



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:19 PM UTC

PDB ID : 1SMR / pdb_00001smr
Title : The 3-d structure of mouse submaxillary renin complexed with a decapeptide inhibitor ch-66 based on the 4-16 fragment of rat angiotensinogen
Authors : Dealwis, C.G.; Blundell, T.L.
Deposited on : 1992-03-11
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

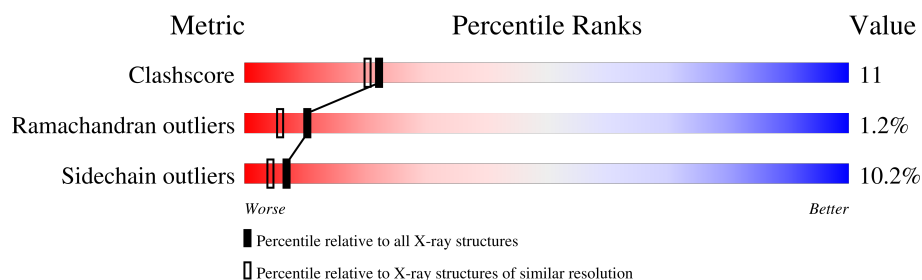
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	33% 50% 13% ..
1	C	335	33% 48% 14% ..
1	E	335	33% 49% 14% ..
1	G	335	33% 48% 15% ..
2	B	9	44% 22% 22% 11%
2	D	9	33% 33% 22% 11%
2	F	9	44% 22% 22% 11%
2	H	9	44% 22% 22% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10560 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 RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2511	1609	409	481	12			
1	C	331	Total	C	N	O	S	0	0	0
			2511	1609	409	481	12			
1	E	331	Total	C	N	O	S	0	0	0
			2511	1609	409	481	12			
1	G	331	Total	C	N	O	S	0	0	0
			2511	1609	409	481	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	GLN	GLU	conflict	UNP P00796
A	173	GLN	GLU	conflict	UNP P00796
C	106	GLN	GLU	conflict	UNP P00796
C	173	GLN	GLU	conflict	UNP P00796
E	106	GLN	GLU	conflict	UNP P00796
E	173	GLN	GLU	conflict	UNP P00796
G	106	GLN	GLU	conflict	UNP P00796
G	173	GLN	GLU	conflict	UNP P00796

- Molecule 2 is a protein called INHIBITOR CH-66.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			90	65	12	13			
2	D	9	Total	C	N	O	0	0	0
			90	65	12	13			
2	F	9	Total	C	N	O	0	0	0
			90	65	12	13			
2	H	9	Total	C	N	O	0	0	0
			90	65	12	13			

- Molecule 3 is water.

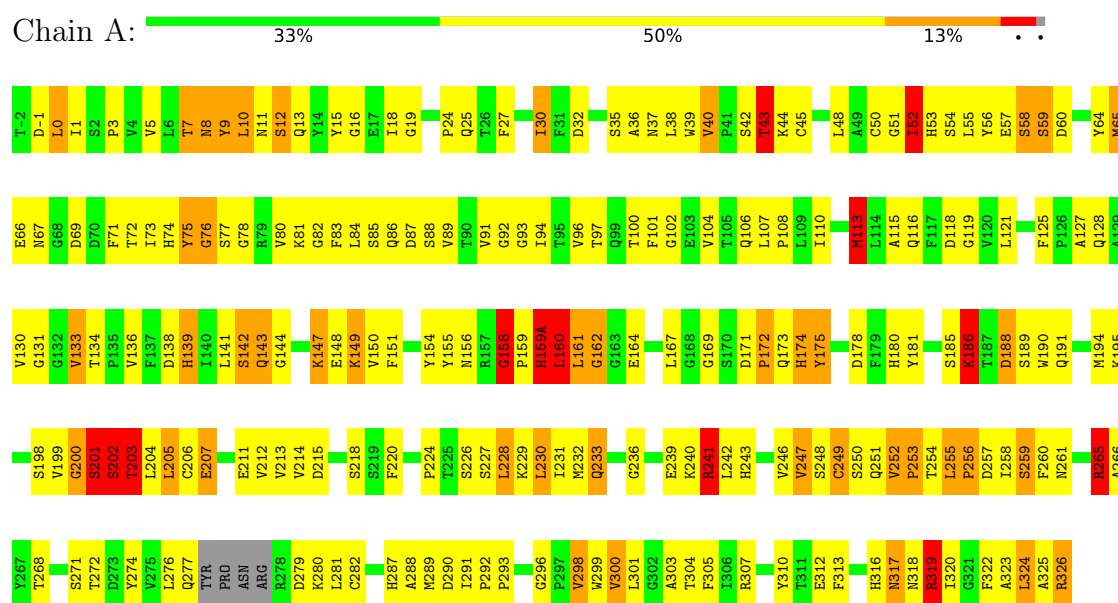
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total 148	O 148	0	0
3	B	5	Total 5	O 5	0	0
3	C	3	Total 3	O 3	0	0

3 Residue-property plots

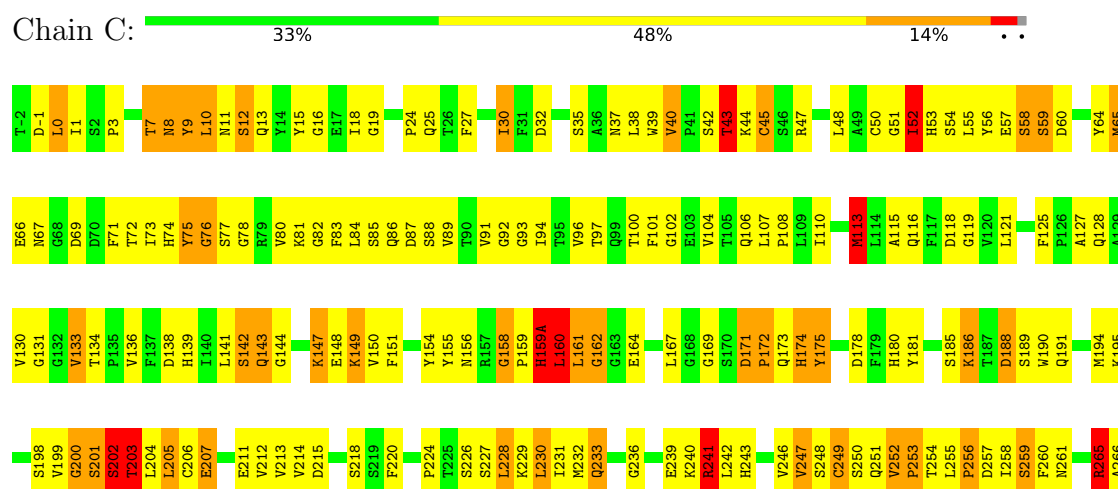
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: RENIN

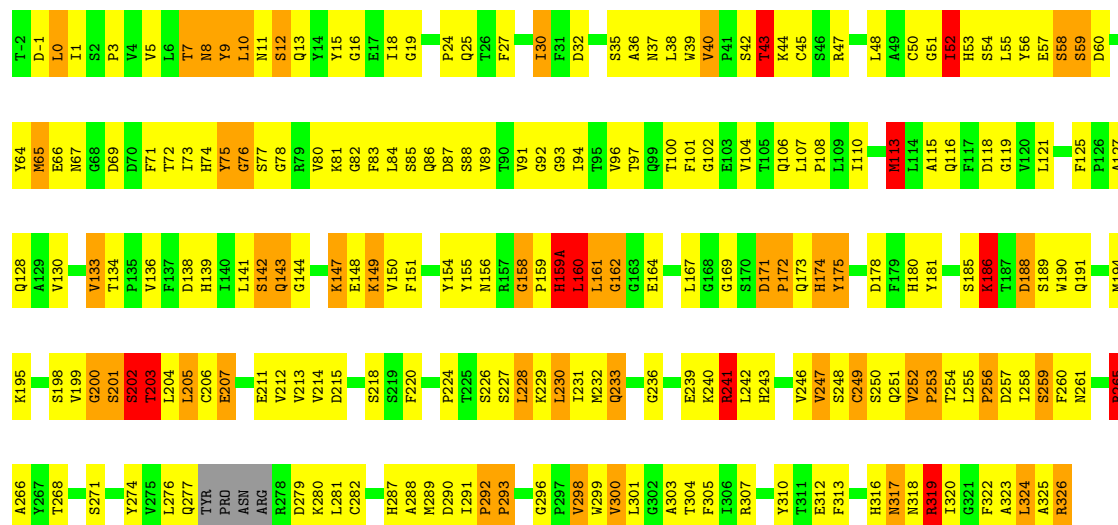


• Molecule 1: RENIN

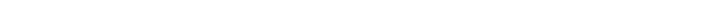


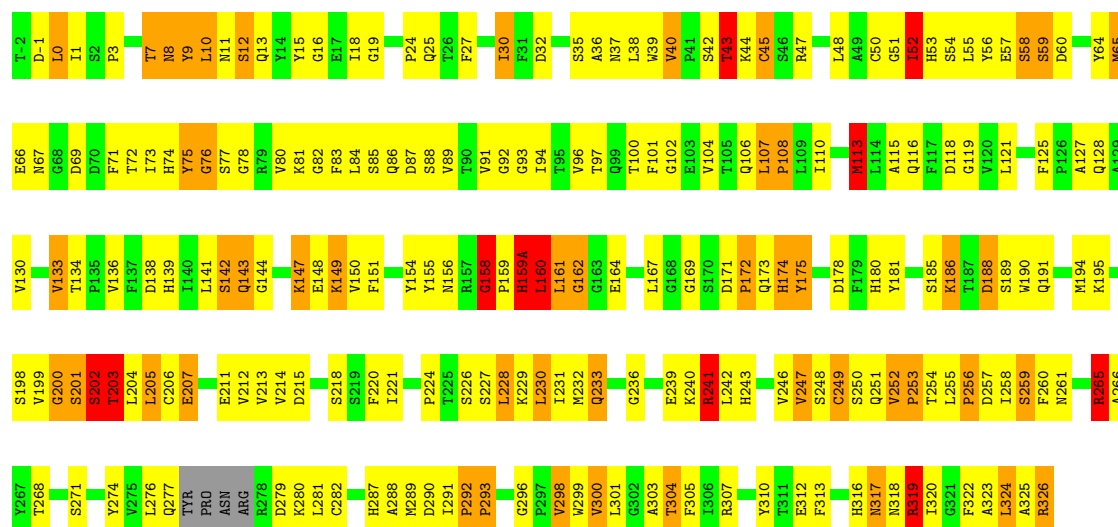
- Molecule 1: RENIN

Chain E:  33% 49% 14% 4%

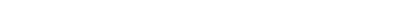


- Molecule 1: RENIN

Chain G:  33% 48% 15% 4%

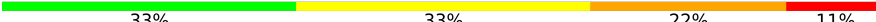


- Molecule 2: INHIBITOR CH-66

Chain B:  44% 22% 22% 11%



- Molecule 2: INHIBITOR CH-66

Chain D:  33% 33% 22% 11%



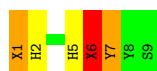
● Molecule 2: INHIBITOR CH-66

Chain F:  44% 22% 22% 11%



● Molecule 2: INHIBITOR CH-66

Chain H:  44% 22% 22% 11%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.34Å 117.76Å 85.88Å 90.00° 101.18° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10560	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.82	51/2572 (2.0%)	3.00	334/3500 (9.5%)
1	C	1.82	50/2572 (1.9%)	3.00	334/3500 (9.5%)
1	E	1.82	51/2572 (2.0%)	3.01	336/3500 (9.6%)
1	G	1.82	50/2572 (1.9%)	3.00	332/3500 (9.5%)
2	B	2.29	4/72 (5.6%)	2.69	7/96 (7.3%)
2	D	2.30	5/72 (6.9%)	2.69	7/96 (7.3%)
2	F	2.29	4/72 (5.6%)	2.69	7/96 (7.3%)
2	H	2.30	4/72 (5.6%)	2.69	7/96 (7.3%)
All	All	1.83	219/10576 (2.1%)	3.00	1364/14384 (9.5%)

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	3
1	C	0	3
1	E	0	3
1	G	0	3
2	B	0	2
2	D	0	2
2	F	0	2
2	H	0	2
All	All	0	20

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	42	SER	CB-OG	-12.89	1.16	1.42
1	G	42	SER	CB-OG	-12.86	1.16	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	SER	CB-OG	-12.85	1.16	1.42
1	C	42	SER	CB-OG	-12.84	1.16	1.42
1	G	180	HIS	CE1-NE2	12.20	1.44	1.32
1	C	180	HIS	CE1-NE2	12.20	1.44	1.32
1	E	180	HIS	CE1-NE2	12.19	1.44	1.32
1	A	180	HIS	CE1-NE2	12.19	1.44	1.32
1	G	43	THR	CB-OG1	-11.66	1.25	1.43
1	C	43	THR	CB-OG1	-11.65	1.25	1.43
1	A	43	THR	CB-OG1	-11.65	1.25	1.43
1	E	43	THR	CB-OG1	-11.62	1.25	1.43
2	D	5	HIS	CE1-NE2	9.90	1.42	1.32
2	H	5	HIS	CE1-NE2	9.88	1.42	1.32
2	B	5	HIS	CE1-NE2	9.87	1.42	1.32
2	F	5	HIS	CE1-NE2	9.87	1.42	1.32
1	E	78	GLY	N-CA	9.26	1.54	1.45
1	A	78	GLY	N-CA	9.25	1.54	1.45
1	C	78	GLY	N-CA	9.24	1.54	1.45
1	G	78	GLY	N-CA	9.23	1.54	1.45
1	E	243	HIS	CE1-NE2	9.21	1.41	1.32
1	A	243	HIS	CE1-NE2	9.16	1.41	1.32
1	C	243	HIS	CE1-NE2	9.15	1.41	1.32
1	G	243	HIS	CE1-NE2	9.12	1.41	1.32
1	C	88	SER	C-N	-8.44	1.22	1.33
1	A	88	SER	C-N	-8.43	1.22	1.33
1	E	88	SER	C-N	-8.43	1.22	1.33
1	G	88	SER	C-N	-8.42	1.22	1.33
1	E	243	HIS	ND1-CE1	8.34	1.40	1.32
1	G	243	HIS	ND1-CE1	8.28	1.40	1.32
1	A	243	HIS	ND1-CE1	8.28	1.40	1.32
1	C	243	HIS	ND1-CE1	8.26	1.40	1.32
1	G	39	TRP	NE1-CE2	-8.09	1.28	1.37
1	A	39	TRP	NE1-CE2	-8.07	1.28	1.37
1	E	139	HIS	ND1-CE1	8.06	1.40	1.32
1	C	39	TRP	NE1-CE2	-8.04	1.28	1.37
1	C	139	HIS	ND1-CE1	8.03	1.40	1.32
1	E	39	TRP	NE1-CE2	-8.03	1.28	1.37
1	G	139	HIS	ND1-CE1	8.00	1.40	1.32
1	A	139	HIS	ND1-CE1	8.00	1.40	1.32
1	C	326	ARG	C-OXT	7.40	1.38	1.23
1	A	326	ARG	C-OXT	7.39	1.38	1.23
1	E	326	ARG	C-OXT	7.39	1.38	1.23
1	G	326	ARG	C-OXT	7.36	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	PRO	C-O	7.28	1.30	1.24
1	E	293	PRO	C-O	7.28	1.30	1.24
1	G	325	ALA	C-N	-7.26	1.23	1.33
1	A	325	ALA	C-N	-7.25	1.23	1.33
1	E	325	ALA	C-N	-7.24	1.23	1.33
1	C	293	PRO	C-O	7.23	1.30	1.24
1	G	293	PRO	C-O	7.22	1.30	1.24
1	C	325	ALA	C-N	-7.22	1.23	1.33
2	D	5	HIS	CD2-NE2	7.15	1.45	1.37
2	F	5	HIS	CD2-NE2	7.14	1.45	1.37
2	H	5	HIS	CD2-NE2	7.08	1.45	1.37
2	B	5	HIS	CD2-NE2	7.08	1.45	1.37
1	C	51	GLY	C-N	-7.07	1.26	1.33
1	A	51	GLY	C-N	-7.05	1.26	1.33
1	G	51	GLY	C-N	-7.02	1.26	1.33
1	C	268	THR	C-O	-7.02	1.15	1.24
1	E	51	GLY	C-N	-7.00	1.26	1.33
1	A	268	THR	C-O	-6.96	1.15	1.24
1	E	268	THR	C-O	-6.95	1.15	1.24
1	A	19	GLY	CA-C	6.95	1.57	1.52
1	E	19	GLY	CA-C	6.94	1.57	1.52
1	G	268	THR	C-O	-6.94	1.15	1.24
1	G	19	GLY	CA-C	6.94	1.57	1.52
1	C	19	GLY	CA-C	6.93	1.57	1.52
1	G	288	ALA	C-O	-6.77	1.15	1.23
2	H	2	HIS	ND1-CE1	6.77	1.39	1.32
1	C	288	ALA	C-O	-6.75	1.15	1.23
1	A	288	ALA	C-O	-6.72	1.15	1.23
2	B	2	HIS	ND1-CE1	6.72	1.39	1.32
1	E	288	ALA	C-O	-6.71	1.15	1.23
1	E	7	THR	C-N	-6.70	1.24	1.33
1	A	7	THR	C-N	-6.69	1.24	1.33
1	G	7	THR	C-N	-6.68	1.24	1.33
2	D	2	HIS	ND1-CE1	6.67	1.39	1.32
2	F	2	HIS	ND1-CE1	6.66	1.39	1.32
1	C	7	THR	C-N	-6.63	1.24	1.33
2	D	2	HIS	CE1-NE2	6.61	1.39	1.32
2	B	2	HIS	CE1-NE2	6.58	1.39	1.32
2	H	2	HIS	CE1-NE2	6.58	1.39	1.32
2	F	2	HIS	CE1-NE2	6.57	1.39	1.32
1	E	303	ALA	C-N	-6.52	1.25	1.33
1	E	162	GLY	CA-C	6.50	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	ALA	C-N	-6.49	1.25	1.33
1	G	162	GLY	CA-C	6.49	1.60	1.51
1	A	162	GLY	CA-C	6.49	1.60	1.51
1	C	162	GLY	CA-C	6.48	1.60	1.51
1	G	303	ALA	C-N	-6.46	1.25	1.33
1	C	303	ALA	C-N	-6.46	1.25	1.33
1	C	313	PHE	C-O	-6.41	1.16	1.24
1	A	313	PHE	C-O	-6.39	1.16	1.24
1	E	180	HIS	CG-CD2	6.36	1.42	1.35
1	G	313	PHE	C-O	-6.35	1.16	1.24
1	E	313	PHE	C-O	-6.34	1.16	1.24
1	A	180	HIS	CG-CD2	6.32	1.42	1.35
1	C	180	HIS	CG-CD2	6.29	1.42	1.35
1	G	180	HIS	CG-CD2	6.24	1.42	1.35
1	C	190	TRP	NE1-CE2	-6.23	1.30	1.37
1	A	190	TRP	NE1-CE2	-6.23	1.30	1.37
1	G	190	TRP	NE1-CE2	-6.22	1.30	1.37
1	E	190	TRP	NE1-CE2	-6.22	1.30	1.37
1	C	100	THR	C-O	6.19	1.31	1.24
1	G	261	ASN	CG-OD1	6.19	1.35	1.23
1	A	261	ASN	CG-OD1	6.16	1.35	1.23
1	E	100	THR	C-O	6.15	1.31	1.24
1	A	100	THR	C-O	6.15	1.31	1.24
1	C	261	ASN	CG-OD1	6.15	1.35	1.23
1	C	74	HIS	ND1-CE1	6.15	1.38	1.32
1	E	74	HIS	ND1-CE1	6.15	1.38	1.32
1	G	100	THR	C-O	6.15	1.31	1.24
1	E	261	ASN	CG-OD1	6.13	1.35	1.23
1	A	74	HIS	ND1-CE1	6.11	1.38	1.32
1	C	180	HIS	ND1-CE1	6.11	1.38	1.32
1	G	55	LEU	C-O	-6.11	1.16	1.24
1	E	316	HIS	CE1-NE2	6.10	1.38	1.32
1	A	180	HIS	ND1-CE1	6.09	1.38	1.32
1	E	180	HIS	ND1-CE1	6.07	1.38	1.32
1	G	180	HIS	ND1-CE1	6.07	1.38	1.32
1	G	74	HIS	ND1-CE1	6.06	1.38	1.32
1	A	316	HIS	CE1-NE2	6.06	1.38	1.32
1	G	316	HIS	CE1-NE2	6.05	1.38	1.32
1	C	74	HIS	CE1-NE2	6.05	1.38	1.32
1	C	316	HIS	CE1-NE2	6.04	1.38	1.32
1	A	55	LEU	C-O	-6.03	1.16	1.24
1	C	287	HIS	CE1-NE2	6.03	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	287	HIS	CE1-NE2	6.03	1.38	1.32
1	C	55	LEU	C-O	-6.01	1.16	1.24
1	E	55	LEU	C-O	-6.00	1.16	1.24
1	G	74	HIS	CE1-NE2	5.99	1.38	1.32
1	A	287	HIS	CE1-NE2	5.99	1.38	1.32
1	C	252	VAL	CA-CB	-5.97	1.51	1.54
1	A	74	HIS	CE1-NE2	5.94	1.38	1.32
1	A	252	VAL	CA-CB	-5.93	1.51	1.54
1	E	287	HIS	CE1-NE2	5.92	1.38	1.32
1	E	19	GLY	N-CA	5.92	1.52	1.46
1	E	74	HIS	CE1-NE2	5.92	1.38	1.32
1	G	37	ASN	C-N	-5.92	1.25	1.33
1	E	252	VAL	CA-CB	-5.91	1.51	1.54
1	C	19	GLY	N-CA	5.91	1.52	1.46
1	C	37	ASN	C-N	-5.90	1.25	1.33
1	A	37	ASN	C-N	-5.89	1.25	1.33
1	A	19	GLY	N-CA	5.87	1.52	1.46
1	E	37	ASN	C-N	-5.87	1.25	1.33
1	G	252	VAL	CA-CB	-5.87	1.51	1.54
1	G	19	GLY	N-CA	5.86	1.52	1.46
1	C	173	GLN	CD-OE1	5.84	1.34	1.23
1	A	173	GLN	CD-OE1	5.81	1.34	1.23
1	G	173	GLN	CD-OE1	5.81	1.34	1.23
1	E	173	GLN	CD-OE1	5.79	1.34	1.23
1	A	316	HIS	ND1-CE1	5.59	1.38	1.32
1	G	316	HIS	ND1-CE1	5.58	1.38	1.32
1	E	316	HIS	ND1-CE1	5.55	1.38	1.32
1	C	316	HIS	ND1-CE1	5.53	1.38	1.32
1	E	290	ASP	C-N	-5.49	1.27	1.33
1	G	290	ASP	C-N	-5.48	1.27	1.33
1	C	290	ASP	C-N	-5.48	1.27	1.33
1	A	290	ASP	C-N	-5.47	1.27	1.33
1	C	42	SER	C-N	-5.43	1.26	1.34
1	C	89	VAL	C-O	-5.43	1.18	1.24
1	E	89	VAL	C-O	-5.42	1.18	1.24
1	G	42	SER	C-N	-5.42	1.26	1.34
1	G	89	VAL	C-O	-5.42	1.18	1.24
1	A	42	SER	C-N	-5.41	1.26	1.34
1	A	89	VAL	C-O	-5.40	1.18	1.24
1	C	317	ASN	CG-OD1	5.38	1.33	1.23
1	E	-1	ASP	C-N	-5.38	1.25	1.33
1	E	42	SER	C-N	-5.37	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-1	ASP	C-N	-5.37	1.25	1.33
1	A	317	ASN	CG-OD1	5.37	1.33	1.23
1	E	317	ASN	CG-OD1	5.36	1.33	1.23
1	C	-1	ASP	C-N	-5.34	1.25	1.33
1	G	317	ASN	CG-OD1	5.32	1.33	1.23
1	G	-1	ASP	C-N	-5.29	1.25	1.33
1	C	243	HIS	CG-CD2	5.29	1.41	1.35
1	C	233	GLN	CD-OE1	5.28	1.33	1.23
1	E	243	HIS	CG-CD2	5.27	1.41	1.35
1	G	233	GLN	CD-OE1	5.26	1.33	1.23
1	A	233	GLN	CD-OE1	5.24	1.33	1.23
1	A	243	HIS	CG-CD2	5.24	1.41	1.35
1	E	233	GLN	CD-OE1	5.21	1.33	1.23
1	G	243	HIS	CG-CD2	5.19	1.41	1.35
1	E	8	ASN	CG-OD1	5.19	1.33	1.23
1	G	8	ASN	CG-OD1	5.19	1.33	1.23
1	C	74	HIS	CG-CD2	5.19	1.41	1.35
1	A	74	HIS	CG-CD2	5.17	1.41	1.35
1	A	8	ASN	CG-OD1	5.16	1.33	1.23
1	G	74	HIS	CG-CD2	5.15	1.41	1.35
1	C	8	ASN	CG-OD1	5.15	1.33	1.23
1	G	143	GLN	CD-OE1	5.14	1.33	1.23
1	E	74	HIS	CG-CD2	5.13	1.41	1.35
1	E	143	GLN	CD-OE1	5.13	1.33	1.23
1	A	143	GLN	CD-OE1	5.12	1.33	1.23
1	C	143	GLN	CD-OE1	5.09	1.33	1.23
1	C	75	TYR	C-O	5.09	1.30	1.23
1	E	251	GLN	CD-OE1	5.08	1.33	1.23
1	C	116	GLN	CD-OE1	5.08	1.33	1.23
1	G	251	GLN	CD-OE1	5.08	1.33	1.23
1	E	71	PHE	C-N	-5.08	1.26	1.33
1	E	75	TYR	C-O	5.07	1.30	1.23
1	A	251	GLN	CD-OE1	5.07	1.33	1.23
1	C	71	PHE	C-N	-5.07	1.26	1.33
1	A	75	TYR	C-O	5.06	1.30	1.23
1	E	116	GLN	CD-OE1	5.06	1.33	1.23
1	G	116	GLN	CD-OE1	5.06	1.33	1.23
1	C	251	GLN	CD-OE1	5.05	1.33	1.23
1	E	36	ALA	C-O	-5.05	1.17	1.24
1	A	116	GLN	CD-OE1	5.05	1.33	1.23
1	G	75	TYR	C-O	5.04	1.30	1.23
1	A	71	PHE	C-N	-5.04	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	3	PRO	C-N	-5.03	1.26	1.33
1	A	36	ALA	C-O	-5.03	1.17	1.24
1	G	71	PHE	C-N	-5.03	1.26	1.33
2	D	4	PHE	C-O	-5.02	1.18	1.24
1	C	3	PRO	C-N	-5.01	1.26	1.33
1	G	36	ALA	C-O	-5.01	1.17	1.24
1	A	3	PRO	C-N	-5.00	1.26	1.33

All (1364) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	160	LEU	O-C-N	19.75	147.76	122.68
1	A	160	LEU	O-C-N	19.74	147.74	122.68
1	G	160	LEU	O-C-N	19.73	147.74	122.68
1	C	160	LEU	O-C-N	19.73	147.74	122.68
1	C	43	THR	CA-CB-OG1	15.66	133.09	109.60
1	G	43	THR	CA-CB-OG1	15.66	133.09	109.60
1	A	43	THR	CA-CB-OG1	15.65	133.08	109.60
1	E	43	THR	CA-CB-OG1	15.63	133.05	109.60
1	C	42	SER	CA-CB-OG	15.12	141.33	111.10
1	E	42	SER	CA-CB-OG	15.11	141.33	111.10
1	A	42	SER	CA-CB-OG	15.11	141.31	111.10
1	G	42	SER	CA-CB-OG	15.09	141.27	111.10
1	G	203	THR	CA-C-N	15.07	145.22	121.26
1	G	203	THR	C-N-CA	15.07	145.22	121.26
1	A	203	THR	CA-C-N	15.07	145.22	121.26
1	A	203	THR	C-N-CA	15.07	145.22	121.26
1	E	203	THR	CA-C-N	15.06	145.21	121.26
1	E	203	THR	C-N-CA	15.06	145.21	121.26
1	C	203	THR	CA-C-N	15.05	145.19	121.26
1	C	203	THR	C-N-CA	15.05	145.19	121.26
1	C	18	ILE	CA-C-N	-15.00	111.38	122.33
1	C	18	ILE	C-N-CA	-15.00	111.38	122.33
1	E	18	ILE	CA-C-N	-14.98	111.39	122.33
1	E	18	ILE	C-N-CA	-14.98	111.39	122.33
1	A	18	ILE	CA-C-N	-14.97	111.40	122.33
1	A	18	ILE	C-N-CA	-14.97	111.40	122.33
1	G	18	ILE	CA-C-N	-14.95	111.42	122.33
1	G	18	ILE	C-N-CA	-14.95	111.42	122.33
1	C	319	ARG	CD-NE-CZ	13.87	143.81	124.40
1	E	319	ARG	CD-NE-CZ	13.87	143.82	124.40
1	G	319	ARG	CD-NE-CZ	13.86	143.81	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ARG	CD-NE-CZ	13.86	143.80	124.40
1	A	171	ASP	CA-C-N	13.38	133.21	119.56
1	A	171	ASP	C-N-CA	13.38	133.21	119.56
1	C	171	ASP	CA-C-N	13.38	133.21	119.56
1	C	171	ASP	C-N-CA	13.38	133.21	119.56
1	E	171	ASP	CA-C-N	13.38	133.21	119.56
1	E	171	ASP	C-N-CA	13.38	133.21	119.56
1	G	171	ASP	CA-C-N	13.35	133.18	119.56
1	G	171	ASP	C-N-CA	13.35	133.18	119.56
1	A	277	GLN	CA-C-N	13.18	145.41	121.70
1	A	277	GLN	C-N-CA	13.18	145.41	121.70
1	G	277	GLN	CA-C-N	13.17	145.41	121.70
1	G	277	GLN	C-N-CA	13.17	145.41	121.70
1	C	277	GLN	CA-C-N	13.16	145.39	121.70
1	C	277	GLN	C-N-CA	13.16	145.39	121.70
1	E	277	GLN	CA-C-N	13.15	145.38	121.70
1	E	277	GLN	C-N-CA	13.15	145.38	121.70
1	G	52	ILE	N-CA-CB	-12.41	97.56	112.33
1	A	52	ILE	N-CA-CB	-12.40	97.57	112.33
1	C	52	ILE	N-CA-CB	-12.40	97.57	112.33
1	E	52	ILE	N-CA-CB	-12.38	97.59	112.33
1	G	7	THR	CA-C-O	-12.20	107.08	120.38
1	A	7	THR	CA-C-O	-12.20	107.09	120.38
1	E	7	THR	CA-C-O	-12.19	107.09	120.38
1	C	7	THR	CA-C-O	-12.15	107.13	120.38
1	C	256	PRO	CA-C-O	12.04	138.04	122.15
1	A	256	PRO	CA-C-O	12.00	137.99	122.15
1	G	256	PRO	CA-C-O	12.00	137.99	122.15
1	E	256	PRO	CA-C-O	12.00	137.99	122.15
1	C	326	ARG	CD-NE-CZ	11.90	141.07	124.40
1	A	326	ARG	CD-NE-CZ	11.88	141.03	124.40
1	E	326	ARG	CD-NE-CZ	11.88	141.03	124.40
1	G	326	ARG	CD-NE-CZ	11.88	141.03	124.40
1	E	43	THR	N-CA-CB	-11.86	91.96	110.22
1	A	43	THR	N-CA-CB	-11.83	92.00	110.22
1	C	43	THR	N-CA-CB	-11.83	92.01	110.22
1	G	43	THR	N-CA-CB	-11.82	92.01	110.22
1	A	13	GLN	OE1-CD-NE2	-11.64	110.96	122.60
1	C	13	GLN	OE1-CD-NE2	-11.63	110.97	122.60
1	E	13	GLN	OE1-CD-NE2	-11.63	110.97	122.60
1	G	13	GLN	OE1-CD-NE2	-11.62	110.98	122.60
1	G	301	LEU	CA-C-O	-11.54	108.92	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	301	LEU	CA-C-O	-11.51	108.95	120.92
1	A	301	LEU	CA-C-O	-11.50	108.96	120.92
1	C	301	LEU	CA-C-O	-11.48	108.98	120.92
1	E	144	GLY	CA-C-N	-11.20	108.52	121.85
1	E	144	GLY	C-N-CA	-11.20	108.52	121.85
1	G	144	GLY	CA-C-N	-11.19	108.54	121.85
1	G	144	GLY	C-N-CA	-11.19	108.54	121.85
1	A	144	GLY	CA-C-N	-11.18	108.54	121.85
1	A	144	GLY	C-N-CA	-11.18	108.54	121.85
1	C	144	GLY	CA-C-N	-11.16	108.57	121.85
1	C	144	GLY	C-N-CA	-11.16	108.57	121.85
1	C	76	GLY	O-C-N	-11.14	111.36	122.17
1	C	43	THR	OG1-CB-CG2	-11.12	87.05	109.30
1	A	43	THR	OG1-CB-CG2	-11.12	87.06	109.30
1	E	43	THR	OG1-CB-CG2	-11.12	87.07	109.30
1	E	76	GLY	O-C-N	-11.12	111.39	122.17
1	G	43	THR	OG1-CB-CG2	-11.11	87.08	109.30
1	A	76	GLY	O-C-N	-11.10	111.41	122.17
1	G	76	GLY	O-C-N	-11.06	111.44	122.17
1	A	159(A)	HIS	CA-C-N	-10.94	106.33	122.41
1	A	159(A)	HIS	C-N-CA	-10.94	106.33	122.41
1	E	159(A)	HIS	CA-C-N	-10.93	106.35	122.41
1	E	159(A)	HIS	C-N-CA	-10.93	106.35	122.41
1	C	159(A)	HIS	CA-C-N	-10.90	106.39	122.41
1	C	159(A)	HIS	C-N-CA	-10.90	106.39	122.41
1	G	159(A)	HIS	CA-C-N	-10.90	106.39	122.41
1	G	159(A)	HIS	C-N-CA	-10.90	106.39	122.41
1	E	174	HIS	CA-CB-CG	-10.80	103.00	113.80
1	G	174	HIS	CA-CB-CG	-10.80	103.00	113.80
1	A	174	HIS	CA-CB-CG	-10.79	103.01	113.80
1	C	174	HIS	CA-CB-CG	-10.78	103.02	113.80
1	E	40	VAL	O-C-N	10.69	129.20	121.72
1	E	77	SER	CA-C-N	-10.66	105.10	121.62
1	E	77	SER	C-N-CA	-10.66	105.10	121.62
1	G	40	VAL	O-C-N	10.65	129.18	121.72
1	A	77	SER	CA-C-N	-10.65	105.12	121.62
1	A	77	SER	C-N-CA	-10.65	105.12	121.62
1	G	77	SER	CA-C-N	-10.64	105.12	121.62
1	G	77	SER	C-N-CA	-10.64	105.12	121.62
1	A	40	VAL	O-C-N	10.63	129.16	121.72
1	C	77	SER	CA-C-N	-10.62	105.15	121.62
1	C	77	SER	C-N-CA	-10.62	105.15	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	VAL	O-C-N	10.58	129.13	121.72
1	E	158	GLY	CA-C-N	10.55	130.65	119.89
1	E	158	GLY	C-N-CA	10.55	130.65	119.89
1	A	203	THR	O-C-N	10.54	136.60	122.59
1	C	203	THR	O-C-N	10.53	136.60	122.59
1	A	158	GLY	CA-C-N	10.53	130.63	119.89
1	A	158	GLY	C-N-CA	10.53	130.63	119.89
1	E	203	THR	O-C-N	10.52	136.59	122.59
1	G	158	GLY	CA-C-N	10.52	130.62	119.89
1	G	158	GLY	C-N-CA	10.52	130.62	119.89
1	G	203	THR	O-C-N	10.52	136.58	122.59
1	C	158	GLY	CA-C-N	10.49	130.59	119.89
1	C	158	GLY	C-N-CA	10.49	130.59	119.89
1	C	260	PHE	CA-CB-CG	-10.48	103.32	113.80
1	E	260	PHE	CA-CB-CG	-10.48	103.32	113.80
1	A	260	PHE	CA-CB-CG	-10.47	103.33	113.80
1	G	260	PHE	CA-CB-CG	-10.47	103.33	113.80
1	E	279	ASP	O-C-N	-10.45	106.28	123.00
1	G	279	ASP	O-C-N	-10.45	106.28	123.00
1	A	279	ASP	O-C-N	-10.43	106.31	123.00
1	C	279	ASP	O-C-N	-10.43	106.31	123.00
1	E	40	VAL	CA-CB-CG2	10.42	128.11	110.40
1	C	40	VAL	CA-CB-CG2	10.41	128.10	110.40
1	A	40	VAL	CA-CB-CG2	10.41	128.10	110.40
1	G	40	VAL	CA-CB-CG2	10.41	128.09	110.40
1	E	293	PRO	CA-C-O	-10.31	112.59	120.73
1	C	128	GLN	OE1-CD-NE2	-10.29	112.31	122.60
1	G	293	PRO	CA-C-O	-10.27	112.61	120.73
1	E	229	LYS	CA-C-O	-10.26	109.67	120.55
1	A	293	PRO	CA-C-O	-10.26	112.63	120.73
1	A	128	GLN	OE1-CD-NE2	-10.25	112.35	122.60
1	A	229	LYS	CA-C-O	-10.25	109.69	120.55
1	G	128	GLN	OE1-CD-NE2	-10.25	112.35	122.60
1	C	229	LYS	CA-C-O	-10.23	109.70	120.55
1	G	229	LYS	CA-C-O	-10.23	109.70	120.55
1	E	128	GLN	OE1-CD-NE2	-10.21	112.39	122.60
1	C	293	PRO	CA-C-O	-10.21	112.66	120.73
1	G	7	THR	O-C-N	10.03	135.12	123.29
1	C	276	LEU	CA-C-N	10.02	136.32	122.19
1	C	276	LEU	C-N-CA	10.02	136.32	122.19
1	E	7	THR	O-C-N	10.02	135.12	123.29
1	G	276	LEU	CA-C-N	10.02	136.31	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	276	LEU	C-N-CA	10.02	136.31	122.19
1	A	7	THR	O-C-N	10.01	135.10	123.29
1	A	276	LEU	CA-C-N	9.99	136.27	122.19
1	A	276	LEU	C-N-CA	9.99	136.27	122.19
1	E	276	LEU	CA-C-N	9.98	136.26	122.19
1	E	276	LEU	C-N-CA	9.98	136.26	122.19
1	C	7	THR	O-C-N	9.97	135.06	123.29
1	E	101	PHE	CA-C-N	-9.78	112.08	121.57
1	E	101	PHE	C-N-CA	-9.78	112.08	121.57
1	G	101	PHE	CA-C-N	-9.76	112.11	121.57
1	G	101	PHE	C-N-CA	-9.76	112.11	121.57
1	A	101	PHE	CA-C-N	-9.75	112.11	121.57
1	A	101	PHE	C-N-CA	-9.75	112.11	121.57
1	C	101	PHE	CA-C-N	-9.74	112.12	121.57
1	C	101	PHE	C-N-CA	-9.74	112.12	121.57
1	C	241	ARG	CA-C-O	-9.69	110.14	120.99
1	E	67	ASN	OD1-CG-ND2	-9.68	112.92	122.60
1	G	241	ARG	CA-C-O	-9.68	110.15	120.99
1	A	241	ARG	CA-C-O	-9.67	110.16	120.99
1	E	241	ARG	CA-C-O	-9.64	110.19	120.99
1	G	67	ASN	OD1-CG-ND2	-9.64	112.96	122.60
1	A	67	ASN	OD1-CG-ND2	-9.63	112.97	122.60
1	E	310	TYR	O-C-N	-9.63	111.01	122.95
1	C	67	ASN	OD1-CG-ND2	-9.62	112.98	122.60
1	G	310	TYR	O-C-N	-9.61	111.04	122.95
1	A	310	TYR	O-C-N	-9.60	111.04	122.95
1	C	205	LEU	CA-C-O	-9.59	110.46	121.58
1	E	205	LEU	CA-C-O	-9.59	110.46	121.58
1	G	205	LEU	CA-C-O	-9.58	110.47	121.58
1	C	310	TYR	O-C-N	-9.57	111.08	122.95
1	A	205	LEU	CA-C-O	-9.57	110.48	121.58
1	E	1	ILE	CA-C-O	-9.54	110.49	120.51
1	A	1	ILE	CA-C-O	-9.54	110.50	120.51
1	G	1	ILE	CA-C-O	-9.52	110.51	120.51
1	E	324	LEU	CA-C-O	-9.51	109.87	120.81
1	G	324	LEU	CA-C-O	-9.51	109.88	120.81
1	A	324	LEU	CA-C-O	-9.50	109.89	120.81
1	C	1	ILE	CA-C-O	-9.50	110.53	120.51
1	C	324	LEU	CA-C-O	-9.45	109.94	120.81
1	C	158	GLY	O-C-N	9.44	131.21	121.77
1	G	158	GLY	O-C-N	9.42	131.19	121.77
1	A	158	GLY	O-C-N	9.41	131.18	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	158	GLY	O-C-N	9.37	131.14	121.77
1	E	9	TYR	CA-C-N	9.37	135.85	122.08
1	E	9	TYR	C-N-CA	9.37	135.85	122.08
1	A	9	TYR	CA-C-N	9.35	135.83	122.08
1	A	9	TYR	C-N-CA	9.35	135.83	122.08
1	E	215	ASP	O-C-N	-9.35	111.37	122.87
1	G	9	TYR	CA-C-N	9.34	135.81	122.08
1	G	9	TYR	C-N-CA	9.34	135.81	122.08
1	C	215	ASP	O-C-N	-9.33	111.39	122.87
1	A	215	ASP	O-C-N	-9.32	111.40	122.87
1	C	9	TYR	CA-C-N	9.32	135.78	122.08
1	C	9	TYR	C-N-CA	9.32	135.78	122.08
1	G	215	ASP	O-C-N	-9.30	111.42	122.87
1	E	1	ILE	O-C-N	9.24	131.68	122.71
1	A	1	ILE	O-C-N	9.22	131.65	122.71
1	C	1	ILE	O-C-N	9.19	131.62	122.71
1	G	1	ILE	O-C-N	9.18	131.62	122.71
1	E	-1	ASP	CA-CB-CG	-9.17	103.43	112.60
1	G	-1	ASP	CA-CB-CG	-9.17	103.43	112.60
1	A	-1	ASP	CA-CB-CG	-9.14	103.45	112.60
1	C	-1	ASP	CA-CB-CG	-9.10	103.50	112.60
2	D	2	HIS	CA-CB-CG	-9.10	104.70	113.80
2	B	2	HIS	CA-CB-CG	-9.08	104.72	113.80
2	F	2	HIS	CA-CB-CG	-9.07	104.73	113.80
2	H	2	HIS	CA-CB-CG	-9.04	104.76	113.80
1	E	27	PHE	CA-CB-CG	-9.04	104.76	113.80
1	C	27	PHE	CA-CB-CG	-9.02	104.78	113.80
1	A	27	PHE	CA-CB-CG	-9.02	104.78	113.80
1	G	27	PHE	CA-CB-CG	-9.00	104.80	113.80
1	E	162	GLY	N-CA-C	-8.99	103.51	114.66
1	C	162	GLY	N-CA-C	-8.96	103.54	114.66
1	A	162	GLY	N-CA-C	-8.96	103.55	114.66
1	G	162	GLY	N-CA-C	-8.95	103.57	114.66
1	G	-1	ASP	CA-C-O	8.81	132.49	122.27
1	C	171	ASP	CA-C-O	8.80	126.84	119.71
1	G	171	ASP	CA-C-O	8.80	126.84	119.71
1	A	171	ASP	CA-C-O	8.79	126.83	119.71
1	A	-1	ASP	CA-C-O	8.78	132.45	122.27
1	E	-1	ASP	CA-C-O	8.78	132.45	122.27
1	C	-1	ASP	CA-C-O	8.76	132.43	122.27
1	E	171	ASP	CA-C-O	8.76	126.81	119.71
1	E	252	VAL	CA-C-O	8.73	125.35	118.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	252	VAL	CA-C-O	8.69	125.31	118.71
1	A	252	VAL	CA-C-O	8.66	125.29	118.71
1	C	252	VAL	CA-C-O	8.63	125.27	118.71
1	E	188	ASP	CA-CB-CG	-8.63	103.97	112.60
1	A	188	ASP	CA-CB-CG	-8.62	103.98	112.60
1	C	188	ASP	CA-CB-CG	-8.60	104.00	112.60
1	G	188	ASP	CA-CB-CG	-8.59	104.01	112.60
1	G	307	ARG	NE-CZ-NH1	-8.55	112.95	121.50
1	E	307	ARG	NE-CZ-NH1	-8.55	112.95	121.50
1	E	32	ASP	CA-C-O	-8.54	111.62	120.84
1	C	32	ASP	CA-C-O	-8.53	111.63	120.84
1	A	307	ARG	NE-CZ-NH1	-8.52	112.98	121.50
1	C	307	ARG	NE-CZ-NH1	-8.52	112.98	121.50
1	A	32	ASP	CA-C-O	-8.51	111.65	120.84
1	G	206	CYS	CA-C-O	-8.50	110.29	120.32
1	C	113	MET	CA-CB-CG	-8.50	97.10	114.10
1	E	206	CYS	CA-C-O	-8.50	110.29	120.32
1	A	206	CYS	CA-C-O	-8.50	110.30	120.32
1	C	206	CYS	CA-C-O	-8.49	110.30	120.32
1	G	32	ASP	CA-C-O	-8.49	111.67	120.84
1	E	113	MET	CA-CB-CG	-8.48	97.13	114.10
1	G	113	MET	CA-CB-CG	-8.48	97.14	114.10
1	A	113	MET	CA-CB-CG	-8.47	97.15	114.10
1	A	134	THR	O-C-N	8.46	128.83	121.30
1	G	276	LEU	CA-C-O	8.45	130.33	120.69
1	A	160	LEU	CA-C-N	8.43	137.65	121.54
1	A	160	LEU	C-N-CA	8.43	137.65	121.54
1	C	276	LEU	CA-C-O	8.43	130.30	120.69
1	G	10	LEU	CA-C-O	-8.43	110.54	121.08
1	G	134	THR	O-C-N	8.43	128.81	121.30
1	A	276	LEU	CA-C-O	8.43	130.30	120.69
1	C	160	LEU	CA-C-N	8.43	137.64	121.54
1	C	160	LEU	C-N-CA	8.43	137.64	121.54
1	E	276	LEU	CA-C-O	8.43	130.30	120.69
1	E	160	LEU	CA-C-N	8.42	137.63	121.54
1	E	160	LEU	C-N-CA	8.42	137.63	121.54
1	G	160	LEU	CA-C-N	8.42	137.63	121.54
1	G	160	LEU	C-N-CA	8.42	137.63	121.54
1	A	10	LEU	CA-C-O	-8.42	110.55	121.08
1	C	10	LEU	CA-C-O	-8.41	110.56	121.08
1	G	85	SER	O-C-N	-8.41	112.22	123.15
1	C	85	SER	O-C-N	-8.40	112.22	123.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	LEU	CA-C-O	-8.40	110.57	121.08
1	E	134	THR	O-C-N	8.40	128.78	121.30
1	A	85	SER	O-C-N	-8.39	112.25	123.15
1	C	134	THR	O-C-N	8.36	128.74	121.30
1	E	80	VAL	O-C-N	-8.36	114.15	123.18
1	E	85	SER	O-C-N	-8.33	112.32	123.15
1	E	150	VAL	CA-CB-CG1	8.32	124.55	110.40
1	C	80	VAL	O-C-N	-8.31	114.20	123.18
1	C	150	VAL	CA-CB-CG1	8.31	124.52	110.40
1	G	80	VAL	O-C-N	-8.31	114.21	123.18
1	A	150	VAL	CA-CB-CG1	8.30	124.51	110.40
1	A	80	VAL	O-C-N	-8.30	114.22	123.18
1	G	8	ASN	CA-CB-CG	-8.28	104.32	112.60
1	G	150	VAL	CA-CB-CG1	8.28	124.48	110.40
1	E	8	ASN	CA-CB-CG	-8.28	104.32	112.60
1	A	8	ASN	CA-CB-CG	-8.26	104.34	112.60
1	E	110	ILE	CA-C-O	-8.26	113.17	119.20
1	C	8	ASN	CA-CB-CG	-8.26	104.34	112.60
1	G	110	ILE	CA-C-O	-8.25	113.18	119.20
1	G	303	ALA	CA-C-O	-8.23	110.98	120.20
1	A	303	ALA	CA-C-O	-8.23	110.98	120.20
1	E	303	ALA	CA-C-O	-8.22	110.99	120.20
1	C	110	ILE	CA-C-O	-8.22	113.20	119.20
1	C	303	ALA	CA-C-O	-8.22	111.00	120.20
1	A	110	ILE	CA-C-O	-8.21	113.20	119.20
1	E	171	ASP	O-C-N	-8.12	112.65	120.85
1	A	171	ASP	O-C-N	-8.12	112.65	120.85
1	G	171	ASP	O-C-N	-8.11	112.66	120.85
1	C	171	ASP	O-C-N	-8.10	112.67	120.85
1	A	13	GLN	CG-CD-NE2	8.03	128.45	116.40
1	G	133	VAL	CA-CB-CG2	8.03	124.05	110.40
1	E	13	GLN	CG-CD-NE2	8.02	128.43	116.40
1	C	13	GLN	CG-CD-NE2	8.01	128.42	116.40
1	E	133	VAL	CA-CB-CG2	8.01	124.02	110.40
1	A	133	VAL	CA-CB-CG2	8.01	124.01	110.40
1	G	13	GLN	CG-CD-NE2	8.01	128.41	116.40
1	C	288	ALA	CA-C-O	-7.98	111.75	120.92
1	C	133	VAL	CA-CB-CG2	7.97	123.95	110.40
1	G	288	ALA	CA-C-O	-7.97	111.75	120.92
1	A	288	ALA	CA-C-O	-7.96	111.76	120.92
1	E	288	ALA	CA-C-O	-7.90	111.83	120.92
1	G	253	PRO	CA-C-N	-7.85	110.09	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	253	PRO	C-N-CA	-7.85	110.09	122.65
1	G	324	LEU	O-C-N	7.84	132.57	122.93
1	C	253	PRO	CA-C-N	-7.83	110.13	122.65
1	C	253	PRO	C-N-CA	-7.83	110.13	122.65
1	A	253	PRO	CA-C-N	-7.82	110.14	122.65
1	A	253	PRO	C-N-CA	-7.82	110.14	122.65
1	A	324	LEU	O-C-N	7.80	132.53	122.93
1	E	253	PRO	CA-C-N	-7.80	110.17	122.65
1	E	253	PRO	C-N-CA	-7.80	110.17	122.65
1	E	324	LEU	O-C-N	7.79	132.50	122.93
1	C	324	LEU	O-C-N	7.77	132.48	122.93
1	C	113	MET	CG-SD-CE	7.73	117.91	100.90
1	E	113	MET	CG-SD-CE	7.72	117.89	100.90
1	A	113	MET	CG-SD-CE	7.72	117.89	100.90
1	E	144	GLY	O-C-N	-7.72	112.66	122.70
1	G	113	MET	CG-SD-CE	7.72	117.88	100.90
1	A	144	GLY	O-C-N	-7.71	112.68	122.70
1	C	144	GLY	O-C-N	-7.70	112.69	122.70
1	G	144	GLY	O-C-N	-7.70	112.70	122.70
1	G	292	PRO	O-C-N	7.69	124.85	121.31
1	A	66	GLU	O-C-N	-7.68	113.79	122.86
1	E	66	GLU	O-C-N	-7.68	113.79	122.86
1	G	66	GLU	O-C-N	-7.68	113.80	122.86
1	A	164	GLU	O-C-N	-7.67	114.89	123.48
1	C	164	GLU	O-C-N	-7.67	114.89	123.48
1	G	288	ALA	O-C-N	7.67	132.06	123.16
1	C	97	THR	O-C-N	7.67	132.13	122.93
1	G	164	GLU	O-C-N	-7.67	114.89	123.48
1	A	292	PRO	O-C-N	7.66	124.83	121.31
1	C	265	ARG	NE-CZ-NH2	7.65	126.09	119.20
1	C	66	GLU	O-C-N	-7.65	113.83	122.86
1	C	288	ALA	O-C-N	7.65	132.04	123.16
1	G	97	THR	O-C-N	7.65	132.11	122.93
1	E	164	GLU	O-C-N	-7.65	114.91	123.48
1	A	288	ALA	O-C-N	7.64	132.02	123.16
1	G	307	ARG	NE-CZ-NH2	7.64	126.07	119.20
1	E	292	PRO	O-C-N	7.63	124.82	121.31
1	A	97	THR	O-C-N	7.63	132.08	122.93
1	A	265	ARG	NE-CZ-NH2	7.62	126.06	119.20
1	G	265	ARG	NE-CZ-NH2	7.62	126.06	119.20
1	G	312	GLU	O-C-N	-7.62	114.30	123.29
1	E	97	THR	O-C-N	7.60	132.05	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	312	GLU	O-C-N	-7.59	114.33	123.29
1	E	326	ARG	CB-CG-CD	7.59	128.76	111.30
1	A	312	GLU	O-C-N	-7.59	114.33	123.29
1	G	322	PHE	CA-C-O	-7.58	112.51	120.70
1	E	288	ALA	O-C-N	7.58	131.96	123.16
1	C	307	ARG	NE-CZ-NH2	7.58	126.02	119.20
1	A	326	ARG	CB-CG-CD	7.58	128.73	111.30
1	C	326	ARG	CB-CG-CD	7.58	128.73	111.30
1	A	307	ARG	NE-CZ-NH2	7.58	126.02	119.20
1	E	265	ARG	NE-CZ-NH2	7.58	126.02	119.20
1	C	15	TYR	O-C-N	-7.57	114.00	123.17
1	E	307	ARG	NE-CZ-NH2	7.57	126.02	119.20
1	G	326	ARG	CB-CG-CD	7.57	128.71	111.30
1	A	322	PHE	CA-C-O	-7.57	112.53	120.70
1	C	312	GLU	O-C-N	-7.56	114.36	123.29
1	G	15	TYR	O-C-N	-7.56	114.02	123.17
1	E	322	PHE	CA-C-O	-7.56	112.53	120.70
1	C	292	PRO	O-C-N	7.56	124.79	121.31
1	G	249	CYS	CA-C-N	7.55	131.79	120.31
1	G	249	CYS	C-N-CA	7.55	131.79	120.31
1	A	15	TYR	O-C-N	-7.54	114.05	123.17
1	E	231	ILE	O-C-N	-7.53	114.07	121.90
1	A	249	CYS	CA-C-N	7.53	131.75	120.31
1	A	249	CYS	C-N-CA	7.53	131.75	120.31
1	C	231	ILE	O-C-N	-7.53	114.07	121.90
1	C	229	LYS	CA-C-N	7.53	130.36	120.28
1	C	229	LYS	C-N-CA	7.53	130.36	120.28
1	E	249	CYS	CA-C-N	7.53	131.75	120.31
1	E	249	CYS	C-N-CA	7.53	131.75	120.31
1	C	322	PHE	CA-C-O	-7.52	112.57	120.70
1	G	255	LEU	CA-C-O	-7.52	112.50	120.70
1	A	255	LEU	CA-C-O	-7.52	112.50	120.70
1	C	215	ASP	CA-C-O	7.52	128.96	120.84
1	E	255	LEU	CA-C-O	-7.52	112.51	120.70
1	A	215	ASP	CA-C-O	7.51	128.96	120.84
1	E	215	ASP	CA-C-O	7.51	128.96	120.84
1	C	249	CYS	CA-C-N	7.51	131.73	120.31
1	C	249	CYS	C-N-CA	7.51	131.73	120.31
1	G	229	LYS	CA-C-N	7.50	130.33	120.28
1	G	229	LYS	C-N-CA	7.50	130.33	120.28
1	C	255	LEU	CA-C-O	-7.50	112.53	120.70
1	E	15	TYR	O-C-N	-7.49	114.11	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	LYS	CA-C-N	7.49	130.31	120.28
1	A	229	LYS	C-N-CA	7.49	130.31	120.28
1	C	128	GLN	CG-CD-NE2	7.49	127.63	116.40
1	A	231	ILE	O-C-N	-7.48	114.12	121.90
1	E	229	LYS	CA-C-N	7.48	130.30	120.28
1	E	229	LYS	C-N-CA	7.48	130.30	120.28
1	E	282	CYS	CA-C-N	7.48	131.42	120.95
1	E	282	CYS	C-N-CA	7.48	131.42	120.95
1	G	215	ASP	CA-C-O	7.48	128.92	120.84
1	G	198	SER	CA-C-N	-7.48	113.40	123.12
1	G	198	SER	C-N-CA	-7.48	113.40	123.12
1	G	128	GLN	CG-CD-NE2	7.47	127.61	116.40
1	G	231	ILE	O-C-N	-7.47	114.13	121.90
1	E	198	SER	CA-C-N	-7.47	113.41	123.12
1	E	198	SER	C-N-CA	-7.47	113.41	123.12
1	C	282	CYS	CA-C-N	7.46	131.40	120.95
1	C	282	CYS	C-N-CA	7.46	131.40	120.95
1	A	198	SER	CA-C-N	-7.46	113.42	123.12
1	A	198	SER	C-N-CA	-7.46	113.42	123.12
1	A	282	CYS	CA-C-N	7.46	131.39	120.95
1	A	282	CYS	C-N-CA	7.46	131.39	120.95
1	A	128	GLN	CG-CD-NE2	7.45	127.58	116.40
1	C	198	SER	CA-C-N	-7.45	113.43	123.12
1	C	198	SER	C-N-CA	-7.45	113.43	123.12
1	G	282	CYS	CA-C-N	7.45	131.38	120.95
1	G	282	CYS	C-N-CA	7.45	131.38	120.95
1	E	128	GLN	CG-CD-NE2	7.44	127.56	116.40
1	C	189	SER	CA-C-O	-7.43	112.72	120.89
1	G	189	SER	CA-C-O	-7.40	112.75	120.89
1	A	106	GLN	CA-C-N	7.39	132.80	122.74
1	A	106	GLN	C-N-CA	7.39	132.80	122.74
1	C	106	GLN	CA-C-N	7.39	132.80	122.74
1	C	106	GLN	C-N-CA	7.39	132.80	122.74
1	C	71	PHE	CA-C-N	7.39	133.42	123.00
1	C	71	PHE	C-N-CA	7.39	133.42	123.00
1	G	106	GLN	CA-C-N	7.39	132.79	122.74
1	G	106	GLN	C-N-CA	7.39	132.79	122.74
1	E	39	TRP	CA-C-O	-7.38	113.35	121.33
1	E	106	GLN	CA-C-N	7.38	132.78	122.74
1	E	106	GLN	C-N-CA	7.38	132.78	122.74
1	A	39	TRP	CA-C-O	-7.38	113.36	121.33
1	A	189	SER	CA-C-O	-7.38	112.77	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	71	PHE	CA-C-N	7.38	133.41	123.00
1	G	71	PHE	C-N-CA	7.38	133.41	123.00
1	E	257	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	71	PHE	CA-C-N	7.37	133.39	123.00
1	A	71	PHE	C-N-CA	7.37	133.39	123.00
1	E	189	SER	CA-C-O	-7.37	112.79	120.89
1	C	72	THR	CA-C-N	-7.37	112.11	122.71
1	C	72	THR	C-N-CA	-7.37	112.11	122.71
1	G	72	THR	CA-C-N	-7.37	112.10	122.71
1	G	72	THR	C-N-CA	-7.37	112.10	122.71
1	G	257	ASP	CA-CB-CG	7.37	119.97	112.60
1	E	71	PHE	CA-C-N	7.36	133.38	123.00
1	E	71	PHE	C-N-CA	7.36	133.38	123.00
1	A	257	ASP	CA-CB-CG	7.36	119.96	112.60
1	C	39	TRP	CA-C-O	-7.35	113.39	121.33
1	E	212	VAL	CA-CB-CG1	7.35	122.90	110.40
1	E	72	THR	CA-C-N	-7.35	112.12	122.71
1	E	72	THR	C-N-CA	-7.35	112.12	122.71
1	C	257	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	72	THR	CA-C-N	-7.35	112.13	122.71
1	A	72	THR	C-N-CA	-7.35	112.13	122.71
1	C	212	VAL	CA-CB-CG1	7.35	122.89	110.40
1	E	252	VAL	O-C-N	-7.34	115.72	120.42
1	E	298	VAL	CA-CB-CG2	7.34	122.89	110.40
1	G	39	TRP	CA-C-O	-7.34	113.40	121.33
1	A	212	VAL	CA-CB-CG1	7.34	122.88	110.40
1	C	252	VAL	O-C-N	-7.34	115.72	120.42
1	A	298	VAL	CA-CB-CG2	7.33	122.87	110.40
1	C	298	VAL	CA-CB-CG2	7.33	122.87	110.40
1	G	212	VAL	CA-CB-CG1	7.32	122.85	110.40
1	G	252	VAL	O-C-N	-7.32	115.73	120.42
1	G	298	VAL	CA-CB-CG2	7.32	122.85	110.40
1	A	252	VAL	O-C-N	-7.32	115.74	120.42
1	C	30	ILE	O-C-N	-7.31	114.70	122.81
1	A	30	ILE	O-C-N	-7.29	114.72	122.81
1	E	30	ILE	O-C-N	-7.26	114.75	122.81
1	G	30	ILE	O-C-N	-7.26	114.75	122.81
1	C	317	ASN	CA-C-O	-7.25	110.87	119.35
1	E	248	SER	CA-CB-OG	-7.24	96.63	111.10
1	A	248	SER	CA-CB-OG	-7.23	96.64	111.10
1	C	248	SER	CA-CB-OG	-7.22	96.66	111.10
1	G	248	SER	CA-CB-OG	-7.22	96.66	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	320	ILE	O-C-N	-7.14	115.55	123.26
1	A	320	ILE	O-C-N	-7.14	115.55	123.26
1	E	40	VAL	CA-C-O	-7.14	112.35	121.13
1	A	40	VAL	CA-C-O	-7.13	112.36	121.13
1	C	40	VAL	CA-C-O	-7.13	112.36	121.13
1	G	320	ILE	O-C-N	-7.13	115.56	123.26
1	G	224	PRO	O-C-N	-7.12	114.18	123.01
1	C	320	ILE	O-C-N	-7.12	115.57	123.26
1	G	40	VAL	CA-C-O	-7.12	112.38	121.13
1	C	133	VAL	CA-C-N	7.11	130.31	120.65
1	C	133	VAL	C-N-CA	7.11	130.31	120.65
1	G	133	VAL	CA-C-N	7.09	130.29	120.65
1	G	133	VAL	C-N-CA	7.09	130.29	120.65
1	A	133	VAL	CA-C-N	7.09	130.29	120.65
1	A	133	VAL	C-N-CA	7.09	130.29	120.65
1	E	224	PRO	O-C-N	-7.08	114.23	123.01
1	E	133	VAL	CA-C-N	7.07	130.27	120.65
1	E	133	VAL	C-N-CA	7.07	130.27	120.65
1	A	224	PRO	O-C-N	-7.07	114.24	123.01
1	G	71	PHE	O-C-N	-7.07	113.79	123.12
1	C	71	PHE	O-C-N	-7.06	113.80	123.12
1	C	293	PRO	N-CA-CB	-7.06	99.55	103.22
1	C	224	PRO	O-C-N	-7.06	114.26	123.01
1	A	71	PHE	O-C-N	-7.06	113.80	123.12
1	G	211	GLU	O-C-N	7.06	131.34	123.16
1	C	186	LYS	CA-C-O	-7.05	111.38	119.98
1	E	186	LYS	CA-C-O	-7.05	111.38	119.98
1	C	160	LEU	CB-CA-C	7.04	123.28	111.30
1	A	186	LYS	CA-C-O	-7.04	111.39	119.98
1	E	211	GLU	O-C-N	7.04	131.33	123.16
1	A	211	GLU	O-C-N	7.04	131.32	123.16
1	E	71	PHE	O-C-N	-7.04	113.83	123.12
1	C	211	GLU	O-C-N	7.03	131.31	123.16
1	A	160	LEU	CB-CA-C	7.03	123.25	111.30
1	E	202	SER	CA-C-N	7.03	134.96	121.54
1	E	202	SER	C-N-CA	7.03	134.96	121.54
1	A	293	PRO	N-CA-CB	-7.02	99.57	103.22
1	G	160	LEU	CB-CA-C	7.02	123.23	111.30
1	G	186	LYS	CA-C-O	-7.02	111.42	119.98
1	C	202	SER	CA-C-N	7.01	134.94	121.54
1	C	202	SER	C-N-CA	7.01	134.94	121.54
1	E	160	LEU	CB-CA-C	7.01	123.22	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	SER	CA-C-N	7.01	134.92	121.54
1	A	202	SER	C-N-CA	7.01	134.92	121.54
1	C	161	LEU	N-CA-CB	7.00	122.33	110.49
1	E	161	LEU	N-CA-CB	7.00	122.33	110.49
1	A	161	LEU	N-CA-CB	7.00	122.32	110.49
1	G	202	SER	CA-C-N	7.00	134.90	121.54
1	G	202	SER	C-N-CA	7.00	134.90	121.54
1	G	293	PRO	N-CA-CB	-6.99	99.59	103.22
1	G	161	LEU	N-CA-CB	6.98	122.29	110.49
1	E	293	PRO	N-CA-CB	-6.98	99.59	103.22
1	C	148	GLU	CB-CG-CD	-6.98	100.74	112.60
1	A	148	GLU	CB-CG-CD	-6.96	100.76	112.60
1	E	148	GLU	CB-CG-CD	-6.96	100.77	112.60
1	G	148	GLU	CB-CG-CD	-6.96	100.77	112.60
1	A	317	ASN	CA-C-O	-6.92	110.91	119.28
1	E	317	ASN	CA-C-O	-6.91	110.92	119.28
2	F	5	HIS	CE1-NE2-CD2	-6.91	102.09	109.00
1	E	326	ARG	CA-CB-CG	6.91	127.92	114.10
1	G	317	ASN	CA-C-O	-6.91	110.92	119.28
1	C	326	ARG	CA-CB-CG	6.90	127.91	114.10
1	C	214	VAL	CA-C-N	6.90	132.44	122.85
1	C	214	VAL	C-N-CA	6.90	132.44	122.85
2	H	5	HIS	CE1-NE2-CD2	-6.90	102.10	109.00
1	A	326	ARG	CA-CB-CG	6.90	127.90	114.10
1	G	326	ARG	CA-CB-CG	6.90	127.90	114.10
2	B	5	HIS	CE1-NE2-CD2	-6.90	102.10	109.00
2	D	5	HIS	CE1-NE2-CD2	-6.90	102.10	109.00
1	C	154	TYR	CA-C-O	6.89	127.68	120.30
1	E	214	VAL	CA-C-N	6.88	132.41	122.85
1	E	214	VAL	C-N-CA	6.88	132.41	122.85
1	A	154	TYR	CA-C-O	6.87	127.65	120.30
1	A	214	VAL	CA-C-N	6.87	132.40	122.85
1	A	214	VAL	C-N-CA	6.87	132.40	122.85
1	G	154	TYR	CA-C-O	6.87	127.65	120.30
1	C	256	PRO	O-C-N	-6.86	114.81	123.04
1	G	214	VAL	CA-C-N	6.86	132.38	122.85
1	G	214	VAL	C-N-CA	6.86	132.38	122.85
1	A	113	MET	O-C-N	-6.86	113.24	122.43
1	E	256	PRO	O-C-N	-6.85	114.82	123.04
1	G	256	PRO	O-C-N	-6.85	114.82	123.04
1	C	113	MET	O-C-N	-6.85	113.25	122.43
1	E	113	MET	O-C-N	-6.85	113.25	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	180	HIS	CB-CG-ND1	6.84	132.96	122.70
1	G	113	MET	O-C-N	-6.83	113.27	122.43
1	E	154	TYR	CA-C-O	6.83	127.61	120.30
1	A	256	PRO	O-C-N	-6.83	114.85	123.04
1	C	180	HIS	CB-CG-ND1	6.83	132.94	122.70
1	G	200	GLY	CA-C-N	6.82	134.09	122.36
1	G	200	GLY	C-N-CA	6.82	134.09	122.36
1	C	259	SER	CA-C-N	6.82	132.59	123.05
1	C	259	SER	C-N-CA	6.82	132.59	123.05
1	A	180	HIS	CB-CG-ND1	6.82	132.92	122.70
1	E	200	GLY	CA-C-N	6.82	134.08	122.36
1	E	200	GLY	C-N-CA	6.82	134.08	122.36
1	A	259	SER	CA-C-N	6.81	132.59	123.05
1	A	259	SER	C-N-CA	6.81	132.59	123.05
1	C	200	GLY	CA-C-N	6.81	134.08	122.36
1	C	200	GLY	C-N-CA	6.81	134.08	122.36
1	E	259	SER	CA-C-N	6.81	132.58	123.05
1	E	259	SER	C-N-CA	6.81	132.58	123.05
1	A	200	GLY	CA-C-N	6.80	134.06	122.36
1	A	200	GLY	C-N-CA	6.80	134.06	122.36
1	E	12	SER	O-C-N	-6.80	114.89	122.10
1	C	42	SER	CA-C-N	6.80	130.07	120.28
1	C	42	SER	C-N-CA	6.80	130.07	120.28
1	G	83	PHE	CA-C-O	-6.80	113.99	121.33
1	G	180	HIS	CB-CG-ND1	6.79	132.89	122.70
1	A	83	PHE	CA-C-O	-6.79	114.00	121.33
1	E	83	PHE	CA-C-O	-6.79	114.00	121.33
1	G	259	SER	CA-C-N	6.79	132.55	123.05
1	G	259	SER	C-N-CA	6.79	132.55	123.05
1	C	12	SER	O-C-N	-6.78	114.91	122.10
1	G	247	VAL	CA-C-O	-6.78	114.76	121.67
1	C	83	PHE	CA-C-O	-6.77	114.02	121.33
1	A	233	GLN	CB-CG-CD	-6.77	101.09	112.60
1	A	42	SER	CA-C-N	6.76	130.02	120.28
1	A	42	SER	C-N-CA	6.76	130.02	120.28
1	C	316	HIS	CA-CB-CG	-6.76	107.04	113.80
1	E	316	HIS	CA-CB-CG	-6.76	107.04	113.80
1	E	233	GLN	CB-CG-CD	-6.76	101.10	112.60
1	G	316	HIS	CA-CB-CG	-6.76	107.04	113.80
1	A	12	SER	O-C-N	-6.76	114.94	122.10
1	G	42	SER	CA-C-N	6.76	130.01	120.28
1	G	42	SER	C-N-CA	6.76	130.01	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	247	VAL	CA-C-O	-6.76	114.78	121.67
1	G	233	GLN	CB-CG-CD	-6.76	101.11	112.60
1	C	233	GLN	CB-CG-CD	-6.76	101.11	112.60
1	A	316	HIS	CA-CB-CG	-6.75	107.05	113.80
1	E	42	SER	CA-C-N	6.75	130.00	120.28
1	E	42	SER	C-N-CA	6.75	130.00	120.28
1	G	12	SER	O-C-N	-6.75	114.95	122.10
1	E	300	VAL	CA-CB-CG2	6.74	121.85	110.40
1	G	300	VAL	CA-CB-CG2	6.73	121.85	110.40
1	A	247	VAL	CA-C-O	-6.72	114.82	121.67
1	G	204	LEU	O-C-N	-6.72	113.87	123.07
1	A	300	VAL	CA-CB-CG2	6.71	121.81	110.40
1	C	190	TRP	CG-CD1-NE1	-6.71	101.48	110.20
1	C	300	VAL	CA-CB-CG2	6.70	121.80	110.40
1	A	204	LEU	O-C-N	-6.70	113.90	123.07
1	E	204	LEU	O-C-N	-6.70	113.90	123.07
1	C	247	VAL	CA-C-O	-6.69	114.84	121.67
1	C	74	HIS	O-C-N	6.68	131.92	123.23
1	G	190	TRP	CG-CD1-NE1	-6.68	101.52	110.20
1	A	74	HIS	O-C-N	6.67	131.91	123.23
1	A	190	TRP	CG-CD1-NE1	-6.67	101.53	110.20
1	E	190	TRP	CG-CD1-NE1	-6.67	101.53	110.20
1	C	204	LEU	O-C-N	-6.65	113.96	123.07
1	G	74	HIS	O-C-N	6.65	131.87	123.23
1	E	74	HIS	O-C-N	6.64	131.87	123.23
1	A	45	CYS	O-C-N	-6.63	114.73	122.95
1	C	155	TYR	O-C-N	-6.62	115.46	123.27
1	C	45	CYS	O-C-N	-6.60	114.77	122.95
1	A	155	TYR	O-C-N	-6.59	115.49	123.27
1	E	155	TYR	O-C-N	-6.59	115.49	123.27
1	G	45	CYS	O-C-N	-6.59	114.78	122.95
1	E	292	PRO	N-CA-CB	-6.58	99.50	103.19
1	E	45	CYS	O-C-N	-6.58	114.79	122.95
1	E	305	PHE	CE1-CZ-CE2	6.58	131.84	120.00
1	E	224	PRO	CA-C-N	6.56	129.37	120.38
1	E	224	PRO	C-N-CA	6.56	129.37	120.38
1	A	305	PHE	CE1-CZ-CE2	6.55	131.79	120.00
1	G	155	TYR	O-C-N	-6.55	115.54	123.27
1	C	305	PHE	CE1-CZ-CE2	6.55	131.78	120.00
1	G	224	PRO	CA-C-N	6.54	129.35	120.38
1	G	224	PRO	C-N-CA	6.54	129.35	120.38
1	G	305	PHE	CE1-CZ-CE2	6.54	131.77	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	PRO	CA-C-N	6.53	129.32	120.38
1	A	224	PRO	C-N-CA	6.53	129.32	120.38
1	C	224	PRO	CA-C-N	6.52	129.31	120.38
1	C	224	PRO	C-N-CA	6.52	129.31	120.38
1	G	292	PRO	N-CA-CB	-6.50	99.55	103.19
1	C	35	SER	CA-C-O	-6.49	114.48	121.36
1	E	128	GLN	CA-C-O	-6.49	111.46	119.18
1	A	292	PRO	N-CA-CB	-6.49	99.56	103.19
1	G	128	GLN	CA-C-O	-6.49	111.46	119.18
1	E	35	SER	CA-C-O	-6.48	114.49	121.36
1	E	174	HIS	O-C-N	-6.48	114.35	122.19
1	C	128	GLN	CA-C-O	-6.48	111.47	119.18
1	A	128	GLN	CA-C-O	-6.47	111.47	119.18
1	E	107	LEU	CA-C-N	6.47	126.50	119.90
1	E	107	LEU	C-N-CA	6.47	126.50	119.90
1	C	133	VAL	CA-C-O	-6.46	112.81	121.02
1	A	133	VAL	CA-C-O	-6.46	112.81	121.02
1	C	288	ALA	CA-C-N	-6.46	112.00	121.76
1	C	288	ALA	C-N-CA	-6.46	112.00	121.76
1	E	133	VAL	CA-C-O	-6.46	112.82	121.02
1	G	288	ALA	CA-C-N	-6.46	112.01	121.76
1	G	288	ALA	C-N-CA	-6.46	112.01	121.76
1	A	35	SER	CA-C-O	-6.45	114.52	121.36
1	A	288	ALA	CA-C-N	-6.45	112.02	121.76
1	A	288	ALA	C-N-CA	-6.45	112.02	121.76
1	C	298	VAL	CA-CB-CG1	6.45	121.37	110.40
1	G	35	SER	CA-C-O	-6.45	114.52	121.36
1	G	298	VAL	CA-CB-CG1	6.45	121.36	110.40
1	E	288	ALA	CA-C-N	-6.45	112.03	121.76
1	E	288	ALA	C-N-CA	-6.45	112.03	121.76
1	C	107	LEU	CA-C-N	6.45	126.47	119.90
1	C	107	LEU	C-N-CA	6.45	126.47	119.90
1	E	298	VAL	CA-CB-CG1	6.44	121.35	110.40
1	A	298	VAL	CA-CB-CG1	6.44	121.35	110.40
1	G	107	LEU	CA-C-N	6.44	126.46	119.90
1	G	107	LEU	C-N-CA	6.44	126.46	119.90
1	A	174	HIS	O-C-N	-6.43	114.40	122.19
1	C	292	PRO	N-CA-CB	-6.43	99.59	103.19
1	G	133	VAL	CA-C-O	-6.43	112.85	121.02
1	G	174	HIS	O-C-N	-6.43	114.41	122.19
1	A	107	LEU	CA-C-N	6.43	126.46	119.90
1	A	107	LEU	C-N-CA	6.43	126.46	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	HIS	O-C-N	-6.42	114.42	122.19
1	E	298	VAL	O-C-N	6.41	130.05	123.00
1	G	73	ILE	CA-C-O	-6.40	113.72	120.76
1	C	73	ILE	CA-C-O	-6.39	113.73	120.76
1	A	298	VAL	O-C-N	6.38	130.02	123.00
1	A	43	THR	CA-CB-CG2	6.38	121.34	110.50
1	G	43	THR	CA-CB-CG2	6.38	121.34	110.50
1	G	298	VAL	O-C-N	6.38	130.01	123.00
1	A	16	GLY	O-C-N	-6.37	118.12	123.73
1	C	43	THR	CA-CB-CG2	6.37	121.33	110.50
1	A	73	ILE	CA-C-O	-6.36	113.76	120.76
1	A	203	THR	CA-C-O	-6.36	111.41	120.51
1	E	43	THR	CA-CB-CG2	6.36	121.31	110.50
1	C	16	GLY	O-C-N	-6.36	118.14	123.73
1	E	203	THR	CA-C-O	-6.36	111.42	120.51
1	C	203	THR	CA-C-O	-6.35	111.42	120.51
1	E	73	ILE	CA-C-O	-6.35	113.77	120.76
1	C	298	VAL	O-C-N	6.35	129.98	123.00
1	G	203	THR	CA-C-O	-6.35	111.43	120.51
1	G	16	GLY	O-C-N	-6.34	118.15	123.73
1	A	58	SER	CA-C-N	6.33	131.30	120.72
1	A	58	SER	C-N-CA	6.33	131.30	120.72
1	E	58	SER	CA-C-N	6.33	131.30	120.72
1	E	58	SER	C-N-CA	6.33	131.30	120.72
1	G	58	SER	CA-C-N	6.33	131.30	120.72
1	G	58	SER	C-N-CA	6.33	131.30	120.72
1	C	58	SER	CA-C-N	6.33	131.29	120.72
1	C	58	SER	C-N-CA	6.33	131.29	120.72
1	C	147	LYS	CA-CB-CG	6.33	126.76	114.10
1	E	16	GLY	O-C-N	-6.33	118.16	123.73
1	A	147	LYS	CA-CB-CG	6.33	126.75	114.10
1	E	104	VAL	CA-C-O	6.32	128.06	120.85
1	G	147	LYS	CA-CB-CG	6.32	126.74	114.10
1	G	143	GLN	CB-CG-CD	-6.30	101.89	112.60
1	C	56	TYR	O-C-N	-6.30	115.18	122.93
1	E	74	HIS	CB-CG-CD2	-6.30	123.02	131.20
1	E	143	GLN	CB-CG-CD	-6.30	101.90	112.60
1	G	56	TYR	O-C-N	-6.29	115.19	122.93
1	E	147	LYS	CA-CB-CG	6.29	126.69	114.10
1	C	143	GLN	CB-CG-CD	-6.29	101.92	112.60
1	A	104	VAL	CA-C-O	6.28	128.01	120.85
1	G	254	THR	CA-C-O	-6.28	112.21	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	GLN	CB-CG-CD	-6.28	101.92	112.60
1	A	56	TYR	O-C-N	-6.28	115.21	122.93
1	C	236	GLY	N-CA-C	-6.27	105.25	114.90
1	E	307	ARG	CA-C-O	6.27	127.19	120.55
1	G	104	VAL	CA-C-O	6.26	127.99	120.85
1	A	74	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	C	104	VAL	CA-C-O	6.26	127.99	120.85
1	E	254	THR	CA-C-O	-6.26	112.24	119.56
1	A	254	THR	CA-C-O	-6.25	112.24	119.56
1	C	74	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	A	236	GLY	N-CA-C	-6.25	105.28	114.90
1	G	169	GLY	CA-C-N	6.25	132.31	122.94
1	G	169	GLY	C-N-CA	6.25	132.31	122.94
1	A	169	GLY	CA-C-N	6.25	132.31	122.94
1	A	169	GLY	C-N-CA	6.25	132.31	122.94
1	E	25	GLN	CA-CB-CG	-6.24	101.62	114.10
1	G	74	HIS	CB-CG-CD2	-6.24	123.08	131.20
1	G	236	GLY	N-CA-C	-6.24	105.29	114.90
1	A	25	GLN	CA-CB-CG	-6.24	101.62	114.10
1	C	254	THR	CA-C-O	-6.24	112.26	119.56
1	E	169	GLY	CA-C-N	6.24	132.30	122.94
1	E	169	GLY	C-N-CA	6.24	132.30	122.94
1	C	266	ALA	CA-C-N	6.24	131.97	123.11
1	C	266	ALA	C-N-CA	6.24	131.97	123.11
1	G	266	ALA	CA-C-N	6.23	131.96	123.11
1	G	266	ALA	C-N-CA	6.23	131.96	123.11
1	E	56	TYR	O-C-N	-6.23	115.27	122.93
1	G	25	GLN	CA-CB-CG	-6.23	101.64	114.10
1	C	169	GLY	CA-C-N	6.23	132.28	122.94
1	C	169	GLY	C-N-CA	6.23	132.28	122.94
1	C	143	GLN	O-C-N	6.22	131.60	122.39
1	E	236	GLY	N-CA-C	-6.22	105.31	114.90
1	C	25	GLN	CA-CB-CG	-6.22	101.65	114.10
1	G	307	ARG	CA-C-O	6.22	127.14	120.55
1	C	307	ARG	CA-C-O	6.22	127.14	120.55
1	A	307	ARG	CA-C-O	6.22	127.14	120.55
1	G	92	GLY	N-CA-C	-6.22	104.16	114.48
1	A	24	PRO	O-C-N	6.21	130.89	123.06
1	E	266	ALA	CA-C-N	6.21	131.94	123.11
1	E	266	ALA	C-N-CA	6.21	131.94	123.11
1	A	92	GLY	N-CA-C	-6.21	104.18	114.48
1	G	24	PRO	O-C-N	6.21	130.88	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	GLN	O-C-N	6.20	131.57	122.39
1	E	92	GLY	N-CA-C	-6.20	104.19	114.48
1	A	266	ALA	CA-C-N	6.20	131.91	123.11
1	A	266	ALA	C-N-CA	6.20	131.91	123.11
1	C	24	PRO	O-C-N	6.20	130.87	123.06
1	G	143	GLN	O-C-N	6.19	131.56	122.39
1	E	24	PRO	O-C-N	6.19	130.86	123.06
1	E	156	ASN	O-C-N	-6.18	115.45	122.68
1	C	92	GLY	N-CA-C	-6.18	104.22	114.48
1	E	218	SER	CA-C-N	6.17	128.46	120.44
1	E	218	SER	C-N-CA	6.17	128.46	120.44
1	G	218	SER	CA-C-N	6.17	128.47	120.44
1	G	218	SER	C-N-CA	6.17	128.47	120.44
1	E	143	GLN	O-C-N	6.17	131.52	122.39
1	A	218	SER	CA-C-N	6.17	128.46	120.44
1	A	218	SER	C-N-CA	6.17	128.46	120.44
1	E	75	TYR	CD1-CG-CD2	6.17	127.35	118.10
1	C	136	VAL	CA-C-O	-6.16	114.86	121.27
1	G	75	TYR	CD1-CG-CD2	6.16	127.34	118.10
1	C	75	TYR	CD1-CG-CD2	6.16	127.34	118.10
1	E	138	ASP	CA-CB-CG	-6.16	106.44	112.60
1	E	318	ASN	CA-C-O	6.16	129.78	122.14
1	A	75	TYR	CD1-CG-CD2	6.16	127.33	118.10
1	G	318	ASN	CA-C-O	6.15	129.77	122.14
1	A	318	ASN	CA-C-O	6.15	129.76	122.14
1	A	156	ASN	O-C-N	-6.14	115.49	122.68
1	A	136	VAL	CA-C-O	-6.14	114.88	121.27
1	C	218	SER	CA-C-N	6.14	128.43	120.44
1	C	218	SER	C-N-CA	6.14	128.43	120.44
1	C	252	VAL	CA-CB-CG1	6.14	120.83	110.40
1	E	252	VAL	CA-CB-CG1	6.14	120.83	110.40
1	G	138	ASP	CA-CB-CG	-6.14	106.46	112.60
1	G	136	VAL	CA-C-O	-6.13	114.89	121.27
1	A	252	VAL	CA-CB-CG1	6.13	120.82	110.40
1	G	156	ASN	O-C-N	-6.13	115.51	122.68
1	G	252	VAL	CA-CB-CG1	6.13	120.81	110.40
1	G	50	CYS	O-C-N	-6.12	114.01	122.46
1	E	136	VAL	CA-C-O	-6.12	114.90	121.27
1	A	138	ASP	CA-CB-CG	-6.12	106.48	112.60
1	C	50	CYS	O-C-N	-6.12	114.02	122.46
1	C	156	ASN	O-C-N	-6.12	115.52	122.68
1	C	318	ASN	CA-C-O	6.11	129.72	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	TYR	CA-C-O	6.11	127.95	120.92
1	E	50	CYS	O-C-N	-6.11	114.03	122.46
1	E	181	TYR	CA-C-O	6.10	127.93	120.92
1	A	141	LEU	CA-C-O	6.09	127.01	120.55
2	B	2	HIS	ND1-CG-CD2	6.09	112.19	106.10
1	G	32	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	50	CYS	O-C-N	-6.09	114.06	122.46
1	E	32	ASP	CA-CB-CG	6.09	118.69	112.60
2	F	2	HIS	ND1-CG-CD2	6.09	112.19	106.10
1	C	108	PRO	CA-C-N	6.08	128.75	120.54
1	C	108	PRO	C-N-CA	6.08	128.75	120.54
1	C	138	ASP	CA-CB-CG	-6.08	106.52	112.60
1	E	141	LEU	CA-C-O	6.08	127.00	120.55
1	C	195	LYS	CA-C-O	-6.08	112.30	120.15
1	G	108	PRO	CA-C-N	6.08	128.75	120.54
1	G	108	PRO	C-N-CA	6.08	128.75	120.54
2	H	2	HIS	ND1-CG-CD2	6.08	112.18	106.10
1	C	181	TYR	CA-C-O	6.08	127.91	120.92
1	A	32	ASP	CA-CB-CG	6.08	118.68	112.60
1	G	181	TYR	CA-C-O	6.07	127.90	120.92
1	A	195	LYS	CA-C-O	-6.07	112.32	120.15
1	E	108	PRO	CA-C-N	6.07	128.74	120.54
1	E	108	PRO	C-N-CA	6.07	128.74	120.54
1	E	195	LYS	CA-C-O	-6.07	112.32	120.15
1	A	108	PRO	CA-C-N	6.07	128.73	120.54
1	A	108	PRO	C-N-CA	6.07	128.73	120.54
1	G	141	LEU	CA-C-O	6.07	126.98	120.55
1	C	32	ASP	CA-CB-CG	6.05	118.66	112.60
1	G	207	GLU	CB-CG-CD	-6.05	102.31	112.60
1	C	141	LEU	CA-C-O	6.05	126.97	120.55
1	A	207	GLU	CB-CG-CD	-6.05	102.32	112.60
1	G	195	LYS	CA-C-O	-6.05	112.35	120.15
1	C	207	GLU	CB-CG-CD	-6.04	102.32	112.60
1	C	318	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	E	207	GLU	CB-CG-CD	-6.04	102.34	112.60
2	D	2	HIS	ND1-CG-CD2	6.04	112.14	106.10
1	A	93	GLY	CA-C-N	6.02	130.95	123.12
1	A	93	GLY	C-N-CA	6.02	130.95	123.12
1	G	178	ASP	CA-C-O	-6.01	114.28	121.56
1	E	93	GLY	CA-C-N	6.01	130.94	123.12
1	E	93	GLY	C-N-CA	6.01	130.94	123.12
1	E	178	ASP	CA-C-O	-6.01	114.29	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	GLY	CA-C-N	6.00	130.93	123.12
1	C	93	GLY	C-N-CA	6.00	130.93	123.12
1	G	93	GLY	CA-C-N	6.00	130.93	123.12
1	G	93	GLY	C-N-CA	6.00	130.93	123.12
1	A	0	LEU	CA-C-N	6.00	130.85	123.17
1	A	0	LEU	C-N-CA	6.00	130.85	123.17
1	E	60	ASP	CA-C-O	-5.99	112.34	119.35
1	G	0	LEU	CA-C-N	5.99	130.84	123.17
1	G	0	LEU	C-N-CA	5.99	130.84	123.17
1	A	10	LEU	O-C-N	5.99	131.88	122.23
1	A	178	ASP	CA-C-O	-5.99	114.31	121.56
1	A	60	ASP	CA-C-O	-5.99	112.34	119.35
1	G	97	THR	CA-C-O	-5.99	114.17	120.58
1	G	318	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	C	10	LEU	O-C-N	5.99	131.87	122.23
1	E	10	LEU	O-C-N	5.99	131.87	122.23
1	A	318	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	G	299	TRP	CA-C-O	-5.98	114.37	121.66
1	G	10	LEU	O-C-N	5.98	131.85	122.23
1	C	97	THR	CA-C-O	-5.97	114.19	120.58
1	G	60	ASP	CA-C-O	-5.97	112.36	119.35
1	C	11	ASN	CA-C-N	-5.97	112.94	122.08
1	C	11	ASN	C-N-CA	-5.97	112.94	122.08
1	C	60	ASP	CA-C-O	-5.97	112.36	119.35
1	E	0	LEU	CA-C-N	5.97	130.81	123.17
1	E	0	LEU	C-N-CA	5.97	130.81	123.17
1	C	299	TRP	CA-C-O	-5.97	114.38	121.66
1	E	318	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	A	299	TRP	CA-C-O	-5.97	114.38	121.66
1	C	178	ASP	CA-C-O	-5.97	114.34	121.56
1	C	0	LEU	CA-C-N	5.96	130.80	123.17
1	C	0	LEU	C-N-CA	5.96	130.80	123.17
1	E	11	ASN	CA-C-N	-5.96	112.96	122.08
1	E	11	ASN	C-N-CA	-5.96	112.96	122.08
1	E	299	TRP	CA-C-O	-5.96	114.39	121.66
1	G	11	ASN	CA-C-N	-5.96	112.96	122.08
1	G	11	ASN	C-N-CA	-5.96	112.96	122.08
1	A	78	GLY	N-CA-C	-5.96	103.87	110.96
1	A	11	ASN	CA-C-N	-5.95	112.97	122.08
1	A	11	ASN	C-N-CA	-5.95	112.97	122.08
1	E	78	GLY	N-CA-C	-5.95	103.87	110.96
1	A	97	THR	CA-C-O	-5.95	114.22	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	78	GLY	N-CA-C	-5.94	103.89	110.96
1	C	78	GLY	N-CA-C	-5.92	103.91	110.96
1	E	97	THR	CA-C-O	-5.91	114.26	120.58
1	G	191	GLN	CA-C-O	5.91	127.08	120.70
1	A	323	ALA	CA-C-O	-5.90	114.73	121.40
1	E	191	GLN	CA-C-O	5.90	127.07	120.70
1	E	323	ALA	CA-C-O	-5.90	114.74	121.40
1	A	191	GLN	CA-C-O	5.88	127.05	120.70
1	C	191	GLN	CA-C-O	5.88	127.05	120.70
1	C	323	ALA	CA-C-O	-5.88	114.75	121.40
1	A	279	ASP	CA-C-N	-5.88	110.31	121.54
1	A	279	ASP	C-N-CA	-5.88	110.31	121.54
1	C	279	ASP	CA-C-N	-5.88	110.32	121.54
1	C	279	ASP	C-N-CA	-5.88	110.32	121.54
1	G	279	ASP	CA-C-N	-5.87	110.32	121.54
1	G	279	ASP	C-N-CA	-5.87	110.32	121.54
1	E	279	ASP	CA-C-N	-5.87	110.33	121.54
1	E	279	ASP	C-N-CA	-5.87	110.33	121.54
1	G	323	ALA	CA-C-O	-5.87	114.77	121.40
1	C	247	VAL	CA-CB-CG2	5.86	120.37	110.40
1	C	96	VAL	CA-CB-CG2	5.85	120.35	110.40
1	G	60	ASP	CA-CB-CG	-5.85	106.75	112.60
1	G	96	VAL	CA-CB-CG2	5.85	120.35	110.40
1	G	134	THR	CA-C-O	-5.85	114.25	119.75
1	A	96	VAL	CA-CB-CG2	5.85	120.35	110.40
1	E	60	ASP	CA-CB-CG	-5.85	106.75	112.60
1	C	265	ARG	CA-CB-CG	5.85	125.79	114.10
1	C	246	VAL	CA-C-O	5.84	127.37	121.64
1	G	265	ARG	CA-CB-CG	5.84	125.79	114.10
1	A	247	VAL	CA-CB-CG2	5.84	120.33	110.40
1	A	60	ASP	CA-CB-CG	-5.84	106.76	112.60
1	A	265	ARG	CA-CB-CG	5.84	125.78	114.10
1	G	39	TRP	CH2-CZ2-CE2	5.84	125.09	117.50
1	C	60	ASP	CA-CB-CG	-5.83	106.77	112.60
1	G	247	VAL	CA-CB-CG2	5.83	120.31	110.40
1	E	247	VAL	CA-CB-CG2	5.83	120.31	110.40
1	G	318	ASN	O-C-N	-5.83	115.69	122.86
1	A	134	THR	CA-C-O	-5.82	114.28	119.75
1	E	265	ARG	CA-CB-CG	5.82	125.74	114.10
1	A	246	VAL	CA-C-O	5.82	127.34	121.64
1	E	246	VAL	CA-C-O	5.82	127.34	121.64
1	E	96	VAL	CA-CB-CG2	5.82	120.29	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	318	ASN	O-C-N	-5.82	115.71	122.86
1	A	318	ASN	O-C-N	-5.81	115.71	122.86
1	C	39	TRP	CH2-CZ2-CE2	5.81	125.06	117.50
1	E	39	TRP	O-C-N	5.81	129.87	123.25
1	G	194	MET	O-C-N	-5.81	116.60	123.22
1	E	134	THR	CA-C-O	-5.80	114.30	119.75
1	A	39	TRP	CH2-CZ2-CE2	5.80	125.04	117.50
1	E	194	MET	O-C-N	-5.80	116.61	123.22
2	D	2	HIS	CA-C-N	-5.79	114.00	120.14
2	D	2	HIS	C-N-CA	-5.79	114.00	120.14
2	B	2	HIS	CA-C-N	-5.79	114.00	120.14
2	B	2	HIS	C-N-CA	-5.79	114.00	120.14
1	C	228	LEU	CA-C-O	-5.79	114.71	120.90
1	C	281	LEU	O-C-N	-5.79	116.73	123.27
1	A	39	TRP	O-C-N	5.79	129.84	123.25
2	H	2	HIS	CA-C-N	-5.79	114.01	120.14
2	H	2	HIS	C-N-CA	-5.79	114.01	120.14
2	F	2	HIS	CA-C-N	-5.78	114.01	120.14
2	F	2	HIS	C-N-CA	-5.78	114.01	120.14
1	C	39	TRP	O-C-N	5.78	129.84	123.25
1	A	118	ASP	CA-C-O	5.78	126.73	120.55
1	C	194	MET	O-C-N	-5.78	116.64	123.22
1	C	318	ASN	O-C-N	-5.78	115.76	122.86
1	G	246	VAL	CA-C-O	5.78	127.30	121.64
1	A	194	MET	O-C-N	-5.77	116.64	123.22
1	E	39	TRP	CH2-CZ2-CE2	5.77	125.00	117.50
1	A	326	ARG	CG-CD-NE	5.77	124.69	112.00
1	C	118	ASP	CA-C-O	5.76	126.72	120.55
1	C	326	ARG	CG-CD-NE	5.76	124.68	112.00
1	A	228	LEU	CA-C-O	-5.76	114.74	120.90
1	G	228	LEU	CA-C-O	-5.76	114.74	120.90
1	G	240	LYS	CA-C-O	5.76	126.48	119.11
1	E	118	ASP	CA-C-O	5.75	126.71	120.55
1	G	39	TRP	O-C-N	5.75	129.81	123.25
1	A	240	LYS	CA-C-O	5.75	126.47	119.11
1	E	228	LEU	CA-C-O	-5.75	114.75	120.90
1	G	326	ARG	CG-CD-NE	5.75	124.65	112.00
1	E	240	LYS	CA-C-O	5.75	126.47	119.11
1	E	326	ARG	CG-CD-NE	5.75	124.64	112.00
1	A	250	SER	CA-C-O	-5.74	113.36	119.97
1	C	134	THR	CA-C-O	-5.74	114.35	119.75
1	E	250	SER	CA-C-O	-5.74	113.37	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	LYS	CA-C-O	5.74	126.45	119.11
1	C	250	SER	CA-C-O	-5.74	113.38	119.97
1	E	139	HIS	O-C-N	-5.73	115.62	122.15
1	A	139	HIS	O-C-N	-5.73	115.62	122.15
1	A	281	LEU	O-C-N	-5.73	116.80	123.27
1	G	250	SER	CA-C-O	-5.73	113.38	119.97
1	G	281	LEU	O-C-N	-5.72	116.80	123.27
1	G	118	ASP	CA-C-O	5.72	126.67	120.55
1	E	281	LEU	O-C-N	-5.72	116.81	123.27
1	C	139	HIS	O-C-N	-5.71	115.64	122.15
1	G	139	HIS	O-C-N	-5.71	115.64	122.15
1	G	159(A)	HIS	O-C-N	-5.70	115.02	122.59
1	E	113	MET	CA-C-N	5.69	132.63	122.06
1	E	113	MET	C-N-CA	5.69	132.63	122.06
1	C	82	GLY	O-C-N	-5.68	115.31	122.70
1	G	289	MET	CA-C-N	-5.68	115.45	122.84
1	G	289	MET	C-N-CA	-5.68	115.45	122.84
1	E	317	ASN	CA-CB-CG	-5.68	106.92	112.60
1	G	82	GLY	O-C-N	-5.68	115.31	122.70
1	A	289	MET	CA-C-N	-5.68	115.46	122.84
1	A	289	MET	C-N-CA	-5.68	115.46	122.84
1	G	317	ASN	CA-CB-CG	-5.68	106.92	112.60
1	A	82	GLY	O-C-N	-5.68	115.32	122.70
1	C	159(A)	HIS	O-C-N	-5.68	115.04	122.59
1	C	113	MET	CA-C-N	5.67	132.62	122.06
1	C	113	MET	C-N-CA	5.67	132.62	122.06
1	C	289	MET	CA-C-N	-5.67	115.47	122.84
1	C	289	MET	C-N-CA	-5.67	115.47	122.84
1	E	82	GLY	O-C-N	-5.67	115.33	122.70
1	A	113	MET	CA-C-N	5.67	132.60	122.06
1	A	113	MET	C-N-CA	5.67	132.60	122.06
1	C	246	VAL	CA-C-N	-5.66	114.77	122.92
1	C	246	VAL	C-N-CA	-5.66	114.77	122.92
1	C	37	ASN	CB-CG-ND2	5.66	124.89	116.40
1	A	317	ASN	CA-CB-CG	-5.66	106.94	112.60
1	G	113	MET	CA-C-N	5.66	132.58	122.06
1	G	113	MET	C-N-CA	5.66	132.58	122.06
1	E	159(A)	HIS	O-C-N	-5.66	115.07	122.59
1	A	159(A)	HIS	O-C-N	-5.66	115.07	122.59
1	E	289	MET	CA-C-N	-5.65	115.49	122.84
1	E	289	MET	C-N-CA	-5.65	115.49	122.84
1	C	317	ASN	CA-CB-CG	-5.65	106.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	37	ASN	CB-CG-ND2	5.64	124.86	116.40
1	A	246	VAL	CA-C-N	-5.64	114.80	122.92
1	A	246	VAL	C-N-CA	-5.64	114.80	122.92
1	G	246	VAL	CA-C-N	-5.64	114.80	122.92
1	G	246	VAL	C-N-CA	-5.64	114.80	122.92
1	E	37	ASN	CB-CG-ND2	5.63	124.85	116.40
1	E	246	VAL	CA-C-N	-5.63	114.81	122.92
1	E	246	VAL	C-N-CA	-5.63	114.81	122.92
1	A	37	ASN	CB-CG-ND2	5.63	124.84	116.40
1	E	304	THR	CA-C-N	5.63	130.11	120.71
1	E	304	THR	C-N-CA	5.63	130.11	120.71
1	G	304	THR	CA-C-N	5.63	130.10	120.71
1	G	304	THR	C-N-CA	5.63	130.10	120.71
1	A	304	THR	CA-C-N	5.62	130.10	120.71
1	A	304	THR	C-N-CA	5.62	130.10	120.71
2	B	7	TYR	CD1-CG-CD2	5.61	126.51	118.10
2	F	7	TYR	CD1-CG-CD2	5.60	126.50	118.10
1	C	304	THR	CA-C-N	5.60	130.06	120.71
1	C	304	THR	C-N-CA	5.60	130.06	120.71
1	G	119	GLY	CA-C-N	5.59	130.77	122.99
1	G	119	GLY	C-N-CA	5.59	130.77	122.99
1	C	119	GLY	CA-C-N	5.59	130.76	122.99
1	C	119	GLY	C-N-CA	5.59	130.76	122.99
1	A	119	GLY	CA-C-N	5.59	130.76	122.99
1	A	119	GLY	C-N-CA	5.59	130.76	122.99
2	D	7	TYR	CD1-CG-CD2	5.59	126.49	118.10
1	A	220	PHE	CA-C-N	-5.59	113.56	122.50
1	A	220	PHE	C-N-CA	-5.59	113.56	122.50
1	C	220	PHE	CA-C-N	-5.59	113.56	122.50
1	C	220	PHE	C-N-CA	-5.59	113.56	122.50
1	E	220	PHE	CA-C-N	-5.58	113.57	122.50
1	E	220	PHE	C-N-CA	-5.58	113.57	122.50
1	G	220	PHE	CA-C-N	-5.58	113.57	122.50
1	G	220	PHE	C-N-CA	-5.58	113.57	122.50
2	H	7	TYR	CD1-CG-CD2	5.58	126.46	118.10
1	C	180	HIS	CB-CG-CD2	-5.57	123.95	131.20
1	E	243	HIS	CB-CG-CD2	-5.57	123.95	131.20
1	C	220	PHE	CA-CB-CG	5.56	119.36	113.80
1	E	119	GLY	CA-C-N	5.56	130.72	122.99
1	E	119	GLY	C-N-CA	5.56	130.72	122.99
1	E	180	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	E	220	PHE	CA-CB-CG	5.55	119.36	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	HIS	CA-C-O	5.55	126.30	120.42
1	A	220	PHE	CA-CB-CG	5.55	119.35	113.80
1	A	243	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	A	180	HIS	CB-CG-CD2	-5.54	123.99	131.20
1	G	220	PHE	CA-CB-CG	5.54	119.34	113.80
1	G	139	HIS	CA-C-O	5.54	126.29	120.42
1	E	139	HIS	CA-C-O	5.53	126.28	120.42
1	C	3	PRO	CA-C-N	5.53	130.54	123.13
1	C	3	PRO	C-N-CA	5.53	130.54	123.13
1	G	243	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	G	180	HIS	CB-CG-CD2	-5.52	124.02	131.20
1	E	3	PRO	CA-C-N	5.52	130.53	123.13
1	E	3	PRO	C-N-CA	5.52	130.53	123.13
1	G	3	PRO	CA-C-N	5.51	130.52	123.13
1	G	3	PRO	C-N-CA	5.51	130.52	123.13
1	C	243	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	A	3	PRO	CA-C-N	5.50	130.50	123.13
1	A	3	PRO	C-N-CA	5.50	130.50	123.13
1	C	139	HIS	CA-C-O	5.50	126.24	120.42
1	C	281	LEU	CA-C-N	5.49	130.73	122.99
1	C	281	LEU	C-N-CA	5.49	130.73	122.99
1	E	215	ASP	CA-C-N	5.49	129.88	120.72
1	E	215	ASP	C-N-CA	5.49	129.88	120.72
1	G	215	ASP	CA-C-N	5.49	129.88	120.72
1	G	215	ASP	C-N-CA	5.49	129.88	120.72
1	A	281	LEU	CA-C-N	5.48	130.72	122.99
1	A	281	LEU	C-N-CA	5.48	130.72	122.99
1	A	215	ASP	CA-C-N	5.47	129.86	120.72
1	A	215	ASP	C-N-CA	5.47	129.86	120.72
1	C	215	ASP	CA-C-N	5.47	129.86	120.72
1	C	215	ASP	C-N-CA	5.47	129.86	120.72
1	E	281	LEU	CA-C-N	5.47	130.71	122.99
1	E	281	LEU	C-N-CA	5.47	130.71	122.99
1	G	281	LEU	CA-C-N	5.47	130.71	122.99
1	G	281	LEU	C-N-CA	5.47	130.71	122.99
1	E	38	LEU	CA-C-O	-5.46	114.48	120.43
1	E	149	LYS	CA-C-N	-5.45	114.95	122.69
1	E	149	LYS	C-N-CA	-5.45	114.95	122.69
1	C	149	LYS	CA-C-N	-5.45	114.95	122.69
1	C	149	LYS	C-N-CA	-5.45	114.95	122.69
1	G	25	GLN	CA-C-O	-5.44	114.50	120.43
1	A	149	LYS	CA-C-N	-5.44	114.97	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	LYS	C-N-CA	-5.44	114.97	122.69
1	E	25	GLN	CA-C-O	-5.43	114.51	120.43
1	G	149	LYS	CA-C-N	-5.43	114.98	122.69
1	G	149	LYS	C-N-CA	-5.43	114.98	122.69
1	A	25	GLN	CA-C-O	-5.41	114.53	120.43
1	C	25	GLN	CA-C-O	-5.41	114.53	120.43
1	G	312	GLU	CA-C-O	5.41	126.28	120.38
1	A	38	LEU	CA-C-O	-5.40	114.54	120.43
1	E	312	GLU	CA-C-O	5.40	126.27	120.38
1	E	300	VAL	CA-CB-CG1	5.40	119.58	110.40
1	C	87	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	38	LEU	CA-C-O	-5.40	114.55	120.43
1	A	300	VAL	CA-CB-CG1	5.39	119.56	110.40
1	G	300	VAL	CA-CB-CG1	5.39	119.56	110.40
1	E	87	ASP	CA-CB-CG	5.39	117.99	112.60
1	C	300	VAL	CA-CB-CG1	5.38	119.55	110.40
1	C	312	GLU	CA-C-O	5.38	126.25	120.38
1	E	141	LEU	O-C-N	-5.38	116.42	122.12
1	A	87	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	312	GLU	CA-C-O	5.38	126.25	120.38
1	G	38	LEU	CA-C-O	-5.38	114.57	120.43
1	G	141	LEU	O-C-N	-5.37	116.42	122.12
1	E	76	GLY	CA-C-N	5.37	132.06	121.58
1	E	76	GLY	C-N-CA	5.37	132.06	121.58
1	G	84	LEU	CA-C-O	5.36	127.09	120.92
1	A	141	LEU	O-C-N	-5.36	116.44	122.12
1	G	239	GLU	CA-C-N	-5.36	111.13	121.58
1	G	239	GLU	C-N-CA	-5.36	111.13	121.58
1	C	141	LEU	O-C-N	-5.35	116.44	122.12
1	C	76	GLY	CA-C-N	5.35	132.02	121.58
1	C	76	GLY	C-N-CA	5.35	132.02	121.58
1	G	87	ASP	CA-CB-CG	5.35	117.95	112.60
1	G	233	GLN	CA-C-O	5.35	126.09	120.42
1	A	239	GLU	CA-C-N	-5.34	111.16	121.58
1	A	239	GLU	C-N-CA	-5.34	111.16	121.58
1	E	239	GLU	CA-C-N	-5.34	111.16	121.58
1	E	239	GLU	C-N-CA	-5.34	111.16	121.58
1	A	76	GLY	CA-C-N	5.34	131.99	121.58
1	A	76	GLY	C-N-CA	5.34	131.99	121.58
1	A	84	LEU	CA-C-O	5.33	127.06	120.92
1	C	164	GLU	CA-C-O	5.33	126.76	120.89
1	A	229	LYS	CA-CB-CG	-5.33	103.44	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	SER	CA-C-O	-5.33	114.97	121.05
1	C	151	PHE	O-C-N	-5.33	116.68	123.24
1	C	239	GLU	CA-C-N	-5.33	111.19	121.58
1	C	239	GLU	C-N-CA	-5.33	111.19	121.58
1	C	84	LEU	CA-C-O	5.33	127.04	120.92
1	E	229	LYS	CA-CB-CG	-5.33	103.45	114.10
1	A	233	GLN	CA-C-O	5.32	126.06	120.42
1	E	233	GLN	CA-C-O	5.32	126.06	120.42
1	E	242	LEU	CA-C-O	-5.32	115.05	120.80
1	G	229	LYS	CA-CB-CG	-5.32	103.46	114.10
1	A	242	LEU	CA-C-O	-5.32	115.06	120.80
1	G	76	GLY	CA-C-N	5.32	131.95	121.58
1	G	76	GLY	C-N-CA	5.32	131.95	121.58
1	E	84	LEU	CA-C-O	5.31	127.03	120.92
1	E	151	PHE	O-C-N	-5.31	116.70	123.24
1	G	213	VAL	CA-C-O	-5.31	114.89	120.57
1	G	261	ASN	CA-C-O	5.31	126.26	120.58
1	A	54	SER	CA-C-O	-5.31	115.00	121.05
1	A	151	PHE	O-C-N	-5.31	116.71	123.24
1	C	229	LYS	CA-CB-CG	-5.30	103.49	114.10
1	C	233	GLN	CA-C-O	5.30	126.04	120.42
1	E	164	GLU	CA-C-O	5.30	126.72	120.89
1	A	164	GLU	CA-C-O	5.29	126.71	120.89
1	E	116	GLN	CA-C-O	5.29	125.46	119.27
1	G	54	SER	CA-C-O	-5.29	115.02	121.05
1	G	151	PHE	O-C-N	-5.29	116.74	123.24
1	C	116	GLN	CA-C-O	5.29	125.45	119.27
1	C	213	VAL	CA-C-O	-5.29	114.91	120.57
1	E	54	SER	CA-C-O	-5.29	115.03	121.05
1	A	116	GLN	CA-C-O	5.28	125.45	119.27
1	A	167	LEU	CA-C-O	-5.28	114.52	120.43
1	A	213	VAL	CA-C-O	-5.28	114.92	120.57
1	G	167	LEU	CA-C-O	-5.28	114.52	120.43
1	G	242	LEU	CA-C-O	-5.28	115.10	120.80
1	G	116	GLN	CA-C-O	5.28	125.44	119.27
1	C	242	LEU	CA-C-O	-5.27	115.11	120.80
1	E	167	LEU	CA-C-O	-5.27	114.53	120.43
1	A	261	ASN	CA-C-O	5.26	126.21	120.58
1	E	213	VAL	CA-C-O	-5.26	114.94	120.57
1	G	164	GLU	CA-C-O	5.26	126.67	120.89
1	C	121	LEU	O-C-N	-5.25	116.18	123.01
1	E	25	GLN	CG-CD-NE2	5.25	124.28	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	25	GLN	CG-CD-NE2	5.25	124.28	116.40
1	G	175	TYR	CA-C-O	5.24	127.14	121.06
1	E	224	PRO	N-CA-CB	-5.24	98.79	103.35
1	C	167	LEU	CA-C-O	-5.24	114.56	120.43
1	A	25	GLN	CG-CD-NE2	5.23	124.25	116.40
1	A	121	LEU	O-C-N	-5.23	116.21	123.01
1	A	175	TYR	CA-C-O	5.23	127.13	121.06
1	C	175	TYR	CA-C-O	5.23	127.13	121.06
1	G	121	LEU	O-C-N	-5.23	116.21	123.01
1	E	175	TYR	CA-C-O	5.23	127.13	121.06
1	C	201	SER	CA-CB-OG	-5.23	100.65	111.10
1	G	201	SER	CA-CB-OG	-5.23	100.65	111.10
1	A	201	SER	CA-CB-OG	-5.22	100.65	111.10
1	E	277	GLN	O-C-N	5.22	129.41	122.41
1	G	224	PRO	N-CA-CB	-5.22	98.81	103.35
1	E	121	LEU	O-C-N	-5.22	116.22	123.01
1	E	261	ASN	CA-C-O	5.22	126.17	120.58
1	E	201	SER	CA-CB-OG	-5.22	100.66	111.10
1	A	224	PRO	N-CA-CB	-5.22	98.81	103.35
1	C	261	ASN	CA-C-O	5.22	126.17	120.58
1	G	305	PHE	CD1-CG-CD2	5.22	126.43	118.60
1	C	91	VAL	CA-C-O	-5.22	114.74	120.43
1	C	25	GLN	CG-CD-NE2	5.21	124.22	116.40
1	C	125	PHE	CG-CD2-CE2	5.21	129.55	120.70
1	G	125	PHE	CG-CD2-CE2	5.21	129.55	120.70
1	G	185	SER	O-C-N	-5.21	115.19	122.37
1	A	125	PHE	CG-CD2-CE2	5.20	129.54	120.70
1	C	268	THR	CA-C-O	5.20	126.05	120.38
1	A	305	PHE	CD1-CG-CD2	5.20	126.40	118.60
1	G	268	THR	CA-C-O	5.19	126.04	120.38
1	A	268	THR	CA-C-O	5.19	126.04	120.38
1	C	224	PRO	N-CA-CB	-5.19	98.83	103.35
1	E	305	PHE	CD1-CG-CD2	5.19	126.39	118.60
1	E	125	PHE	CG-CD2-CE2	5.19	129.52	120.70
1	A	175	TYR	O-C-N	-5.18	117.26	123.27
1	C	81	LYS	CG-CD-CE	-5.18	99.38	111.30
1	G	175	TYR	O-C-N	-5.18	117.26	123.27
1	C	175	TYR	O-C-N	-5.18	117.26	123.27
1	G	312	GLU	CB-CG-CD	-5.18	103.79	112.60
1	A	81	LYS	CG-CD-CE	-5.18	99.39	111.30
1	E	268	THR	CA-C-O	5.18	126.02	120.38
1	A	91	VAL	CA-C-O	-5.17	114.79	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	81	LYS	CG-CD-CE	-5.17	99.40	111.30
1	E	312	GLU	CB-CG-CD	-5.17	103.81	112.60
1	A	185	SER	O-C-N	-5.17	115.23	122.37
1	G	81	LYS	CG-CD-CE	-5.17	99.41	111.30
1	E	52	ILE	CB-CA-C	5.17	116.20	110.62
1	C	305	PHE	CD1-CG-CD2	5.17	126.35	118.60
1	E	91	VAL	CA-C-O	-5.17	114.80	120.43
1	E	185	SER	O-C-N	-5.17	115.24	122.37
1	C	277	GLN	O-C-N	5.16	129.33	122.41
1	E	175	TYR	O-C-N	-5.16	117.28	123.27
1	C	312	GLU	CB-CG-CD	-5.16	103.83	112.60
1	G	52	ILE	CB-CA-C	5.16	116.19	110.62
1	A	277	GLN	O-C-N	5.16	129.32	122.41
1	A	312	GLU	CB-CG-CD	-5.16	103.83	112.60
1	C	52	ILE	CB-CA-C	5.16	116.19	110.62
1	G	277	GLN	O-C-N	5.16	129.32	122.41
1	A	52	ILE	CB-CA-C	5.15	116.19	110.62
1	C	185	SER	O-C-N	-5.15	115.26	122.37
1	A	190	TRP	CB-CG-CD1	-5.14	119.19	126.90
1	G	156	ASN	CB-CG-ND2	-5.14	108.69	116.40
2	B	5	HIS	CG-CD2-NE2	5.14	112.34	107.20
1	C	190	TRP	CB-CG-CD1	-5.14	119.19	126.90
2	F	5	HIS	CG-CD2-NE2	5.14	112.34	107.20
1	E	305	PHE	CA-C-N	5.13	128.58	120.47
1	E	305	PHE	C-N-CA	5.13	128.58	120.47
1	G	190	TRP	CB-CG-CD1	-5.13	119.20	126.90
1	E	142	SER	O-C-N	-5.13	116.30	122.15
1	E	190	TRP	CB-CG-CD1	-5.13	119.21	126.90
1	G	91	VAL	CA-C-O	-5.13	114.84	120.43
1	E	104	VAL	O-C-N	-5.12	117.12	122.81
1	G	305	PHE	CA-C-N	5.12	128.56	120.47
1	G	305	PHE	C-N-CA	5.12	128.56	120.47
1	A	156	ASN	CB-CG-ND2	-5.12	108.72	116.40
2	H	5	HIS	CG-CD2-NE2	5.12	112.32	107.20
1	A	142	SER	O-C-N	-5.12	116.31	122.15
1	A	305	PHE	CA-C-N	5.12	128.56	120.47
1	A	305	PHE	C-N-CA	5.12	128.56	120.47
1	C	69	ASP	CA-CB-CG	-5.12	107.48	112.60
1	C	156	ASN	CB-CG-ND2	-5.12	108.72	116.40
1	G	102	GLY	CA-C-N	5.12	129.93	122.41
1	G	102	GLY	C-N-CA	5.12	129.93	122.41
1	A	211	GLU	CA-C-N	-5.11	115.35	122.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	GLU	C-N-CA	-5.11	115.35	122.71
1	G	69	ASP	CA-CB-CG	-5.11	107.49	112.60
1	G	258	ILE	CA-C-O	-5.11	115.02	120.39
1	C	211	GLU	CA-C-N	-5.11	115.35	122.71
1	C	211	GLU	C-N-CA	-5.11	115.35	122.71
1	C	305	PHE	CA-C-N	5.11	128.54	120.47
1	C	305	PHE	C-N-CA	5.11	128.54	120.47
1	E	211	GLU	CA-C-N	-5.11	115.35	122.71
1	E	211	GLU	C-N-CA	-5.11	115.35	122.71
1	C	76	GLY	N-CA-C	-5.11	106.60	112.83
1	E	156	ASN	CB-CG-ND2	-5.11	108.74	116.40
1	G	104	VAL	O-C-N	-5.11	117.14	122.81
1	E	76	GLY	N-CA-C	-5.10	106.60	112.83
1	G	211	GLU	CA-C-N	-5.10	115.36	122.71
1	G	211	GLU	C-N-CA	-5.10	115.36	122.71
1	G	323	ALA	O-C-N	-5.10	117.00	123.17
1	A	76	GLY	N-CA-C	-5.10	106.61	112.83
1	A	104	VAL	O-C-N	-5.10	117.15	122.81
1	C	55	LEU	CB-CG-CD2	5.10	125.99	110.70
1	G	55	LEU	CB-CG-CD2	5.10	125.99	110.70
1	A	55	LEU	CB-CG-CD2	5.10	125.99	110.70
1	C	102	GLY	CA-C-N	5.09	129.90	122.41
1	C	102	GLY	C-N-CA	5.09	129.90	122.41
1	C	323	ALA	O-C-N	-5.09	117.01	123.17
1	A	258	ILE	CA-C-O	-5.09	115.04	120.39
1	A	102	GLY	CA-C-N	5.09	129.90	122.41
1	A	102	GLY	C-N-CA	5.09	129.90	122.41
1	E	69	ASP	CA-CB-CG	-5.09	107.51	112.60
1	E	323	ALA	O-C-N	-5.09	117.01	123.17
1	C	142	SER	O-C-N	-5.09	116.35	122.15
1	E	55	LEU	CB-CG-CD2	5.09	125.97	110.70
1	A	323	ALA	O-C-N	-5.09	117.01	123.17
1	C	258	ILE	CA-C-O	-5.09	115.05	120.39
1	G	142	SER	O-C-N	-5.09	116.35	122.15
1	C	104	VAL	O-C-N	-5.08	117.17	122.81
1	A	69	ASP	CA-CB-CG	-5.08	107.52	112.60
1	C	172	PRO	CA-C-O	5.08	126.44	119.18
1	A	232	MET	CG-SD-CE	5.08	112.07	100.90
1	E	258	ILE	CA-C-O	-5.08	115.06	120.39
1	E	232	MET	CG-SD-CE	5.07	112.06	100.90
2	D	5	HIS	CG-CD2-NE2	5.07	112.27	107.20
1	E	102	GLY	CA-C-N	5.07	129.87	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	102	GLY	C-N-CA	5.07	129.87	122.41
1	G	232	MET	CG-SD-CE	5.07	112.06	100.90
1	C	232	MET	CG-SD-CE	5.07	112.05	100.90
1	G	76	GLY	N-CA-C	-5.07	106.65	112.83
1	C	24	PRO	CA-N-CD	5.06	119.08	112.00
1	A	172	PRO	CA-C-O	5.05	126.41	119.18
1	G	172	PRO	CA-C-O	5.04	126.39	119.18
1	E	172	PRO	CA-C-O	5.04	126.39	119.18
1	G	198	SER	O-C-N	5.04	129.24	123.29
1	G	77	SER	CA-C-O	-5.04	112.66	119.11
1	A	24	PRO	CA-N-CD	5.04	119.05	112.00
1	C	198	SER	O-C-N	5.03	129.23	123.29
1	E	24	PRO	CA-N-CD	5.03	119.05	112.00
1	E	77	SER	CA-C-O	-5.03	112.67	119.11
1	E	319	ARG	O-C-N	5.03	128.54	123.26
1	G	24	PRO	CA-N-CD	5.03	119.04	112.00
1	E	198	SER	O-C-N	5.02	129.22	123.29
1	C	151	PHE	CA-C-O	-5.02	115.24	121.11
1	A	66	GLU	CA-C-O	5.02	127.03	121.56
1	A	131	GLY	N-CA-C	-5.02	108.33	115.30
1	A	198	SER	O-C-N	5.01	129.21	123.29
1	E	151	PHE	CA-C-O	-5.01	115.24	121.11
1	A	5	VAL	CA-CB-CG1	5.01	118.92	110.40
1	C	131	GLY	N-CA-C	-5.01	108.34	115.30
1	E	5	VAL	CA-CB-CG1	5.01	118.92	110.40
1	E	66	GLU	CA-C-O	5.01	127.02	121.56
1	G	151	PHE	CA-C-O	-5.01	115.25	121.11
1	C	77	SER	CA-C-O	-5.00	112.70	119.11
1	C	250	SER	CA-CB-OG	5.00	121.11	111.10
1	E	250	SER	CA-CB-OG	5.00	121.11	111.10
1	A	151	PHE	CA-C-O	-5.00	115.26	121.11

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	ARG	Sidechain
1	A	265	ARG	Sidechain
1	A	319	ARG	Sidechain
2	B	6	LPL	Mainchain,Peptide
1	C	241	ARG	Sidechain
1	C	265	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	319	ARG	Sidechain
2	D	6	LPL	Mainchain,Peptide
1	E	241	ARG	Sidechain
1	E	265	ARG	Sidechain
1	E	319	ARG	Sidechain
2	F	6	LPL	Mainchain,Peptide
1	G	241	ARG	Sidechain
1	G	265	ARG	Sidechain
1	G	319	ARG	Sidechain
2	H	6	LPL	Mainchain,Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2511	0	2444	54	16
1	C	2511	0	2444	52	19
1	E	2511	0	2444	54	17
1	G	2511	0	2444	54	19
2	B	90	0	86	3	0
2	D	90	0	86	3	0
2	F	90	0	86	3	0
2	H	90	0	86	3	0
3	A	148	0	0	3	1
3	B	5	0	0	0	0
3	C	3	0	0	1	0
All	All	10560	0	10120	218	36

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 11.

All (218) 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:C:199:VAL:HB	1:C:203:THR:HG23	1.44	1.00
1:E:199:VAL:HB	1:E:203:THR:HG23	1.44	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:VAL:HB	1:G:203:THR:HG23	1.44	0.99
1:A:199:VAL:HB	1:A:203:THR:HG23	1.44	0.97
1:A:199:VAL:HB	1:A:203:THR:CG2	2.00	0.92
1:E:199:VAL:HB	1:E:203:THR:CG2	2.00	0.91
1:G:199:VAL:HB	1:G:203:THR:CG2	2.00	0.91
1:C:199:VAL:HB	1:C:203:THR:CG2	2.00	0.90
1:A:65:MET:HG3	1:A:86:GLN:HE21	1.42	0.84
1:E:65:MET:HG3	1:E:86:GLN:HE21	1.42	0.82
1:C:65:MET:HG3	1:C:86:GLN:HE21	1.42	0.81
1:G:65:MET:HG3	1:G:86:GLN:HE21	1.42	0.81
1:G:8:ASN:H	1:G:160:LEU:CD2	1.94	0.81
1:C:8:ASN:H	1:C:160:LEU:CD2	1.94	0.81
1:C:159:PRO:O	1:C:159(A):HIS:CB	2.30	0.80
1:A:8:ASN:H	1:A:160:LEU:CD2	1.94	0.80
1:A:317:ASN:HB2	1:A:319:ARG:HD3	1.64	0.79
1:G:317:ASN:HB2	1:G:319:ARG:HD3	1.64	0.79
1:E:317:ASN:HB2	1:E:319:ARG:HD3	1.64	0.79
1:E:8:ASN:H	1:E:160:LEU:CD2	1.94	0.79
1:E:159:PRO:O	1:E:159(A):HIS:CB	2.30	0.79
1:A:159:PRO:O	1:A:159(A):HIS:CB	2.30	0.79
1:C:159(A):HIS:O	1:C:161:LEU:N	2.16	0.78
1:A:159(A):HIS:O	1:A:161:LEU:N	2.16	0.78
1:A:8:ASN:H	1:A:160:LEU:HD21	1.49	0.78
1:G:159:PRO:O	1:G:159(A):HIS:CB	2.30	0.78
1:C:317:ASN:HB2	1:C:319:ARG:HD3	1.64	0.77
1:C:8:ASN:H	1:C:160:LEU:HD21	1.49	0.77
1:E:8:ASN:H	1:E:160:LEU:HD21	1.49	0.77
1:G:159(A):HIS:O	1:G:161:LEU:N	2.16	0.76
1:G:8:ASN:H	1:G:160:LEU:HD21	1.49	0.75
1:E:159(A):HIS:O	1:E:161:LEU:N	2.16	0.74
1:E:43:THR:HG22	1:E:44:LYS:HD2	1.70	0.74
1:A:43:THR:HG22	1:A:44:LYS:HD2	1.70	0.73
1:C:43:THR:HG22	1:C:44:LYS:HD2	1.70	0.73
1:G:43:THR:HG22	1:G:44:LYS:HD2	1.70	0.72
1:C:203:THR:O	1:C:203:THR:OG1	2.03	0.71
1:G:203:THR:O	1:G:203:THR:OG1	2.03	0.70
1:E:203:THR:O	1:E:203:THR:OG1	2.03	0.70
1:A:48:LEU:O	1:A:48:LEU:HD23	1.92	0.69
1:C:48:LEU:O	1:C:48:LEU:HD23	1.92	0.69
1:A:317:ASN:CB	1:A:319:ARG:HD3	2.23	0.69
1:E:48:LEU:HD23	1:E:48:LEU:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ASN:CB	1:C:319:ARG:HD3	2.23	0.69
1:G:48:LEU:HD23	1:G:48:LEU:O	1.92	0.68
1:A:203:THR:O	1:A:203:THR:OG1	2.03	0.68
1:E:317:ASN:CB	1:E:319:ARG:HD3	2.23	0.67
1:G:317:ASN:CB	1:G:319:ARG:HD3	2.23	0.67
1:E:160:LEU:HD23	1:E:162:GLY:N	2.10	0.67
1:A:160:LEU:HD23	1:A:162:GLY:N	2.10	0.66
1:C:160:LEU:HD23	1:C:162:GLY:N	2.10	0.66
1:G:160:LEU:HD23	1:G:162:GLY:N	2.10	0.66
1:E:202:SER:C	1:E:203:THR:HG22	2.21	0.65
1:E:200:GLY:HA2	1:E:256:PRO:HB2	1.80	0.64
1:C:57:GLU:OE2	1:C:59:SER:HB2	1.98	0.64
1:E:57:GLU:OE2	1:E:59:SER:HB2	1.98	0.64
1:G:57:GLU:OE2	1:G:59:SER:HB2	1.98	0.64
1:G:202:SER:C	1:G:203:THR:HG22	2.21	0.64
1:A:200:GLY:HA2	1:A:256:PRO:HB2	1.80	0.64
1:C:202:SER:C	1:C:203:THR:HG22	2.21	0.64
1:G:200:GLY:HA2	1:G:256:PRO:HB2	1.80	0.64
1:A:202:SER:C	1:A:203:THR:HG22	2.21	0.64
1:C:200:GLY:HA2	1:C:256:PRO:HB2	1.80	0.64
1:A:57:GLU:OE2	1:A:59:SER:HB2	1.98	0.62
1:E:174:HIS:HD2	1:E:326:ARG:OXT	1.83	0.61
1:G:200:GLY:CA	1:G:256:PRO:HB2	2.30	0.61
1:A:200:GLY:CA	1:A:256:PRO:HB2	2.30	0.61
1:C:200:GLY:CA	1:C:256:PRO:HB2	2.30	0.61
1:A:201:SER:HB2	3:A:460:HOH:O	1.99	0.61
1:C:174:HIS:HD2	1:C:326:ARG:OXT	1.83	0.60
1:A:174:HIS:HD2	1:A:326:ARG:OXT	1.83	0.60
1:E:200:GLY:CA	1:E:256:PRO:HB2	2.30	0.60
1:A:53:HIS:HE1	1:A:115:ALA:O	1.85	0.60
1:C:65:MET:HG3	1:C:86:GLN:NE2	2.16	0.60
1:G:174:HIS:HD2	1:G:326:ARG:OXT	1.83	0.59
1:E:53:HIS:HE1	1:E:115:ALA:O	1.85	0.59
1:G:53:HIS:HE1	1:G:115:ALA:O	1.85	0.59
1:A:65:MET:HG3	1:A:86:GLN:NE2	2.16	0.59
1:C:53:HIS:HE1	1:C:115:ALA:O	1.85	0.58
1:G:65:MET:HG3	1:G:86:GLN:NE2	2.16	0.58
1:E:65:MET:HG3	1:E:86:GLN:NE2	2.16	0.57
1:A:139:HIS:HE1	3:A:402:HOH:O	1.87	0.57
1:G:52:ILE:CD1	1:G:113:MET:HG2	2.35	0.56
1:C:8:ASN:C	1:C:8:ASN:OD1	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:CYS:O	1:A:252:VAL:HG23	2.06	0.56
1:A:52:ILE:CD1	1:A:113:MET:HG2	2.35	0.56
1:C:249:CYS:O	1:C:252:VAL:HG23	2.06	0.56
1:E:52:ILE:CD1	1:E:113:MET:HG2	2.35	0.56
1:E:249:CYS:O	1:E:252:VAL:HG23	2.06	0.56
1:C:52:ILE:CD1	1:C:113:MET:HG2	2.35	0.56
1:G:8:ASN:OD1	1:G:8:ASN:C	2.48	0.56
1:G:249:CYS:O	1:G:252:VAL:HG23	2.06	0.56
1:C:202:SER:O	1:C:203:THR:HG22	2.06	0.55
1:A:52:ILE:HG22	1:A:53:HIS:CD2	2.42	0.55
1:G:202:SER:O	1:G:203:THR:HG22	2.06	0.55
1:C:52:ILE:HG22	1:C:53:HIS:CD2	2.42	0.55
1:G:52:ILE:HG22	1:G:53:HIS:CD2	2.42	0.55
1:E:52:ILE:HG22	1:E:53:HIS:CD2	2.42	0.55
1:E:202:SER:O	1:E:203:THR:HG22	2.07	0.55
1:A:8:ASN:C	1:A:8:ASN:OD1	2.48	0.54
1:A:202:SER:O	1:A:203:THR:HG22	2.06	0.54
1:A:205:LEU:HD13	1:A:227:SER:HB3	1.89	0.54
1:C:205:LEU:HD13	1:C:227:SER:HB3	1.89	0.54
1:E:160:LEU:HD23	1:E:162:GLY:CA	2.38	0.54
1:G:160:LEU:HD23	1:G:162:GLY:CA	2.38	0.54
1:C:160:LEU:HD23	1:C:162:GLY:CA	2.38	0.54
1:E:8:ASN:OD1	1:E:8:ASN:C	2.48	0.54
1:G:205:LEU:HD13	1:G:227:SER:HB3	1.89	0.54
1:A:160:LEU:HD23	1:A:162:GLY:CA	2.38	0.53
1:G:252:VAL:HB	1:G:253:PRO:HD3	1.91	0.53
1:E:205:LEU:HD13	1:E:227:SER:HB3	1.89	0.52
1:C:48:LEU:HD23	1:C:48:LEU:C	2.34	0.52
1:E:0:LEU:HD21	1:E:94:ILE:HD11	1.92	0.52
1:A:48:LEU:HD23	1:A:48:LEU:C	2.34	0.52
1:E:7:THR:HA	1:E:160:LEU:HD22	1.92	0.52
1:A:7:THR:HA	1:A:160:LEU:HD22	1.92	0.52
1:A:252:VAL:HB	1:A:253:PRO:HD3	1.91	0.52
1:A:0:LEU:HD21	1:A:94:ILE:HD11	1.92	0.51
1:C:252:VAL:HB	1:C:253:PRO:HD3	1.91	0.51
1:G:48:LEU:HD23	1:G:48:LEU:C	2.34	0.51
1:G:0:LEU:HD21	1:G:94:ILE:HD11	1.92	0.51
1:G:7:THR:HA	1:G:160:LEU:HD22	1.92	0.51
1:E:48:LEU:HD23	1:E:48:LEU:C	2.34	0.51
1:E:252:VAL:HB	1:E:253:PRO:HD3	1.91	0.51
1:A:127:ALA:HB3	1:A:188:ASP:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:THR:HA	1:C:160:LEU:HD22	1.92	0.50
1:G:58:SER:HB2	1:G:64:TYR:CD1	2.47	0.50
1:C:0:LEU:HD21	1:C:94:ILE:HD11	1.92	0.50
1:C:58:SER:HB2	1:C:64:TYR:CD1	2.47	0.50
1:G:127:ALA:HB3	1:G:188:ASP:HB3	1.93	0.50
1:E:58:SER:HB2	1:E:64:TYR:CD1	2.47	0.49
1:E:75:TYR:HA	2:F:6:LPL:O	2.12	0.49
1:C:127:ALA:HB3	1:C:188:ASP:HB3	1.93	0.49
1:G:75:TYR:HA	2:H:6:LPL:O	2.12	0.49
1:A:58:SER:HB2	1:A:64:TYR:CD1	2.47	0.49
1:C:75:TYR:HA	2:D:6:LPL:O	2.12	0.49
1:E:127:ALA:HB3	1:E:188:ASP:HB3	1.93	0.49
1:A:75:TYR:HA	2:B:6:LPL:O	2.12	0.48
1:C:291:ILE:O	1:C:296:GLY:HA3	2.14	0.48
1:A:291:ILE:O	1:A:296:GLY:HA3	2.14	0.48
1:E:159(A):HIS:C	1:E:160:LEU:HG	2.39	0.47
1:G:159(A):HIS:C	1:G:160:LEU:HG	2.39	0.47
1:G:291:ILE:O	1:G:296:GLY:HA3	2.14	0.47
1:C:9:TYR:CE2	1:C:10:LEU:HD12	2.49	0.47
1:A:9:TYR:CE2	1:A:10:LEU:HD12	2.49	0.47
1:C:159(A):HIS:C	1:C:160:LEU:HG	2.39	0.47
1:C:160:LEU:C	3:C:329:HOH:O	2.57	0.47
1:G:9:TYR:CE2	1:G:10:LEU:HD12	2.49	0.47
1:E:9:TYR:CE2	1:E:10:LEU:HD12	2.49	0.47
1:E:291:ILE:O	1:E:296:GLY:HA3	2.14	0.47
1:A:58:SER:HB2	1:A:64:TYR:CG	2.50	0.47
1:E:58:SER:HB2	1:E:64:TYR:CG	2.50	0.47
1:G:199:VAL:HB	1:G:203:THR:HG21	1.94	0.47
1:C:58:SER:HB2	1:C:64:TYR:CG	2.50	0.47
1:G:58:SER:HB2	1:G:64:TYR:CG	2.50	0.47
1:A:159(A):HIS:C	1:A:160:LEU:HG	2.39	0.47
1:A:158:GLY:HA3	1:A:159:PRO:HD2	1.27	0.46
1:A:48:LEU:C	1:A:48:LEU:CD2	2.89	0.46
1:C:48:LEU:C	1:C:48:LEU:CD2	2.89	0.46
1:E:48:LEU:C	1:E:48:LEU:CD2	2.89	0.46
1:A:199:VAL:HB	1:A:203:THR:HG21	1.94	0.46
1:C:271:SER:HA	1:C:274:TYR:CE2	2.51	0.45
1:G:271:SER:HA	1:G:274:TYR:CE2	2.51	0.45
1:A:271:SER:HA	1:A:274:TYR:CE2	2.51	0.45
1:G:8:ASN:HB2	1:G:162:GLY:CA	2.47	0.45
1:G:48:LEU:C	1:G:48:LEU:CD2	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ASN:HB2	1:A:162:GLY:CA	2.47	0.45
1:C:292:PRO:HA	1:C:293:PRO:HD3	1.82	0.45
1:E:271:SER:HA	1:E:274:TYR:CE2	2.51	0.45
1:E:8:ASN:HB2	1:E:162:GLY:CA	2.47	0.45
1:E:172:PRO:HA	1:E:175:TYR:CE1	2.52	0.45
1:A:172:PRO:HA	1:A:175:TYR:CE1	2.52	0.45
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.72	0.45
1:G:172:PRO:HA	1:G:175:TYR:CE1	2.52	0.45
1:C:199:VAL:HB	1:C:203:THR:HG21	1.94	0.44
1:E:171:ASP:HA	1:E:172:PRO:HD2	1.72	0.44
1:C:172:PRO:HA	1:C:175:TYR:CE1	2.52	0.44
1:C:8:ASN:HB2	1:C:162:GLY:CA	2.47	0.44
1:C:161:LEU:HD12	1:C:161:LEU:HA	1.94	0.44
1:C:175:TYR:HA	1:C:324:LEU:O	2.18	0.44
1:E:292:PRO:HA	1:E:293:PRO:HD3	1.81	0.44
1:G:175:TYR:HA	1:G:324:LEU:O	2.18	0.44
1:G:292:PRO:HA	1:G:293:PRO:HD3	1.81	0.44
1:A:272:THR:HG23	3:A:456:HOH:O	2.18	0.44
1:C:171:ASP:HA	1:C:172:PRO:HD2	1.72	0.44
1:A:175:TYR:HA	1:A:324:LEU:O	2.18	0.43
1:E:175:TYR:HA	1:E:324:LEU:O	2.18	0.43
1:A:12:SER:HB3	2:B:1:PIV:C3	2.48	0.43
1:E:12:SER:HB3	2:F:1:PIV:C3	2.49	0.43
2:B:7:TYR:CD1	2:B:7:TYR:C	2.97	0.43
2:D:7:TYR:CD1	2:D:7:TYR:C	2.97	0.43
1:E:199:VAL:HB	1:E:203:THR:HG21	1.94	0.43
1:C:12:SER:HB3	2:D:1:PIV:C3	2.48	0.43
2:F:7:TYR:CD1	2:F:7:TYR:C	2.97	0.43
1:G:158:GLY:HA3	1:G:159:PRO:HD2	1.27	0.42
1:G:230:LEU:HD12	1:G:230:LEU:HA	1.72	0.42
1:A:8:ASN:HB3	1:A:160:LEU:HD21	2.01	0.42
1:E:8:ASN:HB3	1:E:160:LEU:HD21	2.02	0.42
1:G:47:ARG:HH11	1:G:47:ARG:HD3	1.66	0.42
1:G:12:SER:HB3	2:H:1:PIV:C3	2.48	0.42
2:H:7:TYR:CD1	2:H:7:TYR:C	2.97	0.42
1:E:161:LEU:HD12	1:E:161:LEU:HA	1.94	0.42
1:C:230:LEU:HD12	1:C:230:LEU:HA	1.72	0.42
1:G:8:ASN:HB3	1:G:160:LEU:HD21	2.02	0.42
1:A:186:LYS:HB2	1:A:186:LYS:HE3	1.07	0.41
1:G:107:LEU:HA	1:G:108:PRO:HD2	1.82	0.41
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ASN:HB3	1:C:160:LEU:HD21	2.02	0.41
1:C:75:TYR:O	1:C:76:GLY:C	2.64	0.41
1:E:47:ARG:HH11	1:E:47:ARG:HD3	1.66	0.41
1:E:52:ILE:HG22	1:E:53:HIS:NE2	2.36	0.41
1:E:230:LEU:HD12	1:E:230:LEU:HA	1.72	0.41
1:G:221:ILE:HG13	1:G:304:THR:HB	2.03	0.41
1:A:75:TYR:O	1:A:76:GLY:C	2.64	0.41
1:E:186:LYS:HB2	1:E:186:LYS:HE3	1.08	0.41
1:G:75:TYR:O	1:G:76:GLY:C	2.64	0.41
1:E:75:TYR:O	1:E:76:GLY:C	2.64	0.40
1:G:317:ASN:HB3	1:G:319:ARG:HD3	2.03	0.40

All (36) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:MET:CE	1:E:113:MET:CE[1_444]	0.33	1.87
1:E:326:ARG:NE	1:G:326:ARG:NH1[1_565]	0.52	1.68
1:A:326:ARG:NE	1:C:326:ARG:NH1[1_565]	0.63	1.57
1:A:326:ARG:CZ	1:C:326:ARG:CZ[1_565]	0.67	1.53
1:A:113:MET:CE	1:G:113:MET:CE[1_464]	0.69	1.51
1:E:326:ARG:NH1	1:G:326:ARG:CZ[1_565]	0.76	1.44
1:A:326:ARG:NH1	1:C:326:ARG:CZ[1_565]	0.81	1.39
1:E:326:ARG:CZ	1:G:326:ARG:NH1[1_565]	0.86	1.34
1:A:326:ARG:CZ	1:C:326:ARG:NH1[1_565]	0.87	1.33
1:E:326:ARG:CZ	1:G:326:ARG:CZ[1_565]	0.87	1.33
1:A:326:ARG:NH1	1:C:326:ARG:NE[1_565]	0.88	1.32
1:E:326:ARG:NH1	1:G:326:ARG:NE[1_565]	1.01	1.19
1:E:326:ARG:NH1	1:G:326:ARG:NH2[1_565]	1.41	0.79
1:A:326:ARG:NH1	1:C:326:ARG:NH2[1_565]	1.46	0.74
1:A:326:ARG:NE	1:C:326:ARG:CZ[1_565]	1.61	0.59
1:E:326:ARG:NE	1:G:326:ARG:CZ[1_565]	1.65	0.55
1:A:326:ARG:NH2	1:C:326:ARG:NH1[1_565]	1.70	0.50
1:A:326:ARG:CZ	1:C:326:ARG:NH2[1_565]	1.72	0.48
1:A:326:ARG:CZ	1:C:326:ARG:NE[1_565]	1.74	0.46
1:E:326:ARG:CZ	1:G:326:ARG:NH2[1_565]	1.80	0.40
1:E:326:ARG:NH2	1:G:326:ARG:NH1[1_565]	1.85	0.35
1:A:326:ARG:NH2	1:C:326:ARG:CZ[1_565]	1.89	0.31
1:E:326:ARG:CZ	1:G:326:ARG:NE[1_565]	1.90	0.30
1:E:326:ARG:CD	1:G:326:ARG:NH1[1_565]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ARG:NH1	1:G:45:CYS:O[1_455]	1.94	0.26
1:A:113:MET:CE	1:G:113:MET:SD[1_464]	2.00	0.20
1:C:113:MET:SD	1:E:113:MET:CE[1_444]	2.04	0.16
1:C:113:MET:CE	1:E:113:MET:SD[1_444]	2.04	0.16
1:E:326:ARG:NH1	1:G:326:ARG:NH1[1_565]	2.05	0.15
1:E:47:ARG:O	3:A:366:HOH:O[1_657]	2.06	0.14
1:A:113:MET:SD	1:G:113:MET:CE[1_464]	2.07	0.13
1:A:326:ARG:CD	1:C:326:ARG:NH1[1_565]	2.07	0.13
1:E:326:ARG:NH2	1:G:326:ARG:CZ[1_565]	2.11	0.09
1:A:326:ARG:NH1	1:C:326:ARG:NH1[1_565]	2.14	0.06
1:C:45:CYS:O	1:G:47:ARG:NH1[1_455]	2.15	0.05
1:C:45:CYS:O	1:G:47:ARG:NH2[1_455]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/335 (98%)	315 (96%)	8 (2%)	4 (1%)	10	6
1	C	327/335 (98%)	315 (96%)	8 (2%)	4 (1%)	10	6
1	E	327/335 (98%)	315 (96%)	8 (2%)	4 (1%)	10	6
1	G	327/335 (98%)	315 (96%)	8 (2%)	4 (1%)	10	6
2	B	6/9 (67%)	6 (100%)	0	0	100	100
2	D	6/9 (67%)	6 (100%)	0	0	100	100
2	F	6/9 (67%)	6 (100%)	0	0	100	100
2	H	6/9 (67%)	6 (100%)	0	0	100	100
All	All	1332/1376 (97%)	1284 (96%)	32 (2%)	16 (1%)	10	6

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159(A)	HIS
1	A	203	THR
1	A	280	LYS
1	C	159(A)	HIS
1	C	203	THR
1	C	280	LYS
1	E	159(A)	HIS
1	E	203	THR
1	E	280	LYS
1	G	159(A)	HIS
1	G	203	THR
1	G	280	LYS
1	A	158	GLY
1	C	158	GLY
1	E	158	GLY
1	G	158	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/287 (96%)	248 (90%)	29 (10%)	6	4
1	C	277/287 (96%)	248 (90%)	29 (10%)	6	4
1	E	277/287 (96%)	248 (90%)	29 (10%)	6	4
1	G	277/287 (96%)	248 (90%)	29 (10%)	6	4
2	B	7/7 (100%)	7 (100%)	0	100	100
2	D	7/7 (100%)	7 (100%)	0	100	100
2	F	7/7 (100%)	7 (100%)	0	100	100
2	H	7/7 (100%)	7 (100%)	0	100	100
All	All	1136/1176 (97%)	1020 (90%)	116 (10%)	7	4

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	40	VAL
1	A	43	THR
1	A	52	ILE
1	A	59	SER
1	A	65	MET
1	A	113	MET
1	A	130	VAL
1	A	133	VAL
1	A	142	SER
1	A	143	GLN
1	A	147	LYS
1	A	149	LYS
1	A	160	LEU
1	A	186	LYS
1	A	201	SER
1	A	202	SER
1	A	203	THR
1	A	207	GLU
1	A	226	SER
1	A	228	LEU
1	A	230	LEU
1	A	233	GLN
1	A	241	ARG
1	A	247	VAL
1	A	259	SER
1	A	265	ARG
1	A	298	VAL
1	A	300	VAL
1	C	30	ILE
1	C	40	VAL
1	C	43	THR
1	C	52	ILE
1	C	59	SER
1	C	65	MET
1	C	113	MET
1	C	130	VAL
1	C	133	VAL
1	C	142	SER
1	C	143	GLN
1	C	147	LYS
1	C	149	LYS
1	C	160	LEU

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Mol	Chain	Res	Type
1	C	186	LYS
1	C	201	SER
1	C	202	SER
1	C	203	THR
1	C	207	GLU
1	C	226	SER
1	C	228	LEU
1	C	230	LEU
1	C	233	GLN
1	C	241	ARG
1	C	247	VAL
1	C	259	SER
1	C	265	ARG
1	C	298	VAL
1	C	300	VAL
1	E	30	ILE
1	E	40	VAL
1	E	43	THR
1	E	52	ILE
1	E	59	SER
1	E	65	MET
1	E	113	MET
1	E	130	VAL
1	E	133	VAL
1	E	142	SER
1	E	143	GLN
1	E	147	LYS
1	E	149	LYS
1	E	160	LEU
1	E	186	LYS
1	E	201	SER
1	E	202	SER
1	E	203	THR
1	E	207	GLU
1	E	226	SER
1	E	228	LEU
1	E	230	LEU
1	E	233	GLN
1	E	241	ARG
1	E	247	VAL
1	E	259	SER
1	E	265	ARG

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Mol	Chain	Res	Type
1	E	298	VAL
1	E	300	VAL
1	G	30	ILE
1	G	40	VAL
1	G	43	THR
1	G	52	ILE
1	G	59	SER
1	G	65	MET
1	G	113	MET
1	G	130	VAL
1	G	133	VAL
1	G	142	SER
1	G	143	GLN
1	G	147	LYS
1	G	149	LYS
1	G	160	LEU
1	G	186	LYS
1	G	201	SER
1	G	202	SER
1	G	203	THR
1	G	207	GLU
1	G	226	SER
1	G	228	LEU
1	G	230	LEU
1	G	233	GLN
1	G	241	ARG
1	G	247	VAL
1	G	259	SER
1	G	265	ARG
1	G	298	VAL
1	G	300	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	86	GLN
1	A	116	GLN
1	A	174	HIS
1	A	176	GLN
1	A	233	GLN
1	A	261	ASN

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Mol	Chain	Res	Type
1	C	53	HIS
1	C	86	GLN
1	C	174	HIS
1	C	176	GLN
1	C	233	GLN
1	C	261	ASN
1	E	53	HIS
1	E	86	GLN
1	E	116	GLN
1	E	174	HIS
1	E	176	GLN
1	E	233	GLN
1	E	261	ASN
1	G	53	HIS
1	G	86	GLN
1	G	174	HIS
1	G	176	GLN
1	G	233	GLN
1	G	261	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	LPL	D	6	2	15,15,16	1.63	2 (13%)	13,19,21	1.16	1 (7%)
2	PIV	D	1	2	5,5,6	1.38	0	7,7,9	1.94	1 (14%)
2	PIV	F	1	2	5,5,6	1.36	0	7,7,9	1.94	1 (14%)
2	PIV	H	1	2	5,5,6	1.37	0	7,7,9	1.93	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LPL	H	6	2	15,15,16	1.62	2 (13%)	13,19,21	1.17	1 (7%)
2	LPL	F	6	2	15,15,16	1.66	2 (13%)	13,19,21	1.17	1 (7%)
2	PIV	B	1	2	5,5,6	1.36	0	7,7,9	1.93	1 (14%)
2	LPL	B	6	2	15,15,16	1.64	2 (13%)	13,19,21	1.17	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LPL	D	6	2	-	3/18/18/20	-
2	PIV	D	1	2	-	3/3/3/6	-
2	PIV	F	1	2	-	3/3/3/6	-
2	PIV	H	1	2	-	3/3/3/6	-
2	LPL	H	6	2	-	3/18/18/20	-
2	LPL	F	6	2	-	3/18/18/20	-
2	PIV	B	1	2	-	3/3/3/6	-
2	LPL	B	6	2	-	3/18/18/20	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6	LPL	CM-CA1	-4.39	1.50	1.54
2	B	6	LPL	CM-CA1	-4.30	1.50	1.54
2	H	6	LPL	CM-CA1	-4.27	1.50	1.54
2	D	6	LPL	CM-CA1	-4.24	1.50	1.54
2	F	6	LPL	CH-CA	-3.48	1.49	1.53
2	D	6	LPL	CH-CA	-3.45	1.49	1.53
2	B	6	LPL	CH-CA	-3.44	1.49	1.53
2	H	6	LPL	CH-CA	-3.38	1.50	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	PIV	O1-C-CT	-4.74	112.55	124.31
2	H	1	PIV	O1-C-CT	-4.72	112.59	124.31
2	B	1	PIV	O1-C-CT	-4.72	112.59	124.31
2	D	1	PIV	O1-C-CT	-4.72	112.60	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	6	LPL	CB1-CA1-C	-2.19	105.69	110.22
2	F	6	LPL	CB1-CA1-C	-2.19	105.69	110.22
2	B	6	LPL	CB1-CA1-C	-2.18	105.70	110.22
2	D	6	LPL	CB1-CA1-C	-2.16	105.74	110.22

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	PIV	O1-C-CT-C1
2	B	1	PIV	O1-C-CT-C2
2	B	1	PIV	O1-C-CT-C3
2	D	1	PIV	O1-C-CT-C1
2	D	1	PIV	O1-C-CT-C2
2	D	1	PIV	O1-C-CT-C3
2	F	1	PIV	O1-C-CT-C1
2	F	1	PIV	O1-C-CT-C2
2	F	1	PIV	O1-C-CT-C3
2	H	1	PIV	O1-C-CT-C1
2	H	1	PIV	O1-C-CT-C2
2	H	1	PIV	O1-C-CT-C3
2	B	6	LPL	C-CA1-CM-CH
2	D	6	LPL	C-CA1-CM-CH
2	F	6	LPL	C-CA1-CM-CH
2	H	6	LPL	C-CA1-CM-CH
2	B	6	LPL	O-C-CA1-CM
2	B	6	LPL	O-C-CA1-CB1
2	D	6	LPL	O-C-CA1-CM
2	D	6	LPL	O-C-CA1-CB1
2	F	6	LPL	O-C-CA1-CM
2	F	6	LPL	O-C-CA1-CB1
2	H	6	LPL	O-C-CA1-CM
2	H	6	LPL	O-C-CA1-CB1

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	6	LPL	1	0
2	D	1	PIV	1	0
2	F	1	PIV	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	PIV	1	0
2	H	6	LPL	1	0
2	F	6	LPL	1	0
2	B	1	PIV	1	0
2	B	6	LPL	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	C	1
1	E	1
1	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	278:ARG	C	279:ASP	N	9.17
1	C	278:ARG	C	279:ASP	N	9.17
1	E	278:ARG	C	279:ASP	N	9.17
1	G	278:ARG	C	279:ASP	N	9.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.