .
1	J	335	 47% 38% 11% .
1	K	335	 47% 37% 12% .
1	L	335	 47% 39% 11% .

## 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
			Total	C	N	O	S			
1	A	335	2664	1682	466	500	16	0	0	0
1	B	335	2664	1682	466	500	16	0	0	0
1	C	335	2664	1682	466	500	16	0	0	0
1	D	335	2664	1682	466	500	16	0	0	0
1	E	335	2664	1682	466	500	16	0	0	0
1	F	335	2664	1682	466	500	16	0	0	0
1	G	335	2664	1682	466	500	16	0	0	0
1	H	335	2664	1682	466	500	16	0	0	0
1	I	335	2664	1682	466	500	16	0	0	0
1	J	335	2664	1682	466	500	16	0	0	0
1	K	335	2664	1682	466	500	16	0	0	0
1	L	335	2664	1682	466	500	16	0	0	0

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

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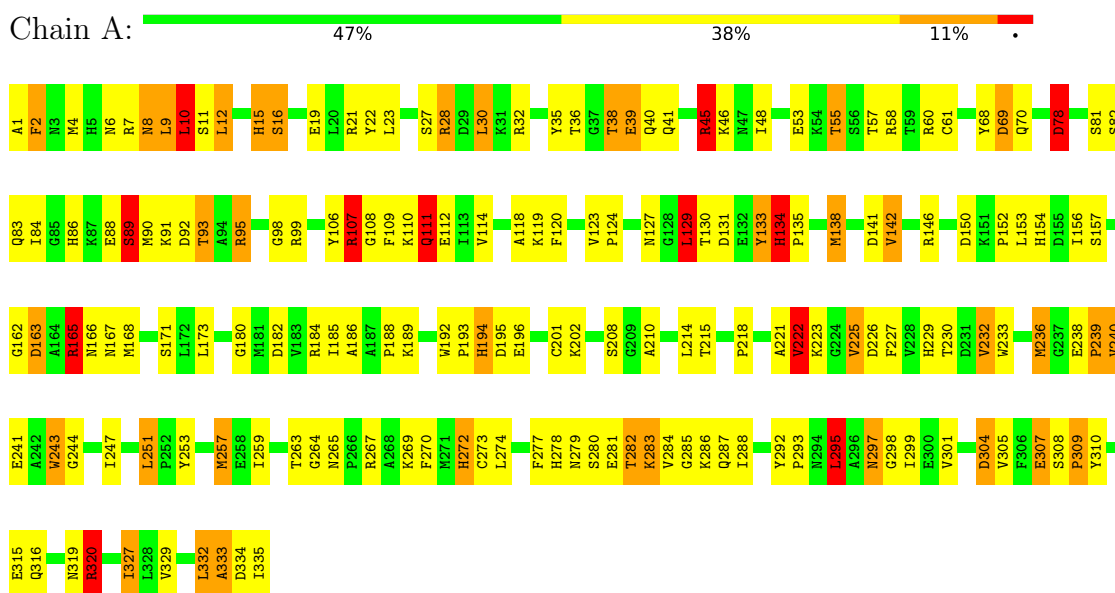
<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
F	105	GLY	GLU	engineered mutation	UNP P08308
G	105	GLY	GLU	engineered mutation	UNP P08308
H	105	GLY	GLU	engineered mutation	UNP P08308
I	105	GLY	GLU	engineered mutation	UNP P08308
J	105	GLY	GLU	engineered mutation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

### 3 Residue-property plots [i](#)

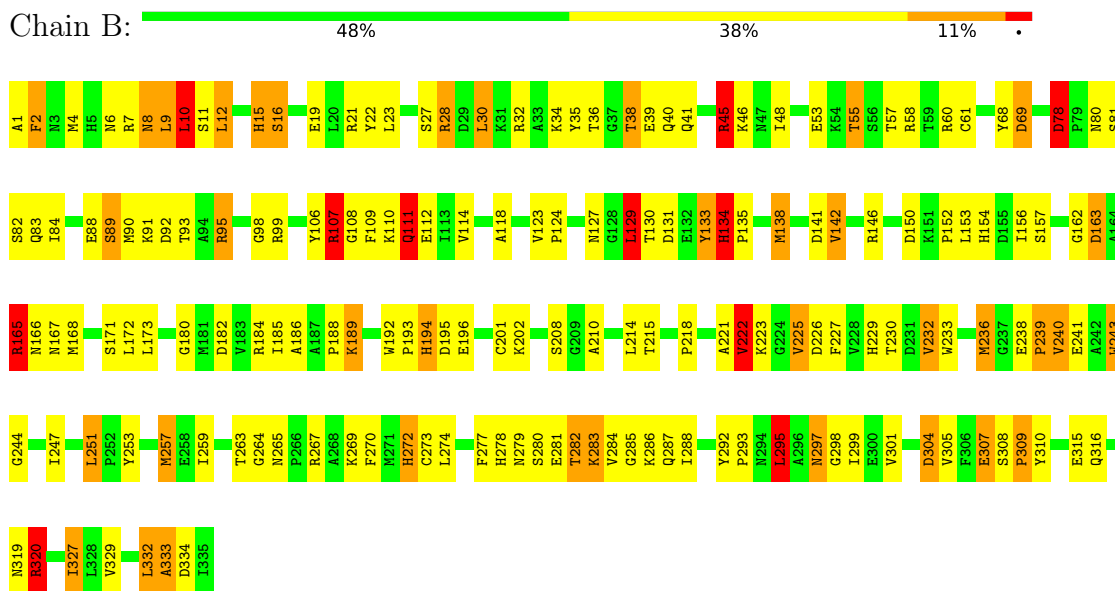
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

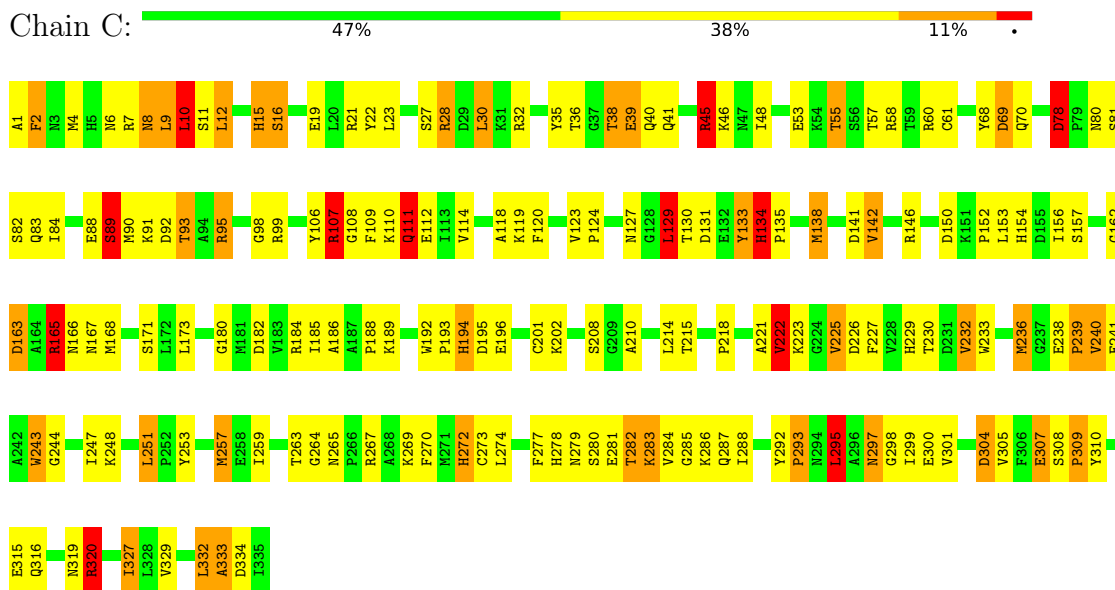
- Molecule 1: ORNITHINE TRANSCARBAMOYLASE



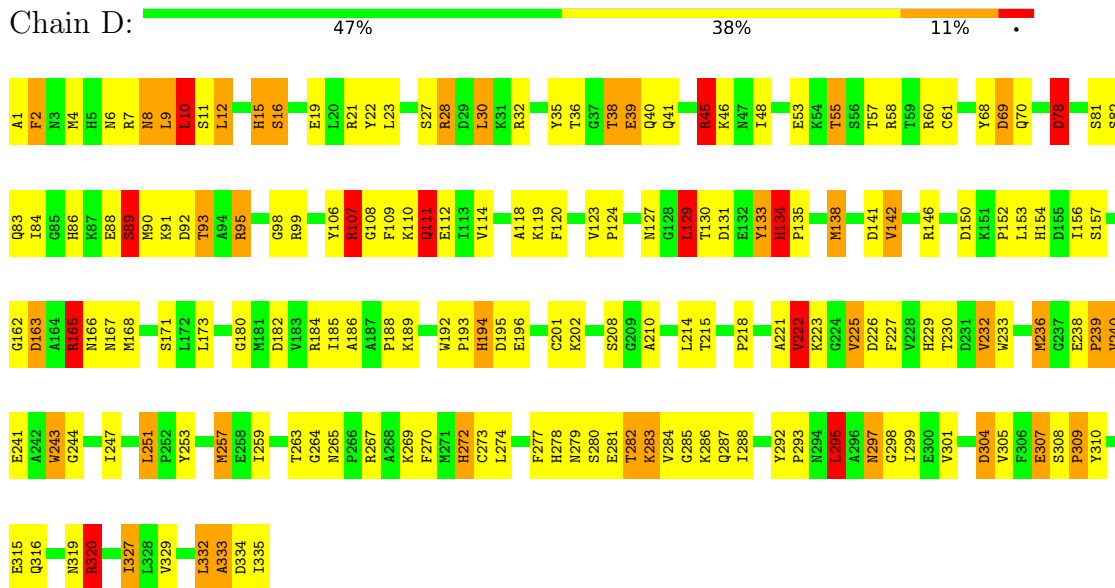
- Molecule 1: ORNITHINE TRANSCARBAMOYLASE



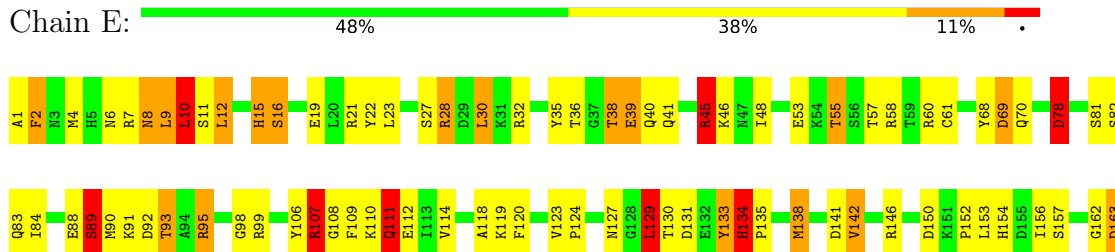
- Molecule 1: ORNITHINE TRANSCARBAMOYLASE

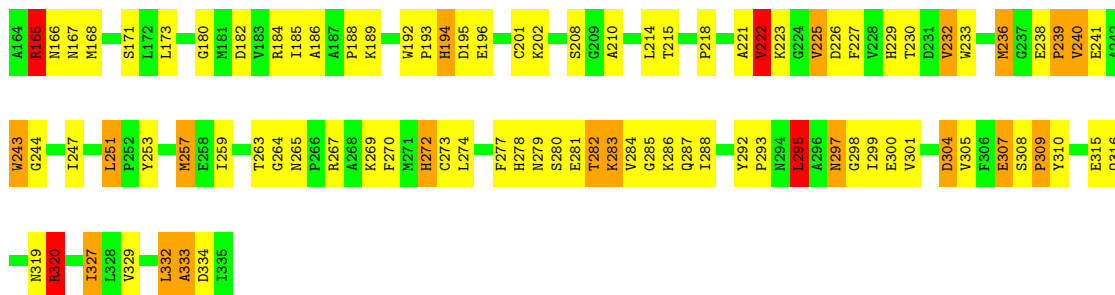


- Molecule 1: ORNITHINE TRANSCARBAMOYLASE

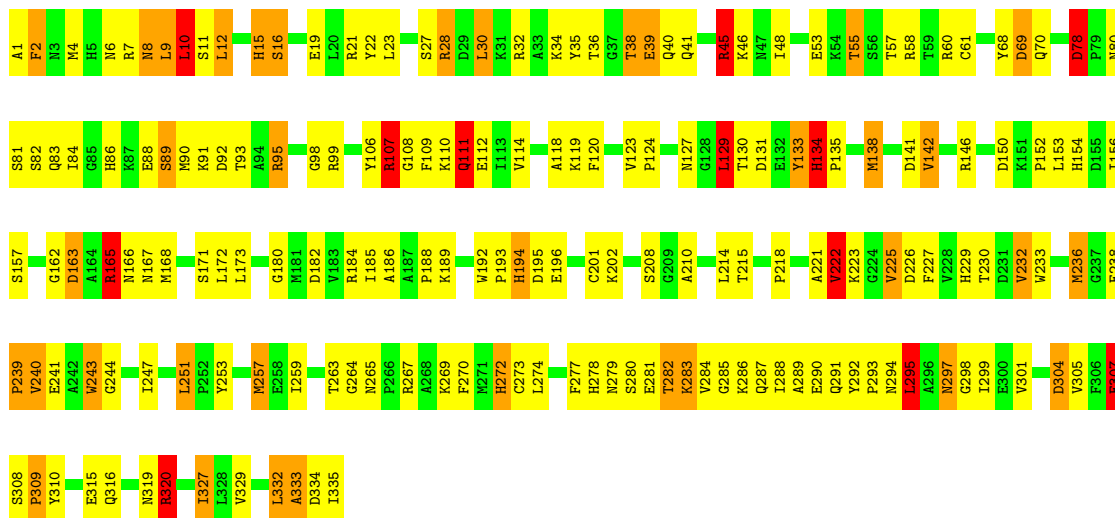


- Molecule 1: ORNITHINE TRANSCARBAMOYLASE

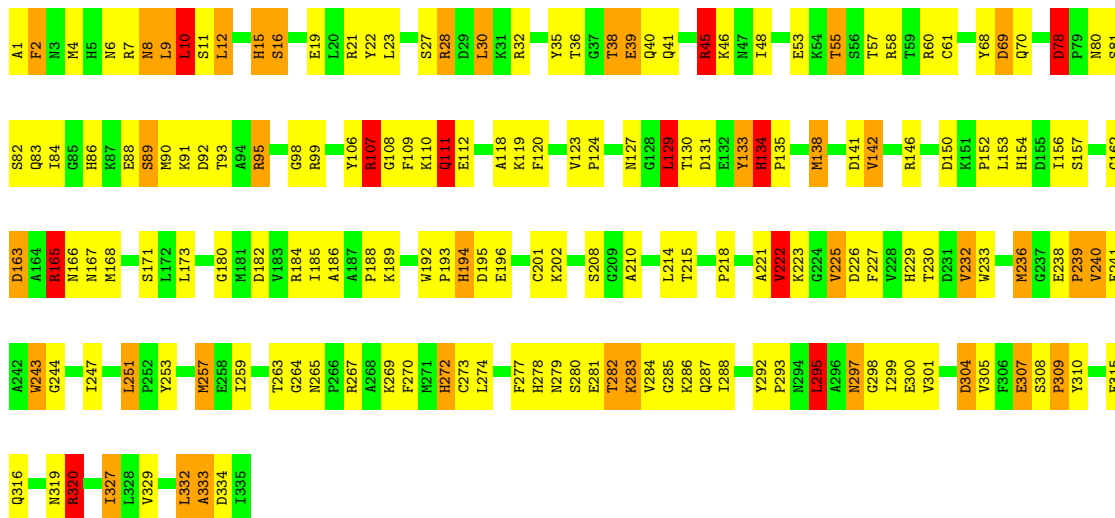




• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

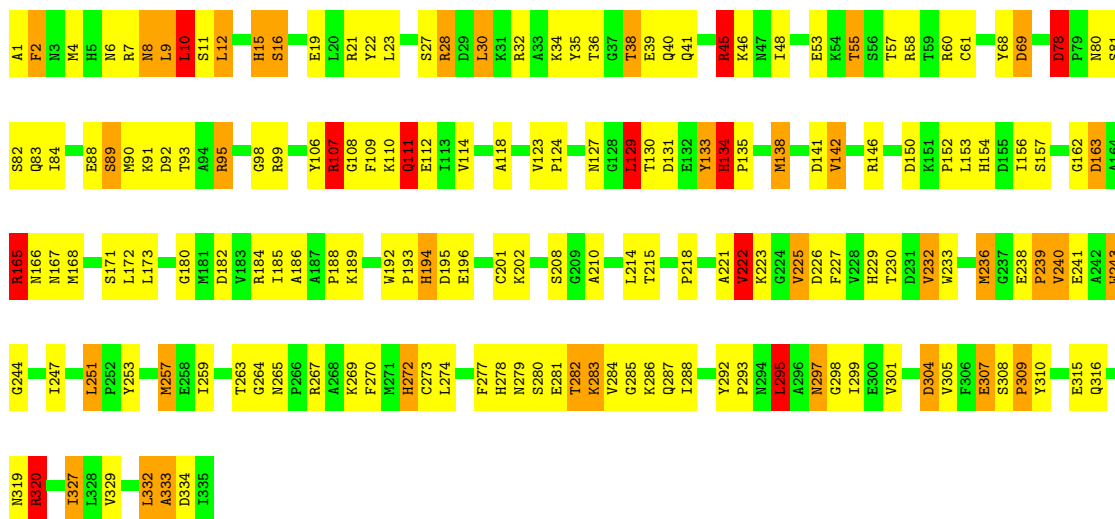


• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

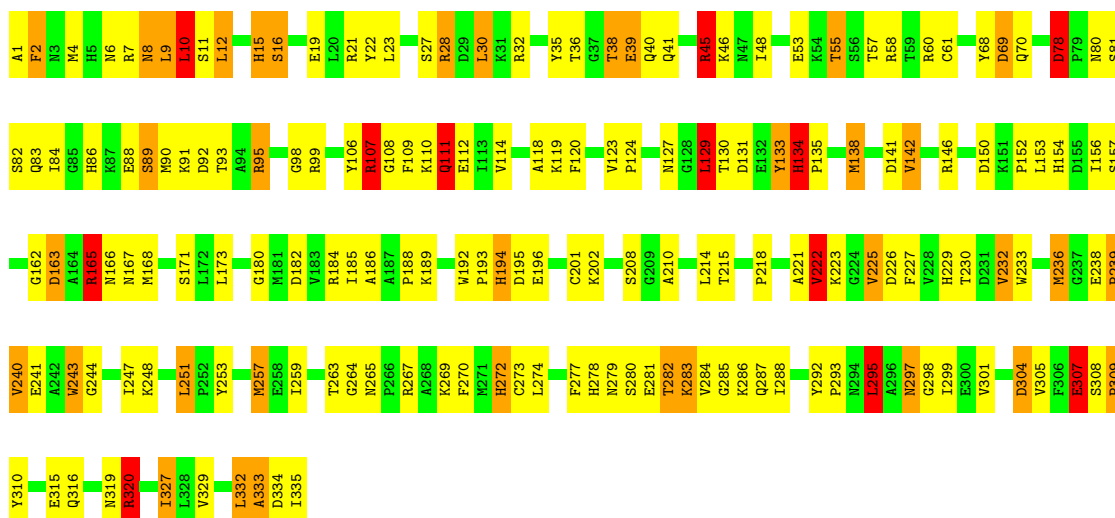


• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

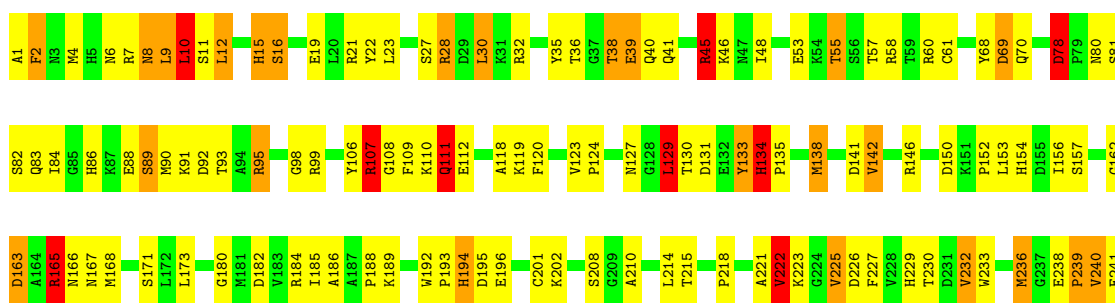


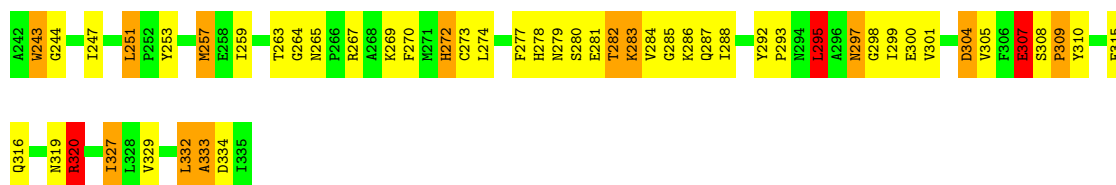


• Molecule 1: ORNITHINE TRANSCARBAMOYLASE



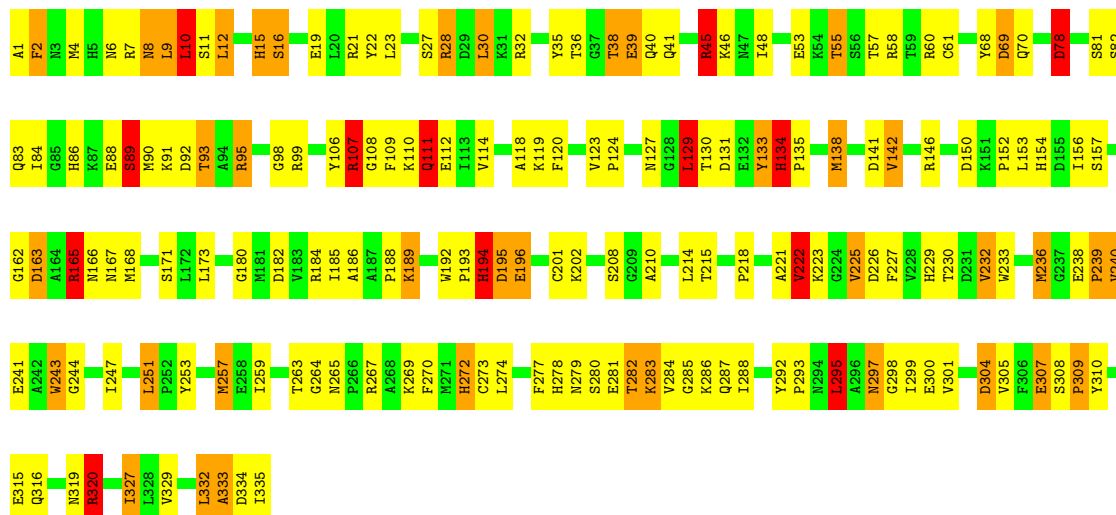
• Molecule 1: ORNITHINE TRANSCARBAMOYLASE





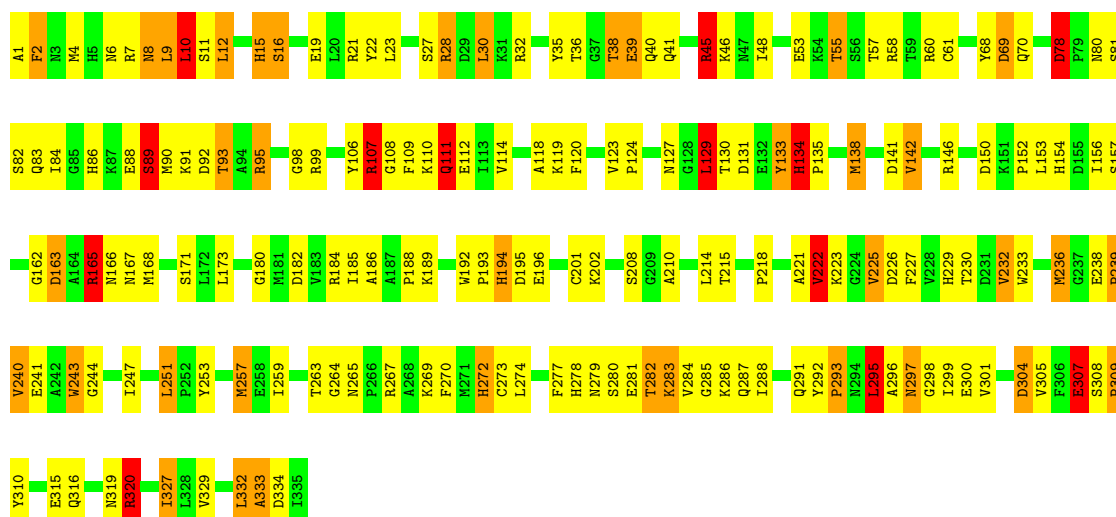
• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

Chain K: 47% 37% 12%



• Molecule 1: ORNITHINE TRANSCARBAMOYLASE

Chain L: 47% 39% 11%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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.	Xtrriage
Total number of atoms	31968	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.93	0/2720	2.00	90/3673 (2.5%)
1	B	0.93	0/2720	2.00	90/3673 (2.5%)
1	C	0.93	0/2720	2.00	90/3673 (2.5%)
1	D	0.93	0/2720	2.00	90/3673 (2.5%)
1	E	0.93	0/2720	2.00	90/3673 (2.5%)
1	F	0.93	0/2720	2.00	90/3673 (2.5%)
1	G	0.93	0/2720	2.00	90/3673 (2.5%)
1	H	0.93	0/2720	2.00	90/3673 (2.5%)
1	I	0.93	0/2720	2.00	90/3673 (2.5%)
1	J	0.93	0/2720	2.00	90/3673 (2.5%)
1	K	0.93	0/2720	2.00	90/3673 (2.5%)
1	L	0.93	0/2720	2.00	90/3673 (2.5%)
All	All	0.93	0/32640	2.00	1080/44076 (2.5%)

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

There are no bond length outliers.

All (1080) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	B	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	C	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	D	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	E	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	F	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	G	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	H	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	I	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	J	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	K	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	L	320	ARG	NE-CZ-NH2	-20.13	110.24	120.30
1	A	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	B	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	C	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	D	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	E	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	F	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	G	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	H	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	I	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	J	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	K	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	L	146	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	A	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	B	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	C	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	D	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	E	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	F	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	G	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	H	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	I	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	J	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	K	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	L	58	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	A	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	B	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	C	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	D	320	ARG	NE-CZ-NH1	10.39	125.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	F	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	G	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	H	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	I	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	J	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	K	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	L	320	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	B	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	C	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	D	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	E	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	F	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	G	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	H	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	I	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	J	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	K	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	L	21	ARG	CA-CB-CG	-10.05	91.30	113.40
1	A	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	B	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	C	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	D	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	E	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	F	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	G	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	H	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	I	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	J	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	K	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	L	95	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	A	134	HIS	N-CA-C	8.64	134.32	111.00
1	B	134	HIS	N-CA-C	8.64	134.32	111.00
1	C	134	HIS	N-CA-C	8.64	134.32	111.00
1	D	134	HIS	N-CA-C	8.64	134.32	111.00
1	E	134	HIS	N-CA-C	8.64	134.32	111.00
1	F	134	HIS	N-CA-C	8.64	134.32	111.00
1	G	134	HIS	N-CA-C	8.64	134.32	111.00
1	H	134	HIS	N-CA-C	8.64	134.32	111.00
1	I	134	HIS	N-CA-C	8.64	134.32	111.00
1	J	134	HIS	N-CA-C	8.64	134.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	134	HIS	N-CA-C	8.64	134.32	111.00
1	L	134	HIS	N-CA-C	8.64	134.32	111.00
1	A	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	B	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	C	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	D	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	E	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	F	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	G	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	H	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	I	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	J	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	K	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	L	243	TRP	CD1-CG-CD2	8.23	112.89	106.30
1	A	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	B	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	C	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	D	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	E	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	F	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	G	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	H	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	I	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	J	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	K	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	L	129	LEU	CA-CB-CG	8.09	133.91	115.30
1	A	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	B	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	C	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	D	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	E	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	F	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	G	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	H	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	I	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	J	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	K	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	L	10	LEU	CA-CB-CG	8.05	133.82	115.30
1	A	12	LEU	CA-C-N	-8.05	99.50	117.20
1	B	12	LEU	CA-C-N	-8.05	99.50	117.20
1	C	12	LEU	CA-C-N	-8.05	99.50	117.20
1	D	12	LEU	CA-C-N	-8.05	99.50	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	12	LEU	CA-C-N	-8.05	99.50	117.20
1	F	12	LEU	CA-C-N	-8.05	99.50	117.20
1	G	12	LEU	CA-C-N	-8.05	99.50	117.20
1	H	12	LEU	CA-C-N	-8.05	99.50	117.20
1	I	12	LEU	CA-C-N	-8.05	99.50	117.20
1	J	12	LEU	CA-C-N	-8.05	99.50	117.20
1	K	12	LEU	CA-C-N	-8.05	99.50	117.20
1	L	12	LEU	CA-C-N	-8.05	99.50	117.20
1	A	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	B	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	D	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	E	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	F	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	G	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	H	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	I	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	J	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	K	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	L	95	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	2	PHE	N-CA-CB	7.87	124.77	110.60
1	B	2	PHE	N-CA-CB	7.87	124.77	110.60
1	C	2	PHE	N-CA-CB	7.87	124.77	110.60
1	D	2	PHE	N-CA-CB	7.87	124.77	110.60
1	E	2	PHE	N-CA-CB	7.87	124.77	110.60
1	F	2	PHE	N-CA-CB	7.87	124.77	110.60
1	G	2	PHE	N-CA-CB	7.87	124.77	110.60
1	H	2	PHE	N-CA-CB	7.87	124.77	110.60
1	I	2	PHE	N-CA-CB	7.87	124.77	110.60
1	J	2	PHE	N-CA-CB	7.87	124.77	110.60
1	K	2	PHE	N-CA-CB	7.87	124.77	110.60
1	L	2	PHE	N-CA-CB	7.87	124.77	110.60
1	A	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	B	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	C	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	D	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	E	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	F	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	G	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	H	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	I	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	J	45	ARG	CA-CB-CG	7.79	130.54	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	L	45	ARG	CA-CB-CG	7.79	130.54	113.40
1	A	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	B	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	C	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	D	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	E	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	F	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	G	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	H	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	I	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	J	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	K	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	L	22	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	A	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	B	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	D	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	E	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	F	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	G	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	H	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	I	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	J	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	K	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	L	165	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	B	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	C	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	D	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	E	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	F	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	G	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	H	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	I	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	J	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	K	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	L	305	VAL	CA-CB-CG2	-7.68	99.38	110.90
1	A	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	B	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	C	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	D	233	TRP	CD1-CG-CD2	7.53	112.33	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	F	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	G	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	H	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	I	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	J	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	K	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	L	233	TRP	CD1-CG-CD2	7.53	112.33	106.30
1	A	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	B	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	C	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	D	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	E	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	F	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	G	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	H	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	I	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	J	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	K	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	L	165	ARG	CB-CG-CD	-7.39	92.39	111.60
1	A	226	ASP	CA-C-N	7.34	133.36	117.20
1	B	226	ASP	CA-C-N	7.34	133.36	117.20
1	C	226	ASP	CA-C-N	7.34	133.36	117.20
1	D	226	ASP	CA-C-N	7.34	133.36	117.20
1	E	226	ASP	CA-C-N	7.34	133.36	117.20
1	F	226	ASP	CA-C-N	7.34	133.36	117.20
1	G	226	ASP	CA-C-N	7.34	133.36	117.20
1	H	226	ASP	CA-C-N	7.34	133.36	117.20
1	I	226	ASP	CA-C-N	7.34	133.36	117.20
1	J	226	ASP	CA-C-N	7.34	133.36	117.20
1	K	226	ASP	CA-C-N	7.34	133.36	117.20
1	L	226	ASP	CA-C-N	7.34	133.36	117.20
1	A	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	B	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	C	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	D	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	E	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	F	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	G	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	H	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	I	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	J	6	ASN	CA-CB-CG	-7.32	97.29	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	L	6	ASN	CA-CB-CG	-7.32	97.29	113.40
1	A	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	B	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	C	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	D	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	E	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	F	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	G	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	H	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	I	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	J	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	K	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	L	69	ASP	CB-CG-OD1	7.32	124.88	118.30
1	A	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	B	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	C	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	D	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	E	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	F	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	G	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	H	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	I	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	J	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	K	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	L	88	GLU	CA-CB-CG	-7.24	97.47	113.40
1	A	12	LEU	N-CA-C	7.23	130.52	111.00
1	B	12	LEU	N-CA-C	7.23	130.52	111.00
1	C	12	LEU	N-CA-C	7.23	130.52	111.00
1	D	12	LEU	N-CA-C	7.23	130.52	111.00
1	E	12	LEU	N-CA-C	7.23	130.52	111.00
1	F	12	LEU	N-CA-C	7.23	130.52	111.00
1	G	12	LEU	N-CA-C	7.23	130.52	111.00
1	H	12	LEU	N-CA-C	7.23	130.52	111.00
1	I	12	LEU	N-CA-C	7.23	130.52	111.00
1	J	12	LEU	N-CA-C	7.23	130.52	111.00
1	K	12	LEU	N-CA-C	7.23	130.52	111.00
1	L	12	LEU	N-CA-C	7.23	130.52	111.00
1	A	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	B	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	C	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	D	192	TRP	CD1-CG-CD2	7.19	112.05	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	F	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	G	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	H	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	I	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	J	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	K	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	L	192	TRP	CD1-CG-CD2	7.19	112.05	106.30
1	A	2	PHE	N-CA-C	-7.17	91.64	111.00
1	B	2	PHE	N-CA-C	-7.17	91.64	111.00
1	C	2	PHE	N-CA-C	-7.17	91.64	111.00
1	D	2	PHE	N-CA-C	-7.17	91.64	111.00
1	E	2	PHE	N-CA-C	-7.17	91.64	111.00
1	F	2	PHE	N-CA-C	-7.17	91.64	111.00
1	G	2	PHE	N-CA-C	-7.17	91.64	111.00
1	H	2	PHE	N-CA-C	-7.17	91.64	111.00
1	I	2	PHE	N-CA-C	-7.17	91.64	111.00
1	J	2	PHE	N-CA-C	-7.17	91.64	111.00
1	K	2	PHE	N-CA-C	-7.17	91.64	111.00
1	L	2	PHE	N-CA-C	-7.17	91.64	111.00
1	A	133	TYR	CA-C-N	-7.12	101.53	117.20
1	B	133	TYR	CA-C-N	-7.12	101.53	117.20
1	C	133	TYR	CA-C-N	-7.12	101.53	117.20
1	D	133	TYR	CA-C-N	-7.12	101.53	117.20
1	E	133	TYR	CA-C-N	-7.12	101.53	117.20
1	F	133	TYR	CA-C-N	-7.12	101.53	117.20
1	G	133	TYR	CA-C-N	-7.12	101.53	117.20
1	H	133	TYR	CA-C-N	-7.12	101.53	117.20
1	I	133	TYR	CA-C-N	-7.12	101.53	117.20
1	J	133	TYR	CA-C-N	-7.12	101.53	117.20
1	K	133	TYR	CA-C-N	-7.12	101.53	117.20
1	L	133	TYR	CA-C-N	-7.12	101.53	117.20
1	A	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	B	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	C	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	D	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	E	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	F	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	G	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	H	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	I	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	J	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	L	146	ARG	NH1-CZ-NH2	7.09	127.20	119.40
1	A	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	B	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	C	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	D	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	E	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	F	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	G	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	H	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	I	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	J	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	K	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	L	99	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	272	HIS	CA-C-N	6.91	132.41	117.20
1	B	272	HIS	CA-C-N	6.91	132.41	117.20
1	C	272	HIS	CA-C-N	6.91	132.41	117.20
1	D	272	HIS	CA-C-N	6.91	132.41	117.20
1	E	272	HIS	CA-C-N	6.91	132.41	117.20
1	F	272	HIS	CA-C-N	6.91	132.41	117.20
1	G	272	HIS	CA-C-N	6.91	132.41	117.20
1	H	272	HIS	CA-C-N	6.91	132.41	117.20
1	I	272	HIS	CA-C-N	6.91	132.41	117.20
1	J	272	HIS	CA-C-N	6.91	132.41	117.20
1	K	272	HIS	CA-C-N	6.91	132.41	117.20
1	L	272	HIS	CA-C-N	6.91	132.41	117.20
1	A	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	C	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	D	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	E	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	F	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	G	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	H	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	I	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	J	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	K	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	L	58	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	B	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	C	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	99	ARG	NE-CZ-NH1	6.76	123.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	F	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	G	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	H	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	I	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	J	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	K	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	L	99	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	78	ASP	N-CA-C	6.64	128.93	111.00
1	B	78	ASP	N-CA-C	6.64	128.93	111.00
1	C	78	ASP	N-CA-C	6.64	128.93	111.00
1	D	78	ASP	N-CA-C	6.64	128.93	111.00
1	E	78	ASP	N-CA-C	6.64	128.93	111.00
1	F	78	ASP	N-CA-C	6.64	128.93	111.00
1	G	78	ASP	N-CA-C	6.64	128.93	111.00
1	H	78	ASP	N-CA-C	6.64	128.93	111.00
1	I	78	ASP	N-CA-C	6.64	128.93	111.00
1	J	78	ASP	N-CA-C	6.64	128.93	111.00
1	K	78	ASP	N-CA-C	6.64	128.93	111.00
1	L	78	ASP	N-CA-C	6.64	128.93	111.00
1	A	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	C	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	D	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	E	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	F	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	G	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	H	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	I	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	J	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	K	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	L	267	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	B	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	C	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	D	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	E	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	F	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	G	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	H	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	I	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	J	99	ARG	CA-CB-CG	-6.41	99.30	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	L	99	ARG	CA-CB-CG	-6.41	99.30	113.40
1	A	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	B	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	C	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	D	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	E	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	F	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	G	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	H	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	I	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	J	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	K	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	L	297	ASN	CA-CB-CG	-6.38	99.37	113.40
1	A	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	B	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	C	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	D	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	E	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	F	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	G	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	H	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	I	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	J	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	K	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	L	192	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	A	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	B	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	C	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	D	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	E	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	F	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	G	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	H	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	I	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	J	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	K	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	L	57	THR	CA-CB-CG2	6.26	121.16	112.40
1	A	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	B	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	C	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	D	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	F	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	G	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	H	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	I	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	J	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	K	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	L	243	TRP	CE2-CD2-CG	-6.23	102.32	107.30
1	A	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	B	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	C	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	D	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	E	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	F	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	G	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	H	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	I	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	J	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	K	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	L	57	THR	CA-CB-OG1	-6.19	95.99	109.00
1	A	133	TYR	C-N-CA	6.13	137.04	121.70
1	B	133	TYR	C-N-CA	6.13	137.04	121.70
1	C	133	TYR	C-N-CA	6.13	137.04	121.70
1	D	133	TYR	C-N-CA	6.13	137.04	121.70
1	E	133	TYR	C-N-CA	6.13	137.04	121.70
1	F	133	TYR	C-N-CA	6.13	137.04	121.70
1	G	133	TYR	C-N-CA	6.13	137.04	121.70
1	H	133	TYR	C-N-CA	6.13	137.04	121.70
1	I	133	TYR	C-N-CA	6.13	137.04	121.70
1	J	133	TYR	C-N-CA	6.13	137.04	121.70
1	K	133	TYR	C-N-CA	6.13	137.04	121.70
1	L	133	TYR	C-N-CA	6.13	137.04	121.70
1	A	193	PRO	CA-C-N	6.07	130.55	117.20
1	B	193	PRO	CA-C-N	6.07	130.55	117.20
1	C	193	PRO	CA-C-N	6.07	130.55	117.20
1	D	193	PRO	CA-C-N	6.07	130.55	117.20
1	E	193	PRO	CA-C-N	6.07	130.55	117.20
1	F	193	PRO	CA-C-N	6.07	130.55	117.20
1	G	193	PRO	CA-C-N	6.07	130.55	117.20
1	H	193	PRO	CA-C-N	6.07	130.55	117.20
1	I	193	PRO	CA-C-N	6.07	130.55	117.20
1	J	193	PRO	CA-C-N	6.07	130.55	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	193	PRO	CA-C-N	6.07	130.55	117.20
1	L	193	PRO	CA-C-N	6.07	130.55	117.20
1	A	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	B	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	C	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	D	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	E	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	F	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	G	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	H	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	I	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	J	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	K	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	L	310	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	A	82	SER	N-CA-C	-5.97	94.89	111.00
1	B	82	SER	N-CA-C	-5.97	94.89	111.00
1	C	82	SER	N-CA-C	-5.97	94.89	111.00
1	D	82	SER	N-CA-C	-5.97	94.89	111.00
1	E	82	SER	N-CA-C	-5.97	94.89	111.00
1	F	82	SER	N-CA-C	-5.97	94.89	111.00
1	G	82	SER	N-CA-C	-5.97	94.89	111.00
1	H	82	SER	N-CA-C	-5.97	94.89	111.00
1	I	82	SER	N-CA-C	-5.97	94.89	111.00
1	J	82	SER	N-CA-C	-5.97	94.89	111.00
1	K	82	SER	N-CA-C	-5.97	94.89	111.00
1	L	82	SER	N-CA-C	-5.97	94.89	111.00
1	A	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	B	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	C	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	D	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	E	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	F	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	G	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	H	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	I	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	J	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	K	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	L	229	HIS	CB-CA-C	-5.94	98.52	110.40
1	A	241	GLU	CA-C-N	-5.84	104.35	117.20
1	B	241	GLU	CA-C-N	-5.84	104.35	117.20
1	C	241	GLU	CA-C-N	-5.84	104.35	117.20
1	D	241	GLU	CA-C-N	-5.84	104.35	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	241	GLU	CA-C-N	-5.84	104.35	117.20
1	F	241	GLU	CA-C-N	-5.84	104.35	117.20
1	G	241	GLU	CA-C-N	-5.84	104.35	117.20
1	H	241	GLU	CA-C-N	-5.84	104.35	117.20
1	I	241	GLU	CA-C-N	-5.84	104.35	117.20
1	J	241	GLU	CA-C-N	-5.84	104.35	117.20
1	K	241	GLU	CA-C-N	-5.84	104.35	117.20
1	L	241	GLU	CA-C-N	-5.84	104.35	117.20
1	A	333	ALA	N-CA-C	5.84	126.76	111.00
1	B	333	ALA	N-CA-C	5.84	126.76	111.00
1	C	333	ALA	N-CA-C	5.84	126.76	111.00
1	D	333	ALA	N-CA-C	5.84	126.76	111.00
1	E	333	ALA	N-CA-C	5.84	126.76	111.00
1	F	333	ALA	N-CA-C	5.84	126.76	111.00
1	G	333	ALA	N-CA-C	5.84	126.76	111.00
1	H	333	ALA	N-CA-C	5.84	126.76	111.00
1	I	333	ALA	N-CA-C	5.84	126.76	111.00
1	J	333	ALA	N-CA-C	5.84	126.76	111.00
1	K	333	ALA	N-CA-C	5.84	126.76	111.00
1	L	333	ALA	N-CA-C	5.84	126.76	111.00
1	A	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	B	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	C	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	D	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	E	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	F	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	G	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	H	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	I	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	J	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	K	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	L	243	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	A	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	B	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	C	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	D	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	E	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	F	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	G	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	H	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	I	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	J	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	L	233	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	A	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	A	309	PRO	N-CA-C	5.76	127.08	112.10
1	B	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	B	309	PRO	N-CA-C	5.76	127.08	112.10
1	C	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	C	309	PRO	N-CA-C	5.76	127.08	112.10
1	D	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	D	309	PRO	N-CA-C	5.76	127.08	112.10
1	E	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	E	309	PRO	N-CA-C	5.76	127.08	112.10
1	F	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	F	309	PRO	N-CA-C	5.76	127.08	112.10
1	G	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	G	309	PRO	N-CA-C	5.76	127.08	112.10
1	H	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	H	309	PRO	N-CA-C	5.76	127.08	112.10
1	I	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	I	309	PRO	N-CA-C	5.76	127.08	112.10
1	J	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	J	309	PRO	N-CA-C	5.76	127.08	112.10
1	K	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	K	309	PRO	N-CA-C	5.76	127.08	112.10
1	L	60	ARG	CB-CG-CD	-5.76	96.62	111.60
1	L	309	PRO	N-CA-C	5.76	127.08	112.10
1	A	163	ASP	N-CA-CB	5.74	120.94	110.60
1	B	163	ASP	N-CA-CB	5.74	120.94	110.60
1	C	163	ASP	N-CA-CB	5.74	120.94	110.60
1	D	163	ASP	N-CA-CB	5.74	120.94	110.60
1	E	163	ASP	N-CA-CB	5.74	120.94	110.60
1	F	163	ASP	N-CA-CB	5.74	120.94	110.60
1	G	163	ASP	N-CA-CB	5.74	120.94	110.60
1	H	163	ASP	N-CA-CB	5.74	120.94	110.60
1	I	163	ASP	N-CA-CB	5.74	120.94	110.60
1	J	163	ASP	N-CA-CB	5.74	120.94	110.60
1	K	163	ASP	N-CA-CB	5.74	120.94	110.60
1	L	163	ASP	N-CA-CB	5.74	120.94	110.60
1	A	38	THR	N-CA-CB	-5.73	99.41	110.30
1	B	38	THR	N-CA-CB	-5.73	99.41	110.30
1	C	38	THR	N-CA-CB	-5.73	99.41	110.30
1	D	38	THR	N-CA-CB	-5.73	99.41	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	38	THR	N-CA-CB	-5.73	99.41	110.30
1	F	38	THR	N-CA-CB	-5.73	99.41	110.30
1	G	38	THR	N-CA-CB	-5.73	99.41	110.30
1	H	38	THR	N-CA-CB	-5.73	99.41	110.30
1	I	38	THR	N-CA-CB	-5.73	99.41	110.30
1	J	38	THR	N-CA-CB	-5.73	99.41	110.30
1	K	38	THR	N-CA-CB	-5.73	99.41	110.30
1	L	38	THR	N-CA-CB	-5.73	99.41	110.30
1	A	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	B	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	C	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	D	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	E	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	F	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	G	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	H	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	I	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	J	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	K	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	L	123	VAL	N-CA-CB	-5.70	98.96	111.50
1	A	194	HIS	CA-C-N	-5.60	104.87	117.20
1	B	194	HIS	CA-C-N	-5.60	104.87	117.20
1	C	194	HIS	CA-C-N	-5.60	104.87	117.20
1	D	194	HIS	CA-C-N	-5.60	104.87	117.20
1	E	194	HIS	CA-C-N	-5.60	104.87	117.20
1	F	194	HIS	CA-C-N	-5.60	104.87	117.20
1	G	194	HIS	CA-C-N	-5.60	104.87	117.20
1	H	194	HIS	CA-C-N	-5.60	104.87	117.20
1	I	194	HIS	CA-C-N	-5.60	104.87	117.20
1	J	194	HIS	CA-C-N	-5.60	104.87	117.20
1	K	194	HIS	CA-C-N	-5.60	104.87	117.20
1	L	194	HIS	CA-C-N	-5.60	104.87	117.20
1	A	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	B	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	C	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	D	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	E	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	F	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	G	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	H	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	I	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	J	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	L	39	GLU	OE1-CD-OE2	-5.58	116.61	123.30
1	A	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	B	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	C	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	D	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	E	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	F	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	G	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	H	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	I	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	J	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	K	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	L	61	CYS	CA-CB-SG	-5.57	103.97	114.00
1	A	12	LEU	O-C-N	5.54	131.57	122.70
1	B	12	LEU	O-C-N	5.54	131.57	122.70
1	C	12	LEU	O-C-N	5.54	131.57	122.70
1	D	12	LEU	O-C-N	5.54	131.57	122.70
1	E	12	LEU	O-C-N	5.54	131.57	122.70
1	F	12	LEU	O-C-N	5.54	131.57	122.70
1	G	12	LEU	O-C-N	5.54	131.57	122.70
1	H	12	LEU	O-C-N	5.54	131.57	122.70
1	I	12	LEU	O-C-N	5.54	131.57	122.70
1	J	12	LEU	O-C-N	5.54	131.57	122.70
1	K	12	LEU	O-C-N	5.54	131.57	122.70
1	L	12	LEU	O-C-N	5.54	131.57	122.70
1	A	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	B	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	C	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	D	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	E	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	F	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	G	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	H	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	I	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	J	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	K	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	L	225	VAL	N-CA-CB	-5.47	99.47	111.50
1	A	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	B	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	C	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	D	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	F	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	G	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	H	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	I	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	J	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	K	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	L	307	GLU	OE1-CD-OE2	-5.46	116.75	123.30
1	A	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	D	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	E	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	F	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	G	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	H	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	I	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	J	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	K	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	L	165	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	B	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	C	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	D	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	E	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	F	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	G	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	H	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	I	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	J	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	K	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	L	8	ASN	CB-CA-C	-5.44	99.51	110.40
1	A	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	B	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	C	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	D	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	E	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	F	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	G	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	H	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	I	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	J	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	L	192	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	A	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	B	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	C	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	D	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	E	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	F	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	G	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	H	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	I	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	J	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	K	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	L	83	GLN	CA-CB-CG	5.40	125.27	113.40
1	A	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	C	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	D	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	E	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	F	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	G	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	H	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	I	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	J	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	K	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	L	21	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	166	ASN	N-CA-C	-5.39	96.45	111.00
1	B	166	ASN	N-CA-C	-5.39	96.45	111.00
1	C	166	ASN	N-CA-C	-5.39	96.45	111.00
1	D	166	ASN	N-CA-C	-5.39	96.45	111.00
1	E	166	ASN	N-CA-C	-5.39	96.45	111.00
1	F	166	ASN	N-CA-C	-5.39	96.45	111.00
1	G	166	ASN	N-CA-C	-5.39	96.45	111.00
1	H	166	ASN	N-CA-C	-5.39	96.45	111.00
1	I	166	ASN	N-CA-C	-5.39	96.45	111.00
1	J	166	ASN	N-CA-C	-5.39	96.45	111.00
1	K	166	ASN	N-CA-C	-5.39	96.45	111.00
1	L	166	ASN	N-CA-C	-5.39	96.45	111.00
1	A	329	VAL	CA-C-N	5.37	129.02	117.20
1	B	329	VAL	CA-C-N	5.37	129.02	117.20
1	C	329	VAL	CA-C-N	5.37	129.02	117.20
1	D	329	VAL	CA-C-N	5.37	129.02	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	329	VAL	CA-C-N	5.37	129.02	117.20
1	F	329	VAL	CA-C-N	5.37	129.02	117.20
1	G	329	VAL	CA-C-N	5.37	129.02	117.20
1	H	329	VAL	CA-C-N	5.37	129.02	117.20
1	I	329	VAL	CA-C-N	5.37	129.02	117.20
1	J	329	VAL	CA-C-N	5.37	129.02	117.20
1	K	329	VAL	CA-C-N	5.37	129.02	117.20
1	L	329	VAL	CA-C-N	5.37	129.02	117.20
1	A	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	B	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	C	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	D	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	E	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	F	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	G	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	H	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	I	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	J	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	K	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	L	141	ASP	CB-CA-C	-5.37	99.67	110.40
1	A	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	B	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	C	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	D	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	E	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	F	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	G	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	H	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	I	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	J	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	K	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	L	35	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	A	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	D	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	E	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	F	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	G	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	H	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	I	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	J	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	L	28	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	332	LEU	CA-C-N	5.31	128.89	117.20
1	B	332	LEU	CA-C-N	5.31	128.89	117.20
1	C	332	LEU	CA-C-N	5.31	128.89	117.20
1	D	332	LEU	CA-C-N	5.31	128.89	117.20
1	E	332	LEU	CA-C-N	5.31	128.89	117.20
1	F	332	LEU	CA-C-N	5.31	128.89	117.20
1	G	332	LEU	CA-C-N	5.31	128.89	117.20
1	H	332	LEU	CA-C-N	5.31	128.89	117.20
1	I	332	LEU	CA-C-N	5.31	128.89	117.20
1	J	332	LEU	CA-C-N	5.31	128.89	117.20
1	K	332	LEU	CA-C-N	5.31	128.89	117.20
1	L	332	LEU	CA-C-N	5.31	128.89	117.20
1	A	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	B	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	C	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	D	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	E	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	F	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	G	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	H	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	I	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	J	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	K	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	L	305	VAL	CA-CB-CG1	5.30	118.85	110.90
1	A	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	B	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	C	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	D	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	E	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	F	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	G	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	H	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	I	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	J	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	K	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	L	233	TRP	CE2-CD2-CG	-5.26	103.09	107.30
1	A	214	LEU	N-CA-C	-5.26	96.80	111.00
1	B	214	LEU	N-CA-C	-5.26	96.80	111.00
1	C	214	LEU	N-CA-C	-5.26	96.80	111.00
1	D	214	LEU	N-CA-C	-5.26	96.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	214	LEU	N-CA-C	-5.26	96.80	111.00
1	F	214	LEU	N-CA-C	-5.26	96.80	111.00
1	G	214	LEU	N-CA-C	-5.26	96.80	111.00
1	H	214	LEU	N-CA-C	-5.26	96.80	111.00
1	I	214	LEU	N-CA-C	-5.26	96.80	111.00
1	J	214	LEU	N-CA-C	-5.26	96.80	111.00
1	K	214	LEU	N-CA-C	-5.26	96.80	111.00
1	L	214	LEU	N-CA-C	-5.26	96.80	111.00
1	A	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	B	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	C	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	D	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	E	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	F	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	G	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	H	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	I	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	J	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	K	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	L	327	ILE	CG1-CB-CG2	-5.26	99.83	111.40
1	A	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	B	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	C	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	D	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	E	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	F	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	G	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	H	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	I	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	J	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	K	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	L	301	VAL	CB-CA-C	-5.26	101.41	111.40
1	A	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	B	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	C	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	D	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	E	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	F	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	G	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	H	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	I	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	J	68	TYR	CD1-CG-CD2	5.25	123.68	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	L	68	TYR	CD1-CG-CD2	5.25	123.68	117.90
1	A	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	D	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	E	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	F	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	G	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	H	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	I	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	J	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	K	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	L	7	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	295	LEU	CA-C-N	5.23	128.70	117.20
1	B	295	LEU	CA-C-N	5.23	128.70	117.20
1	C	295	LEU	CA-C-N	5.23	128.70	117.20
1	D	295	LEU	CA-C-N	5.23	128.70	117.20
1	E	295	LEU	CA-C-N	5.23	128.70	117.20
1	F	295	LEU	CA-C-N	5.23	128.70	117.20
1	G	295	LEU	CA-C-N	5.23	128.70	117.20
1	H	295	LEU	CA-C-N	5.23	128.70	117.20
1	I	295	LEU	CA-C-N	5.23	128.70	117.20
1	J	295	LEU	CA-C-N	5.23	128.70	117.20
1	K	295	LEU	CA-C-N	5.23	128.70	117.20
1	L	295	LEU	CA-C-N	5.23	128.70	117.20
1	A	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	B	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	C	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	D	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	E	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	F	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	G	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	H	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	I	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	J	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	K	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	L	309	PRO	CA-N-CD	-5.18	104.25	111.50
1	A	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	B	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	C	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	D	68	TYR	CB-CG-CD2	-5.15	117.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	F	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	G	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	H	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	I	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	J	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	K	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	L	68	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	A	208	SER	CA-C-N	5.13	126.45	116.20
1	B	208	SER	CA-C-N	5.13	126.45	116.20
1	C	208	SER	CA-C-N	5.13	126.45	116.20
1	D	208	SER	CA-C-N	5.13	126.45	116.20
1	E	208	SER	CA-C-N	5.13	126.45	116.20
1	F	208	SER	CA-C-N	5.13	126.45	116.20
1	G	208	SER	CA-C-N	5.13	126.45	116.20
1	H	208	SER	CA-C-N	5.13	126.45	116.20
1	I	208	SER	CA-C-N	5.13	126.45	116.20
1	J	208	SER	CA-C-N	5.13	126.45	116.20
1	K	208	SER	CA-C-N	5.13	126.45	116.20
1	L	208	SER	CA-C-N	5.13	126.45	116.20
1	A	16	SER	CA-C-N	5.11	128.45	117.20
1	B	16	SER	CA-C-N	5.11	128.45	117.20
1	C	16	SER	CA-C-N	5.11	128.45	117.20
1	D	16	SER	CA-C-N	5.11	128.45	117.20
1	E	16	SER	CA-C-N	5.11	128.45	117.20
1	F	16	SER	CA-C-N	5.11	128.45	117.20
1	G	16	SER	CA-C-N	5.11	128.45	117.20
1	H	16	SER	CA-C-N	5.11	128.45	117.20
1	I	16	SER	CA-C-N	5.11	128.45	117.20
1	J	16	SER	CA-C-N	5.11	128.45	117.20
1	K	16	SER	CA-C-N	5.11	128.45	117.20
1	L	16	SER	CA-C-N	5.11	128.45	117.20
1	A	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	B	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	C	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	D	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	E	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	F	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	G	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	H	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	I	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	J	40	GLN	CG-CD-NE2	5.11	128.96	116.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	L	40	GLN	CG-CD-NE2	5.11	128.96	116.70
1	A	89	SER	N-CA-CB	5.10	118.15	110.50
1	B	89	SER	N-CA-CB	5.10	118.15	110.50
1	C	89	SER	N-CA-CB	5.10	118.15	110.50
1	D	89	SER	N-CA-CB	5.10	118.15	110.50
1	E	89	SER	N-CA-CB	5.10	118.15	110.50
1	F	89	SER	N-CA-CB	5.10	118.15	110.50
1	G	89	SER	N-CA-CB	5.10	118.15	110.50
1	H	89	SER	N-CA-CB	5.10	118.15	110.50
1	I	89	SER	N-CA-CB	5.10	118.15	110.50
1	J	89	SER	N-CA-CB	5.10	118.15	110.50
1	K	89	SER	N-CA-CB	5.10	118.15	110.50
1	L	89	SER	N-CA-CB	5.10	118.15	110.50
1	A	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	B	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	C	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	D	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	E	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	F	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	G	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	H	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	I	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	J	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	K	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	L	112	GLU	CA-CB-CG	5.09	124.60	113.40
1	A	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	B	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	C	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	D	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	E	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	F	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	G	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	H	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	I	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	J	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	K	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	L	78	ASP	CA-CB-CG	-5.07	102.24	113.40
1	A	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	B	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	C	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	D	107	ARG	CB-CG-CD	-5.05	98.47	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	F	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	G	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	H	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	I	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	J	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	K	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	L	107	ARG	CB-CG-CD	-5.05	98.47	111.60
1	A	226	ASP	O-C-N	-5.04	114.63	122.70
1	B	226	ASP	O-C-N	-5.04	114.63	122.70
1	C	226	ASP	O-C-N	-5.04	114.63	122.70
1	D	226	ASP	O-C-N	-5.04	114.63	122.70
1	E	226	ASP	O-C-N	-5.04	114.63	122.70
1	F	226	ASP	O-C-N	-5.04	114.63	122.70
1	G	226	ASP	O-C-N	-5.04	114.63	122.70
1	H	226	ASP	O-C-N	-5.04	114.63	122.70
1	I	226	ASP	O-C-N	-5.04	114.63	122.70
1	J	226	ASP	O-C-N	-5.04	114.63	122.70
1	K	226	ASP	O-C-N	-5.04	114.63	122.70
1	L	226	ASP	O-C-N	-5.04	114.63	122.70
1	A	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	B	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	C	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	D	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	E	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	F	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	G	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	H	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	I	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	J	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	K	222	VAL	CA-CB-CG2	-5.03	103.35	110.90
1	L	222	VAL	CA-CB-CG2	-5.03	103.35	110.90

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
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
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

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Mol	Chain	Res	Type	Group
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
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	96	0
1	B	2664	0	2637	92	5
1	C	2664	0	2637	97	4
1	D	2664	0	2637	94	0
1	E	2664	0	2637	95	0
1	F	2664	0	2637	100	40
1	G	2664	0	2637	91	0
1	H	2664	0	2637	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2664	0	2637	97	5
1	J	2664	0	2637	92	0
1	K	2664	0	2637	96	40
1	L	2664	0	2637	98	4
All	All	31968	0	31644	1020	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 16.

All (1020) 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
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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:138:MET:SD	1:B:171:SER:HB3	2.39	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:B:251:LEU:HD21	1:B:295:LEU:HD11	1.82	0.62
1:H:251:LEU:HD21	1:H:295:LEU:HD11	1.82	0.62
1:D:283:LYS:HZ3	1:D:283:LYS:HB3	1.65	0.61
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:K:11:SER:HA	1:K:135:PRO:HG3	1.84	0.60

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:11:SER:HA	1:A:135:PRO:HG3	1.84	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:G:138:MET:HE3	1:G:138:MET:HA	1.85	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:A:81:SER:HB2	1:E:55:THR:CG2	2.33	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: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:H:107:ARG:NH1	1:H:129:LEU:HD11	2.18	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:J:138:MET:HE3	1:J: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:I:107:ARG:HH11	1:I:129:LEU:HD11	1.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:138:MET:HE3	1:C:138:MET:HA	1.88	0.55
1:E:138:MET:HA	1:E:138:MET:CE	2.36	0.55
1:L:138:MET:HE3	1:L:138:MET:HA	1.88	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:D:138:MET:HA	1:D:138:MET:HE3	1.88	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:MET:HA	1:I:138:MET:HE3	1.89	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:F:283:LYS:HZ3	1:F:283:LYS:HB3	1.74	0.53
1:H:157:SER:HB3	1:H:182:ASP:HB3	1.90	0.53
1:I:283:LYS:HZ3	1:I:283:LYS:HB3	1.74	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
1:C:45:ARG:NH1	1:C:45:ARG:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:HIS:CE1	1:K:283:LYS:HZ2	2.27	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:L:283:LYS:HB3	1:L:283:LYS:HZ3	1.74	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:G:283:LYS:HZ2	1:I:86:HIS:CE1	2.28	0.52
1:B:138:MET:CE	1:B:138:MET:HA	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:K:138:MET:HA	1:K:138:MET:HE3	1.92	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:E:138:MET:HA	1:E:138:MET:HE3	1.92	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:A:86:HIS:CE1	1:E:283:LYS:HZ2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:86:HIS:CE1	1:J:283:LYS:HZ2	2.29	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:C:283:LYS:HZ2	1:K:86:HIS:CE1	2.30	0.49
1:A:53:GLU:HG3	1:A:106:TYR:OH	2.12	0.49
1:B:283:LYS:HZ2	1:J:86:HIS:CE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:86:HIS:CE1	1:H:283:LYS:HZ2	2.30	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
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:A:138:MET:HA	1:A:138:MET:HE3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:273:CYS:SG	1:D:273:CYS:O	2.72	0.48
1:K:273:CYS:SG	1:K:273:CYS:O	2.72	0.48
1:K:280:SER:O	1:K:286:LYS:HG3	2.13	0.48
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: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: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: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

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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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:283:LYS:HB3	1:A:283:LYS:HZ3	1.80	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	1:I:283:LYS:NZ	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:HB3	1:F:283:LYS:NZ	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:283:LYS:HB3	1:L:283:LYS:NZ	2.31	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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:283:LYS:HZ2	1:L:86:HIS:CE1	2.35	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:F:53:GLU:HB2	1:F:108:GLY:HA2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:288:ILE:HD13	1:A:299:ILE:HD11	2.02	0.42
1:B:138:MET:HE2	1:B:172:LEU:HA	2.00	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:F:288:ILE:HD13	1:F:299:ILE:HD11	2.02	0.42
1:H:138:MET:HE2	1:H:172:LEU:HA	2.00	0.42
1:I:288:ILE:HD13	1:I:299:ILE:HD11	2.02	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:H:334:ASP:O	1:K:45:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:272:HIS:H	1:I:316:GLN:HE22	1.67	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:I:111:GLN:HA	1:I:130:THR:HG21	2.02	0.42
1:L:240:VAL:HA	1:L:243:TRP:CD1	2.55	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: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:A:10:LEU:HD22	1:A:10:LEU:O	2.20	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
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: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: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:L:4:MET:SD	1:L:19:GLU:OE1	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:138:MET:HA	1:F:138:MET:HE3	2.02	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
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:138:MET:HE2	1:F:172:LEU:HA	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:LYS:HB3	1:C:283:LYS:HZ3	1.86	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
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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:34:LYS:NZ	1:B:69:ASP:OD2	2.53	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
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:H:34:LYS:NZ	1:H:69:ASP:OD2	2.53	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:34:LYS:NZ	1:F:69:ASP:OD2	2.53	0.40
1:F:243:TRP:CZ3	1:F:288:ILE:HG12	2.57	0.40

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
1	B	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
1	C	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
1	D	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
1	E	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
1	G	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
1	H	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
1	I	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
1	J	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
1	K	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
1	L	333/335 (99%)	270 (81%)	45 (14%)	18 (5%)	2	11
All	All	3996/4020 (99%)	3240 (81%)	540 (14%)	216 (5%)	2	11

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
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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Mol	Chain	Res	Type
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 [i](#)

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%)	235 (83%)	49 (17%)	2	10
1	B	284/284 (100%)	235 (83%)	49 (17%)	2	10
1	C	284/284 (100%)	235 (83%)	49 (17%)	2	10
1	D	284/284 (100%)	235 (83%)	49 (17%)	2	10
1	E	284/284 (100%)	235 (83%)	49 (17%)	2	10
1	F	284/284 (100%)	235 (83%)	49 (17%)	2	10
1	G	284/284 (100%)	235 (83%)	49 (17%)	2	10
1	H	284/284 (100%)	235 (83%)	49 (17%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	284/284 (100%)	235 (83%)	49 (17%)	2	10
1	J	284/284 (100%)	235 (83%)	49 (17%)	2	10
1	K	284/284 (100%)	235 (83%)	49 (17%)	2	10
1	L	284/284 (100%)	235 (83%)	49 (17%)	2	10
All	All	3408/3408 (100%)	2820 (83%)	588 (17%)	2	10

All (588) 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	46	LYS
1	A	48	ILE
1	A	55	THR
1	A	84	ILE
1	A	90	MET
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
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	232	VAL
1	A	236	MET
1	A	239	PRO
1	A	251	LEU
1	A	257	MET
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	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	46	LYS
1	B	48	ILE
1	B	55	THR
1	B	84	ILE
1	B	90	MET
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	265	ASN
1	B	281	GLU
1	B	282	THR
1	B	283	LYS
1	B	293	PRO
1	B	295	LEU
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
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	46	LYS
1	C	48	ILE
1	C	55	THR
1	C	84	ILE
1	C	90	MET
1	C	93	THR
1	C	107	ARG
1	C	111	GLN
1	C	124	PRO
1	C	129	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	265	ASN
1	C	281	GLU
1	C	282	THR
1	C	283	LYS
1	C	293	PRO
1	C	295	LEU
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	46	LYS
1	D	48	ILE
1	D	55	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	84	ILE
1	D	90	MET
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
1	D	251	LEU
1	D	257	MET
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	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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	27	SER
1	E	30	LEU
1	E	38	THR
1	E	45	ARG
1	E	46	LYS
1	E	48	ILE
1	E	55	THR
1	E	84	ILE
1	E	90	MET
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
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	265	ASN
1	E	281	GLU
1	E	282	THR
1	E	283	LYS
1	E	293	PRO
1	E	295	LEU
1	E	304	ASP
1	E	307	GLU
1	E	315	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	46	LYS
1	F	48	ILE
1	F	55	THR
1	F	84	ILE
1	F	90	MET
1	F	93	THR
1	F	107	ARG
1	F	111	GLN
1	F	124	PRO
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	265	ASN
1	F	281	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	282	THR
1	F	283	LYS
1	F	293	PRO
1	F	295	LEU
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
1	G	45	ARG
1	G	46	LYS
1	G	48	ILE
1	G	55	THR
1	G	84	ILE
1	G	90	MET
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	232	VAL
1	G	236	MET
1	G	239	PRO
1	G	251	LEU
1	G	257	MET
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	304	ASP
1	G	307	GLU
1	G	315	GLU
1	G	320	ARG
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	46	LYS
1	H	48	ILE
1	H	55	THR
1	H	84	ILE
1	H	90	MET
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	265	ASN
1	H	281	GLU
1	H	282	THR
1	H	283	LYS
1	H	293	PRO
1	H	295	LEU
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	46	LYS
1	I	48	ILE
1	I	55	THR
1	I	84	ILE
1	I	90	MET
1	I	93	THR
1	I	107	ARG
1	I	111	GLN
1	I	124	PRO
1	I	129	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
1	I	232	VAL
1	I	236	MET
1	I	239	PRO
1	I	251	LEU
1	I	257	MET
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	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	46	LYS
1	J	48	ILE
1	J	55	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	J	84	ILE
1	J	90	MET
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
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	265	ASN
1	J	281	GLU
1	J	282	THR
1	J	283	LYS
1	J	293	PRO
1	J	295	LEU
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	27	SER
1	K	30	LEU
1	K	38	THR
1	K	45	ARG
1	K	46	LYS
1	K	48	ILE
1	K	55	THR
1	K	84	ILE
1	K	90	MET
1	K	93	THR
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	265	ASN
1	K	281	GLU
1	K	282	THR
1	K	283	LYS
1	K	293	PRO
1	K	295	LEU
1	K	304	ASP
1	K	307	GLU
1	K	315	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
1	L	27	SER
1	L	30	LEU
1	L	38	THR
1	L	45	ARG
1	L	46	LYS
1	L	48	ILE
1	L	55	THR
1	L	84	ILE
1	L	90	MET
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	265	ASN
1	L	281	GLU

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Mol	Chain	Res	Type
1	L	282	THR
1	L	283	LYS
1	L	293	PRO
1	L	295	LEU
1	L	304	ASP
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 (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	47	ASN
1	A	80	ASN
1	A	86	HIS
1	A	127	ASN
1	A	229	HIS
1	A	272	HIS
1	A	278	HIS
1	A	311	ASN
1	A	316	GLN
1	B	8	ASN
1	B	47	ASN
1	B	80	ASN
1	B	86	HIS
1	B	127	ASN
1	B	229	HIS
1	B	272	HIS
1	B	278	HIS
1	B	311	ASN
1	B	316	GLN
1	C	8	ASN
1	C	47	ASN
1	C	80	ASN
1	C	86	HIS
1	C	127	ASN
1	C	229	HIS
1	C	272	HIS
1	C	278	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	311	ASN
1	C	316	GLN
1	D	8	ASN
1	D	47	ASN
1	D	80	ASN
1	D	86	HIS
1	D	127	ASN
1	D	229	HIS
1	D	272	HIS
1	D	278	HIS
1	D	311	ASN
1	D	316	GLN
1	E	8	ASN
1	E	47	ASN
1	E	80	ASN
1	E	86	HIS
1	E	127	ASN
1	E	229	HIS
1	E	272	HIS
1	E	278	HIS
1	E	311	ASN
1	E	316	GLN
1	F	8	ASN
1	F	47	ASN
1	F	80	ASN
1	F	86	HIS
1	F	127	ASN
1	F	229	HIS
1	F	272	HIS
1	F	278	HIS
1	F	311	ASN
1	F	316	GLN
1	G	5	HIS
1	G	8	ASN
1	G	47	ASN
1	G	80	ASN
1	G	86	HIS
1	G	127	ASN
1	G	229	HIS
1	G	272	HIS
1	G	278	HIS
1	G	311	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	316	GLN
1	H	8	ASN
1	H	47	ASN
1	H	80	ASN
1	H	86	HIS
1	H	127	ASN
1	H	229	HIS
1	H	272	HIS
1	H	278	HIS
1	H	311	ASN
1	H	316	GLN
1	I	8	ASN
1	I	47	ASN
1	I	80	ASN
1	I	86	HIS
1	I	127	ASN
1	I	229	HIS
1	I	272	HIS
1	I	278	HIS
1	I	311	ASN
1	I	316	GLN
1	J	5	HIS
1	J	8	ASN
1	J	47	ASN
1	J	80	ASN
1	J	86	HIS
1	J	127	ASN
1	J	229	HIS
1	J	272	HIS
1	J	278	HIS
1	J	311	ASN
1	J	316	GLN
1	K	8	ASN
1	K	47	ASN
1	K	80	ASN
1	K	86	HIS
1	K	127	ASN
1	K	229	HIS
1	K	272	HIS
1	K	278	HIS
1	K	311	ASN
1	K	316	GLN

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Mol	Chain	Res	Type
1	L	8	ASN
1	L	47	ASN
1	L	80	ASN
1	L	86	HIS
1	L	127	ASN
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 monosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.