



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:35 PM BST

PDB ID : 4BP7  
EMDB ID: : EMD-2365  
Title : Asymmetric structure of a virus-receptor complex  
Authors : Dent, K.C.; Thompson, R.; Barker, A.M.; Barr, J.N.; Hiscox, J.A.; Stockley, P.G.; Ranson, N.A.  
Deposited on : 2013-07-17  
Resolution : 39.00 Å(reported)  
Based on PDB ID : 2MS2

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

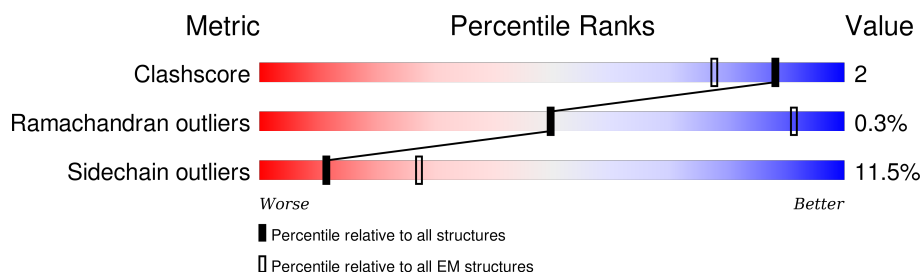
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 39.00 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.
















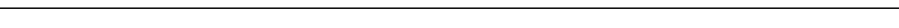











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A0	129	77% 17% 5% .
1	A1	129	78% 16% 5% .
1	A2	129	77% 17% 5% .
1	A3	129	77% 17% 5% .
1	A4	129	78% 16% 5% .
1	A5	129	78% 16% 5% .
1	A6	129	78% 16% 5% .
1	A7	129	77% 17% 5% .
1	A8	129	77% 17% 5% .












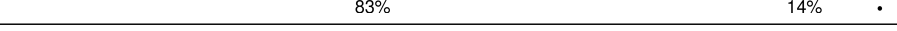







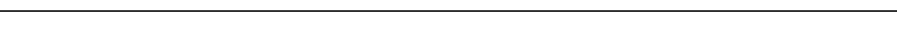

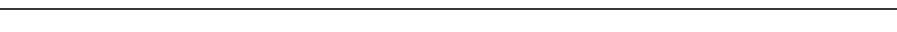
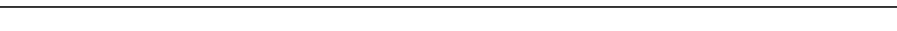


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Mol	Chain	Length	Quality of chain
1	A9	129	 77% 17% 5% .
1	AA	129	 78% 16% 5% .
1	AB	129	 77% 17% 5% .
1	AC	129	 78% 16% 5% .
1	AD	129	 77% 17% 5% .
1	AE	129	 78% 16% 5% .
1	AF	129	 77% 17% 5% .
1	AG	129	 77% 17% 5% .
1	AH	129	 77% 17% 5% .
1	AI	129	 78% 16% 5% .
1	AJ	129	 77% 17% 5% .
1	AK	129	 77% 17% 5% .
1	AL	129	 77% 17% 5% .
1	AM	129	 78% 16% 5% .
1	AN	129	 77% 17% 5% .
1	AO	129	 77% 17% 5% .
1	AP	129	 77% 17% 5% .
1	AQ	129	 77% 17% 5% .
1	AR	129	 77% 17% 5% .
1	AS	129	 78% 16% 5% .
1	AT	129	 77% 17% 5% .
1	AU	129	 77% 17% 5% .
1	AV	129	 78% 16% 5% .
1	AW	129	 77% 17% 5% .
1	AX	129	 77% 17% 5% .

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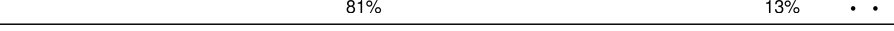







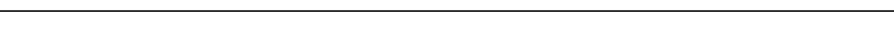

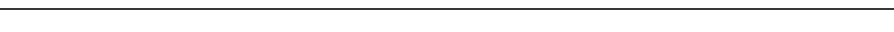
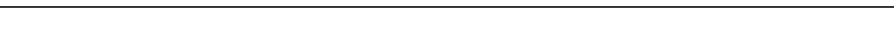


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Mol	Chain	Length	Quality of chain
1	AY	129	 77% 17% 5% •
1	AZ	129	 77% 17% 5% •
1	Aa	129	 83% 14% •
1	Ab	129	 83% 14% •
1	Ac	129	 83% 14% •
1	Ad	129	 83% 14% •
1	Ae	129	 83% 14% •
1	Af	129	 83% 14% •
1	Ag	129	 83% 14% •
1	Ah	129	 83% 14% •
1	Ai	129	 83% 14% •
1	Aj	129	 83% 14% •
1	Ak	129	 83% 14% •
1	Al	129	 83% 14% •
1	Am	129	 83% 14% •
1	An	129	 83% 14% •
1	Ao	129	 83% 14% •
1	Ap	129	 83% 14% •
1	Aq	129	 83% 14% •
1	Ar	129	 83% 14% •
1	As	129	 83% 14% •
1	At	129	 83% 14% •
1	Au	129	 83% 14% •
1	Av	129	 83% 14% •
1	Aw	129	 83% 14% •

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Mol	Chain	Length	Quality of chain
1	Ax	129	 83% 14% . .
1	B0	129	 82% 12% . .
1	B1	129	 82% 12% . .
1	B2	129	 82% 12% . .
1	B3	129	 82% 12% . .
1	B4	129	 81% 13% . .
1	B5	129	 81% 14% . .
1	B6	129	 82% 12% . .
1	B7	129	 81% 13% . .
1	B8	129	 81% 13% . .
1	B9	129	 81% 13% . .
1	BA	129	 81% 13% . .
1	BB	129	 81% 13% . .
1	BC	129	 81% 13% . .
1	BD	129	 82% 12% . .
1	BE	129	 81% 13% . .
1	BF	129	 81% 13% . .
1	BG	129	 81% 13% . .
1	BH	129	 81% 13% . .
1	BI	129	 81% 13% . .
1	BJ	129	 81% 13% . .
1	BK	129	 82% 12% . .
1	BL	129	 81% 14% . .
1	BM	129	 82% 12% . .
1	BN	129	 82% 12% . .














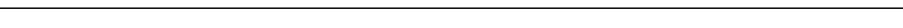











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Mol	Chain	Length	Quality of chain
1	BO	129	 81% 14% . .
1	BP	129	 81% 13% . .
1	BQ	129	 82% 12% . .
1	BR	129	 81% 13% . .
1	BS	129	 81% 14% . .
1	BT	129	 81% 13% . .
1	BU	129	 81% 13% . .
1	BV	129	 82% 12% . .
1	BW	129	 81% 13% . .
1	BX	129	 81% 13% . .
1	BY	129	 82% 12% . .
1	BZ	129	 81% 13% . .
1	Ba	129	 88% 9% .
1	Bb	129	 87% 9% .
1	Bc	129	 88% 9% .
1	Bd	129	 87% 9% .
1	Be	129	 87% 9% .
1	Bf	129	 88% 9% .
1	Bg	129	 87% 9% .
1	Bh	129	 87% 9% .
1	Bi	129	 87% 9% .
1	Bj	129	 87% 9% .
1	Bk	129	 88% 9% .
1	Bl	129	 88% 9% .
1	Bm	129	 87% 9% .














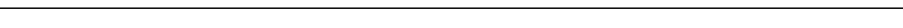











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Mol	Chain	Length	Quality of chain
1	Bn	129	 88% 9% .
1	Bo	129	 88% 9% .
1	Bp	129	 88% 9% .
1	Bq	129	 87% 9% .
1	Br	129	 87% 9% .
1	Bs	129	 87% 9% .
1	Bt	129	 88% 9% .
1	Bu	129	 88% 9% .
1	Bv	129	 88% 9% .
1	Bw	129	 88% 9% .
1	Bx	129	 87% 9% .
1	C0	129	 79% 16% 5% .
1	C1	129	 80% 15% 5% .
1	C2	129	 81% 14% 5% .
1	C3	129	 80% 16% . .
1	C4	129	 80% 16% . .
1	C5	129	 81% 14% . .
1	C6	129	 78% 16% 5% .
1	C7	129	 81% 14% . .
1	C8	129	 80% 15% 5% .
1	C9	129	 80% 15% 5% .
1	CA	129	 78% 16% 5% .
1	CB	129	 80% 15% 5% .
1	CC	129	 79% 16% . .
1	CD	129	 80% 15% 5% .













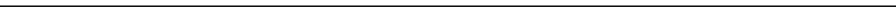
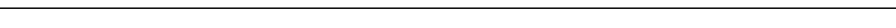







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Mol	Chain	Length	Quality of chain
1	CE	129	 78% 16% 5% •
1	CF	129	 79% 16% 5% •
1	CG	129	 79% 16% 5% •
1	CH	129	 78% 16% 5% •
1	CI	129	 80% 15% 5% •
1	CJ	129	 79% 16% 5% •
1	CK	129	 81% 14% 5% •
1	CL	129	 81% 15% • •
1	CM	129	 81% 14% 5% •
1	CN	129	 78% 16% 5% •
1	CO	129	 79% 16% 5% •
1	CP	129	 78% 16% 5% •
1	CQ	129	 78% 16% 5% •
1	CR	129	 81% 14% 5% •
1	CS	129	 78% 16% 5% •
1	CT	129	 78% 16% 5% •
1	CU	129	 79% 16% 5% •
1	CV	129	 78% 16% 5% •
1	CW	129	 80% 15% 5% •
1	CX	129	 79% 16% 5% •
1	CY	129	 80% 15% 5% •
1	CZ	129	 81% 15% • •
1	Ca	129	 84% 13% •
1	Cb	129	 84% 12% •
1	Cc	129	 84% 12% •

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Mol	Chain	Length	Quality of chain
1	Cd	129	 84% 13% .
1	Ce	129	 84% 12% .
1	Cf	129	 84% 13% .
1	Cg	129	 84% 12% .
1	Ch	129	 84% 12% .
1	Ci	129	 84% 12% .
1	Cj	129	 84% 12% .
1	Ck	129	 84% 13% .
1	Cl	129	 84% 12% .
1	Cm	129	 84% 12% .
1	Cn	129	 84% 12% .
1	Co	129	 84% 12% .
1	Cp	129	 84% 13% .
1	Cq	129	 84% 13% .
1	Cr	129	 84% 12% .
1	Cs	129	 84% 12% .
1	Ct	129	 84% 13% .
1	Cu	129	 84% 13% .
1	Cv	129	 84% 13% .
1	Cw	129	 84% 12% .
1	Cx	129	 84% 13% .

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 173700 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 COAT PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A1	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A2	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A3	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A4	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A5	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A6	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A7	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A8	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	A9	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AA	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AB	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AC	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AD	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AE	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AF	129	Total	C	N	O	S	0	0
			965	606	165	190	4		
1	AG	129	Total	C	N	O	S	0	0
			965	606	165	190	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	AH	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AI	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AJ	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AK	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AL	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AM	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AN	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AO	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AP	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AQ	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AR	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AS	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AT	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AU	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AV	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AW	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AX	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AY	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	AZ	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Aa	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ab	129	Total 965	C 606	N 165	O 190	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ac	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ad	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ae	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Af	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ag	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ah	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ai	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Aj	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ak	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Al	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Am	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	An	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ao	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ap	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Aq	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ar	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	As	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	At	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Au	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Av	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Aw	129	Total 965	C 606	N 165	O 190	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ax	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	B0	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	B1	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	B2	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	B3	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	B4	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	B5	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	B6	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	B7	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	B8	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	B9	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BA	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BB	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BC	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BD	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BE	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BF	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BG	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BH	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BI	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BJ	129	Total 965	C 606	N 165	O 190	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	BK	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BL	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BM	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BN	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BO	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BP	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BQ	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BR	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BS	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BT	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BU	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BV	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BW	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BX	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BY	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	BZ	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ba	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bb	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bc	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bd	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Be	129	Total 965	C 606	N 165	O 190	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bf	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bg	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bh	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bi	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bj	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bk	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bl	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bm	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bn	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bo	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bp	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bq	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Br	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bs	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bt	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bu	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bv	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bw	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Bx	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	C0	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	C1	129	Total 965	C 606	N 165	O 190	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	C2	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	C3	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	C4	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	C5	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	C6	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	C7	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	C8	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	C9	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CA	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CB	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CC	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CD	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CE	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CF	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CG	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CH	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CI	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CJ	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CK	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CL	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CM	129	Total 965	C 606	N 165	O 190	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CN	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CO	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CP	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CQ	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CR	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CS	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CT	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CU	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CV	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CW	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CX	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CY	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	CZ	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ca	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cb	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cc	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cd	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ce	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cf	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cg	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ch	129	Total 965	C 606	N 165	O 190	S 4	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ci	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cj	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ck	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cl	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cm	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cn	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Co	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cp	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cq	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cr	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cs	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Ct	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cu	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cv	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cw	129	Total 965	C 606	N 165	O 190	S 4	0	0
1	Cx	129	Total 965	C 606	N 165	O 190	S 4	0	0

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


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

- Molecule 1: COAT PROTEIN

Chain A0: 




- Molecule 1: COAT PROTEIN

Chain A1: 




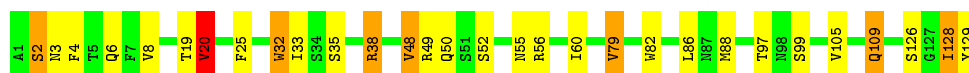
- Molecule 1: COAT PROTEIN

Chain A2: 




- Molecule 1: COAT PROTEIN

Chain A3: 




- Molecule 1: COAT PROTEIN

Chain A4: 




- Molecule 1: COAT PROTEIN


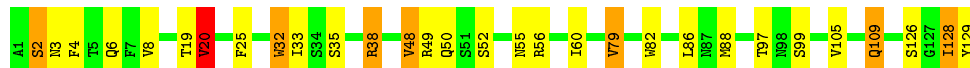
Chain A5: 




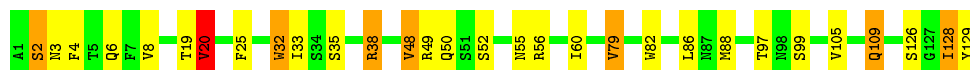
## • Molecule 1: COAT PROTEIN

Chain A6:  78% 16% 5%


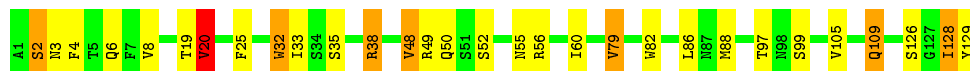
## • Molecule 1: COAT PROTEIN

Chain A7:  77% 17% 5%


## • Molecule 1: COAT PROTEIN

Chain A8:  77% 17% 5%


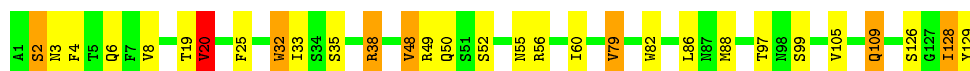
## • Molecule 1: COAT PROTEIN

Chain A9:  77% 17% 5%


## • Molecule 1: COAT PROTEIN

Chain AA:  78% 16% 5%


## • Molecule 1: COAT PROTEIN

Chain AB:  77% 17% 5%

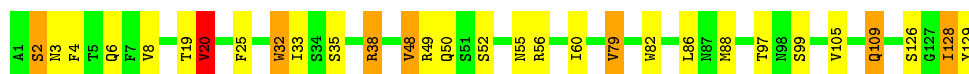
## • Molecule 1: COAT PROTEIN

Chain AC:  78% 16% 5%

## • Molecule 1: COAT PROTEIN

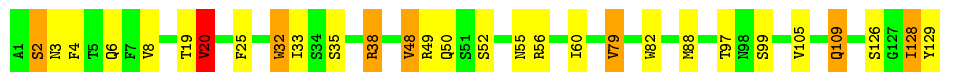
Chain AD:  77% 17% 5%





- Molecule 1: COAT PROTEIN

Chain AE: 78% 16% 5%



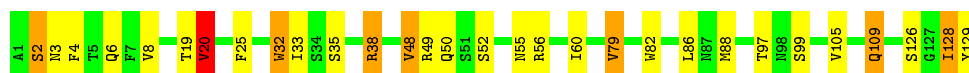
- Molecule 1: COAT PROTEIN

Chain AF: 77% 17% 5%



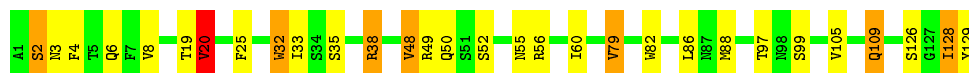
- Molecule 1: COAT PROTEIN

Chain AG: 77% 17% 5%



- Molecule 1: COAT PROTEIN

Chain AH: 77% 17% 5%



- Molecule 1: COAT PROTEIN

Chain AI: 78% 16% 5%



- Molecule 1: COAT PROTEIN

Chain AJ: 77% 17% 5%




- Molecule 1: COAT PROTEIN

Chain AK: 77% 17% 5%




- Molecule 1: COAT PROTEIN

Chain AL:  77% 17% 5%




• Molecule 1: COAT PROTEIN

Chain AM:  78% 16% 5%




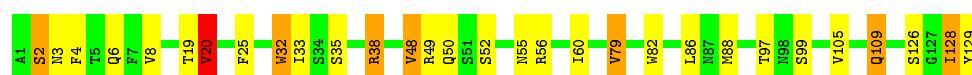
• Molecule 1: COAT PROTEIN

Chain AN:  77% 17% 5%




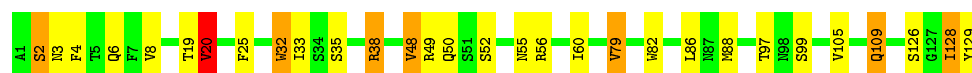
• Molecule 1: COAT PROTEIN

Chain AO:  77% 17% 5%




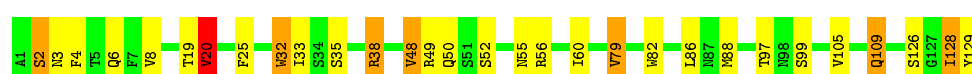
• Molecule 1: COAT PROTEIN

Chain AP:  77% 17% 5%




• Molecule 1: COAT PROTEIN

Chain AQ:  77% 17% 5%




• Molecule 1: COAT PROTEIN

Chain AR:  77% 17% 5%

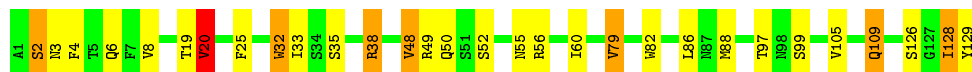
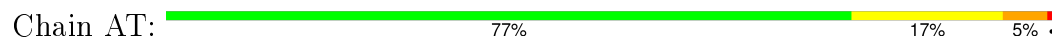


• Molecule 1: COAT PROTEIN

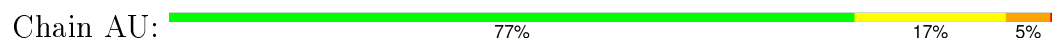
Chain AS:  78% 16% 5%



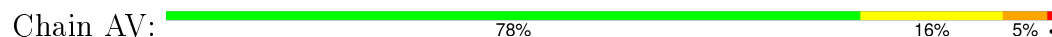
- Molecule 1: COAT PROTEIN



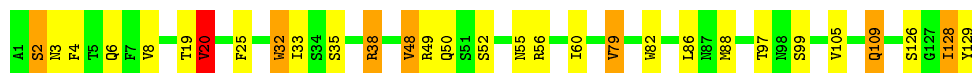
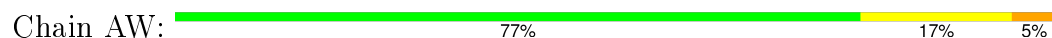
- Molecule 1: COAT PROTEIN



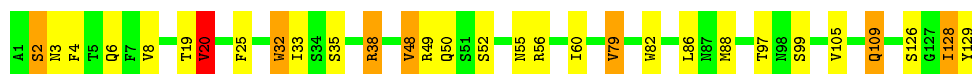
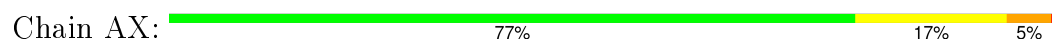
- Molecule 1: COAT PROTEIN



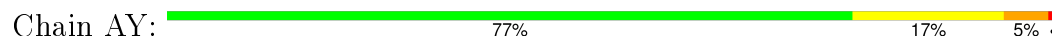
- Molecule 1: COAT PROTEIN



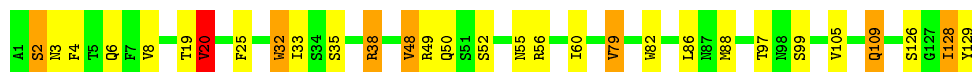
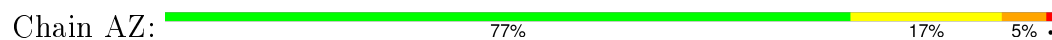
- Molecule 1: COAT PROTEIN




- Molecule 1: COAT PROTEIN



- Molecule 1: COAT PROTEIN




- Molecule 1: COAT PROTEIN

Chain Aa:  83% 14% .




- Molecule 1: COAT PROTEIN

Chain Ab:  83% 14% .




- Molecule 1: COAT PROTEIN

Chain Ac:  83% 14% .




- Molecule 1: COAT PROTEIN

Chain Ad:  83% 14% .




- Molecule 1: COAT PROTEIN

Chain Ae:  83% 14% .




- Molecule 1: COAT PROTEIN

Chain Af:  83% 14% .




- Molecule 1: COAT PROTEIN

Chain Ag:  83% 14% .




- Molecule 1: COAT PROTEIN

Chain Ah:  83% 14% .




- Molecule 1: COAT PROTEIN

Chain Ai:  83% 14% •




- Molecule 1: COAT PROTEIN

Chain Aj:  83% 14% •




- Molecule 1: COAT PROTEIN

Chain Ak:  83% 14% •




- Molecule 1: COAT PROTEIN

Chain Al:  83% 14% •




- Molecule 1: COAT PROTEIN

Chain Am:  83% 14% •




- Molecule 1: COAT PROTEIN

Chain An:  83% 14% •




- Molecule 1: COAT PROTEIN


Chain Ao:  83% 14% •




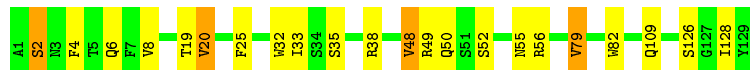
## • Molecule 1: COAT PROTEIN

Chain Ap:  83% 14%


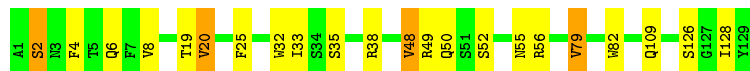
## • Molecule 1: COAT PROTEIN

Chain Aq:  83% 14%


## • Molecule 1: COAT PROTEIN

Chain Ar:  83% 14%


## • Molecule 1: COAT PROTEIN

Chain As:  83% 14%


## • Molecule 1: COAT PROTEIN

Chain At:  83% 14%


## • Molecule 1: COAT PROTEIN

Chain Au:  83% 14%

## • Molecule 1: COAT PROTEIN

Chain Av:  83% 14%

## • Molecule 1: COAT PROTEIN

Chain Aw:  83% 14%



- Molecule 1: COAT PROTEIN

Chain Ax: 83% 14% •



- Molecule 1: COAT PROTEIN

Chain B0: 82% 12% • •



- Molecule 1: COAT PROTEIN

Chain B1: 82% 12% • •



- Molecule 1: COAT PROTEIN

Chain B2: 82% 12% • •



- Molecule 1: COAT PROTEIN

Chain B3: 82% 12% • •



- Molecule 1: COAT PROTEIN

Chain B4: 81% 13% • •




- Molecule 1: COAT PROTEIN

Chain B5: 81% 14% • •




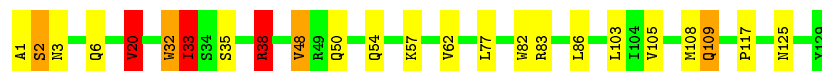
- Molecule 1: COAT PROTEIN

Chain B6:  82% 12% . .




• Molecule 1: COAT PROTEIN

Chain B7:  81% 13% . .




• Molecule 1: COAT PROTEIN

Chain B8:  81% 13% . .




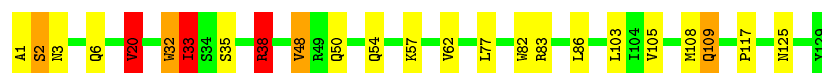
• Molecule 1: COAT PROTEIN

Chain B9:  81% 13% . .




• Molecule 1: COAT PROTEIN

Chain BA:  81% 13% . .




• Molecule 1: COAT PROTEIN

Chain BB:  81% 13% . .




• Molecule 1: COAT PROTEIN

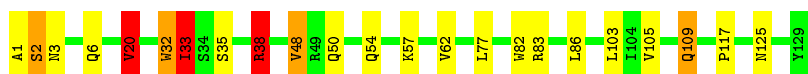
Chain BC:  81% 13% . .




• Molecule 1: COAT PROTEIN

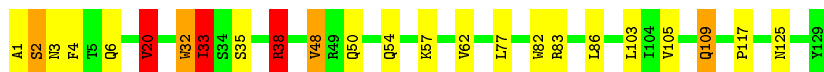
Chain BD:  82% 12% . .






- Molecule 1: COAT PROTEIN

Chain BE:  81% 13% • •




- Molecule 1: COAT PROTEIN

Chain BF:  81% 13% • •




- Molecule 1: COAT PROTEIN

Chain BG:  81% 13% • •




- Molecule 1: COAT PROTEIN

Chain BH:  81% 13% • •




- Molecule 1: COAT PROTEIN

Chain BI:  81% 13% • •




- Molecule 1: COAT PROTEIN

Chain BJ:  81% 13% • •




- Molecule 1: COAT PROTEIN

Chain BK:  82% 12% • •




- Molecule 1: COAT PROTEIN

Chain BL:  81% 14% . .




• Molecule 1: COAT PROTEIN

Chain BM:  82% 12% . .




• Molecule 1: COAT PROTEIN

Chain BN:  82% 12% . .




• Molecule 1: COAT PROTEIN

Chain BO:  81% 14% . .




• Molecule 1: COAT PROTEIN

Chain BP:  81% 13% . .




• Molecule 1: COAT PROTEIN

Chain BQ:  82% 12% . .




• Molecule 1: COAT PROTEIN

Chain BR:  81% 13% . .



• Molecule 1: COAT PROTEIN

Chain BS:  81% 14% . .



- Molecule 1: COAT PROTEIN

Chain BT: 81% 13% . .



- Molecule 1: COAT PROTEIN

Chain BU: 81% 13% . .



- Molecule 1: COAT PROTEIN

Chain BV: 82% 12% . .



- Molecule 1: COAT PROTEIN

Chain BW: 81% 13% . .



- Molecule 1: COAT PROTEIN

Chain BX: 81% 13% . .



- Molecule 1: COAT PROTEIN

Chain BY: 82% 12% . .




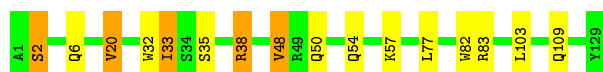
- Molecule 1: COAT PROTEIN

Chain BZ: 81% 13% . .




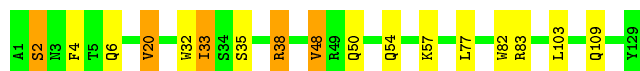
- Molecule 1: COAT PROTEIN

Chain Ba:  88% 9% .




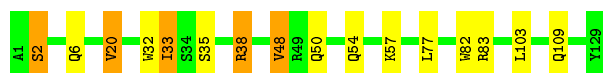
- Molecule 1: COAT PROTEIN

Chain Bb:  87% 9% .




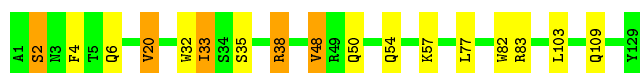
- Molecule 1: COAT PROTEIN

Chain Bc:  88% 9% .



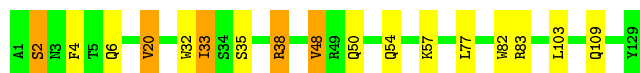
- Molecule 1: COAT PROTEIN

Chain Bd:  87% 9% .



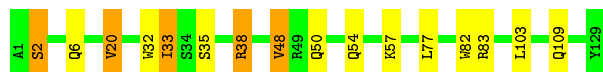
- Molecule 1: COAT PROTEIN

Chain Be:  87% 9% .




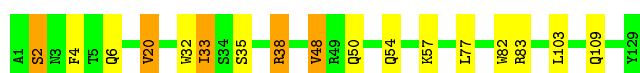
- Molecule 1: COAT PROTEIN

Chain Bf:  88% 9% .



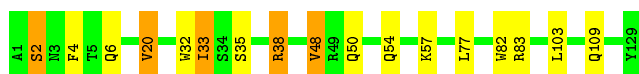
- Molecule 1: COAT PROTEIN

Chain Bg:  87% 9% .



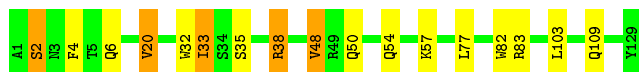
- Molecule 1: COAT PROTEIN

Chain Bh:  87% 9% .



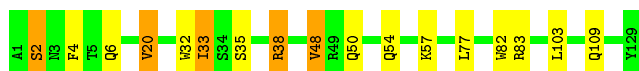
- Molecule 1: COAT PROTEIN

Chain Bi: 87% 9% .



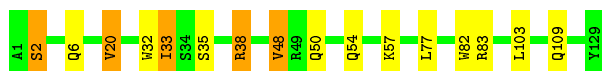
- Molecule 1: COAT PROTEIN

Chain Bj: 87% 9% .



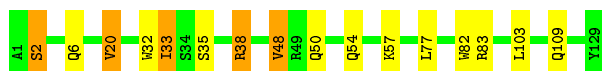
- Molecule 1: COAT PROTEIN

Chain Bk: 88% 9% .



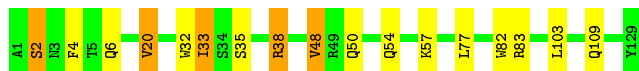
- Molecule 1: COAT PROTEIN

Chain Bl: 88% 9% .



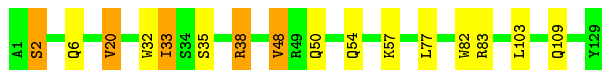
- Molecule 1: COAT PROTEIN

Chain Bm: 87% 9% .



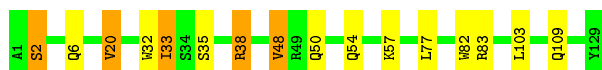
- Molecule 1: COAT PROTEIN

Chain Bn: 88% 9% .


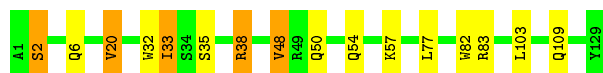


- Molecule 1: COAT PROTEIN


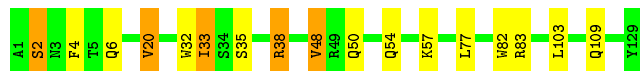
Chain Bo: 88% 9% .




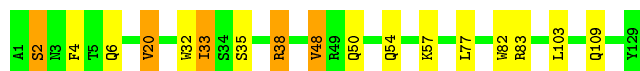
## • Molecule 1: COAT PROTEIN

Chain Bp:  88% 9% .

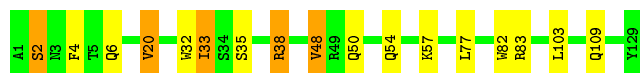
## • Molecule 1: COAT PROTEIN

Chain Bq:  87% 9% .

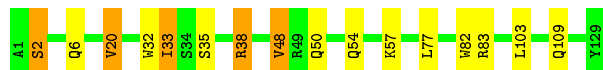
## • Molecule 1: COAT PROTEIN

Chain Br:  87% 9% .

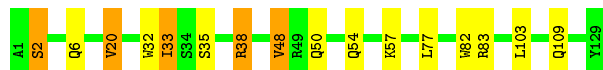
## • Molecule 1: COAT PROTEIN

Chain Bs:  87% 9% .


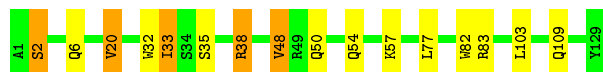
## • Molecule 1: COAT PROTEIN

Chain Bt:  88% 9% .

## • Molecule 1: COAT PROTEIN

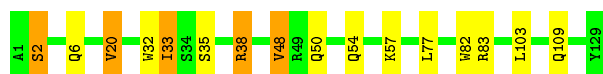
Chain Bu:  88% 9% .

## • Molecule 1: COAT PROTEIN

Chain Bv:  88% 9% .

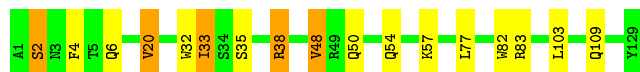
## • Molecule 1: COAT PROTEIN

Chain Bw:  88% 9% .



- Molecule 1: COAT PROTEIN

Chain Bx: 87% 9% .



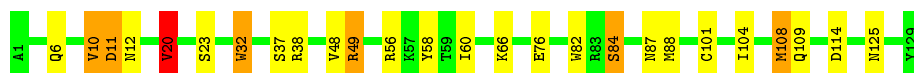
- Molecule 1: COAT PROTEIN

Chain C0: 79% 16% 5% .



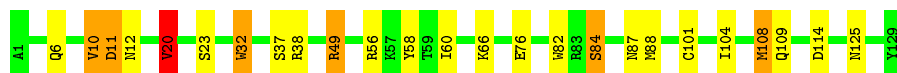
- Molecule 1: COAT PROTEIN

Chain C1: 80% 15% 5% .



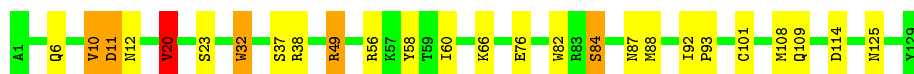
- Molecule 1: COAT PROTEIN

Chain C2: 81% 14% 5% .



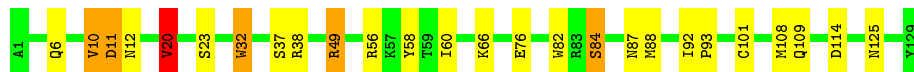
- Molecule 1: COAT PROTEIN

Chain C3: 80% 16% . .



- Molecule 1: COAT PROTEIN

Chain C4: 80% 16% . .

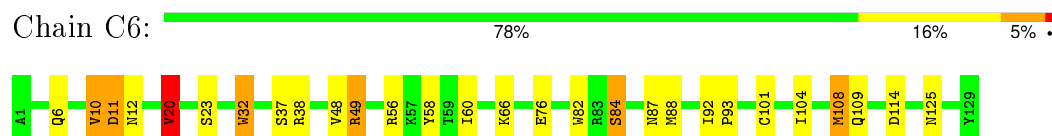


- Molecule 1: COAT PROTEIN

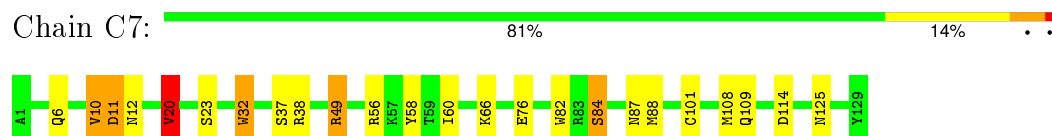
Chain C5: 81% 14% . .



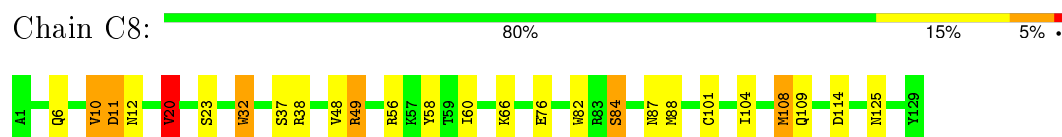
- Molecule 1: COAT PROTEIN



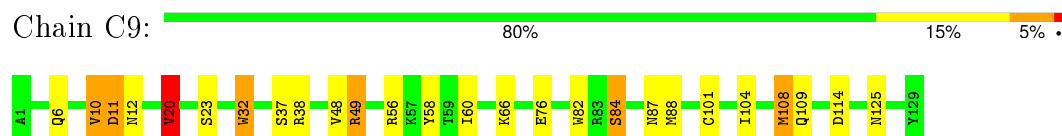
- Molecule 1: COAT PROTEIN



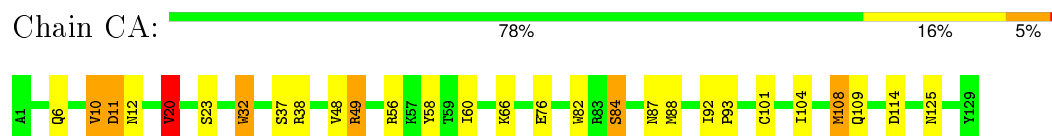
- Molecule 1: COAT PROTEIN



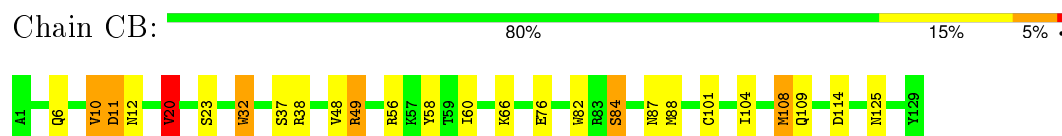
- Molecule 1: COAT PROTEIN



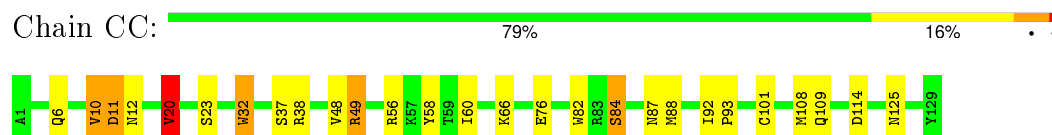
- Molecule 1: COAT PROTEIN



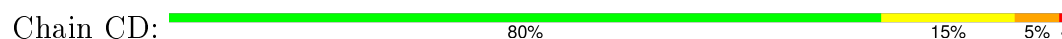
- Molecule 1: COAT PROTEIN



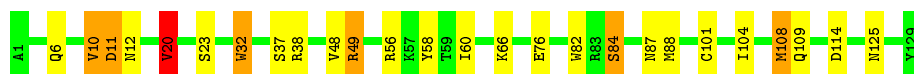
- Molecule 1: COAT PROTEIN



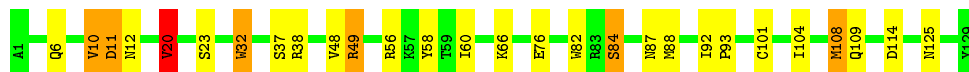
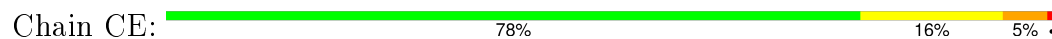
- Molecule 1: COAT PROTEIN



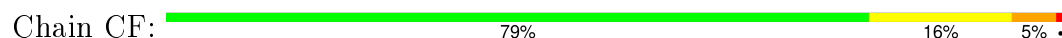




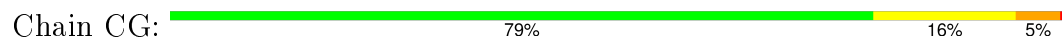
- Molecule 1: COAT PROTEIN



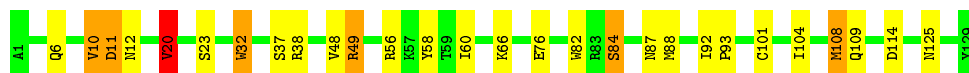
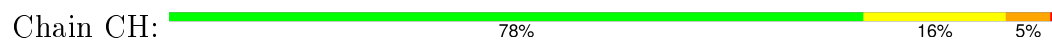
- Molecule 1: COAT PROTEIN



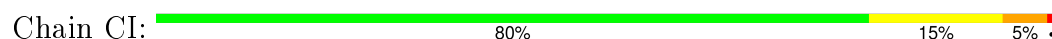
- Molecule 1: COAT PROTEIN



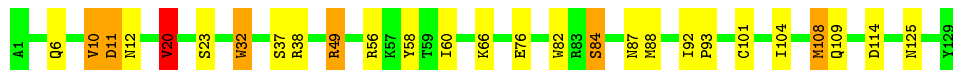
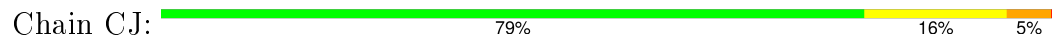
- Molecule 1: COAT PROTEIN



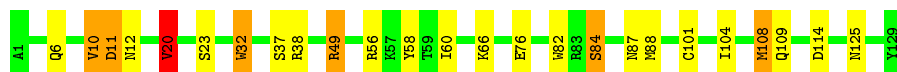
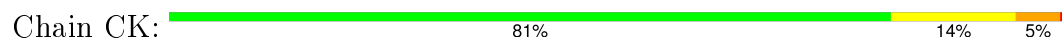
- Molecule 1: COAT PROTEIN



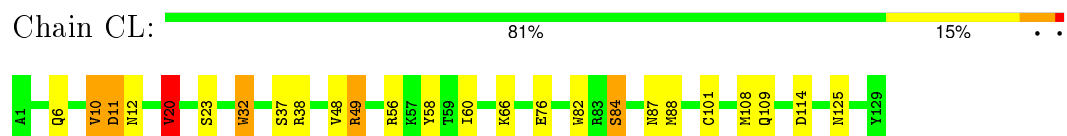
- Molecule 1: COAT PROTEIN



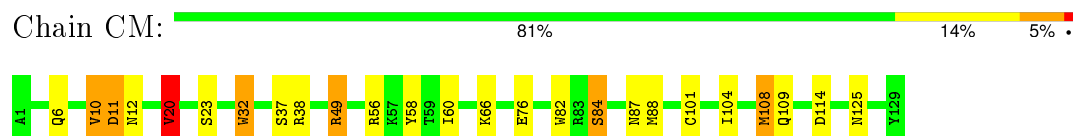
- Molecule 1: COAT PROTEIN



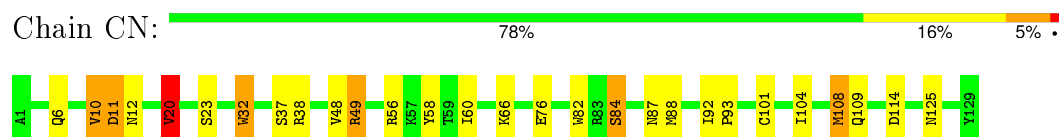
- Molecule 1: COAT PROTEIN



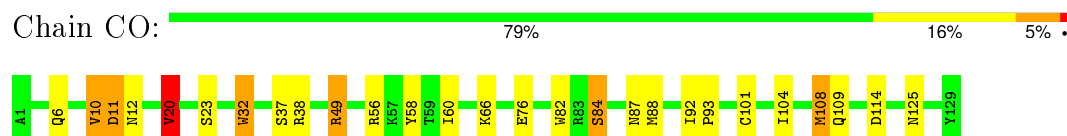
• Molecule 1: COAT PROTEIN



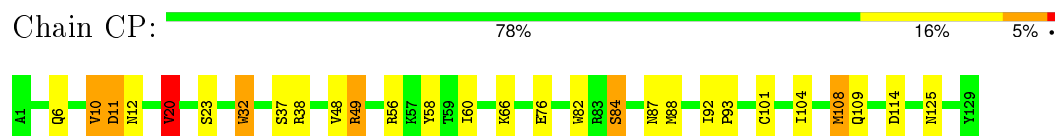
• Molecule 1: COAT PROTEIN



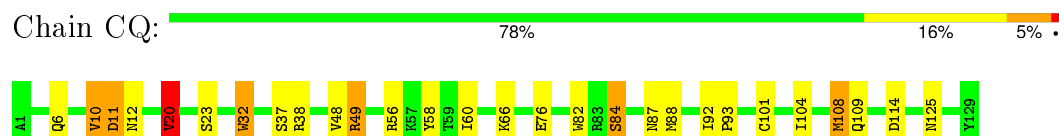
• Molecule 1: COAT PROTEIN



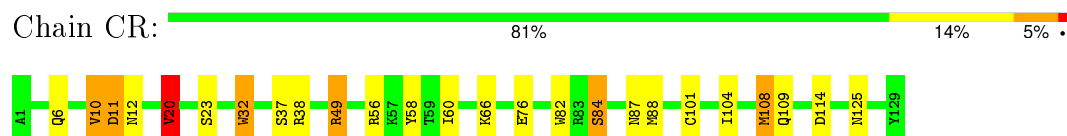
• Molecule 1: COAT PROTEIN



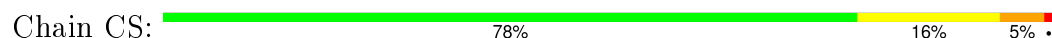
• Molecule 1: COAT PROTEIN

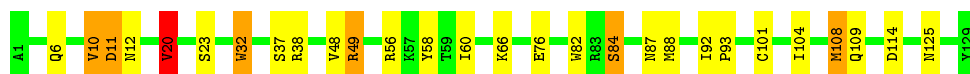


• Molecule 1: COAT PROTEIN



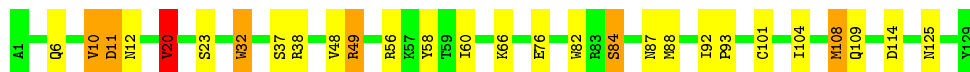
• Molecule 1: COAT PROTEIN





- Molecule 1: COAT PROTEIN

Chain CT: 78% 16% 5%



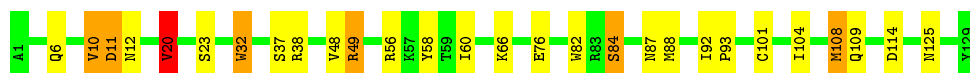
- Molecule 1: COAT PROTEIN

Chain CU: 79% 16% 5%



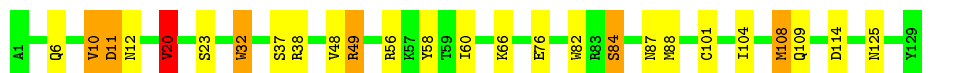
- Molecule 1: COAT PROTEIN

Chain CV: 78% 16% 5%



- Molecule 1: COAT PROTEIN

Chain CW: 80% 15% 5%



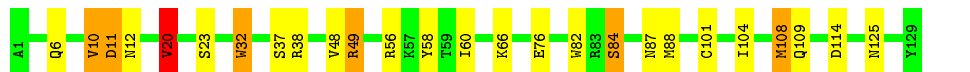
- Molecule 1: COAT PROTEIN

Chain CX: 79% 16% 5%



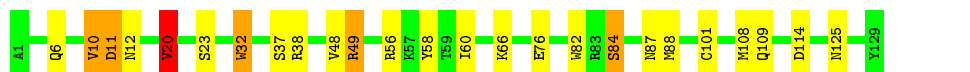
- Molecule 1: COAT PROTEIN

Chain CY: 80% 15% 5%




- Molecule 1: COAT PROTEIN

Chain CZ: 81% 15%




- Molecule 1: COAT PROTEIN

Chain Ca:  84% 13% •




• Molecule 1: COAT PROTEIN

Chain Cb:  84% 12% •




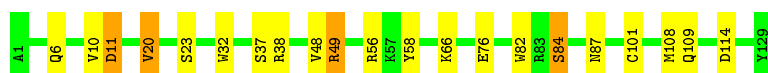
• Molecule 1: COAT PROTEIN

Chain Cc:  84% 12% •




• Molecule 1: COAT PROTEIN

Chain Cd:  84% 13% •




• Molecule 1: COAT PROTEIN

Chain Ce:  84% 12% •




• Molecule 1: COAT PROTEIN

Chain Cf:  84% 13% •




• Molecule 1: COAT PROTEIN

Chain Cg:  84% 12% •



• Molecule 1: COAT PROTEIN

Chain Ch:  84% 12% •



- Molecule 1: COAT PROTEIN

Chain Ci: 84% 12% .



- Molecule 1: COAT PROTEIN

Chain Cj: 84% 12% .



- Molecule 1: COAT PROTEIN

Chain Ck: 84% 13% .



- Molecule 1: COAT PROTEIN

Chain Cl: 84% 12% .



- Molecule 1: COAT PROTEIN

Chain Cm: 84% 12% .



- Molecule 1: COAT PROTEIN

Chain Cn: 84% 12% .




- Molecule 1: COAT PROTEIN


Chain Co: 84% 12% .




## • Molecule 1: COAT PROTEIN

Chain Cp:  84% 13%


## • Molecule 1: COAT PROTEIN

Chain Cq:  84% 13%


## • Molecule 1: COAT PROTEIN

Chain Cr:  84% 12%


## • Molecule 1: COAT PROTEIN

Chain Cs:  84% 12%


## • Molecule 1: COAT PROTEIN

Chain Ct:  84% 13%


## • Molecule 1: COAT PROTEIN

Chain Cu:  84% 13%

## • Molecule 1: COAT PROTEIN

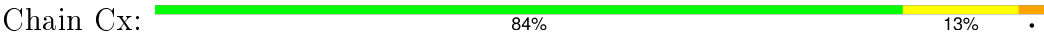
Chain Cv:  84% 13%

## • Molecule 1: COAT PROTEIN

Chain Cw:  84% 12%



● Molecule 1: COAT PROTEIN



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	23000	Depositor
Image detector	GATAN US1000XP	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A0	1.01	0/982	1.65	19/1337 (1.4%)
1	A1	1.01	0/982	1.65	19/1337 (1.4%)
1	A2	1.01	0/982	1.65	19/1337 (1.4%)
1	A3	1.01	0/982	1.65	19/1337 (1.4%)
1	A4	1.01	0/982	1.65	19/1337 (1.4%)
1	A5	1.01	0/982	1.65	19/1337 (1.4%)
1	A6	1.01	0/982	1.65	19/1337 (1.4%)
1	A7	1.01	0/982	1.65	19/1337 (1.4%)
1	A8	1.01	0/982	1.65	19/1337 (1.4%)
1	A9	1.01	0/982	1.65	19/1337 (1.4%)
1	AA	1.01	0/982	1.65	19/1337 (1.4%)
1	AB	1.01	0/982	1.65	19/1337 (1.4%)
1	AC	1.01	0/982	1.65	19/1337 (1.4%)
1	AD	1.01	0/982	1.65	19/1337 (1.4%)
1	AE	1.01	0/982	1.65	19/1337 (1.4%)
1	AF	1.01	0/982	1.65	19/1337 (1.4%)
1	AG	1.01	0/982	1.65	19/1337 (1.4%)
1	AH	1.01	0/982	1.65	19/1337 (1.4%)
1	AI	1.01	0/982	1.65	19/1337 (1.4%)
1	AJ	1.01	0/982	1.65	19/1337 (1.4%)
1	AK	1.01	0/982	1.65	19/1337 (1.4%)
1	AL	1.01	0/982	1.65	19/1337 (1.4%)
1	AM	1.01	0/982	1.65	19/1337 (1.4%)
1	AN	1.01	0/982	1.65	19/1337 (1.4%)
1	AO	1.01	0/982	1.65	19/1337 (1.4%)
1	AP	1.01	0/982	1.65	19/1337 (1.4%)
1	AQ	1.01	0/982	1.65	19/1337 (1.4%)
1	AR	1.01	0/982	1.65	19/1337 (1.4%)
1	AS	1.01	0/982	1.65	19/1337 (1.4%)
1	AT	1.01	0/982	1.65	19/1337 (1.4%)
1	AU	1.01	0/982	1.65	19/1337 (1.4%)
1	AV	1.01	0/982	1.65	19/1337 (1.4%)
1	AW	1.01	0/982	1.65	19/1337 (1.4%)
1	AX	1.01	0/982	1.65	19/1337 (1.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	AY	1.01	0/982	1.65	19/1337 (1.4%)
1	AZ	1.01	0/982	1.65	19/1337 (1.4%)
1	Aa	1.01	0/982	1.65	19/1337 (1.4%)
1	Ab	1.01	0/982	1.65	19/1337 (1.4%)
1	Ac	1.01	0/982	1.65	19/1337 (1.4%)
1	Ad	1.01	0/982	1.65	19/1337 (1.4%)
1	Ae	1.01	0/982	1.65	19/1337 (1.4%)
1	Af	1.01	0/982	1.65	19/1337 (1.4%)
1	Ag	1.01	0/982	1.65	19/1337 (1.4%)
1	Ah	1.01	0/982	1.65	19/1337 (1.4%)
1	Ai	1.01	0/982	1.65	19/1337 (1.4%)
1	Aj	1.01	0/982	1.65	19/1337 (1.4%)
1	Ak	1.01	0/982	1.65	19/1337 (1.4%)
1	Al	1.01	0/982	1.65	19/1337 (1.4%)
1	Am	1.01	0/982	1.65	19/1337 (1.4%)
1	An	1.01	0/982	1.65	19/1337 (1.4%)
1	Ao	1.01	0/982	1.65	19/1337 (1.4%)
1	Ap	1.01	0/982	1.65	19/1337 (1.4%)
1	Aq	1.01	0/982	1.65	19/1337 (1.4%)
1	Ar	1.01	0/982	1.65	19/1337 (1.4%)
1	As	1.01	0/982	1.65	19/1337 (1.4%)
1	At	1.01	0/982	1.65	19/1337 (1.4%)
1	Au	1.01	0/982	1.65	19/1337 (1.4%)
1	Av	1.01	0/982	1.65	19/1337 (1.4%)
1	Aw	1.01	0/982	1.65	19/1337 (1.4%)
1	Ax	1.01	0/982	1.65	19/1337 (1.4%)
1	B0	1.02	0/982	1.52	18/1337 (1.3%)
1	B1	1.02	0/982	1.52	19/1337 (1.4%)
1	B2	1.02	0/982	1.52	19/1337 (1.4%)
1	B3	1.02	0/982	1.52	18/1337 (1.3%)
1	B4	1.02	0/982	1.52	19/1337 (1.4%)
1	B5	1.02	0/982	1.52	18/1337 (1.3%)
1	B6	1.02	0/982	1.52	19/1337 (1.4%)
1	B7	1.02	0/982	1.52	18/1337 (1.3%)
1	B8	1.02	0/982	1.52	18/1337 (1.3%)
1	B9	1.02	0/982	1.52	18/1337 (1.3%)
1	BA	1.02	0/982	1.52	18/1337 (1.3%)
1	BB	1.02	0/982	1.52	18/1337 (1.3%)
1	BC	1.02	0/982	1.52	18/1337 (1.3%)
1	BD	1.02	0/982	1.52	18/1337 (1.3%)
1	BE	1.02	0/982	1.52	18/1337 (1.3%)
1	BF	1.02	0/982	1.52	18/1337 (1.3%)
1	BG	1.02	0/982	1.52	18/1337 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	BH	1.02	0/982	1.52	18/1337 (1.3%)
1	BI	1.02	0/982	1.52	18/1337 (1.3%)
1	BJ	1.02	0/982	1.52	18/1337 (1.3%)
1	BK	1.02	0/982	1.52	18/1337 (1.3%)
1	BL	1.02	0/982	1.52	19/1337 (1.4%)
1	BM	1.02	0/982	1.52	19/1337 (1.4%)
1	BN	1.02	0/982	1.52	18/1337 (1.3%)
1	BO	1.02	0/982	1.52	18/1337 (1.3%)
1	BP	1.02	0/982	1.52	18/1337 (1.3%)
1	BQ	1.02	0/982	1.52	18/1337 (1.3%)
1	BR	1.02	0/982	1.52	18/1337 (1.3%)
1	BS	1.02	0/982	1.52	19/1337 (1.4%)
1	BT	1.02	0/982	1.52	18/1337 (1.3%)
1	BU	1.02	0/982	1.52	18/1337 (1.3%)
1	BV	1.02	0/982	1.52	18/1337 (1.3%)
1	BW	1.02	0/982	1.52	18/1337 (1.3%)
1	BX	1.02	0/982	1.52	18/1337 (1.3%)
1	BY	1.02	0/982	1.52	18/1337 (1.3%)
1	BZ	1.02	0/982	1.52	18/1337 (1.3%)
1	Ba	1.02	0/982	1.52	18/1337 (1.3%)
1	Bb	1.02	0/982	1.52	19/1337 (1.4%)
1	Bc	1.02	0/982	1.52	18/1337 (1.3%)
1	Bd	1.02	0/982	1.52	18/1337 (1.3%)
1	Be	1.02	0/982	1.52	18/1337 (1.3%)
1	Bf	1.02	0/982	1.52	18/1337 (1.3%)
1	Bg	1.02	0/982	1.52	19/1337 (1.4%)
1	Bh	1.02	0/982	1.52	18/1337 (1.3%)
1	Bi	1.02	0/982	1.52	18/1337 (1.3%)
1	Bj	1.02	0/982	1.52	18/1337 (1.3%)
1	Bk	1.02	0/982	1.52	18/1337 (1.3%)
1	Bl	1.02	0/982	1.52	18/1337 (1.3%)
1	Bm	1.02	0/982	1.52	18/1337 (1.3%)
1	Bn	1.02	0/982	1.52	18/1337 (1.3%)
1	Bo	1.02	0/982	1.52	18/1337 (1.3%)
1	Bp	1.02	0/982	1.52	18/1337 (1.3%)
1	Bq	1.02	0/982	1.52	19/1337 (1.4%)
1	Br	1.02	0/982	1.52	19/1337 (1.4%)
1	Bs	1.02	0/982	1.52	18/1337 (1.3%)
1	Bt	1.02	0/982	1.52	18/1337 (1.3%)
1	Bu	1.02	0/982	1.52	18/1337 (1.3%)
1	Bv	1.02	0/982	1.52	18/1337 (1.3%)
1	Bw	1.02	0/982	1.52	18/1337 (1.3%)
1	Bx	1.02	0/982	1.52	18/1337 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	C0	0.94	0/982	1.67	22/1337 (1.6%)
1	C1	0.94	0/982	1.67	22/1337 (1.6%)
1	C2	0.94	0/982	1.67	22/1337 (1.6%)
1	C3	0.94	0/982	1.66	21/1337 (1.6%)
1	C4	0.94	0/982	1.66	21/1337 (1.6%)
1	C5	0.94	0/982	1.67	21/1337 (1.6%)
1	C6	0.94	0/982	1.67	22/1337 (1.6%)
1	C7	0.94	0/982	1.67	21/1337 (1.6%)
1	C8	0.94	0/982	1.67	22/1337 (1.6%)
1	C9	0.94	0/982	1.67	22/1337 (1.6%)
1	CA	0.94	0/982	1.67	22/1337 (1.6%)
1	CB	0.94	0/982	1.66	22/1337 (1.6%)
1	CC	0.94	0/982	1.67	22/1337 (1.6%)
1	CD	0.94	0/982	1.67	22/1337 (1.6%)
1	CE	0.94	0/982	1.67	22/1337 (1.6%)
1	CF	0.94	0/982	1.67	22/1337 (1.6%)
1	CG	0.94	0/982	1.67	21/1337 (1.6%)
1	CH	0.94	0/982	1.67	22/1337 (1.6%)
1	CI	0.94	0/982	1.66	22/1337 (1.6%)
1	CJ	0.94	0/982	1.67	21/1337 (1.6%)
1	CK	0.94	0/982	1.66	21/1337 (1.6%)
1	CL	0.94	0/982	1.67	22/1337 (1.6%)
1	CM	0.94	0/982	1.67	21/1337 (1.6%)
1	CN	0.94	0/982	1.67	22/1337 (1.6%)
1	CO	0.94	0/982	1.67	21/1337 (1.6%)
1	CP	0.94	0/982	1.67	23/1337 (1.7%)
1	CQ	0.94	0/982	1.67	22/1337 (1.6%)
1	CR	0.94	0/982	1.67	21/1337 (1.6%)
1	CS	0.94	0/982	1.66	22/1337 (1.6%)
1	CT	0.94	0/982	1.67	22/1337 (1.6%)
1	CU	0.94	0/982	1.66	21/1337 (1.6%)
1	CV	0.94	0/982	1.67	22/1337 (1.6%)
1	CW	0.94	0/982	1.67	22/1337 (1.6%)
1	CX	0.94	0/982	1.67	21/1337 (1.6%)
1	CY	0.94	0/982	1.67	22/1337 (1.6%)
1	CZ	0.94	0/982	1.67	22/1337 (1.6%)
1	Ca	0.94	0/982	1.67	22/1337 (1.6%)
1	Cb	0.94	0/982	1.67	21/1337 (1.6%)
1	Cc	0.94	0/982	1.67	21/1337 (1.6%)
1	Cd	0.94	0/982	1.67	22/1337 (1.6%)
1	Ce	0.94	0/982	1.67	21/1337 (1.6%)
1	Cf	0.94	0/982	1.67	22/1337 (1.6%)
1	Cg	0.94	0/982	1.67	21/1337 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
1	Ch	0.94	0/982	1.67	21/1337 (1.6%)
1	Ci	0.94	0/982	1.66	21/1337 (1.6%)
1	Cj	0.94	0/982	1.67	21/1337 (1.6%)
1	Ck	0.94	0/982	1.67	22/1337 (1.6%)
1	Cl	0.94	0/982	1.66	21/1337 (1.6%)
1	Cm	0.94	0/982	1.67	21/1337 (1.6%)
1	Cn	0.94	0/982	1.67	21/1337 (1.6%)
1	Co	0.94	0/982	1.67	21/1337 (1.6%)
1	Cp	0.94	0/982	1.67	22/1337 (1.6%)
1	Cq	0.94	0/982	1.67	22/1337 (1.6%)
1	Cr	0.94	0/982	1.67	21/1337 (1.6%)
1	Cs	0.94	0/982	1.66	21/1337 (1.6%)
1	Ct	0.94	0/982	1.67	22/1337 (1.6%)
1	Cu	0.94	0/982	1.67	22/1337 (1.6%)
1	Cv	0.94	0/982	1.67	22/1337 (1.6%)
1	Cw	0.94	0/982	1.67	21/1337 (1.6%)
1	Cx	0.94	0/982	1.67	22/1337 (1.6%)
All	All	0.99	0/176760	1.61	3526/240660 (1.5%)

There are no bond length outliers.

All (3526) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ac	56	ARG	NE-CZ-NH2	-20.60	110.00	120.30
1	A1	56	ARG	NE-CZ-NH2	-20.59	110.00	120.30
1	A3	56	ARG	NE-CZ-NH2	-20.56	110.02	120.30
1	AW	56	ARG	NE-CZ-NH2	-20.54	110.03	120.30
1	A9	56	ARG	NE-CZ-NH2	-20.54	110.03	120.30
1	AN	56	ARG	NE-CZ-NH2	-20.53	110.03	120.30
1	Av	56	ARG	NE-CZ-NH2	-20.52	110.04	120.30
1	Ax	56	ARG	NE-CZ-NH2	-20.51	110.05	120.30
1	Ar	56	ARG	NE-CZ-NH2	-20.50	110.05	120.30
1	AV	56	ARG	NE-CZ-NH2	-20.50	110.05	120.30
1	Ad	56	ARG	NE-CZ-NH2	-20.50	110.05	120.30
1	AA	56	ARG	NE-CZ-NH2	-20.49	110.05	120.30
1	AZ	56	ARG	NE-CZ-NH2	-20.49	110.05	120.30
1	As	56	ARG	NE-CZ-NH2	-20.49	110.06	120.30
1	A5	56	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	AD	56	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	Al	56	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	An	56	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	Ak	56	ARG	NE-CZ-NH2	-20.47	110.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A4	56	ARG	NE-CZ-NH2	-20.47	110.07	120.30
1	AT	56	ARG	NE-CZ-NH2	-20.47	110.07	120.30
1	Aw	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	Aj	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	Am	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	Ab	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	Au	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	AF	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	AU	56	ARG	NE-CZ-NH2	-20.46	110.07	120.30
1	Af	56	ARG	NE-CZ-NH2	-20.45	110.07	120.30
1	AB	56	ARG	NE-CZ-NH2	-20.45	110.07	120.30
1	A7	56	ARG	NE-CZ-NH2	-20.45	110.08	120.30
1	AH	56	ARG	NE-CZ-NH2	-20.45	110.08	120.30
1	AE	56	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	A6	56	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	Ae	56	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	A8	56	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	AM	56	ARG	NE-CZ-NH2	-20.44	110.08	120.30
1	AR	56	ARG	NE-CZ-NH2	-20.43	110.08	120.30
1	AX	56	ARG	NE-CZ-NH2	-20.43	110.08	120.30
1	A0	56	ARG	NE-CZ-NH2	-20.43	110.08	120.30
1	AI	56	ARG	NE-CZ-NH2	-20.43	110.08	120.30
1	A2	56	ARG	NE-CZ-NH2	-20.43	110.09	120.30
1	Ag	56	ARG	NE-CZ-NH2	-20.42	110.09	120.30
1	AK	56	ARG	NE-CZ-NH2	-20.42	110.09	120.30
1	Aa	56	ARG	NE-CZ-NH2	-20.40	110.10	120.30
1	AC	56	ARG	NE-CZ-NH2	-20.40	110.10	120.30
1	AL	56	ARG	NE-CZ-NH2	-20.40	110.10	120.30
1	Ap	56	ARG	NE-CZ-NH2	-20.40	110.10	120.30
1	AG	56	ARG	NE-CZ-NH2	-20.40	110.10	120.30
1	AO	56	ARG	NE-CZ-NH2	-20.39	110.10	120.30
1	Ah	56	ARG	NE-CZ-NH2	-20.39	110.11	120.30
1	AJ	56	ARG	NE-CZ-NH2	-20.39	110.11	120.30
1	AQ	56	ARG	NE-CZ-NH2	-20.38	110.11	120.30
1	Ao	56	ARG	NE-CZ-NH2	-20.37	110.11	120.30
1	AY	56	ARG	NE-CZ-NH2	-20.37	110.11	120.30
1	At	56	ARG	NE-CZ-NH2	-20.36	110.12	120.30
1	AP	56	ARG	NE-CZ-NH2	-20.36	110.12	120.30
1	Aq	56	ARG	NE-CZ-NH2	-20.33	110.14	120.30
1	AS	56	ARG	NE-CZ-NH2	-20.33	110.14	120.30
1	Ai	56	ARG	NE-CZ-NH2	-20.26	110.17	120.30
1	CR	11	ASP	CB-CA-C	-10.60	89.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CJ	11	ASP	CB-CA-C	-10.60	89.20	110.40
1	CV	11	ASP	CB-CA-C	-10.59	89.22	110.40
1	Cr	11	ASP	CB-CA-C	-10.59	89.22	110.40
1	Cg	11	ASP	CB-CA-C	-10.59	89.22	110.40
1	CL	11	ASP	CB-CA-C	-10.59	89.22	110.40
1	Cf	11	ASP	CB-CA-C	-10.59	89.23	110.40
1	Cp	11	ASP	CB-CA-C	-10.59	89.23	110.40
1	C5	11	ASP	CB-CA-C	-10.58	89.23	110.40
1	Cs	11	ASP	CB-CA-C	-10.58	89.23	110.40
1	CD	11	ASP	CB-CA-C	-10.58	89.24	110.40
1	C1	11	ASP	CB-CA-C	-10.58	89.24	110.40
1	CB	11	ASP	CB-CA-C	-10.58	89.24	110.40
1	CC	11	ASP	CB-CA-C	-10.58	89.24	110.40
1	CI	11	ASP	CB-CA-C	-10.58	89.25	110.40
1	Cd	11	ASP	CB-CA-C	-10.58	89.25	110.40
1	Ci	11	ASP	CB-CA-C	-10.58	89.25	110.40
1	Ck	11	ASP	CB-CA-C	-10.58	89.25	110.40
1	Co	11	ASP	CB-CA-C	-10.58	89.25	110.40
1	Cl	11	ASP	CB-CA-C	-10.57	89.25	110.40
1	CU	11	ASP	CB-CA-C	-10.57	89.25	110.40
1	CS	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	CT	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	Cc	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	Ch	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	Cj	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	Cq	11	ASP	CB-CA-C	-10.57	89.26	110.40
1	CF	11	ASP	CB-CA-C	-10.57	89.27	110.40
1	Cn	11	ASP	CB-CA-C	-10.57	89.27	110.40
1	C0	11	ASP	CB-CA-C	-10.56	89.27	110.40
1	CQ	11	ASP	CB-CA-C	-10.56	89.27	110.40
1	CA	11	ASP	CB-CA-C	-10.56	89.27	110.40
1	C3	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	Ct	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	C6	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	CH	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	CK	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	CO	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	Ca	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	Cw	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	C9	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	CM	11	ASP	CB-CA-C	-10.56	89.28	110.40
1	CZ	11	ASP	CB-CA-C	-10.56	89.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C2	11	ASP	CB-CA-C	-10.56	89.29	110.40
1	C4	11	ASP	CB-CA-C	-10.56	89.29	110.40
1	C8	11	ASP	CB-CA-C	-10.55	89.29	110.40
1	CE	11	ASP	CB-CA-C	-10.55	89.29	110.40
1	CY	11	ASP	CB-CA-C	-10.55	89.29	110.40
1	Cv	11	ASP	CB-CA-C	-10.55	89.29	110.40
1	Cx	11	ASP	CB-CA-C	-10.55	89.29	110.40
1	C7	11	ASP	CB-CA-C	-10.55	89.30	110.40
1	CN	11	ASP	CB-CA-C	-10.55	89.30	110.40
1	CP	11	ASP	CB-CA-C	-10.54	89.31	110.40
1	Cm	11	ASP	CB-CA-C	-10.54	89.31	110.40
1	Cu	11	ASP	CB-CA-C	-10.54	89.32	110.40
1	CG	11	ASP	CB-CA-C	-10.54	89.32	110.40
1	CW	11	ASP	CB-CA-C	-10.54	89.32	110.40
1	CX	11	ASP	CB-CA-C	-10.54	89.32	110.40
1	Cb	11	ASP	CB-CA-C	-10.54	89.33	110.40
1	Ce	11	ASP	CB-CA-C	-10.52	89.35	110.40
1	CF	11	ASP	N-CA-CB	10.22	129.00	110.60
1	CG	11	ASP	N-CA-CB	10.22	129.00	110.60
1	Cn	11	ASP	N-CA-CB	10.22	128.99	110.60
1	CM	11	ASP	N-CA-CB	10.22	128.99	110.60
1	Cb	11	ASP	N-CA-CB	10.21	128.99	110.60
1	Cf	11	ASP	N-CA-CB	10.21	128.98	110.60
1	Ce	11	ASP	N-CA-CB	10.21	128.97	110.60
1	Ct	11	ASP	N-CA-CB	10.21	128.97	110.60
1	CI	11	ASP	N-CA-CB	10.20	128.96	110.60
1	CX	11	ASP	N-CA-CB	10.20	128.97	110.60
1	C7	11	ASP	N-CA-CB	10.20	128.96	110.60
1	C2	11	ASP	N-CA-CB	10.20	128.95	110.60
1	CH	11	ASP	N-CA-CB	10.20	128.95	110.60
1	C0	11	ASP	N-CA-CB	10.19	128.95	110.60
1	CE	11	ASP	N-CA-CB	10.19	128.95	110.60
1	CA	11	ASP	N-CA-CB	10.19	128.94	110.60
1	Cj	11	ASP	N-CA-CB	10.19	128.94	110.60
1	Ck	11	ASP	N-CA-CB	10.19	128.94	110.60
1	CT	11	ASP	N-CA-CB	10.19	128.94	110.60
1	CC	11	ASP	N-CA-CB	10.19	128.93	110.60
1	CD	11	ASP	N-CA-CB	10.19	128.93	110.60
1	CN	11	ASP	N-CA-CB	10.19	128.93	110.60
1	Ch	11	ASP	N-CA-CB	10.19	128.93	110.60
1	C1	11	ASP	N-CA-CB	10.18	128.93	110.60
1	C3	11	ASP	N-CA-CB	10.18	128.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C9	11	ASP	N-CA-CB	10.18	128.93	110.60
1	CZ	11	ASP	N-CA-CB	10.18	128.93	110.60
1	Cm	11	ASP	N-CA-CB	10.18	128.93	110.60
1	Cc	11	ASP	N-CA-CB	10.18	128.93	110.60
1	Cx	11	ASP	N-CA-CB	10.18	128.93	110.60
1	C4	11	ASP	N-CA-CB	10.18	128.92	110.60
1	CO	11	ASP	N-CA-CB	10.18	128.92	110.60
1	C6	11	ASP	N-CA-CB	10.18	128.92	110.60
1	CP	11	ASP	N-CA-CB	10.18	128.92	110.60
1	C5	11	ASP	N-CA-CB	10.17	128.91	110.60
1	CK	11	ASP	N-CA-CB	10.17	128.91	110.60
1	CU	11	ASP	N-CA-CB	10.17	128.91	110.60
1	Cu	11	ASP	N-CA-CB	10.17	128.91	110.60
1	CW	11	ASP	N-CA-CB	10.17	128.91	110.60
1	Cw	11	ASP	N-CA-CB	10.17	128.91	110.60
1	C8	11	ASP	N-CA-CB	10.17	128.90	110.60
1	CB	11	ASP	N-CA-CB	10.17	128.90	110.60
1	CQ	11	ASP	N-CA-CB	10.17	128.90	110.60
1	CV	11	ASP	N-CA-CB	10.17	128.90	110.60
1	Cp	11	ASP	N-CA-CB	10.17	128.90	110.60
1	Cg	11	ASP	N-CA-CB	10.16	128.89	110.60
1	Cl	11	ASP	N-CA-CB	10.16	128.90	110.60
1	Cs	11	ASP	N-CA-CB	10.16	128.90	110.60
1	CR	11	ASP	N-CA-CB	10.16	128.89	110.60
1	Cq	11	ASP	N-CA-CB	10.16	128.89	110.60
1	Ci	11	ASP	N-CA-CB	10.16	128.89	110.60
1	Co	11	ASP	N-CA-CB	10.16	128.89	110.60
1	Cd	11	ASP	N-CA-CB	10.15	128.88	110.60
1	Cv	11	ASP	N-CA-CB	10.15	128.87	110.60
1	CY	11	ASP	N-CA-CB	10.15	128.87	110.60
1	Ca	11	ASP	N-CA-CB	10.15	128.87	110.60
1	Cr	11	ASP	N-CA-CB	10.15	128.86	110.60
1	CL	11	ASP	N-CA-CB	10.14	128.86	110.60
1	CJ	11	ASP	N-CA-CB	10.13	128.84	110.60
1	CS	11	ASP	N-CA-CB	10.12	128.82	110.60
1	AV	56	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	Aj	56	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	Ax	56	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	AB	56	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	Af	56	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	Ac	56	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	A1	56	ARG	NE-CZ-NH1	9.16	124.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	56	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	Ao	56	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	As	56	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	Ah	56	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	Av	56	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	AT	56	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	Ag	56	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	AJ	56	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	Ab	56	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	AU	56	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	An	56	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	A0	56	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	AK	56	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	Au	56	ARG	NE-CZ-NH1	9.11	124.85	120.30
1	AW	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	Aw	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	AN	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	Ad	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A5	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	AC	56	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A9	56	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	Al	56	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	Ar	56	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	AQ	56	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	AM	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	AF	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	AO	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	Am	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A4	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A7	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	Ak	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	Aq	56	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A2	56	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	AZ	56	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A3	56	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	At	56	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	AI	56	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	Ap	56	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	AL	56	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	AP	56	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A8	56	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	AX	56	ARG	NE-CZ-NH1	9.04	124.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AE	56	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	AG	56	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	AA	56	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	AD	56	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A6	56	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	AH	56	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	AS	56	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	AY	56	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	Ae	56	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	Aa	56	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	Ai	56	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	Ck	56	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	Co	32	TRP	CE2-CD2-CG	-8.76	100.29	107.30
1	C0	32	TRP	CE2-CD2-CG	-8.76	100.30	107.30
1	Cm	32	TRP	CE2-CD2-CG	-8.76	100.30	107.30
1	CQ	56	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	Cx	32	TRP	CE2-CD2-CG	-8.74	100.31	107.30
1	CN	32	TRP	CE2-CD2-CG	-8.73	100.31	107.30
1	Ct	56	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	CH	32	TRP	CE2-CD2-CG	-8.73	100.32	107.30
1	Cd	32	TRP	CE2-CD2-CG	-8.73	100.32	107.30
1	CX	32	TRP	CE2-CD2-CG	-8.73	100.32	107.30
1	Cf	56	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	Cn	56	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	Ca	32	TRP	CE2-CD2-CG	-8.72	100.32	107.30
1	Ce	32	TRP	CE2-CD2-CG	-8.72	100.32	107.30
1	CL	32	TRP	CE2-CD2-CG	-8.72	100.32	107.30
1	C6	56	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	CE	32	TRP	CE2-CD2-CG	-8.72	100.33	107.30
1	CO	32	TRP	CE2-CD2-CG	-8.72	100.33	107.30
1	CV	32	TRP	CE2-CD2-CG	-8.72	100.33	107.30
1	C7	32	TRP	CE2-CD2-CG	-8.71	100.33	107.30
1	C5	32	TRP	CE2-CD2-CG	-8.71	100.33	107.30
1	CZ	32	TRP	CE2-CD2-CG	-8.71	100.33	107.30
1	CJ	32	TRP	CE2-CD2-CG	-8.71	100.33	107.30
1	CK	56	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	CT	32	TRP	CE2-CD2-CG	-8.71	100.33	107.30
1	C5	56	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	CD	32	TRP	CE2-CD2-CG	-8.70	100.34	107.30
1	CP	32	TRP	CE2-CD2-CG	-8.70	100.34	107.30
1	CM	32	TRP	CE2-CD2-CG	-8.70	100.34	107.30
1	CY	32	TRP	CE2-CD2-CG	-8.70	100.34	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Cv	32	TRP	CE2-CD2-CG	-8.70	100.34	107.30
1	Cp	32	TRP	CE2-CD2-CG	-8.69	100.34	107.30
1	C1	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	C9	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CA	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CC	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	Ch	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	Cr	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CI	56	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	Cj	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CH	56	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	CQ	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	Ca	56	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	Cc	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CK	32	TRP	CE2-CD2-CG	-8.69	100.35	107.30
1	CB	32	TRP	CE2-CD2-CG	-8.68	100.35	107.30
1	C8	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	Cn	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	Cq	56	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	Cu	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	C2	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	CW	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	Cb	32	TRP	CE2-CD2-CG	-8.68	100.36	107.30
1	CS	32	TRP	CE2-CD2-CG	-8.67	100.36	107.30
1	Cj	56	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	Cw	56	ARG	NE-CZ-NH2	-8.67	115.96	120.30
1	Ci	32	TRP	CE2-CD2-CG	-8.67	100.36	107.30
1	C3	32	TRP	CE2-CD2-CG	-8.67	100.37	107.30
1	CR	32	TRP	CE2-CD2-CG	-8.67	100.37	107.30
1	Cw	32	TRP	CE2-CD2-CG	-8.67	100.36	107.30
1	C4	32	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	CG	32	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	CA	56	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	C6	32	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	Cf	32	TRP	CE2-CD2-CG	-8.66	100.37	107.30
1	CF	32	TRP	CE2-CD2-CG	-8.65	100.38	107.30
1	CV	56	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	Cq	32	TRP	CE2-CD2-CG	-8.65	100.38	107.30
1	C9	56	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	Ck	32	TRP	CE2-CD2-CG	-8.65	100.38	107.30
1	CC	56	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	Cg	32	TRP	CE2-CD2-CG	-8.65	100.38	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CW	56	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	CY	56	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	Cs	32	TRP	CE2-CD2-CG	-8.65	100.38	107.30
1	CT	56	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	Cl	32	TRP	CE2-CD2-CG	-8.64	100.39	107.30
1	CR	56	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	CX	56	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	C0	56	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	CU	32	TRP	CE2-CD2-CG	-8.63	100.39	107.30
1	C4	56	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	CP	56	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	Co	56	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	Ct	32	TRP	CE2-CD2-CG	-8.63	100.40	107.30
1	Ce	56	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	CJ	56	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	C7	56	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	CG	56	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	Ci	56	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	Cb	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	CL	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	Cr	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	CD	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	CF	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	Cc	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	CN	56	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	C8	56	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	CI	32	TRP	CE2-CD2-CG	-8.59	100.43	107.30
1	Ch	56	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	Cm	56	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	Cx	56	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	Cs	56	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	C3	56	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	CE	56	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	Cu	56	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	Cg	56	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	CU	56	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	Cv	56	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	CO	56	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	CS	56	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	C1	56	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	Cd	56	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	Cl	56	ARG	NE-CZ-NH2	-8.52	116.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C2	56	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	CB	56	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	CZ	56	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	Cp	56	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	CM	56	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B9	32	TRP	CD1-CG-CD2	8.35	112.98	106.30
1	Bw	32	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	B0	32	TRP	CD1-CG-CD2	8.29	112.94	106.30
1	Bv	32	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	BN	32	TRP	CD1-CG-CD2	8.29	112.93	106.30
1	BH	32	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	BP	32	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	BW	32	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	Ba	32	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	Bu	32	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	Bc	32	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	Bf	32	TRP	CD1-CG-CD2	8.26	112.91	106.30
1	B4	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	BD	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	B5	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	BA	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	B6	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	BY	32	TRP	CD1-CG-CD2	8.25	112.90	106.30
1	BF	32	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	B7	32	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	Bs	32	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	BG	32	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	Bn	32	TRP	CD1-CG-CD2	8.24	112.89	106.30
1	Bo	32	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	Bb	32	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	B2	32	TRP	CD1-CG-CD2	8.23	112.88	106.30
1	BS	32	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	Bx	32	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	B3	32	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	Bd	32	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	BT	32	TRP	CD1-CG-CD2	8.22	112.88	106.30
1	BQ	32	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	Bp	32	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	B1	32	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	BI	32	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	Bl	32	TRP	CD1-CG-CD2	8.21	112.87	106.30
1	Cm	49	ARG	NE-CZ-NH2	-8.21	116.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BV	32	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	Bm	32	TRP	CD1-CG-CD2	8.20	112.86	106.30
1	BX	32	TRP	CD1-CG-CD2	8.19	112.86	106.30
1	Bk	32	TRP	CD1-CG-CD2	8.19	112.86	106.30
1	Be	32	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	Bh	32	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	B8	32	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	BK	32	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	CA	49	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	Bt	32	TRP	CD1-CG-CD2	8.18	112.85	106.30
1	BB	32	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	Bj	32	TRP	CD1-CG-CD2	8.18	112.84	106.30
1	Bg	32	TRP	CD1-CG-CD2	8.17	112.84	106.30
1	BC	32	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	BZ	32	TRP	CD1-CG-CD2	8.17	112.83	106.30
1	Br	32	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	BJ	32	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	BO	32	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	Bi	32	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	CZ	49	ARG	NE-CZ-NH2	-8.15	116.23	120.30
1	BL	32	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	Cj	49	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	AO	32	TRP	CD1-CG-CD2	8.14	112.81	106.30
1	A7	32	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	BU	32	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	Co	49	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	BE	32	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	BR	32	TRP	CD1-CG-CD2	8.13	112.81	106.30
1	BM	32	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	Ca	49	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	Bq	32	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	C1	49	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	AP	32	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	Au	32	TRP	CD1-CG-CD2	8.12	112.80	106.30
1	CO	49	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	CW	49	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	Cl	49	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	C2	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	C3	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A3	32	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	C7	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	C8	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	32	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	AX	32	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	CG	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	CX	49	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	At	32	TRP	CD1-CG-CD2	8.09	112.78	106.30
1	AB	32	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	A9	32	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	AR	32	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	Cb	49	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	Ax	32	TRP	CD1-CG-CD2	8.08	112.77	106.30
1	CM	49	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	Aj	32	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	Ak	32	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	AF	32	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	BX	83	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	CE	49	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	CY	49	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	AA	32	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	AD	32	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	Cd	49	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	Ar	32	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	AN	32	TRP	CD1-CG-CD2	8.07	112.75	106.30
1	AW	32	TRP	CD1-CG-CD2	8.07	112.75	106.30
1	Ab	32	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	CF	49	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	AS	32	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	C9	49	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	AJ	32	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	Ac	32	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	Ap	32	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	CP	49	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A0	32	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	A6	32	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	AV	32	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	C5	49	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	Al	32	TRP	CD1-CG-CD2	8.05	112.74	106.30
1	C0	49	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	Cf	49	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	AZ	32	TRP	CD1-CG-CD2	8.04	112.74	106.30
1	Af	32	TRP	CD1-CG-CD2	8.04	112.74	106.30
1	Av	32	TRP	CD1-CG-CD2	8.04	112.74	106.30
1	Aw	32	TRP	CD1-CG-CD2	8.04	112.73	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	AY	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	CD	49	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	CT	49	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	Cp	49	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A4	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	AQ	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	A8	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	AL	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	AM	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	Ao	32	TRP	CD1-CG-CD2	8.03	112.73	106.30
1	As	32	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	C4	49	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	Cw	49	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	Cx	49	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	AE	32	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	AT	32	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	Aa	32	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	AC	32	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	Am	32	TRP	CD1-CG-CD2	8.03	112.72	106.30
1	CC	49	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	Cn	49	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	Cu	49	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	CN	49	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	Cc	49	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	Aq	32	TRP	CD1-CG-CD2	8.02	112.72	106.30
1	Ce	49	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	Ad	32	TRP	CD1-CG-CD2	8.02	112.71	106.30
1	Ae	32	TRP	CD1-CG-CD2	8.02	112.71	106.30
1	AK	32	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	AI	32	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	A5	32	TRP	CD1-CG-CD2	8.01	112.70	106.30
1	Ah	32	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	AH	32	TRP	CD1-CG-CD2	8.00	112.70	106.30
1	Cv	49	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B4	83	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	CR	49	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	AG	32	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	AU	32	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	CB	49	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	Cq	49	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	Bi	83	ARG	NE-CZ-NH2	-7.98	116.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bo	83	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	CQ	49	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	BB	83	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	Ag	32	TRP	CD1-CG-CD2	7.98	112.68	106.30
1	An	32	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	B6	83	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	BL	83	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	CH	49	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	Ai	32	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	Bt	83	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	CJ	49	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	CL	49	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	Cs	49	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	Cg	49	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	Bx	83	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	Ci	49	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	BU	83	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	C6	49	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B7	83	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	Ct	49	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	CK	49	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	BR	83	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	CV	49	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	Ck	49	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	BM	83	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	Ch	49	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	CS	49	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	Bg	83	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	CP	32	TRP	CG-CD2-CE3	7.94	141.05	133.90
1	BQ	83	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	Cr	49	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	Be	83	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	Bp	83	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	CJ	32	TRP	CG-CD2-CE3	7.93	141.04	133.90
1	BG	83	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	C9	32	TRP	CG-CD2-CE3	7.93	141.03	133.90
1	CU	49	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	Br	83	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	Co	32	TRP	CG-CD2-CE3	7.92	141.03	133.90
1	B1	83	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	Bh	83	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	Bb	83	ARG	NE-CZ-NH2	-7.92	116.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CL	32	TRP	CG-CD2-CE3	7.92	141.03	133.90
1	CN	32	TRP	CG-CD2-CE3	7.92	141.03	133.90
1	Ca	32	TRP	CG-CD2-CE3	7.92	141.03	133.90
1	CB	32	TRP	CG-CD2-CE3	7.92	141.02	133.90
1	Bf	83	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	BV	83	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	Cq	32	TRP	CG-CD2-CE3	7.91	141.02	133.90
1	C1	32	TRP	CG-CD2-CE3	7.91	141.02	133.90
1	CY	32	TRP	CG-CD2-CE3	7.91	141.02	133.90
1	BF	83	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	BI	83	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	CI	49	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	Cm	32	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	B2	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	BS	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	Bc	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	CA	32	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	Ch	32	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	BZ	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	BO	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	Cd	32	TRP	CG-CD2-CE3	7.90	141.01	133.90
1	CS	32	TRP	CG-CD2-CE3	7.89	141.00	133.90
1	Bq	83	ARG	NE-CZ-NH2	-7.89	116.35	120.30
1	Cv	32	TRP	CG-CD2-CE3	7.89	141.00	133.90
1	CD	32	TRP	CG-CD2-CE3	7.89	141.00	133.90
1	BJ	83	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	B5	83	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	BP	83	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	BT	83	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	Bj	83	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	BZ	82	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	Bs	82	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	C0	32	TRP	CG-CD2-CE3	7.88	140.99	133.90
1	CO	32	TRP	CG-CD2-CE3	7.88	140.99	133.90
1	Cc	32	TRP	CG-CD2-CE3	7.88	140.99	133.90
1	BH	82	TRP	CD1-CG-CD2	7.88	112.60	106.30
1	Cg	32	TRP	CG-CD2-CE3	7.88	140.99	133.90
1	Bs	83	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	CU	32	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	Ct	32	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	Cw	32	TRP	CG-CD2-CE3	7.87	140.99	133.90
1	CE	32	TRP	CG-CD2-CE3	7.87	140.98	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CH	32	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	CR	32	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	Bu	83	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	CZ	32	TRP	CG-CD2-CE3	7.87	140.98	133.90
1	BA	83	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	CT	32	TRP	CG-CD2-CE3	7.86	140.98	133.90
1	AN	82	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	BY	83	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	Bm	83	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C2	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	C4	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	Ci	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	BA	82	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	BC	82	TRP	CD1-CG-CD2	7.86	112.59	106.30
1	Cp	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	BE	82	TRP	CD1-CG-CD2	7.86	112.58	106.30
1	BE	83	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C6	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	Cu	32	TRP	CG-CD2-CE3	7.86	140.97	133.90
1	Bj	82	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	B8	83	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	BH	83	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	AJ	82	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	Bp	82	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	AR	82	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	C3	32	TRP	CG-CD2-CE3	7.85	140.96	133.90
1	Bl	83	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	CX	32	TRP	CG-CD2-CE3	7.84	140.96	133.90
1	Cr	32	TRP	CG-CD2-CE3	7.84	140.96	133.90
1	BF	82	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	Bd	83	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	C8	32	TRP	CG-CD2-CE3	7.84	140.96	133.90
1	CQ	32	TRP	CG-CD2-CE3	7.84	140.96	133.90
1	Cj	32	TRP	CG-CD2-CE3	7.84	140.95	133.90
1	Ao	82	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	C7	32	TRP	CG-CD2-CE3	7.84	140.95	133.90
1	B4	82	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	Bm	82	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	Bn	83	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	C5	32	TRP	CG-CD2-CE3	7.83	140.95	133.90
1	CM	32	TRP	CG-CD2-CE3	7.83	140.95	133.90
1	Cb	32	TRP	CG-CD2-CE3	7.83	140.95	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BB	82	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	BD	82	TRP	CD1-CG-CD2	7.83	112.57	106.30
1	Au	82	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	B3	83	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	BK	83	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	CV	32	TRP	CG-CD2-CE3	7.83	140.95	133.90
1	At	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	Ba	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	Bk	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	Bk	83	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	Ah	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	B2	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	AB	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	AD	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	Bf	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	CG	32	TRP	CG-CD2-CE3	7.82	140.94	133.90
1	B9	82	TRP	CD1-CG-CD2	7.82	112.56	106.30
1	Ce	32	TRP	CG-CD2-CE3	7.82	140.94	133.90
1	Cx	32	TRP	CG-CD2-CE3	7.82	140.94	133.90
1	Ax	82	TRP	CD1-CG-CD2	7.82	112.55	106.30
1	Bd	82	TRP	CD1-CG-CD2	7.82	112.55	106.30
1	CF	32	TRP	CG-CD2-CE3	7.82	140.94	133.90
1	CW	32	TRP	CG-CD2-CE3	7.82	140.94	133.90
1	Cs	32	TRP	CG-CD2-CE3	7.82	140.93	133.90
1	AQ	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	B0	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	BI	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	BX	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Br	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Bo	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	CK	32	TRP	CG-CD2-CE3	7.81	140.93	133.90
1	BO	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Bn	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	CI	32	TRP	CG-CD2-CE3	7.81	140.93	133.90
1	AA	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Ar	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	BJ	82	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	BN	83	ARG	NE-CZ-NH2	-7.81	116.40	120.30
1	CA	32	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Cd	32	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	Ap	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	BG	82	TRP	CD1-CG-CD2	7.80	112.54	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BM	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	BV	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Bg	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	CC	32	TRP	CG-CD2-CE3	7.80	140.92	133.90
1	CE	32	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Ck	32	TRP	CG-CD2-CE3	7.80	140.92	133.90
1	B6	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	BN	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	BW	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Cl	32	TRP	CG-CD2-CE3	7.80	140.92	133.90
1	AU	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Av	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	B3	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Be	82	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	Af	82	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	B5	82	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	Bv	82	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	CL	32	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	B7	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	B8	82	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	B9	83	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	Bh	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Bt	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	C0	32	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	CH	32	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Co	32	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	A4	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	B1	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	AE	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Ag	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Bc	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Cf	32	TRP	CG-CD2-CE3	7.79	140.91	133.90
1	Cm	32	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	AF	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Ac	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	B0	83	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	Bq	82	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	CO	32	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	Cn	32	TRP	CG-CD2-CE3	7.79	140.91	133.90
1	BP	82	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	CJ	32	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	A7	82	TRP	CD1-CG-CD2	7.78	112.53	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BT	82	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	Ca	32	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	A2	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	AW	82	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	AZ	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	BS	82	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	Bl	82	TRP	CD1-CG-CD2	7.78	112.53	106.30
1	Bu	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A8	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	BL	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	Bx	82	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A1	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	Bb	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	AH	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	Ba	83	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	Aw	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	A3	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	AS	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	BY	82	TRP	CD1-CG-CD2	7.77	112.52	106.30
1	BD	83	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	AP	82	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	BQ	82	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	BU	82	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	C6	32	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	CV	32	TRP	CD1-CG-CD2	7.77	112.51	106.30
1	CZ	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Ch	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A6	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	C7	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	CG	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Ce	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Cj	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	C1	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	CY	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	AV	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	BR	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	AT	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Bi	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	CB	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Cv	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	AG	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	AI	82	TRP	CD1-CG-CD2	7.76	112.50	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BK	82	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Bw	83	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	C5	32	TRP	CD1-CG-CD2	7.76	112.50	106.30
1	Cx	32	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	Cc	32	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	C9	32	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	Aq	82	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	CM	32	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	Aa	82	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	Ad	82	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	BC	83	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	Cq	32	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A9	82	TRP	CD1-CG-CD2	7.74	112.50	106.30
1	Ai	82	TRP	CD1-CG-CD2	7.74	112.50	106.30
1	Ak	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	Al	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	CN	32	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	AY	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	An	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	Bv	83	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	Cg	32	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	AK	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	Cb	32	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	AL	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	Bw	82	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	CT	32	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	Cw	32	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	AO	82	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	C2	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	CX	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	Ct	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	Ae	82	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	C4	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	CC	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	CD	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	CU	32	TRP	CD1-CG-CD2	7.73	112.48	106.30
1	Am	82	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	As	82	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	Ci	32	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	CP	32	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	Cx	82	TRP	CD1-CG-CD2	7.72	112.48	106.30
1	BW	83	ARG	NE-CZ-NH2	-7.72	116.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CS	32	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	CW	32	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	Cf	32	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	Ck	32	TRP	CD1-CG-CD2	7.72	112.47	106.30
1	C2	82	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	CK	32	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	Au	32	TRP	CE2-CD2-CG	-7.71	101.13	107.30
1	C3	32	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	C6	82	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	CF	32	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	Ce	82	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	AX	82	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	CR	32	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	C8	32	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	Cr	32	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	Cs	32	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A5	82	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	CQ	32	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	CR	82	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	C9	82	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A0	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	C8	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Cp	32	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	As	32	TRP	CE2-CD2-CG	-7.69	101.15	107.30
1	CD	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Cn	32	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Cu	32	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	AM	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	CI	32	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	CP	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	CX	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Ca	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Ch	82	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	Cr	82	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	A9	32	TRP	CE2-CD2-CG	-7.68	101.15	107.30
1	CJ	82	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	CW	82	TRP	CD1-CG-CD2	7.68	112.45	106.30
1	Cw	82	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	CM	82	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	Ct	82	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	Cl	32	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	AC	32	TRP	CE2-CD2-CG	-7.67	101.16	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AN	32	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	At	32	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	Cl	82	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	AD	32	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	CG	82	TRP	CD1-CG-CD2	7.67	112.44	106.30
1	A5	32	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	AP	32	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	CS	82	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	CF	82	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	CN	82	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	Cb	82	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	Cm	82	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	Cv	82	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	AW	32	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	A3	32	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	Cp	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	Ab	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	Aj	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	C0	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	Cq	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	Ap	32	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	CA	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	C1	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	C4	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	Ci	82	TRP	CD1-CG-CD2	7.65	112.42	106.30
1	AC	82	TRP	CD1-CG-CD2	7.64	112.42	106.30
1	AT	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	Ae	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	Aj	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	CL	82	TRP	CD1-CG-CD2	7.64	112.42	106.30
1	Cg	82	TRP	CD1-CG-CD2	7.64	112.42	106.30
1	Cn	82	TRP	CD1-CG-CD2	7.64	112.42	106.30
1	AB	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	Ar	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	Ax	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	C5	82	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	CY	82	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	Cf	82	TRP	CD1-CG-CD2	7.64	112.41	106.30
1	Am	32	TRP	CE2-CD2-CG	-7.64	101.19	107.30
1	A8	32	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	Cj	82	TRP	CD1-CG-CD2	7.63	112.41	106.30
1	CO	82	TRP	CD1-CG-CD2	7.63	112.41	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Av	32	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	AO	32	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	A7	32	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	Ac	32	TRP	CE2-CD2-CG	-7.63	101.20	107.30
1	CH	82	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	CU	82	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	Co	82	TRP	CD1-CG-CD2	7.63	112.40	106.30
1	CZ	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	AJ	32	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	Cc	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	Cu	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	AI	32	TRP	CE2-CD2-CG	-7.62	101.20	107.30
1	C3	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	CT	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	CV	82	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	AS	32	TRP	CE2-CD2-CG	-7.62	101.21	107.30
1	Ao	32	TRP	CE2-CD2-CG	-7.62	101.21	107.30
1	CC	82	TRP	CD1-CG-CD2	7.62	112.39	106.30
1	AV	32	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	Cd	82	TRP	CD1-CG-CD2	7.61	112.39	106.30
1	Af	32	TRP	CE2-CD2-CG	-7.61	101.22	107.30
1	A0	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	AQ	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	CE	82	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	A2	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A4	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	AA	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	AF	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	Ck	82	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	AM	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	AK	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	AR	32	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	Ab	32	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	Ak	32	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	Aw	32	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	AX	32	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	C7	82	TRP	CD1-CG-CD2	7.58	112.37	106.30
1	A1	32	TRP	CE2-CD2-CG	-7.58	101.23	107.30
1	CB	82	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	AL	32	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	AZ	32	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	AU	32	TRP	CE2-CD2-CG	-7.58	101.24	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aq	32	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	CK	82	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	CQ	82	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	AH	32	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	Cs	82	TRP	CD1-CG-CD2	7.57	112.35	106.30
1	CI	82	TRP	CD1-CG-CD2	7.57	112.35	106.30
1	Ag	32	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	Ad	32	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	B9	32	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	Ah	32	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	An	32	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A6	32	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	AE	32	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	BH	32	TRP	CE2-CD2-CG	-7.55	101.26	107.30
1	BY	32	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	AG	32	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	AY	32	TRP	CE2-CD2-CG	-7.54	101.27	107.30
1	Aa	32	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	Bf	32	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	BV	32	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	BN	32	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	Bw	32	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	Al	32	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	Bn	32	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	Ai	32	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	Bc	32	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	BC	32	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	Bv	32	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	Ba	32	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	B0	32	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	BD	32	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	BF	32	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	BW	32	TRP	CE2-CD2-CG	-7.48	101.32	107.30
1	B4	32	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	BK	32	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	BP	32	TRP	CE2-CD2-CG	-7.47	101.32	107.30
1	Bu	32	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	BQ	32	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	Br	32	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	BT	32	TRP	CE2-CD2-CG	-7.46	101.34	107.30
1	Bj	32	TRP	CE2-CD2-CG	-7.46	101.34	107.30
1	B7	32	TRP	CE2-CD2-CG	-7.45	101.34	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B8	32	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	Bg	32	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	BA	32	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	B6	32	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	B2	32	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	Bd	32	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	Bk	32	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	B5	32	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	BG	32	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	BL	32	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	Bb	32	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	Bh	32	TRP	CE2-CD2-CG	-7.43	101.35	107.30
1	BX	32	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	Bp	32	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	BB	32	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	BI	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	Bo	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	Be	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	Bt	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	BS	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	Bq	32	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	CE	32	TRP	CB-CG-CD1	-7.42	117.36	127.00
1	Cd	32	TRP	CB-CG-CD1	-7.42	117.36	127.00
1	BZ	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	Bs	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	Bx	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	CG	32	TRP	CB-CG-CD1	-7.41	117.36	127.00
1	CW	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	Ca	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	Ct	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	B3	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	BM	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	Bm	32	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	Cj	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	CH	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	Co	32	TRP	CB-CG-CD1	-7.41	117.37	127.00
1	B1	32	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	Cx	32	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	BR	32	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	CA	32	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	Bl	32	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	C5	32	TRP	CB-CG-CD1	-7.40	117.38	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C6	32	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	CI	32	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	Cs	32	TRP	CB-CG-CD1	-7.40	117.38	127.00
1	BE	32	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	CZ	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	Cl	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	Bi	32	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	CY	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	Ck	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	CT	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	CU	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	CV	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	C7	32	TRP	CB-CG-CD1	-7.39	117.39	127.00
1	Ch	32	TRP	CB-CG-CD1	-7.39	117.40	127.00
1	Cq	32	TRP	CB-CG-CD1	-7.39	117.40	127.00
1	C4	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	CC	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	C3	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	Ce	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	CM	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	Cc	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	Cm	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	Cv	32	TRP	CB-CG-CD1	-7.38	117.40	127.00
1	C1	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	CQ	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	BJ	32	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	C0	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	C9	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	CX	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	Cb	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	Cf	32	TRP	CB-CG-CD1	-7.38	117.41	127.00
1	C2	32	TRP	CB-CG-CD1	-7.37	117.41	127.00
1	Ci	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	C8	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	CK	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	CS	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	Cg	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	BU	32	TRP	CE2-CD2-CG	-7.37	101.41	107.30
1	CF	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	CO	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	Cn	32	TRP	CB-CG-CD1	-7.37	117.42	127.00
1	CD	32	TRP	CB-CG-CD1	-7.37	117.43	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CR	32	TRP	CB-CG-CD1	-7.37	117.43	127.00
1	Cp	32	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	Cr	32	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	CJ	32	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	Cw	32	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	Cu	32	TRP	CB-CG-CD1	-7.36	117.43	127.00
1	Cr	108	MET	CG-SD-CE	-7.36	88.43	100.20
1	CL	32	TRP	CB-CG-CD1	-7.35	117.44	127.00
1	CB	32	TRP	CB-CG-CD1	-7.35	117.44	127.00
1	BO	32	TRP	CE2-CD2-CG	-7.35	101.42	107.30
1	CP	32	TRP	CB-CG-CD1	-7.34	117.45	127.00
1	Ck	108	MET	CG-SD-CE	-7.34	88.45	100.20
1	CN	32	TRP	CB-CG-CD1	-7.34	117.46	127.00
1	CS	108	MET	CG-SD-CE	-7.34	88.46	100.20
1	CI	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	CM	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	CR	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	CU	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	Ci	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	Cn	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	C4	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	C6	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	Ch	108	MET	CG-SD-CE	-7.33	88.47	100.20
1	CV	108	MET	CG-SD-CE	-7.33	88.48	100.20
1	Cd	108	MET	CG-SD-CE	-7.33	88.48	100.20
1	Cg	108	MET	CG-SD-CE	-7.33	88.48	100.20
1	Ct	108	MET	CG-SD-CE	-7.33	88.48	100.20
1	C3	108	MET	CG-SD-CE	-7.32	88.48	100.20
1	CL	108	MET	CG-SD-CE	-7.32	88.48	100.20
1	Cc	108	MET	CG-SD-CE	-7.32	88.48	100.20
1	Cp	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	CZ	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	Ce	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	C0	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	C5	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	CY	108	MET	CG-SD-CE	-7.32	88.49	100.20
1	C1	108	MET	CG-SD-CE	-7.32	88.50	100.20
1	Cs	108	MET	CG-SD-CE	-7.32	88.50	100.20
1	C8	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	C7	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	CG	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	CH	108	MET	CG-SD-CE	-7.31	88.50	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CQ	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	Cu	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	CA	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	CF	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	CP	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	Ca	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	Cv	108	MET	CG-SD-CE	-7.31	88.50	100.20
1	C2	108	MET	CG-SD-CE	-7.31	88.51	100.20
1	Cb	108	MET	CG-SD-CE	-7.31	88.51	100.20
1	Cf	108	MET	CG-SD-CE	-7.31	88.51	100.20
1	Cw	108	MET	CG-SD-CE	-7.31	88.51	100.20
1	CC	108	MET	CG-SD-CE	-7.31	88.51	100.20
1	CK	108	MET	CG-SD-CE	-7.30	88.51	100.20
1	Cl	108	MET	CG-SD-CE	-7.30	88.51	100.20
1	Cm	108	MET	CG-SD-CE	-7.30	88.51	100.20
1	CJ	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CB	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CE	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CO	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CT	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	Cx	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CW	108	MET	CG-SD-CE	-7.30	88.52	100.20
1	CX	108	MET	CG-SD-CE	-7.30	88.53	100.20
1	Cj	108	MET	CG-SD-CE	-7.30	88.53	100.20
1	Cq	108	MET	CG-SD-CE	-7.29	88.53	100.20
1	Co	108	MET	CG-SD-CE	-7.29	88.53	100.20
1	C9	108	MET	CG-SD-CE	-7.29	88.53	100.20
1	CD	108	MET	CG-SD-CE	-7.29	88.53	100.20
1	CN	108	MET	CG-SD-CE	-7.29	88.53	100.20
1	AW	2	SER	N-CA-C	-7.27	91.37	111.00
1	A3	2	SER	N-CA-C	-7.27	91.38	111.00
1	Ag	2	SER	N-CA-C	-7.27	91.38	111.00
1	AD	2	SER	N-CA-C	-7.26	91.39	111.00
1	Ax	2	SER	N-CA-C	-7.26	91.39	111.00
1	AU	2	SER	N-CA-C	-7.26	91.39	111.00
1	AN	2	SER	N-CA-C	-7.26	91.39	111.00
1	AH	2	SER	N-CA-C	-7.26	91.40	111.00
1	A5	2	SER	N-CA-C	-7.26	91.41	111.00
1	Av	2	SER	N-CA-C	-7.26	91.41	111.00
1	A7	2	SER	N-CA-C	-7.25	91.42	111.00
1	An	2	SER	N-CA-C	-7.25	91.42	111.00
1	Ao	2	SER	N-CA-C	-7.25	91.42	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AL	2	SER	N-CA-C	-7.25	91.42	111.00
1	A0	2	SER	N-CA-C	-7.25	91.42	111.00
1	A2	2	SER	N-CA-C	-7.25	91.42	111.00
1	A8	2	SER	N-CA-C	-7.25	91.43	111.00
1	A9	2	SER	N-CA-C	-7.25	91.43	111.00
1	AE	2	SER	N-CA-C	-7.25	91.43	111.00
1	AP	2	SER	N-CA-C	-7.25	91.42	111.00
1	A1	2	SER	N-CA-C	-7.25	91.43	111.00
1	Aa	2	SER	N-CA-C	-7.25	91.43	111.00
1	Ah	2	SER	N-CA-C	-7.25	91.43	111.00
1	As	2	SER	N-CA-C	-7.25	91.43	111.00
1	At	2	SER	N-CA-C	-7.25	91.43	111.00
1	Au	2	SER	N-CA-C	-7.25	91.43	111.00
1	AB	2	SER	N-CA-C	-7.25	91.43	111.00
1	Ad	2	SER	N-CA-C	-7.25	91.43	111.00
1	Ap	2	SER	N-CA-C	-7.25	91.43	111.00
1	Ac	2	SER	N-CA-C	-7.25	91.44	111.00
1	Ak	2	SER	N-CA-C	-7.25	91.44	111.00
1	AJ	2	SER	N-CA-C	-7.24	91.44	111.00
1	AK	2	SER	N-CA-C	-7.24	91.44	111.00
1	Aw	2	SER	N-CA-C	-7.24	91.44	111.00
1	AF	2	SER	N-CA-C	-7.24	91.45	111.00
1	AS	2	SER	N-CA-C	-7.24	91.45	111.00
1	AZ	2	SER	N-CA-C	-7.24	91.45	111.00
1	Ae	2	SER	N-CA-C	-7.24	91.45	111.00
1	Af	2	SER	N-CA-C	-7.24	91.45	111.00
1	Aj	2	SER	N-CA-C	-7.24	91.45	111.00
1	Ar	2	SER	N-CA-C	-7.24	91.45	111.00
1	AY	2	SER	N-CA-C	-7.24	91.45	111.00
1	Aq	2	SER	N-CA-C	-7.24	91.45	111.00
1	AG	2	SER	N-CA-C	-7.24	91.45	111.00
1	AI	2	SER	N-CA-C	-7.24	91.46	111.00
1	AR	2	SER	N-CA-C	-7.24	91.46	111.00
1	AV	2	SER	N-CA-C	-7.24	91.46	111.00
1	Ai	2	SER	N-CA-C	-7.24	91.46	111.00
1	AQ	2	SER	N-CA-C	-7.24	91.47	111.00
1	AX	2	SER	N-CA-C	-7.24	91.46	111.00
1	Ab	2	SER	N-CA-C	-7.23	91.47	111.00
1	Al	2	SER	N-CA-C	-7.23	91.47	111.00
1	Am	2	SER	N-CA-C	-7.23	91.47	111.00
1	A6	2	SER	N-CA-C	-7.23	91.47	111.00
1	AA	2	SER	N-CA-C	-7.23	91.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AM	2	SER	N-CA-C	-7.23	91.47	111.00
1	AO	2	SER	N-CA-C	-7.23	91.47	111.00
1	A4	2	SER	N-CA-C	-7.23	91.48	111.00
1	AT	2	SER	N-CA-C	-7.23	91.48	111.00
1	CM	82	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	AC	2	SER	N-CA-C	-7.22	91.50	111.00
1	Cx	82	TRP	CE2-CD2-CG	-7.22	101.52	107.30
1	AD	82	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	At	82	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	Cb	82	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	AN	82	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	Au	82	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	CG	82	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	Cm	82	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	CX	82	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	Ah	82	TRP	CE2-CD2-CG	-7.19	101.55	107.30
1	A4	82	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	AH	82	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	C7	82	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	AE	82	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	Cc	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	CC	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	CO	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	A9	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	AW	82	TRP	CE2-CD2-CG	-7.16	101.57	107.30
1	CR	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	Ao	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	C2	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	Ax	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A7	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	AQ	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	AS	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	CZ	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	Cn	82	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	Ap	82	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	Av	82	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	CT	82	TRP	CE2-CD2-CG	-7.14	101.58	107.30
1	An	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	C6	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	AA	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	CJ	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	Cr	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CV	82	TRP	CE2-CD2-CG	-7.14	101.59	107.30
1	Ch	82	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	Cp	82	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	CQ	82	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	BZ	48	VAL	CB-CA-C	-7.13	97.85	111.40
1	Cj	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	AB	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	Ag	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	BS	48	VAL	CB-CA-C	-7.13	97.86	111.40
1	C8	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	Ce	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	Cg	82	TRP	CE2-CD2-CG	-7.13	101.60	107.30
1	C3	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	Ck	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	A2	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	AL	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	AP	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	Be	48	VAL	CB-CA-C	-7.12	97.87	111.40
1	Ct	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	CS	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	Cq	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	AJ	82	TRP	CE2-CD2-CG	-7.12	101.60	107.30
1	Ar	82	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	BU	48	VAL	CB-CA-C	-7.12	97.88	111.40
1	A1	82	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	A3	82	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	Bq	48	VAL	CB-CA-C	-7.12	97.88	111.40
1	Bx	48	VAL	CB-CA-C	-7.12	97.88	111.40
1	CD	82	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	AF	82	TRP	CE2-CD2-CG	-7.12	101.61	107.30
1	BE	48	VAL	CB-CA-C	-7.12	97.88	111.40
1	Bj	48	VAL	CB-CA-C	-7.12	97.88	111.40
1	BX	48	VAL	CB-CA-C	-7.11	97.88	111.40
1	C1	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	Ci	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	C5	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A8	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	BO	48	VAL	CB-CA-C	-7.11	97.89	111.40
1	CI	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	Ca	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	Cf	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	B2	48	VAL	CB-CA-C	-7.11	97.90	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BR	48	VAL	CB-CA-C	-7.11	97.90	111.40
1	CE	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	CK	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	AU	82	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	Af	82	TRP	CE2-CD2-CG	-7.11	101.62	107.30
1	Br	48	VAL	CB-CA-C	-7.11	97.90	111.40
1	Co	82	TRP	CE2-CD2-CG	-7.11	101.62	107.30
1	AO	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	Bb	48	VAL	CB-CA-C	-7.10	97.90	111.40
1	B7	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	Ba	48	VAL	CB-CA-C	-7.10	97.90	111.40
1	Bh	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	Bp	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	CW	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	Bi	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	Bm	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	Bv	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	CL	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	AT	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	B4	48	VAL	CB-CA-C	-7.10	97.91	111.40
1	BA	48	VAL	CB-CA-C	-7.10	97.92	111.40
1	BJ	48	VAL	CB-CA-C	-7.10	97.92	111.40
1	Bc	48	VAL	CB-CA-C	-7.10	97.92	111.40
1	CF	82	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	BN	48	VAL	CB-CA-C	-7.09	97.92	111.40
1	Bg	48	VAL	CB-CA-C	-7.09	97.92	111.40
1	C9	82	TRP	CE2-CD2-CG	-7.09	101.62	107.30
1	CB	82	TRP	CE2-CD2-CG	-7.09	101.62	107.30
1	CU	82	TRP	CE2-CD2-CG	-7.09	101.62	107.30
1	BL	48	VAL	CB-CA-C	-7.09	97.92	111.40
1	Bf	48	VAL	CB-CA-C	-7.09	97.92	111.40
1	Ad	82	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	Bl	48	VAL	CB-CA-C	-7.09	97.92	111.40
1	AR	82	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	B0	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	B8	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	BG	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	BM	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	Bt	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	Cw	82	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	AZ	82	TRP	CE2-CD2-CG	-7.09	101.63	107.30
1	Aw	82	TRP	CE2-CD2-CG	-7.09	101.63	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BF	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	BP	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	Bo	48	VAL	CB-CA-C	-7.09	97.93	111.40
1	B1	48	VAL	CB-CA-C	-7.09	97.94	111.40
1	BC	48	VAL	CB-CA-C	-7.09	97.94	111.40
1	Bk	48	VAL	CB-CA-C	-7.09	97.94	111.40
1	Bu	48	VAL	CB-CA-C	-7.09	97.94	111.40
1	B5	48	VAL	CB-CA-C	-7.08	97.94	111.40
1	B6	48	VAL	CB-CA-C	-7.08	97.94	111.40
1	Cv	82	TRP	CE2-CD2-CG	-7.08	101.63	107.30
1	BK	48	VAL	CB-CA-C	-7.08	97.94	111.40
1	BW	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	BY	48	VAL	CB-CA-C	-7.08	97.94	111.40
1	AV	82	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	Ak	82	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	CA	82	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	B9	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	BB	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	BD	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	Bd	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	Bs	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	As	82	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	B3	48	VAL	CB-CA-C	-7.08	97.95	111.40
1	BH	48	VAL	CB-CA-C	-7.08	97.96	111.40
1	BQ	48	VAL	CB-CA-C	-7.07	97.96	111.40
1	BV	48	VAL	CB-CA-C	-7.07	97.96	111.40
1	Bw	48	VAL	CB-CA-C	-7.07	97.96	111.40
1	Bn	48	VAL	CB-CA-C	-7.07	97.96	111.40
1	BI	48	VAL	CB-CA-C	-7.07	97.97	111.40
1	C4	82	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	AI	82	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	BT	48	VAL	CB-CA-C	-7.07	97.98	111.40
1	Ac	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Al	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	CN	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Cd	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Cl	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Ai	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Am	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	AG	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	Aq	82	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	CP	82	TRP	CE2-CD2-CG	-7.06	101.66	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ab	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A6	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	Aa	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	Cu	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	CH	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	AK	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	AY	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	Ae	82	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	CY	82	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	AM	82	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	C0	82	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	A0	82	TRP	CE2-CD2-CG	-7.04	101.67	107.30
1	AX	82	TRP	CE2-CD2-CG	-7.03	101.67	107.30
1	Aj	82	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	AC	82	TRP	CE2-CD2-CG	-7.03	101.68	107.30
1	Cs	82	TRP	CE2-CD2-CG	-7.02	101.68	107.30
1	A5	82	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	CW	58	TYR	CB-CG-CD2	-7.00	116.80	121.00
1	CN	58	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	Cg	58	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	Ca	58	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	CH	58	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	Cu	58	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	Cd	58	TYR	CB-CG-CD2	-6.96	116.83	121.00
1	CL	58	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	Cr	58	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	Ci	58	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	Cp	58	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	CR	58	TYR	CB-CG-CD2	-6.93	116.84	121.00
1	CP	58	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	Co	58	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	CA	58	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	CB	58	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	CF	58	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	CJ	58	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	C0	58	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	C9	58	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	C8	58	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	Cw	58	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	Ch	58	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	C7	58	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	Cs	58	TYR	CB-CG-CD2	-6.87	116.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CY	58	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	Cv	58	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	CS	58	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	CC	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	CO	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	Ce	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	C1	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	CK	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	CT	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	Cb	58	TYR	CB-CG-CD2	-6.86	116.88	121.00
1	C3	58	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	CU	58	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	Cn	58	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	C6	58	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	CD	58	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	CI	58	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	Cl	58	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	Cx	58	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	CG	58	TYR	CB-CG-CD2	-6.84	116.90	121.00
1	Cm	58	TYR	CB-CG-CD2	-6.84	116.90	121.00
1	CZ	58	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	C5	58	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	C2	58	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	CQ	58	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	C4	58	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	CX	58	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	Cq	58	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	CE	58	TYR	CB-CG-CD2	-6.81	116.92	121.00
1	Cc	58	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	Cj	58	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	CV	58	TYR	CB-CG-CD2	-6.78	116.94	121.00
1	Cf	58	TYR	CB-CG-CD2	-6.77	116.94	121.00
1	Ck	58	TYR	CB-CG-CD2	-6.77	116.94	121.00
1	CM	58	TYR	CB-CG-CD2	-6.76	116.94	121.00
1	Ct	58	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	BZ	82	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	BE	82	TRP	CE2-CD2-CG	-6.72	101.92	107.30
1	Bj	82	TRP	CE2-CD2-CG	-6.70	101.94	107.30
1	BX	82	TRP	CE2-CD2-CG	-6.69	101.95	107.30
1	BO	82	TRP	CE2-CD2-CG	-6.69	101.95	107.30
1	BJ	82	TRP	CE2-CD2-CG	-6.68	101.95	107.30
1	BC	82	TRP	CE2-CD2-CG	-6.68	101.95	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BG	82	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	Bs	82	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	Bq	82	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	B4	82	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	B8	82	TRP	CE2-CD2-CG	-6.68	101.96	107.30
1	BI	82	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	Be	82	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	B6	82	TRP	CE2-CD2-CG	-6.67	101.96	107.30
1	CT	20	VAL	N-CA-CB	-6.67	96.83	111.50
1	CB	20	VAL	N-CA-CB	-6.67	96.83	111.50
1	Bk	82	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	Bp	82	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	BH	82	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	Bh	82	TRP	CE2-CD2-CG	-6.66	101.97	107.30
1	CK	20	VAL	N-CA-CB	-6.66	96.85	111.50
1	BV	82	TRP	CE2-CD2-CG	-6.66	101.98	107.30
1	Cr	20	VAL	N-CA-CB	-6.66	96.86	111.50
1	BS	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	BU	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	Bc	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	C6	20	VAL	N-CA-CB	-6.65	96.87	111.50
1	Cq	20	VAL	N-CA-CB	-6.65	96.87	111.50
1	Ch	20	VAL	N-CA-CB	-6.65	96.87	111.50
1	Cp	20	VAL	N-CA-CB	-6.65	96.87	111.50
1	BR	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	Br	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	CG	20	VAL	N-CA-CB	-6.65	96.88	111.50
1	CM	20	VAL	N-CA-CB	-6.65	96.88	111.50
1	CV	20	VAL	N-CA-CB	-6.65	96.88	111.50
1	CW	20	VAL	N-CA-CB	-6.65	96.88	111.50
1	Cd	20	VAL	N-CA-CB	-6.65	96.87	111.50
1	Bm	82	TRP	CE2-CD2-CG	-6.65	101.98	107.30
1	CD	20	VAL	N-CA-CB	-6.65	96.88	111.50
1	BB	82	TRP	CE2-CD2-CG	-6.64	101.98	107.30
1	CI	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	CP	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	Ca	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	Cf	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	Cm	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	Cx	20	VAL	N-CA-CB	-6.64	96.88	111.50
1	BF	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	C1	20	VAL	N-CA-CB	-6.64	96.89	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CC	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Co	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Bl	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	CR	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Bn	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	CX	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	CY	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Ci	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Ck	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Ct	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Cu	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	Cw	20	VAL	N-CA-CB	-6.64	96.89	111.50
1	B9	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	Cl	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	B3	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	BQ	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	Bd	82	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	C2	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	CH	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	CL	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	CU	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	Cb	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	Cc	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	Cj	20	VAL	N-CA-CB	-6.64	96.90	111.50
1	CE	20	VAL	N-CA-CB	-6.63	96.90	111.50
1	CJ	20	VAL	N-CA-CB	-6.63	96.91	111.50
1	CQ	20	VAL	N-CA-CB	-6.63	96.90	111.50
1	CS	20	VAL	N-CA-CB	-6.63	96.90	111.50
1	Cg	20	VAL	N-CA-CB	-6.63	96.91	111.50
1	Cn	20	VAL	N-CA-CB	-6.63	96.90	111.50
1	Bf	82	TRP	CE2-CD2-CG	-6.63	101.99	107.30
1	C9	20	VAL	N-CA-CB	-6.63	96.91	111.50
1	CO	20	VAL	N-CA-CB	-6.63	96.91	111.50
1	Cv	20	VAL	N-CA-CB	-6.63	96.91	111.50
1	BL	82	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	C7	20	VAL	N-CA-CB	-6.63	96.92	111.50
1	B2	82	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	Bg	82	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	Bx	82	TRP	CE2-CD2-CG	-6.63	102.00	107.30
1	Ce	20	VAL	N-CA-CB	-6.63	96.92	111.50
1	CN	20	VAL	N-CA-CB	-6.63	96.92	111.50
1	BM	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BW	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	C5	20	VAL	N-CA-CB	-6.62	96.92	111.50
1	BA	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	Ba	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	BK	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	BT	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	Bt	82	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	C8	20	VAL	N-CA-CB	-6.62	96.93	111.50
1	CZ	20	VAL	N-CA-CB	-6.62	96.93	111.50
1	B0	82	TRP	CE2-CD2-CG	-6.62	102.01	107.30
1	BN	82	TRP	CE2-CD2-CG	-6.62	102.01	107.30
1	C3	20	VAL	N-CA-CB	-6.62	96.94	111.50
1	CF	20	VAL	N-CA-CB	-6.62	96.95	111.50
1	B5	82	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	C4	20	VAL	N-CA-CB	-6.61	96.95	111.50
1	Cs	20	VAL	N-CA-CB	-6.61	96.95	111.50
1	C0	20	VAL	N-CA-CB	-6.61	96.96	111.50
1	CA	20	VAL	N-CA-CB	-6.61	96.96	111.50
1	BP	82	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	Bb	82	TRP	CE2-CD2-CG	-6.61	102.02	107.30
1	Bu	82	TRP	CE2-CD2-CG	-6.61	102.02	107.30
1	BD	82	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	B7	82	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	B1	82	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	Bi	82	TRP	CE2-CD2-CG	-6.59	102.02	107.30
1	Bo	82	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	BY	82	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	Bv	82	TRP	CE2-CD2-CG	-6.59	102.03	107.30
1	Bw	82	TRP	CE2-CD2-CG	-6.57	102.04	107.30
1	A6	49	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	AE	49	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	BB	20	VAL	N-CA-CB	-6.49	97.22	111.50
1	BK	20	VAL	N-CA-CB	-6.49	97.22	111.50
1	Bu	20	VAL	N-CA-CB	-6.49	97.23	111.50
1	BS	20	VAL	N-CA-CB	-6.49	97.23	111.50
1	BT	20	VAL	N-CA-CB	-6.49	97.23	111.50
1	Bq	20	VAL	N-CA-CB	-6.49	97.23	111.50
1	B4	20	VAL	N-CA-CB	-6.48	97.24	111.50
1	BR	20	VAL	N-CA-CB	-6.48	97.24	111.50
1	B1	20	VAL	N-CA-CB	-6.48	97.24	111.50
1	BL	20	VAL	N-CA-CB	-6.48	97.24	111.50
1	Bo	20	VAL	N-CA-CB	-6.48	97.24	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B6	20	VAL	N-CA-CB	-6.48	97.25	111.50
1	Bn	20	VAL	N-CA-CB	-6.48	97.25	111.50
1	Bw	20	VAL	N-CA-CB	-6.48	97.25	111.50
1	BC	20	VAL	N-CA-CB	-6.47	97.26	111.50
1	BY	20	VAL	N-CA-CB	-6.47	97.25	111.50
1	B2	20	VAL	N-CA-CB	-6.47	97.26	111.50
1	B9	20	VAL	N-CA-CB	-6.47	97.26	111.50
1	BQ	20	VAL	N-CA-CB	-6.47	97.26	111.50
1	Bb	20	VAL	N-CA-CB	-6.47	97.26	111.50
1	B5	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	Bh	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	Br	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	B3	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	BI	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	BJ	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	Bp	20	VAL	N-CA-CB	-6.47	97.27	111.50
1	AM	49	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	Bg	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	Bk	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	Bs	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	B7	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	BV	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	AG	49	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	BD	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	BO	20	VAL	N-CA-CB	-6.46	97.28	111.50
1	BZ	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Ba	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Bi	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	BA	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	B0	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	BP	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	BU	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Bc	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Bj	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Bt	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	BG	20	VAL	N-CA-CB	-6.46	97.30	111.50
1	Bl	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	Bx	20	VAL	N-CA-CB	-6.46	97.29	111.50
1	BF	20	VAL	N-CA-CB	-6.45	97.30	111.50
1	BX	20	VAL	N-CA-CB	-6.45	97.30	111.50
1	BN	20	VAL	N-CA-CB	-6.45	97.31	111.50
1	Bf	20	VAL	N-CA-CB	-6.45	97.31	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bd	20	VAL	N-CA-CB	-6.45	97.31	111.50
1	BE	20	VAL	N-CA-CB	-6.45	97.31	111.50
1	Bv	20	VAL	N-CA-CB	-6.45	97.31	111.50
1	B8	20	VAL	N-CA-CB	-6.45	97.32	111.50
1	BW	20	VAL	N-CA-CB	-6.45	97.32	111.50
1	BM	20	VAL	N-CA-CB	-6.44	97.32	111.50
1	Bm	20	VAL	N-CA-CB	-6.44	97.33	111.50
1	Aw	49	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	BH	20	VAL	N-CA-CB	-6.44	97.33	111.50
1	Be	20	VAL	N-CA-CB	-6.44	97.34	111.50
1	AO	49	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	Au	49	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	Ad	49	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	Ao	49	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	AH	49	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	AR	49	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	Ai	49	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	AX	49	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	Ag	49	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	Aa	49	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	Ah	49	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	Al	49	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	AY	49	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	AU	49	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	Ak	49	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	Bf	2	SER	N-CA-C	-6.36	93.84	111.00
1	Am	49	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A4	49	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	BH	2	SER	N-CA-C	-6.35	93.85	111.00
1	BV	2	SER	N-CA-C	-6.35	93.85	111.00
1	Bg	2	SER	N-CA-C	-6.35	93.85	111.00
1	BB	2	SER	N-CA-C	-6.35	93.85	111.00
1	Bw	2	SER	N-CA-C	-6.35	93.86	111.00
1	AS	49	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	BJ	2	SER	N-CA-C	-6.35	93.86	111.00
1	BS	2	SER	N-CA-C	-6.35	93.86	111.00
1	BY	2	SER	N-CA-C	-6.35	93.86	111.00
1	BK	2	SER	N-CA-C	-6.35	93.86	111.00
1	BR	2	SER	N-CA-C	-6.35	93.86	111.00
1	Bc	2	SER	N-CA-C	-6.35	93.86	111.00
1	BD	2	SER	N-CA-C	-6.34	93.87	111.00
1	BZ	2	SER	N-CA-C	-6.34	93.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ba	2	SER	N-CA-C	-6.34	93.87	111.00
1	Bk	2	SER	N-CA-C	-6.34	93.87	111.00
1	Bm	2	SER	N-CA-C	-6.34	93.87	111.00
1	Br	2	SER	N-CA-C	-6.34	93.87	111.00
1	Bv	2	SER	N-CA-C	-6.34	93.87	111.00
1	B0	2	SER	N-CA-C	-6.34	93.87	111.00
1	Bi	2	SER	N-CA-C	-6.34	93.88	111.00
1	B7	2	SER	N-CA-C	-6.34	93.88	111.00
1	BE	2	SER	N-CA-C	-6.34	93.88	111.00
1	BL	2	SER	N-CA-C	-6.34	93.88	111.00
1	BP	2	SER	N-CA-C	-6.34	93.88	111.00
1	Be	2	SER	N-CA-C	-6.34	93.88	111.00
1	Bh	2	SER	N-CA-C	-6.34	93.88	111.00
1	Bn	2	SER	N-CA-C	-6.34	93.88	111.00
1	Bp	2	SER	N-CA-C	-6.34	93.88	111.00
1	Ap	49	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	BN	2	SER	N-CA-C	-6.34	93.88	111.00
1	BW	2	SER	N-CA-C	-6.34	93.88	111.00
1	B8	2	SER	N-CA-C	-6.34	93.89	111.00
1	Bt	2	SER	N-CA-C	-6.34	93.89	111.00
1	B2	2	SER	N-CA-C	-6.34	93.89	111.00
1	BC	2	SER	N-CA-C	-6.34	93.89	111.00
1	BM	2	SER	N-CA-C	-6.34	93.89	111.00
1	BT	2	SER	N-CA-C	-6.34	93.89	111.00
1	Bl	2	SER	N-CA-C	-6.34	93.89	111.00
1	Bq	2	SER	N-CA-C	-6.34	93.89	111.00
1	B3	2	SER	N-CA-C	-6.33	93.89	111.00
1	BG	2	SER	N-CA-C	-6.33	93.90	111.00
1	BQ	2	SER	N-CA-C	-6.33	93.90	111.00
1	Bo	2	SER	N-CA-C	-6.33	93.90	111.00
1	Bb	2	SER	N-CA-C	-6.33	93.90	111.00
1	Aq	49	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B4	2	SER	N-CA-C	-6.33	93.91	111.00
1	BO	2	SER	N-CA-C	-6.33	93.90	111.00
1	BX	2	SER	N-CA-C	-6.33	93.91	111.00
1	B6	2	SER	N-CA-C	-6.33	93.91	111.00
1	BI	2	SER	N-CA-C	-6.33	93.91	111.00
1	B5	2	SER	N-CA-C	-6.33	93.91	111.00
1	Bx	2	SER	N-CA-C	-6.33	93.92	111.00
1	Ar	49	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	BA	2	SER	N-CA-C	-6.33	93.92	111.00
1	AN	49	ARG	NE-CZ-NH1	6.32	123.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BF	2	SER	N-CA-C	-6.32	93.93	111.00
1	BU	2	SER	N-CA-C	-6.32	93.92	111.00
1	Bd	2	SER	N-CA-C	-6.32	93.93	111.00
1	Bj	2	SER	N-CA-C	-6.32	93.92	111.00
1	Bu	2	SER	N-CA-C	-6.32	93.92	111.00
1	AJ	49	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	AV	49	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B1	2	SER	N-CA-C	-6.32	93.94	111.00
1	Bs	2	SER	N-CA-C	-6.32	93.94	111.00
1	B9	2	SER	N-CA-C	-6.32	93.94	111.00
1	A3	49	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	AL	49	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A7	49	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	AI	49	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A1	49	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	Ae	49	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	BZ	33	ILE	CA-CB-CG1	-6.29	99.05	111.00
1	Be	33	ILE	CA-CB-CG1	-6.29	99.05	111.00
1	Br	33	ILE	CA-CB-CG1	-6.29	99.05	111.00
1	AF	49	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	BJ	33	ILE	CA-CB-CG1	-6.29	99.05	111.00
1	Bq	33	ILE	CA-CB-CG1	-6.29	99.05	111.00
1	B4	33	ILE	CA-CB-CG1	-6.29	99.06	111.00
1	BD	33	ILE	CA-CB-CG1	-6.29	99.06	111.00
1	BH	33	ILE	CA-CB-CG1	-6.29	99.06	111.00
1	BP	33	ILE	CA-CB-CG1	-6.29	99.06	111.00
1	Bx	33	ILE	CA-CB-CG1	-6.29	99.06	111.00
1	B9	33	ILE	CA-CB-CG1	-6.28	99.06	111.00
1	BR	33	ILE	CA-CB-CG1	-6.28	99.06	111.00
1	A2	49	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	BX	33	ILE	CA-CB-CG1	-6.28	99.06	111.00
1	AD	49	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	BB	33	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	Bb	33	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	Bf	33	ILE	CA-CB-CG1	-6.28	99.06	111.00
1	Bi	33	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	Bu	33	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	Bv	33	ILE	CA-CB-CG1	-6.28	99.06	111.00
1	Av	49	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	Bs	33	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	Ac	49	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	Bd	33	ILE	CA-CB-CG1	-6.28	99.07	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	33	ILE	CA-CB-CG1	-6.28	99.08	111.00
1	Bh	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	B6	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	BL	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	BU	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	BW	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	BY	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	Bo	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	B1	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	B8	33	ILE	CA-CB-CG1	-6.27	99.08	111.00
1	BO	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	Bp	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	AZ	49	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B0	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	BM	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	BV	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	B2	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	BF	33	ILE	CA-CB-CG1	-6.27	99.09	111.00
1	Aj	49	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	BK	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	BG	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	Bj	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	B3	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	Bm	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	Bn	33	ILE	CA-CB-CG1	-6.26	99.10	111.00
1	AC	49	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	BN	33	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	B5	33	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	Bl	33	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	Bt	33	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	Bw	33	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	AQ	49	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	BI	33	ILE	CA-CB-CG1	-6.25	99.11	111.00
1	AT	49	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	An	49	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B7	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	BT	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	Ba	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	Bc	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	BS	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	Bk	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	AB	49	ARG	NE-CZ-NH1	6.25	123.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BQ	33	ILE	CA-CB-CG1	-6.25	99.12	111.00
1	At	49	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	AW	49	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	Bg	33	ILE	CA-CB-CG1	-6.24	99.14	111.00
1	BC	33	ILE	CA-CB-CG1	-6.24	99.14	111.00
1	BE	33	ILE	CA-CB-CG1	-6.24	99.14	111.00
1	AA	49	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A0	49	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	Ax	49	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	As	49	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A8	49	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	Af	49	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	AK	49	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	Ae	20	VAL	N-CA-CB	-6.21	97.85	111.50
1	Aw	20	VAL	N-CA-CB	-6.20	97.85	111.50
1	A5	49	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	Ab	20	VAL	N-CA-CB	-6.20	97.86	111.50
1	Ac	20	VAL	N-CA-CB	-6.19	97.87	111.50
1	AP	49	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A9	49	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	AI	20	VAL	N-CA-CB	-6.19	97.89	111.50
1	AK	20	VAL	N-CA-CB	-6.19	97.89	111.50
1	As	20	VAL	N-CA-CB	-6.19	97.89	111.50
1	A3	20	VAL	N-CA-CB	-6.18	97.89	111.50
1	A5	20	VAL	N-CA-CB	-6.18	97.89	111.50
1	Aq	20	VAL	N-CA-CB	-6.18	97.89	111.50
1	AB	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	Ap	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	AQ	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	AT	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	Ab	49	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A4	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	A7	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	AU	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	AV	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	Ad	20	VAL	N-CA-CB	-6.18	97.90	111.50
1	Av	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	A1	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	AR	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	AZ	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	Af	20	VAL	N-CA-CB	-6.18	97.91	111.50
1	Ai	20	VAL	N-CA-CB	-6.18	97.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AE	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	AM	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	Ah	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	Aj	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	Ak	20	VAL	N-CA-CB	-6.17	97.91	111.50
1	An	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	Al	20	VAL	N-CA-CB	-6.17	97.92	111.50
1	AA	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	AO	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	AX	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	Aa	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	A6	20	VAL	N-CA-CB	-6.17	97.94	111.50
1	AC	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	Am	20	VAL	N-CA-CB	-6.17	97.93	111.50
1	Ar	20	VAL	N-CA-CB	-6.17	97.94	111.50
1	AG	20	VAL	N-CA-CB	-6.17	97.94	111.50
1	A0	20	VAL	N-CA-CB	-6.16	97.94	111.50
1	AJ	20	VAL	N-CA-CB	-6.16	97.94	111.50
1	AL	20	VAL	N-CA-CB	-6.16	97.94	111.50
1	Ax	20	VAL	N-CA-CB	-6.16	97.94	111.50
1	A2	20	VAL	N-CA-CB	-6.16	97.94	111.50
1	AF	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	Ag	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	AP	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	AS	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	A9	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	AH	20	VAL	N-CA-CB	-6.16	97.95	111.50
1	AW	20	VAL	N-CA-CB	-6.16	97.96	111.50
1	AN	20	VAL	N-CA-CB	-6.15	97.96	111.50
1	AY	20	VAL	N-CA-CB	-6.15	97.96	111.50
1	Ao	20	VAL	N-CA-CB	-6.15	97.96	111.50
1	At	20	VAL	N-CA-CB	-6.15	97.96	111.50
1	AD	20	VAL	N-CA-CB	-6.15	97.97	111.50
1	Au	20	VAL	N-CA-CB	-6.14	97.99	111.50
1	A8	20	VAL	N-CA-CB	-6.13	98.00	111.50
1	CK	10	VAL	CA-C-N	6.07	130.55	117.20
1	Cf	10	VAL	CA-C-N	6.06	130.53	117.20
1	CY	10	VAL	CA-C-N	6.06	130.53	117.20
1	CV	10	VAL	CA-C-N	6.06	130.53	117.20
1	Cn	10	VAL	CA-C-N	6.06	130.53	117.20
1	Ck	10	VAL	CA-C-N	6.05	130.52	117.20
1	CI	10	VAL	CA-C-N	6.05	130.52	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CH	10	VAL	CA-C-N	6.05	130.51	117.20
1	Cc	10	VAL	CA-C-N	6.05	130.50	117.20
1	Cu	10	VAL	CA-C-N	6.05	130.50	117.20
1	C6	10	VAL	CA-C-N	6.04	130.50	117.20
1	CF	10	VAL	CA-C-N	6.04	130.50	117.20
1	CT	10	VAL	CA-C-N	6.04	130.50	117.20
1	CW	10	VAL	CA-C-N	6.04	130.50	117.20
1	Cb	10	VAL	CA-C-N	6.04	130.50	117.20
1	Ct	10	VAL	CA-C-N	6.04	130.50	117.20
1	Cw	10	VAL	CA-C-N	6.04	130.49	117.20
1	CC	10	VAL	CA-C-N	6.04	130.49	117.20
1	Cs	10	VAL	CA-C-N	6.04	130.49	117.20
1	CN	10	VAL	CA-C-N	6.04	130.48	117.20
1	Ce	10	VAL	CA-C-N	6.04	130.48	117.20
1	C1	10	VAL	CA-C-N	6.03	130.47	117.20
1	C7	10	VAL	CA-C-N	6.03	130.47	117.20
1	CP	10	VAL	CA-C-N	6.03	130.47	117.20
1	CR	10	VAL	CA-C-N	6.03	130.47	117.20
1	C8	10	VAL	CA-C-N	6.03	130.47	117.20
1	C9	10	VAL	CA-C-N	6.03	130.47	117.20
1	CX	10	VAL	CA-C-N	6.03	130.47	117.20
1	Ca	10	VAL	CA-C-N	6.03	130.47	117.20
1	Ch	10	VAL	CA-C-N	6.03	130.46	117.20
1	C4	10	VAL	CA-C-N	6.03	130.46	117.20
1	CQ	10	VAL	CA-C-N	6.03	130.46	117.20
1	Cl	10	VAL	CA-C-N	6.03	130.46	117.20
1	Cx	10	VAL	CA-C-N	6.03	130.46	117.20
1	CG	10	VAL	CA-C-N	6.03	130.46	117.20
1	CM	10	VAL	CA-C-N	6.03	130.46	117.20
1	CA	10	VAL	CA-C-N	6.02	130.45	117.20
1	CO	10	VAL	CA-C-N	6.02	130.45	117.20
1	Cv	10	VAL	CA-C-N	6.02	130.45	117.20
1	Av	79	VAL	N-CA-CB	-6.02	98.25	111.50
1	C3	10	VAL	CA-C-N	6.02	130.45	117.20
1	CU	10	VAL	CA-C-N	6.02	130.45	117.20
1	CZ	10	VAL	CA-C-N	6.02	130.45	117.20
1	Cg	10	VAL	CA-C-N	6.02	130.45	117.20
1	C2	10	VAL	CA-C-N	6.02	130.45	117.20
1	Cm	10	VAL	CA-C-N	6.02	130.44	117.20
1	Cp	10	VAL	CA-C-N	6.02	130.45	117.20
1	Cj	10	VAL	CA-C-N	6.02	130.44	117.20
1	An	79	VAL	N-CA-CB	-6.02	98.26	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Co	10	VAL	CA-C-N	6.02	130.44	117.20
1	CE	10	VAL	CA-C-N	6.02	130.44	117.20
1	Au	79	VAL	N-CA-CB	-6.01	98.27	111.50
1	C0	10	VAL	CA-C-N	6.01	130.43	117.20
1	CD	10	VAL	CA-C-N	6.01	130.43	117.20
1	CJ	10	VAL	CA-C-N	6.01	130.43	117.20
1	Cr	10	VAL	CA-C-N	6.01	130.43	117.20
1	AE	79	VAL	N-CA-CB	-6.01	98.28	111.50
1	AN	79	VAL	N-CA-CB	-6.01	98.28	111.50
1	C5	10	VAL	CA-C-N	6.01	130.42	117.20
1	CB	10	VAL	CA-C-N	6.01	130.42	117.20
1	Ci	10	VAL	CA-C-N	6.01	130.42	117.20
1	Cq	10	VAL	CA-C-N	6.01	130.42	117.20
1	A9	79	VAL	N-CA-CB	-6.01	98.28	111.50
1	AP	79	VAL	N-CA-CB	-6.01	98.29	111.50
1	AU	79	VAL	N-CA-CB	-6.00	98.29	111.50
1	AW	79	VAL	N-CA-CB	-6.00	98.29	111.50
1	At	79	VAL	N-CA-CB	-6.00	98.29	111.50
1	CL	10	VAL	CA-C-N	6.00	130.41	117.20
1	Aw	79	VAL	N-CA-CB	-6.00	98.29	111.50
1	CS	10	VAL	CA-C-N	6.00	130.41	117.20
1	A7	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	AK	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	Aj	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	AT	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	Cd	10	VAL	CA-C-N	6.00	130.40	117.20
1	A1	32	TRP	CB-CG-CD1	-6.00	119.20	127.00
1	A2	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	A4	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	A8	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	AH	79	VAL	N-CA-CB	-6.00	98.30	111.50
1	AD	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	AF	32	TRP	CB-CG-CD1	-6.00	119.20	127.00
1	AL	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	AR	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	Ax	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	A1	79	VAL	N-CA-CB	-6.00	98.31	111.50
1	A3	79	VAL	N-CA-CB	-5.99	98.31	111.50
1	A6	79	VAL	N-CA-CB	-5.99	98.31	111.50
1	AQ	79	VAL	N-CA-CB	-5.99	98.31	111.50
1	Ab	79	VAL	N-CA-CB	-5.99	98.31	111.50
1	Ag	79	VAL	N-CA-CB	-5.99	98.31	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ak	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AC	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AX	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AZ	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AA	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AG	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	AI	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	Ac	79	VAL	N-CA-CB	-5.99	98.32	111.50
1	AV	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	Aa	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	Ae	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	Ak	32	TRP	CB-CG-CD1	-5.99	119.22	127.00
1	Al	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	Ap	79	VAL	N-CA-CB	-5.99	98.33	111.50
1	At	32	TRP	CB-CG-CD1	-5.99	119.22	127.00
1	AM	79	VAL	N-CA-CB	-5.98	98.33	111.50
1	AS	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	AY	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	Ad	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	AJ	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	Ar	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	As	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	A0	79	VAL	N-CA-CB	-5.98	98.34	111.50
1	A6	32	TRP	CB-CG-CD1	-5.98	119.23	127.00
1	AO	32	TRP	CB-CG-CD1	-5.98	119.23	127.00
1	Am	79	VAL	N-CA-CB	-5.98	98.35	111.50
1	Aq	79	VAL	N-CA-CB	-5.98	98.35	111.50
1	Ac	32	TRP	CB-CG-CD1	-5.98	119.23	127.00
1	Af	79	VAL	N-CA-CB	-5.98	98.35	111.50
1	A5	79	VAL	N-CA-CB	-5.97	98.36	111.50
1	AF	79	VAL	N-CA-CB	-5.97	98.35	111.50
1	AO	79	VAL	N-CA-CB	-5.97	98.36	111.50
1	Ah	79	VAL	N-CA-CB	-5.97	98.36	111.50
1	AB	79	VAL	N-CA-CB	-5.97	98.36	111.50
1	A3	32	TRP	CB-CG-CD1	-5.97	119.24	127.00
1	AA	32	TRP	CB-CG-CD1	-5.97	119.24	127.00
1	An	32	TRP	CB-CG-CD1	-5.97	119.24	127.00
1	Ao	79	VAL	N-CA-CB	-5.96	98.38	111.50
1	Ai	79	VAL	N-CA-CB	-5.96	98.39	111.50
1	A7	32	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	Ax	32	TRP	CB-CG-CD1	-5.96	119.25	127.00
1	AR	32	TRP	CB-CG-CD1	-5.96	119.26	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AX	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	Ab	32	TRP	CB-CG-CD1	-5.95	119.26	127.00
1	A0	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	Ar	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	AP	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	Au	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	AB	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	AY	32	TRP	CB-CG-CD1	-5.95	119.27	127.00
1	AE	32	TRP	CB-CG-CD1	-5.94	119.27	127.00
1	Af	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	Aa	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	Aw	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	AQ	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	Ad	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	Al	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	AW	32	TRP	CB-CG-CD1	-5.94	119.28	127.00
1	A2	32	TRP	CB-CG-CD1	-5.93	119.28	127.00
1	AH	32	TRP	CB-CG-CD1	-5.93	119.28	127.00
1	AV	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	Aj	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	A8	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	AI	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	AL	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	AZ	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	Av	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	Bb	32	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A9	32	TRP	CB-CG-CD1	-5.93	119.29	127.00
1	Ao	32	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	AD	32	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	A4	32	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	AG	32	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	AU	32	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	Bm	32	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	AJ	32	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	AS	32	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	Ag	32	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	B9	32	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	AK	32	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	Ai	32	TRP	CB-CG-CD1	-5.92	119.31	127.00
1	B5	32	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	AM	32	TRP	CB-CG-CD1	-5.91	119.31	127.00
1	Ae	32	TRP	CB-CG-CD1	-5.91	119.32	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AN	32	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	Aq	32	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	Am	32	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	AT	32	TRP	CB-CG-CD1	-5.91	119.32	127.00
1	As	32	TRP	CB-CG-CD1	-5.90	119.33	127.00
1	Ap	32	TRP	CB-CG-CD1	-5.90	119.34	127.00
1	Bp	32	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	Ah	32	TRP	CB-CG-CD1	-5.89	119.34	127.00
1	BX	32	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	AC	32	TRP	CB-CG-CD1	-5.89	119.34	127.00
1	BA	32	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	Bs	32	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	A5	32	TRP	CB-CG-CD1	-5.89	119.34	127.00
1	Bl	32	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	BH	32	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	B3	32	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	BS	32	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	B6	32	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	BJ	32	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	B8	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	BB	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	Bd	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	Bv	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	Bx	50	GLN	CA-CB-CG	-5.87	100.48	113.40
1	B9	50	GLN	CA-CB-CG	-5.87	100.49	113.40
1	B4	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	BG	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	BP	50	GLN	CA-CB-CG	-5.87	100.50	113.40
1	BZ	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	Bo	32	TRP	CG-CD1-NE1	-5.87	104.23	110.10
1	B1	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BL	50	GLN	CA-CB-CG	-5.86	100.50	113.40
1	BR	50	GLN	CA-CB-CG	-5.86	100.50	113.40
1	Bf	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BI	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BP	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BQ	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BZ	50	GLN	CA-CB-CG	-5.86	100.51	113.40
1	Ba	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	Bk	50	GLN	CA-CB-CG	-5.86	100.51	113.40
1	Bx	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BI	50	GLN	CA-CB-CG	-5.86	100.51	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bc	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	B0	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	BK	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	BO	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	Ba	50	GLN	CA-CB-CG	-5.86	100.51	113.40
1	Bc	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	Bg	50	GLN	CA-CB-CG	-5.86	100.51	113.40
1	BA	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	BJ	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	BS	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	Bm	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	Br	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	Bu	32	TRP	CG-CD1-NE1	-5.86	104.24	110.10
1	Bu	50	GLN	CA-CB-CG	-5.86	100.52	113.40
1	BM	50	GLN	CA-CB-CG	-5.85	100.52	113.40
1	BV	50	GLN	CA-CB-CG	-5.85	100.52	113.40
1	Bi	50	GLN	CA-CB-CG	-5.85	100.52	113.40
1	BG	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	BO	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	BW	50	GLN	CA-CB-CG	-5.85	100.52	113.40
1	BY	50	GLN	CA-CB-CG	-5.85	100.52	113.40
1	Bh	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	B2	32	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	BH	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	BF	32	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	Bs	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	Bw	32	TRP	CG-CD1-NE1	-5.85	104.25	110.10
1	B7	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	Be	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	Bj	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	Bn	50	GLN	CA-CB-CG	-5.85	100.54	113.40
1	Bt	50	GLN	CA-CB-CG	-5.85	100.53	113.40
1	B3	50	GLN	CA-CB-CG	-5.85	100.54	113.40
1	BX	50	GLN	CA-CB-CG	-5.85	100.54	113.40
1	Bq	50	GLN	CA-CB-CG	-5.85	100.54	113.40
1	B8	50	GLN	CA-CB-CG	-5.84	100.54	113.40
1	Bi	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	B0	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	BT	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	Bo	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	B4	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	BE	50	GLN	CA-CB-CG	-5.84	100.55	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BN	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	Bp	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	B2	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	B5	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	B7	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	BC	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	BQ	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	Bb	50	GLN	CA-CB-CG	-5.84	100.55	113.40
1	BU	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	Bw	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	B1	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	BD	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	BN	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	BU	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	Be	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	Bg	32	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	Bl	50	GLN	CA-CB-CG	-5.84	100.56	113.40
1	BM	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	Bf	50	GLN	CA-CB-CG	-5.83	100.57	113.40
1	Bj	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	BE	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	BB	50	GLN	CA-CB-CG	-5.83	100.58	113.40
1	BD	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	BF	50	GLN	CA-CB-CG	-5.83	100.58	113.40
1	BY	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	Bv	50	GLN	CA-CB-CG	-5.83	100.58	113.40
1	BR	32	TRP	CG-CD1-NE1	-5.83	104.28	110.10
1	Bd	50	GLN	CA-CB-CG	-5.83	100.58	113.40
1	Bh	32	TRP	CG-CD1-NE1	-5.83	104.27	110.10
1	BW	32	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	B6	50	GLN	CA-CB-CG	-5.82	100.60	113.40
1	BT	32	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	Br	32	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	BL	32	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	Bn	32	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	Bt	32	TRP	CG-CD1-NE1	-5.81	104.29	110.10
1	BV	32	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	Bq	32	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	Bk	32	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	BC	32	TRP	CG-CD1-NE1	-5.79	104.31	110.10
1	BK	32	TRP	CG-CD1-NE1	-5.78	104.32	110.10
1	Bf	82	TRP	CG-CD1-NE1	-5.71	104.39	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bk	82	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	B2	82	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	Bd	82	TRP	CG-CD1-NE1	-5.71	104.39	110.10
1	BA	82	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	Bm	82	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	B4	82	TRP	CG-CD1-NE1	-5.70	104.40	110.10
1	BD	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	BF	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	Bn	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	BW	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	Bs	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	A9	32	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	BJ	38	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	Bf	38	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	B5	82	TRP	CG-CD1-NE1	-5.69	104.41	110.10
1	BH	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	BX	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	BY	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	BC	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	BV	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	B0	82	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	At	32	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	BF	20	VAL	CB-CA-C	5.68	122.19	111.40
1	BJ	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	BZ	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	B9	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	BE	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	B7	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	AP	32	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	BO	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	A7	32	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	Au	32	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	B4	20	VAL	CB-CA-C	5.67	122.17	111.40
1	B7	38	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	BI	38	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	Bt	82	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	B3	20	VAL	CB-CA-C	5.66	122.16	111.40
1	B6	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	Bb	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	Bo	20	VAL	CB-CA-C	5.66	122.16	111.40
1	BB	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	BK	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bn	38	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	CW	11	ASP	CA-CB-CG	5.66	125.85	113.40
1	BP	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	Bg	38	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	Bo	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	Bp	20	VAL	CB-CA-C	5.66	122.15	111.40
1	Bf	20	VAL	CB-CA-C	5.66	122.15	111.40
1	Cm	11	ASP	CA-CB-CG	5.66	125.85	113.40
1	Ax	32	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	B1	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	Bj	82	TRP	CG-CD1-NE1	-5.66	104.44	110.10
1	BQ	82	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Bt	20	VAL	CB-CA-C	5.65	122.14	111.40
1	CY	11	ASP	CA-CB-CG	5.65	125.84	113.40
1	A1	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	AO	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Ba	82	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Bp	82	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Bu	82	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	AB	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Ab	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	BE	20	VAL	CB-CA-C	5.65	122.14	111.40
1	BG	20	VAL	CB-CA-C	5.65	122.14	111.40
1	Bd	20	VAL	CB-CA-C	5.65	122.14	111.40
1	Bi	38	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	Cb	11	ASP	CA-CB-CG	5.65	125.83	113.40
1	Ak	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	BA	20	VAL	CB-CA-C	5.65	122.13	111.40
1	BD	20	VAL	CB-CA-C	5.65	122.13	111.40
1	AX	32	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Bi	20	VAL	CB-CA-C	5.65	122.13	111.40
1	Bl	82	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	Cv	11	ASP	CA-CB-CG	5.65	125.83	113.40
1	B7	20	VAL	CB-CA-C	5.65	122.13	111.40
1	BF	38	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	Bg	20	VAL	CB-CA-C	5.65	122.13	111.40
1	Bq	20	VAL	CB-CA-C	5.65	122.13	111.40
1	Cu	11	ASP	CA-CB-CG	5.65	125.82	113.40
1	AA	32	TRP	CG-CD1-NE1	-5.64	104.45	110.10
1	BI	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	BO	20	VAL	CB-CA-C	5.64	122.12	111.40
1	Bn	20	VAL	CB-CA-C	5.64	122.12	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C6	56	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	Cn	56	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B2	20	VAL	CB-CA-C	5.64	122.12	111.40
1	BB	20	VAL	CB-CA-C	5.64	122.12	111.40
1	BK	20	VAL	CB-CA-C	5.64	122.12	111.40
1	Be	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	Br	20	VAL	CB-CA-C	5.64	122.12	111.40
1	AF	32	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	Be	20	VAL	CB-CA-C	5.64	122.12	111.40
1	Bw	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	C8	11	ASP	CA-CB-CG	5.64	125.81	113.40
1	B8	20	VAL	CB-CA-C	5.64	122.11	111.40
1	BV	20	VAL	CB-CA-C	5.64	122.12	111.40
1	Bh	20	VAL	CB-CA-C	5.64	122.11	111.40
1	CG	11	ASP	CA-CB-CG	5.64	125.81	113.40
1	BM	20	VAL	CB-CA-C	5.64	122.11	111.40
1	Bc	20	VAL	CB-CA-C	5.64	122.11	111.40
1	Bc	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	Bx	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	C4	11	ASP	CA-CB-CG	5.64	125.80	113.40
1	A6	32	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	Ad	55	ASN	CB-CA-C	-5.64	99.13	110.40
1	BL	20	VAL	CB-CA-C	5.64	122.11	111.40
1	BM	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	BS	20	VAL	CB-CA-C	5.64	122.11	111.40
1	BS	82	TRP	CG-CD1-NE1	-5.64	104.46	110.10
1	Bw	20	VAL	CB-CA-C	5.64	122.11	111.40
1	C1	11	ASP	CA-CB-CG	5.64	125.80	113.40
1	CK	11	ASP	CA-CB-CG	5.64	125.80	113.40
1	Av	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	B1	20	VAL	CB-CA-C	5.63	122.11	111.40
1	BC	20	VAL	CB-CA-C	5.63	122.11	111.40
1	BJ	20	VAL	CB-CA-C	5.63	122.11	111.40
1	BN	82	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	BP	20	VAL	CB-CA-C	5.63	122.11	111.40
1	BU	20	VAL	CB-CA-C	5.63	122.11	111.40
1	BX	20	VAL	CB-CA-C	5.63	122.11	111.40
1	Bg	82	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	Bl	20	VAL	CB-CA-C	5.63	122.11	111.40
1	CX	11	ASP	CA-CB-CG	5.63	125.79	113.40
1	Cq	11	ASP	CA-CB-CG	5.63	125.80	113.40
1	AD	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AY	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	B3	82	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	BQ	20	VAL	CB-CA-C	5.63	122.10	111.40
1	BT	20	VAL	CB-CA-C	5.63	122.10	111.40
1	Bx	20	VAL	CB-CA-C	5.63	122.10	111.40
1	BH	32	TRP	CG-CD2-CE3	5.63	138.97	133.90
1	BR	20	VAL	CB-CA-C	5.63	122.10	111.40
1	Bs	20	VAL	CB-CA-C	5.63	122.10	111.40
1	CO	11	ASP	CA-CB-CG	5.63	125.79	113.40
1	CP	11	ASP	CA-CB-CG	5.63	125.79	113.40
1	Ca	11	ASP	CA-CB-CG	5.63	125.79	113.40
1	Cw	11	ASP	CA-CB-CG	5.63	125.79	113.40
1	B7	32	TRP	CG-CD2-CE3	5.63	138.97	133.90
1	BN	20	VAL	CB-CA-C	5.63	122.10	111.40
1	CS	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	A3	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	A8	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	AD	55	ASN	CB-CA-C	-5.63	99.14	110.40
1	AG	55	ASN	CB-CA-C	-5.63	99.14	110.40
1	AO	55	ASN	CB-CA-C	-5.63	99.14	110.40
1	AT	32	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	Ar	55	ASN	CB-CA-C	-5.63	99.14	110.40
1	B8	82	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	B9	20	VAL	CB-CA-C	5.63	122.09	111.40
1	Bc	38	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	Bi	82	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	Bu	20	VAL	CB-CA-C	5.63	122.09	111.40
1	Bv	20	VAL	CB-CA-C	5.63	122.09	111.40
1	C0	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	C2	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	CX	56	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	Ce	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	AW	55	ASN	CB-CA-C	-5.63	99.14	110.40
1	AY	55	ASN	CB-CA-C	-5.63	99.15	110.40
1	Au	55	ASN	CB-CA-C	-5.63	99.15	110.40
1	B6	20	VAL	CB-CA-C	5.63	122.09	111.40
1	BH	20	VAL	CB-CA-C	5.63	122.09	111.40
1	BZ	20	VAL	CB-CA-C	5.63	122.09	111.40
1	Bb	20	VAL	CB-CA-C	5.63	122.09	111.40
1	C3	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	C6	11	ASP	CA-CB-CG	5.63	125.78	113.40
1	Cj	11	ASP	CA-CB-CG	5.63	125.78	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AW	32	TRP	CG-CD1-NE1	-5.62	104.47	110.10
1	Ai	55	ASN	CB-CA-C	-5.62	99.15	110.40
1	B5	20	VAL	CB-CA-C	5.62	122.09	111.40
1	BI	20	VAL	CB-CA-C	5.62	122.09	111.40
1	BY	20	VAL	CB-CA-C	5.62	122.09	111.40
1	Bc	32	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	Bj	20	VAL	CB-CA-C	5.62	122.09	111.40
1	Bk	32	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	Cr	11	ASP	CA-CB-CG	5.62	125.78	113.40
1	A0	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	Am	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	B9	32	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	BG	82	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	CJ	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	CM	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	CN	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	CV	56	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A2	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	A4	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	A6	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	A7	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	AE	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	AS	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	Ac	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	Ap	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	As	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	Bk	20	VAL	CB-CA-C	5.62	122.08	111.40
1	CF	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	Cd	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	Co	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	Cs	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	A8	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	AF	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	AR	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	C9	11	ASP	CA-CB-CG	5.62	125.77	113.40
1	Cl	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	AI	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	AK	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	AN	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	Ac	55	ASN	CB-CA-C	-5.62	99.16	110.40
1	Aj	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	Ak	55	ASN	CB-CA-C	-5.62	99.16	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B0	20	VAL	CB-CA-C	5.62	122.07	111.40
1	BL	38	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	BQ	38	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	BT	32	TRP	CG-CD2-CE3	5.62	138.96	133.90
1	BT	82	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	C7	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	CZ	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	Cx	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	Bh	82	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	Bm	20	VAL	CB-CA-C	5.62	122.07	111.40
1	Br	82	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	CE	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	CQ	11	ASP	CA-CB-CG	5.62	125.76	113.40
1	AH	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	AH	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	AL	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	AV	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	Af	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	Al	32	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	At	55	ASN	CB-CA-C	-5.62	99.17	110.40
1	BY	38	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	Ba	20	VAL	CB-CA-C	5.62	122.07	111.40
1	Ch	11	ASP	CA-CB-CG	5.62	125.75	113.40
1	A5	55	ASN	CB-CA-C	-5.61	99.17	110.40
1	AA	55	ASN	CB-CA-C	-5.61	99.17	110.40
1	AQ	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	AZ	55	ASN	CB-CA-C	-5.61	99.17	110.40
1	Aa	55	ASN	CB-CA-C	-5.61	99.17	110.40
1	Ar	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	AG	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	AK	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	AX	55	ASN	CB-CA-C	-5.61	99.17	110.40
1	Ad	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	BS	38	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	BU	82	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	BW	20	VAL	CB-CA-C	5.61	122.06	111.40
1	A0	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	AV	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	Av	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	BK	32	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	BN	32	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	Bf	32	TRP	CG-CD2-CE3	5.61	138.95	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bq	82	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	Bv	82	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	CA	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	CL	11	ASP	CA-CB-CG	5.61	125.75	113.40
1	CT	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	Cp	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	AJ	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	Ab	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	Ax	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	CH	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	AC	55	ASN	CB-CA-C	-5.61	99.18	110.40
1	AE	55	ASN	CB-CA-C	-5.61	99.19	110.40
1	AI	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	AP	55	ASN	CB-CA-C	-5.61	99.19	110.40
1	Aq	55	ASN	CB-CA-C	-5.61	99.19	110.40
1	As	32	TRP	CG-CD1-NE1	-5.61	104.49	110.10
1	Bn	32	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	CU	11	ASP	CA-CB-CG	5.61	125.73	113.40
1	Cc	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	Ci	11	ASP	CA-CB-CG	5.61	125.74	113.40
1	Aw	55	ASN	CB-CA-C	-5.61	99.19	110.40
1	Br	38	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	CD	11	ASP	CA-CB-CG	5.61	125.73	113.40
1	CR	11	ASP	CA-CB-CG	5.61	125.73	113.40
1	Ck	11	ASP	CA-CB-CG	5.61	125.73	113.40
1	A1	55	ASN	CB-CA-C	-5.60	99.19	110.40
1	A9	55	ASN	CB-CA-C	-5.60	99.19	110.40
1	AM	55	ASN	CB-CA-C	-5.60	99.19	110.40
1	Am	55	ASN	CB-CA-C	-5.60	99.19	110.40
1	Ck	56	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A2	55	ASN	CB-CA-C	-5.60	99.19	110.40
1	AM	32	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	Ao	55	ASN	CB-CA-C	-5.60	99.20	110.40
1	B0	32	TRP	CG-CD2-CE3	5.60	138.94	133.90
1	Bp	38	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	CI	11	ASP	CA-CB-CG	5.60	125.72	113.40
1	Cn	11	ASP	CA-CB-CG	5.60	125.73	113.40
1	Ct	11	ASP	CA-CB-CG	5.60	125.73	113.40
1	AN	32	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	An	55	ASN	CB-CA-C	-5.60	99.20	110.40
1	Aa	32	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	Aw	32	TRP	CG-CD1-NE1	-5.60	104.50	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bt	38	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	CC	11	ASP	CA-CB-CG	5.60	125.72	113.40
1	CV	11	ASP	CA-CB-CG	5.60	125.72	113.40
1	Cg	11	ASP	CA-CB-CG	5.60	125.72	113.40
1	AB	55	ASN	CB-CA-C	-5.60	99.20	110.40
1	AR	55	ASN	CB-CA-C	-5.60	99.21	110.40
1	AU	55	ASN	CB-CA-C	-5.60	99.20	110.40
1	C5	11	ASP	CA-CB-CG	5.60	125.72	113.40
1	AT	55	ASN	CB-CA-C	-5.60	99.21	110.40
1	Ae	55	ASN	CB-CA-C	-5.60	99.21	110.40
1	Al	55	ASN	CB-CA-C	-5.60	99.21	110.40
1	Bo	38	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	CQ	56	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A3	55	ASN	CB-CA-C	-5.59	99.21	110.40
1	Ae	32	TRP	CG-CD1-NE1	-5.59	104.50	110.10
1	Aj	55	ASN	CB-CA-C	-5.59	99.21	110.40
1	Bh	38	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	CC	56	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	CI	56	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	Ag	55	ASN	CB-CA-C	-5.59	99.21	110.40
1	AZ	32	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	Bw	32	TRP	CG-CD2-CE3	5.59	138.93	133.90
1	CB	11	ASP	CA-CB-CG	5.59	125.70	113.40
1	CI	20	VAL	CB-CA-C	5.59	122.02	111.40
1	CW	20	VAL	CB-CA-C	5.59	122.02	111.40
1	AJ	32	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	An	32	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	BK	38	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	BT	38	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	CK	56	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	Cw	20	VAL	CB-CA-C	5.59	122.02	111.40
1	AL	32	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	A5	32	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	C8	20	VAL	CB-CA-C	5.59	122.02	111.40
1	A4	32	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	Ah	55	ASN	CB-CA-C	-5.58	99.23	110.40
1	BL	82	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	BW	32	TRP	CG-CD2-CE3	5.58	138.93	133.90
1	Cn	20	VAL	CB-CA-C	5.58	122.01	111.40
1	Ct	20	VAL	CB-CA-C	5.58	122.01	111.40
1	Aq	32	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	Ba	32	TRP	CG-CD2-CE3	5.58	138.92	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C4	20	VAL	CB-CA-C	5.58	122.00	111.40
1	CL	20	VAL	CB-CA-C	5.58	122.00	111.40
1	CS	20	VAL	CB-CA-C	5.58	122.01	111.40
1	CV	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Ce	56	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	AU	32	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	BR	82	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	Bx	38	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	CP	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Cu	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Ah	32	TRP	CG-CD1-NE1	-5.58	104.52	110.10
1	BR	38	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	CM	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Cc	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Ap	32	TRP	CG-CD1-NE1	-5.58	104.53	110.10
1	BM	38	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	Bk	38	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C0	56	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	CJ	20	VAL	CB-CA-C	5.58	122.00	111.40
1	Ck	20	VAL	CB-CA-C	5.58	121.99	111.40
1	AQ	55	ASN	CB-CA-C	-5.57	99.25	110.40
1	Af	32	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	BY	32	TRP	CG-CD2-CE3	5.57	138.92	133.90
1	C0	20	VAL	CB-CA-C	5.57	121.99	111.40
1	C2	20	VAL	CB-CA-C	5.57	121.99	111.40
1	CO	20	VAL	CB-CA-C	5.57	121.99	111.40
1	CR	20	VAL	CB-CA-C	5.57	121.99	111.40
1	CT	56	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	CU	20	VAL	CB-CA-C	5.57	121.99	111.40
1	Cp	20	VAL	CB-CA-C	5.57	121.99	111.40
1	AC	32	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	Ai	32	TRP	CG-CD1-NE1	-5.57	104.53	110.10
1	Cg	20	VAL	CB-CA-C	5.57	121.99	111.40
1	Co	20	VAL	CB-CA-C	5.57	121.99	111.40
1	BI	32	TRP	CG-CD2-CE3	5.57	138.91	133.90
1	CB	20	VAL	CB-CA-C	5.57	121.98	111.40
1	CC	20	VAL	CB-CA-C	5.57	121.98	111.40
1	CQ	20	VAL	CB-CA-C	5.57	121.98	111.40
1	Cq	20	VAL	CB-CA-C	5.57	121.98	111.40
1	C1	20	VAL	CB-CA-C	5.57	121.98	111.40
1	BV	32	TRP	CG-CD2-CE3	5.57	138.91	133.90
1	CD	20	VAL	CB-CA-C	5.57	121.98	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CN	20	VAL	CB-CA-C	5.57	121.98	111.40
1	Cf	11	ASP	CA-CB-CG	5.57	125.65	113.40
1	Cf	20	VAL	CB-CA-C	5.57	121.98	111.40
1	C7	56	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C9	20	VAL	CB-CA-C	5.57	121.97	111.40
1	CF	20	VAL	CB-CA-C	5.57	121.97	111.40
1	CK	20	VAL	CB-CA-C	5.57	121.97	111.40
1	Cd	20	VAL	CB-CA-C	5.57	121.97	111.40
1	Cs	20	VAL	CB-CA-C	5.57	121.97	111.40
1	B2	32	TRP	CG-CD2-CE3	5.56	138.91	133.90
1	CA	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Ci	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Cl	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Cv	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Ao	32	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	BP	32	TRP	CG-CD2-CE3	5.56	138.91	133.90
1	BX	32	TRP	CG-CD2-CE3	5.56	138.91	133.90
1	C6	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Ch	20	VAL	CB-CA-C	5.56	121.97	111.40
1	Cj	20	VAL	CB-CA-C	5.56	121.97	111.40
1	BC	32	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	Bx	32	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	BQ	32	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	CH	20	VAL	CB-CA-C	5.56	121.96	111.40
1	AS	32	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	Ag	32	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	Bl	32	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	CX	20	VAL	CB-CA-C	5.55	121.95	111.40
1	CZ	20	VAL	CB-CA-C	5.55	121.95	111.40
1	B4	38	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	BD	32	TRP	CG-CD2-CE3	5.55	138.90	133.90
1	Ca	20	VAL	CB-CA-C	5.55	121.95	111.40
1	Cm	20	VAL	CB-CA-C	5.55	121.95	111.40
1	Cx	20	VAL	CB-CA-C	5.55	121.95	111.40
1	B1	38	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	B6	32	TRP	CG-CD2-CE3	5.55	138.90	133.90
1	CO	56	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	CT	20	VAL	CB-CA-C	5.55	121.95	111.40
1	BG	32	TRP	CG-CD2-CE3	5.55	138.90	133.90
1	BV	38	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	C5	56	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	CY	20	VAL	CB-CA-C	5.55	121.94	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ce	20	VAL	CB-CA-C	5.55	121.95	111.40
1	Cr	20	VAL	CB-CA-C	5.55	121.94	111.40
1	Bd	38	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	Bt	32	TRP	CG-CD2-CE3	5.55	138.89	133.90
1	C5	20	VAL	CB-CA-C	5.55	121.94	111.40
1	BF	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	Bo	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	Bp	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	Bs	38	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	Bu	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	C3	20	VAL	CB-CA-C	5.54	121.93	111.40
1	BB	38	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	Bs	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	CN	56	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	BS	32	TRP	CG-CD2-CE3	5.54	138.89	133.90
1	Bg	32	TRP	CG-CD2-CE3	5.54	138.88	133.90
1	C2	56	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	Cj	56	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	CG	20	VAL	CB-CA-C	5.54	121.92	111.40
1	Be	32	TRP	CG-CD2-CE3	5.54	138.88	133.90
1	CE	20	VAL	CB-CA-C	5.54	121.92	111.40
1	B1	32	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	BX	38	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	Bl	38	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C4	56	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	B4	32	TRP	CG-CD2-CE3	5.53	138.88	133.90
1	C7	20	VAL	CB-CA-C	5.53	121.91	111.40
1	Cb	20	VAL	CB-CA-C	5.53	121.91	111.40
1	Ct	56	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	CZ	56	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B8	32	TRP	CG-CD2-CE3	5.53	138.87	133.90
1	BZ	38	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	CA	56	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B2	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B6	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	BC	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	BU	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	Cl	56	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	Bd	32	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	Bj	32	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	Bq	32	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	CW	56	ARG	NE-CZ-NH1	5.52	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ca	56	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	BN	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	Bb	32	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	B3	32	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	BD	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B3	38	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	BB	32	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	Cb	56	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	Br	32	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	CF	56	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	Bm	38	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C3	56	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B5	32	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	Ba	38	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	Bh	32	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	BO	38	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	BA	32	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	BA	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	CL	56	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B5	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	BJ	32	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	BW	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Bv	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	BZ	32	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	Bu	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Bv	32	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	Cc	56	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	Co	56	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	BL	32	TRP	CG-CD2-CE3	5.50	138.85	133.90
1	Bq	38	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	Bw	38	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	Bi	32	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	Bv	32	TRP	CB-CG-CD1	-5.49	119.86	127.00
1	Cf	56	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	BH	38	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	BO	32	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	BU	32	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	Cm	56	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	Cx	56	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B8	38	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B9	38	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	Bm	32	TRP	CG-CD2-CE3	5.48	138.83	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AB	32	TRP	CG-CD2-CE3	5.48	138.83	133.90
1	Bj	38	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	Cs	56	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	BR	32	TRP	CG-CD2-CE3	5.48	138.83	133.90
1	BM	32	TRP	CG-CD2-CE3	5.47	138.83	133.90
1	BE	32	TRP	CG-CD2-CE3	5.47	138.82	133.90
1	Cv	56	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	BS	32	TRP	CB-CG-CD1	-5.46	119.89	127.00
1	Ch	56	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B3	32	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	BB	32	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	B5	32	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	B6	32	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	A2	35	SER	N-CA-CB	-5.46	102.31	110.50
1	Bb	32	TRP	CB-CG-CD1	-5.46	119.90	127.00
1	Cr	56	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	AE	35	SER	N-CA-CB	-5.46	102.31	110.50
1	AG	35	SER	N-CA-CB	-5.46	102.32	110.50
1	B9	32	TRP	CB-CG-CD1	-5.46	119.91	127.00
1	CJ	56	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A7	35	SER	N-CA-CB	-5.45	102.32	110.50
1	Ai	35	SER	N-CA-CB	-5.45	102.32	110.50
1	CM	56	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	CY	56	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	AD	35	SER	N-CA-CB	-5.45	102.32	110.50
1	AJ	32	TRP	CG-CD2-CE3	5.45	138.81	133.90
1	Ab	35	SER	N-CA-CB	-5.45	102.33	110.50
1	An	35	SER	N-CA-CB	-5.45	102.32	110.50
1	Ar	35	SER	N-CA-CB	-5.45	102.32	110.50
1	BP	32	TRP	CB-CG-CD1	-5.45	119.91	127.00
1	Bx	32	TRP	CB-CG-CD1	-5.45	119.91	127.00
1	A6	38	ARG	CG-CD-NE	-5.45	100.36	111.80
1	AA	35	SER	N-CA-CB	-5.45	102.33	110.50
1	AE	38	ARG	CG-CD-NE	-5.45	100.36	111.80
1	Ak	35	SER	N-CA-CB	-5.45	102.33	110.50
1	Ap	32	TRP	CG-CD2-CE3	5.45	138.80	133.90
1	At	35	SER	N-CA-CB	-5.45	102.33	110.50
1	Cu	56	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	Bm	32	TRP	CB-CG-CD1	-5.45	119.92	127.00
1	Cd	56	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	Bp	32	TRP	CB-CG-CD1	-5.45	119.92	127.00
1	CE	56	ARG	NE-CZ-NH1	5.45	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A0	35	SER	N-CA-CB	-5.44	102.33	110.50
1	Ak	38	ARG	CG-CD-NE	-5.44	100.37	111.80
1	A1	38	ARG	CG-CD-NE	-5.44	100.37	111.80
1	AN	35	SER	N-CA-CB	-5.44	102.33	110.50
1	AO	35	SER	N-CA-CB	-5.44	102.33	110.50
1	AY	35	SER	N-CA-CB	-5.44	102.34	110.50
1	AY	38	ARG	CG-CD-NE	-5.44	100.37	111.80
1	Ac	35	SER	N-CA-CB	-5.44	102.33	110.50
1	BF	32	TRP	CB-CG-CD1	-5.44	119.92	127.00
1	Bi	32	TRP	CB-CG-CD1	-5.44	119.92	127.00
1	A9	38	ARG	CG-CD-NE	-5.44	100.37	111.80
1	AG	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	AZ	35	SER	N-CA-CB	-5.44	102.34	110.50
1	As	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	BA	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	BO	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	Bo	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	CS	101	CYS	CA-CB-SG	-5.44	104.21	114.00
1	AC	35	SER	N-CA-CB	-5.44	102.34	110.50
1	AO	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	Ad	35	SER	N-CA-CB	-5.44	102.34	110.50
1	B1	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	Bl	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	Cq	56	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	AM	35	SER	N-CA-CB	-5.44	102.34	110.50
1	AQ	35	SER	N-CA-CB	-5.44	102.34	110.50
1	AR	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	Aa	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	Ai	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	Av	35	SER	N-CA-CB	-5.44	102.34	110.50
1	CD	101	CYS	CA-CB-SG	-5.44	104.21	114.00
1	A2	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	A3	35	SER	N-CA-CB	-5.44	102.35	110.50
1	AL	38	ARG	CG-CD-NE	-5.44	100.38	111.80
1	Ah	38	ARG	CG-CD-NE	-5.44	100.39	111.80
1	BN	32	TRP	CB-CG-CD1	-5.44	119.93	127.00
1	AM	38	ARG	CG-CD-NE	-5.43	100.39	111.80
1	Ag	38	ARG	CG-CD-NE	-5.43	100.39	111.80
1	B0	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	B4	32	TRP	CB-CG-CD1	-5.43	119.93	127.00
1	C8	56	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	CG	101	CYS	CA-CB-SG	-5.43	104.22	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CU	101	CYS	CA-CB-SG	-5.43	104.22	114.00
1	AZ	38	ARG	CG-CD-NE	-5.43	100.39	111.80
1	Ad	38	ARG	CG-CD-NE	-5.43	100.39	111.80
1	Au	35	SER	N-CA-CB	-5.43	102.35	110.50
1	BL	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	Bb	38	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	CJ	101	CYS	CA-CB-SG	-5.43	104.22	114.00
1	CR	56	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	Cw	56	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	Aw	35	SER	N-CA-CB	-5.43	102.35	110.50
1	BW	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	C3	101	CYS	CA-CB-SG	-5.43	104.22	114.00
1	C9	56	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	Ci	101	CYS	CA-CB-SG	-5.43	104.22	114.00
1	A5	35	SER	N-CA-CB	-5.43	102.36	110.50
1	AA	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	AC	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	AI	35	SER	N-CA-CB	-5.43	102.36	110.50
1	AX	35	SER	N-CA-CB	-5.43	102.36	110.50
1	Af	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	Ao	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	Ax	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	BX	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	Bd	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	CN	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cp	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cv	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cw	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	A1	35	SER	N-CA-CB	-5.43	102.36	110.50
1	Ag	35	SER	N-CA-CB	-5.43	102.36	110.50
1	Au	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	Bu	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	CB	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Ct	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	AF	35	SER	N-CA-CB	-5.43	102.36	110.50
1	AH	38	ARG	CG-CD-NE	-5.43	100.41	111.80
1	AS	32	TRP	CG-CD2-CE3	5.43	138.78	133.90
1	AS	38	ARG	CG-CD-NE	-5.43	100.41	111.80
1	Aa	35	SER	N-CA-CB	-5.43	102.36	110.50
1	An	38	ARG	CG-CD-NE	-5.43	100.40	111.80
1	BG	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	BJ	32	TRP	CB-CG-CD1	-5.43	119.94	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BQ	32	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	C4	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cc	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cm	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cq	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	Cx	101	CYS	CA-CB-SG	-5.43	104.23	114.00
1	AB	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	AH	35	SER	N-CA-CB	-5.42	102.36	110.50
1	AX	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	Al	35	SER	N-CA-CB	-5.42	102.36	110.50
1	Ap	35	SER	N-CA-CB	-5.42	102.36	110.50
1	Ap	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	B8	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	BR	57	LYS	CB-CA-C	-5.42	99.55	110.40
1	BU	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	BZ	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	Bf	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	CH	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	CR	101	CYS	CA-CB-SG	-5.42	104.23	114.00
1	CT	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	CU	56	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A3	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	AJ	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	AW	35	SER	N-CA-CB	-5.42	102.36	110.50
1	Aj	35	SER	N-CA-CB	-5.42	102.37	110.50
1	Ax	35	SER	N-CA-CB	-5.42	102.37	110.50
1	B1	57	LYS	CB-CA-C	-5.42	99.55	110.40
1	Ba	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	Bg	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	Bs	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	CE	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Ch	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Cj	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	AP	35	SER	N-CA-CB	-5.42	102.37	110.50
1	AU	38	ARG	CG-CD-NE	-5.42	100.41	111.80
1	Ac	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	Af	32	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	B8	57	LYS	CB-CA-C	-5.42	99.56	110.40
1	Bq	57	LYS	CB-CA-C	-5.42	99.56	110.40
1	Bw	32	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	C7	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	CF	101	CYS	CA-CB-SG	-5.42	104.24	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CP	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Cn	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Cp	56	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	Cs	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Cu	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	Ah	32	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	BZ	57	LYS	CB-CA-C	-5.42	99.56	110.40
1	Be	38	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C5	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	CL	101	CYS	CA-CB-SG	-5.42	104.24	114.00
1	A0	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	A8	35	SER	N-CA-CB	-5.42	102.37	110.50
1	Aq	35	SER	N-CA-CB	-5.42	102.37	110.50
1	Aq	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	As	35	SER	N-CA-CB	-5.42	102.37	110.50
1	Av	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	BH	32	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	Be	32	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	C8	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	C9	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	CW	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	CX	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	CY	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	Cg	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	A4	35	SER	N-CA-CB	-5.42	102.38	110.50
1	AF	38	ARG	CG-CD-NE	-5.42	100.43	111.80
1	AL	32	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	AW	32	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	Af	35	SER	N-CA-CB	-5.42	102.38	110.50
1	Ar	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	Aw	38	ARG	CG-CD-NE	-5.42	100.42	111.80
1	Bt	32	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	CA	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	CK	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	CM	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	BD	57	LYS	CB-CA-C	-5.42	99.57	110.40
1	BI	32	TRP	CB-CG-CD1	-5.42	119.96	127.00
1	Bm	57	LYS	CB-CA-C	-5.42	99.57	110.40
1	C1	56	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	CI	101	CYS	CA-CB-SG	-5.42	104.25	114.00
1	AA	32	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	AL	35	SER	N-CA-CB	-5.41	102.38	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BD	32	TRP	CB-CG-CD1	-5.41	119.96	127.00
1	C0	101	CYS	CA-CB-SG	-5.41	104.25	114.00
1	CZ	101	CYS	CA-CB-SG	-5.41	104.25	114.00
1	Ck	101	CYS	CA-CB-SG	-5.41	104.25	114.00
1	Cr	101	CYS	CA-CB-SG	-5.41	104.25	114.00
1	A8	38	ARG	CG-CD-NE	-5.41	100.43	111.80
1	A9	35	SER	N-CA-CB	-5.41	102.38	110.50
1	AR	35	SER	N-CA-CB	-5.41	102.38	110.50
1	BH	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	A4	38	ARG	CG-CD-NE	-5.41	100.44	111.80
1	Am	35	SER	N-CA-CB	-5.41	102.38	110.50
1	BE	38	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	BU	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	BY	32	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	Bj	32	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	Bj	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	Bl	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	Bo	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	C2	101	CYS	CA-CB-SG	-5.41	104.26	114.00
1	CB	56	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	CG	56	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	AC	32	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	AK	35	SER	N-CA-CB	-5.41	102.39	110.50
1	AP	38	ARG	CG-CD-NE	-5.41	100.44	111.80
1	Ao	32	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	BG	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	Be	57	LYS	CB-CA-C	-5.41	99.58	110.40
1	CO	101	CYS	CA-CB-SG	-5.41	104.27	114.00
1	Ce	101	CYS	CA-CB-SG	-5.41	104.26	114.00
1	A3	32	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	A7	32	TRP	CG-CD2-CE3	5.41	138.77	133.90
1	AI	38	ARG	CG-CD-NE	-5.41	100.45	111.80
1	AQ	38	ARG	CG-CD-NE	-5.41	100.44	111.80
1	BE	57	LYS	CB-CA-C	-5.41	99.59	110.40
1	BL	57	LYS	CB-CA-C	-5.41	99.59	110.40
1	A7	38	ARG	CG-CD-NE	-5.41	100.45	111.80
1	AS	35	SER	N-CA-CB	-5.41	102.39	110.50
1	Ab	38	ARG	CG-CD-NE	-5.41	100.45	111.80
1	At	38	ARG	CG-CD-NE	-5.41	100.45	111.80
1	BR	32	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	Bc	32	TRP	CB-CG-CD1	-5.41	119.97	127.00
1	CQ	101	CYS	CA-CB-SG	-5.41	104.27	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Cb	101	CYS	CA-CB-SG	-5.41	104.27	114.00
1	Cd	101	CYS	CA-CB-SG	-5.41	104.27	114.00
1	Cf	101	CYS	CA-CB-SG	-5.41	104.27	114.00
1	Cl	101	CYS	CA-CB-SG	-5.41	104.27	114.00
1	AN	32	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	AV	38	ARG	CG-CD-NE	-5.40	100.45	111.80
1	Al	38	ARG	CG-CD-NE	-5.40	100.45	111.80
1	BE	32	TRP	CB-CG-CD1	-5.40	119.97	127.00
1	BX	57	LYS	CB-CA-C	-5.40	99.59	110.40
1	A5	38	ARG	CG-CD-NE	-5.40	100.45	111.80
1	AJ	35	SER	N-CA-CB	-5.40	102.40	110.50
1	AT	38	ARG	CG-CD-NE	-5.40	100.46	111.80
1	AW	38	ARG	CG-CD-NE	-5.40	100.45	111.80
1	Ae	35	SER	N-CA-CB	-5.40	102.39	110.50
1	Ae	38	ARG	CG-CD-NE	-5.40	100.46	111.80
1	B0	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	BG	38	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	BM	32	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	Bh	32	TRP	CB-CG-CD1	-5.40	119.97	127.00
1	Bk	32	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	Bn	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	CH	56	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	Ca	101	CYS	CA-CB-SG	-5.40	104.28	114.00
1	AB	35	SER	N-CA-CB	-5.40	102.40	110.50
1	BB	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	BF	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	Br	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	Bu	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	A6	35	SER	N-CA-CB	-5.40	102.40	110.50
1	AD	38	ARG	CG-CD-NE	-5.40	100.46	111.80
1	B9	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	Bb	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	Br	32	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	Bx	57	LYS	CB-CA-C	-5.40	99.60	110.40
1	CV	101	CYS	CA-CB-SG	-5.40	104.28	114.00
1	AN	38	ARG	CG-CD-NE	-5.40	100.47	111.80
1	BT	32	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	C6	101	CYS	CA-CB-SG	-5.40	104.28	114.00
1	Am	38	ARG	CG-CD-NE	-5.40	100.47	111.80
1	BC	32	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	Bn	32	TRP	CB-CG-CD1	-5.40	119.99	127.00
1	Aj	38	ARG	CG-CD-NE	-5.39	100.47	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ak	32	TRP	CG-CD2-CE3	5.39	138.76	133.90
1	Am	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	BJ	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	Ba	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	Bd	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	Bh	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	Bq	32	TRP	CB-CG-CD1	-5.39	119.99	127.00
1	CC	101	CYS	CA-CB-SG	-5.39	104.29	114.00
1	AR	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	Aq	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	B2	32	TRP	CB-CG-CD1	-5.39	119.99	127.00
1	B2	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	B3	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	B4	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	BO	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	BS	57	LYS	CB-CA-C	-5.39	99.61	110.40
1	AP	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	BY	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	Bg	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	Bw	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	A0	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	A4	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	AD	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	AT	35	SER	N-CA-CB	-5.39	102.42	110.50
1	AX	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	B7	32	TRP	CB-CG-CD1	-5.39	120.00	127.00
1	BP	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	Bi	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	Bv	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	C1	101	CYS	CA-CB-SG	-5.39	104.30	114.00
1	AK	38	ARG	CG-CD-NE	-5.39	100.49	111.80
1	AV	35	SER	N-CA-CB	-5.39	102.42	110.50
1	Bs	57	LYS	CB-CA-C	-5.39	99.62	110.40
1	AF	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	Ah	35	SER	N-CA-CB	-5.39	102.42	110.50
1	Aw	32	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	BM	57	LYS	CB-CA-C	-5.39	99.63	110.40
1	A9	32	TRP	CG-CD2-CE3	5.38	138.75	133.90
1	Au	32	TRP	CG-CD2-CE3	5.38	138.75	133.90
1	BT	57	LYS	CB-CA-C	-5.38	99.63	110.40
1	BV	32	TRP	CB-CG-CD1	-5.38	120.00	127.00
1	Co	101	CYS	CA-CB-SG	-5.38	104.31	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ab	32	TRP	CG-CD2-CE3	5.38	138.75	133.90
1	Aj	32	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	B5	57	LYS	CB-CA-C	-5.38	99.63	110.40
1	B7	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	BC	57	LYS	CB-CA-C	-5.38	99.63	110.40
1	Ci	56	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B6	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	BI	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	BA	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	Bc	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	A5	32	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	BN	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	BV	57	LYS	CB-CA-C	-5.38	99.64	110.40
1	Ao	35	SER	N-CA-CB	-5.38	102.44	110.50
1	AU	35	SER	N-CA-CB	-5.38	102.44	110.50
1	Bf	57	LYS	CB-CA-C	-5.38	99.65	110.40
1	AO	32	TRP	CG-CD2-CE3	5.37	138.74	133.90
1	Ar	32	TRP	CG-CD2-CE3	5.37	138.74	133.90
1	At	32	TRP	CG-CD2-CE3	5.37	138.74	133.90
1	BK	32	TRP	CB-CG-CD1	-5.37	120.02	127.00
1	Bk	57	LYS	CB-CA-C	-5.37	99.66	110.40
1	Bp	57	LYS	CB-CA-C	-5.37	99.66	110.40
1	AZ	32	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	Ag	32	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	BK	57	LYS	CB-CA-C	-5.37	99.66	110.40
1	BW	57	LYS	CB-CA-C	-5.37	99.66	110.40
1	Bt	57	LYS	CB-CA-C	-5.37	99.66	110.40
1	A8	32	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	AV	32	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	Ax	32	TRP	CG-CD2-CE3	5.37	138.73	133.90
1	CS	56	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	BP	38	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	Ct	49	ARG	N-CA-CB	-5.36	100.94	110.60
1	AK	32	TRP	CG-CD2-CE3	5.36	138.73	133.90
1	A1	32	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	AT	32	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	Ac	32	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	BQ	57	LYS	CB-CA-C	-5.36	99.68	110.40
1	Cg	56	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A2	32	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	AI	32	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	AQ	32	TRP	CG-CD2-CE3	5.36	138.72	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CD	56	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	Al	32	TRP	CG-CD2-CE3	5.35	138.72	133.90
1	CR	49	ARG	N-CA-CB	-5.35	100.96	110.60
1	CV	49	ARG	N-CA-CB	-5.35	100.96	110.60
1	Cd	49	ARG	N-CA-CB	-5.35	100.96	110.60
1	AM	32	TRP	CG-CD2-CE3	5.35	138.72	133.90
1	Ad	32	TRP	CG-CD2-CE3	5.35	138.72	133.90
1	C6	49	ARG	N-CA-CB	-5.35	100.97	110.60
1	CP	56	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	Cu	49	ARG	N-CA-CB	-5.35	100.96	110.60
1	CC	49	ARG	N-CA-CB	-5.35	100.97	110.60
1	C0	49	ARG	N-CA-CB	-5.35	100.97	110.60
1	CH	49	ARG	N-CA-CB	-5.35	100.97	110.60
1	CP	49	ARG	N-CA-CB	-5.35	100.97	110.60
1	CI	49	ARG	N-CA-CB	-5.35	100.98	110.60
1	Cg	49	ARG	N-CA-CB	-5.35	100.98	110.60
1	As	32	TRP	CG-CD2-CE3	5.35	138.71	133.90
1	CW	49	ARG	N-CA-CB	-5.35	100.98	110.60
1	Cc	49	ARG	N-CA-CB	-5.35	100.98	110.60
1	Cl	49	ARG	N-CA-CB	-5.34	100.98	110.60
1	Cv	49	ARG	N-CA-CB	-5.34	100.98	110.60
1	Cw	49	ARG	N-CA-CB	-5.34	100.98	110.60
1	Av	32	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	Cf	49	ARG	N-CA-CB	-5.34	100.99	110.60
1	Cq	49	ARG	N-CA-CB	-5.34	100.98	110.60
1	CT	49	ARG	N-CA-CB	-5.34	100.99	110.60
1	Cr	49	ARG	N-CA-CB	-5.34	100.99	110.60
1	Ae	32	TRP	CG-CD2-CE3	5.34	138.70	133.90
1	Ch	49	ARG	N-CA-CB	-5.34	100.99	110.60
1	AE	32	TRP	CG-CD2-CE3	5.33	138.70	133.90
1	C5	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	C4	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	C9	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	CK	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	CL	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	CS	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	C3	49	ARG	N-CA-CB	-5.33	101.00	110.60
1	CN	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	B0	38	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C2	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	C7	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	C8	49	ARG	N-CA-CB	-5.33	101.01	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CF	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	CJ	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	CY	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	Ci	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	Cn	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	Cp	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	Ca	49	ARG	N-CA-CB	-5.33	101.01	110.60
1	AU	32	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	CX	49	ARG	N-CA-CB	-5.32	101.02	110.60
1	Ck	49	ARG	N-CA-CB	-5.32	101.02	110.60
1	AY	32	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	CU	49	ARG	N-CA-CB	-5.32	101.02	110.60
1	CO	49	ARG	N-CA-CB	-5.32	101.02	110.60
1	Cb	49	ARG	N-CA-CB	-5.32	101.02	110.60
1	Cs	49	ARG	N-CA-CB	-5.32	101.03	110.60
1	Cj	49	ARG	N-CA-CB	-5.32	101.03	110.60
1	Cm	49	ARG	N-CA-CB	-5.32	101.03	110.60
1	Cl	49	ARG	N-CA-CB	-5.32	101.03	110.60
1	AH	32	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	CE	49	ARG	N-CA-CB	-5.31	101.03	110.60
1	An	32	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	CZ	49	ARG	N-CA-CB	-5.31	101.04	110.60
1	Aa	32	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	Ai	32	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	CA	49	ARG	N-CA-CB	-5.31	101.04	110.60
1	CB	49	ARG	N-CA-CB	-5.31	101.04	110.60
1	Co	49	ARG	N-CA-CB	-5.31	101.04	110.60
1	AG	32	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	CG	49	ARG	N-CA-CB	-5.31	101.05	110.60
1	CQ	49	ARG	N-CA-CB	-5.31	101.05	110.60
1	Cx	49	ARG	N-CA-CB	-5.31	101.05	110.60
1	A6	32	TRP	CG-CD2-CE3	5.30	138.67	133.90
1	CD	49	ARG	N-CA-CB	-5.30	101.06	110.60
1	Ce	49	ARG	N-CA-CB	-5.30	101.06	110.60
1	Ba	6	GLN	N-CA-CB	-5.30	101.06	110.60
1	CM	49	ARG	N-CA-CB	-5.30	101.07	110.60
1	Bv	6	GLN	N-CA-CB	-5.29	101.07	110.60
1	BN	6	GLN	N-CA-CB	-5.29	101.07	110.60
1	Bu	6	GLN	N-CA-CB	-5.29	101.07	110.60
1	BD	6	GLN	N-CA-CB	-5.29	101.08	110.60
1	Bn	6	GLN	N-CA-CB	-5.29	101.07	110.60
1	Bw	6	GLN	N-CA-CB	-5.29	101.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B7	6	GLN	N-CA-CB	-5.29	101.09	110.60
1	BH	6	GLN	N-CA-CB	-5.29	101.09	110.60
1	B0	6	GLN	N-CA-CB	-5.28	101.09	110.60
1	BI	6	GLN	N-CA-CB	-5.28	101.09	110.60
1	Bc	6	GLN	N-CA-CB	-5.28	101.09	110.60
1	BO	6	GLN	N-CA-CB	-5.28	101.09	110.60
1	Bk	6	GLN	N-CA-CB	-5.28	101.09	110.60
1	Bq	6	GLN	N-CA-CB	-5.28	101.10	110.60
1	B4	6	GLN	N-CA-CB	-5.28	101.10	110.60
1	Bf	6	GLN	N-CA-CB	-5.28	101.10	110.60
1	BG	6	GLN	N-CA-CB	-5.28	101.10	110.60
1	BC	6	GLN	N-CA-CB	-5.28	101.10	110.60
1	BY	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	C2	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	Ce	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	B9	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	BP	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	Bt	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	Bp	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	B5	6	GLN	N-CA-CB	-5.27	101.11	110.60
1	BV	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	BK	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	BX	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	C3	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	CD	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	CM	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	B6	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	B8	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	C7	6	GLN	N-CA-CB	-5.27	101.12	110.60
1	Bo	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	Bs	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	C0	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	CG	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	CX	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	Cg	6	GLN	N-CA-CB	-5.26	101.12	110.60
1	BE	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	CC	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Ca	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Cc	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Bl	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Bx	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Co	6	GLN	N-CA-CB	-5.26	101.13	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ct	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Bj	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	CU	6	GLN	N-CA-CB	-5.26	101.13	110.60
1	Cs	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	B2	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	BT	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	BU	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	Bd	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	Bh	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	Bi	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	Bm	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	C4	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	C8	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	C9	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	CA	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	CE	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	CO	6	GLN	N-CA-CB	-5.26	101.14	110.60
1	BA	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	BB	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	BW	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	BL	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	BS	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	C6	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	CI	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	CQ	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	CS	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	Cn	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	Cw	6	GLN	N-CA-CB	-5.25	101.14	110.60
1	CK	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	Cb	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	Cj	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	BM	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	BQ	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	CW	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	CY	6	GLN	N-CA-CB	-5.25	101.15	110.60
1	CJ	6	GLN	N-CA-CB	-5.25	101.16	110.60
1	Cf	6	GLN	N-CA-CB	-5.25	101.16	110.60
1	C5	6	GLN	N-CA-CB	-5.25	101.16	110.60
1	Cp	6	GLN	N-CA-CB	-5.25	101.16	110.60
1	Cx	6	GLN	N-CA-CB	-5.25	101.16	110.60
1	BZ	6	GLN	N-CA-CB	-5.24	101.16	110.60
1	Bb	6	GLN	N-CA-CB	-5.24	101.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Be	6	GLN	N-CA-CB	-5.24	101.16	110.60
1	CZ	6	GLN	N-CA-CB	-5.24	101.16	110.60
1	Cq	6	GLN	N-CA-CB	-5.24	101.16	110.60
1	Cv	6	GLN	N-CA-CB	-5.24	101.16	110.60
1	Ck	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	BJ	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	BR	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	CN	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	Cd	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	Cl	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	Br	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	CL	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	CP	6	GLN	N-CA-CB	-5.24	101.17	110.60
1	CH	6	GLN	N-CA-CB	-5.24	101.18	110.60
1	Ch	6	GLN	N-CA-CB	-5.24	101.18	110.60
1	CT	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	Cm	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	B3	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	BF	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	Bg	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	CF	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	CV	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	Ci	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	Cr	6	GLN	N-CA-CB	-5.23	101.18	110.60
1	Cu	6	GLN	N-CA-CB	-5.23	101.19	110.60
1	B1	6	GLN	N-CA-CB	-5.23	101.19	110.60
1	CB	6	GLN	N-CA-CB	-5.23	101.19	110.60
1	C1	6	GLN	N-CA-CB	-5.22	101.19	110.60
1	A3	56	ARG	NH1-CZ-NH2	5.22	125.14	119.40
1	CR	6	GLN	N-CA-CB	-5.22	101.21	110.60
1	AD	56	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	AJ	82	TRP	CB-CG-CD1	-5.21	120.22	127.00
1	Ae	56	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	AA	56	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	CM	84	SER	N-CA-CB	5.21	118.31	110.50
1	Aa	56	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	AH	56	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	A9	56	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	AW	56	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	AB	82	TRP	CB-CG-CD1	-5.20	120.25	127.00
1	AN	56	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	Ac	56	ARG	NH1-CZ-NH2	5.20	125.11	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Cp	84	SER	N-CA-CB	5.20	118.29	110.50
1	A1	56	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	A6	56	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	AZ	56	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	CA	84	SER	N-CA-CB	5.19	118.28	110.50
1	Ar	56	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	AR	82	TRP	CB-CG-CD1	-5.19	120.26	127.00
1	CR	84	SER	N-CA-CB	5.19	118.28	110.50
1	CX	84	SER	N-CA-CB	5.18	118.28	110.50
1	AE	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	AU	82	TRP	CB-CG-CD1	-5.18	120.26	127.00
1	Ad	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	AY	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	Ak	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	CE	84	SER	N-CA-CB	5.18	118.27	110.50
1	Ce	84	SER	N-CA-CB	5.18	118.27	110.50
1	A4	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	A8	56	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	Al	56	ARG	NH1-CZ-NH2	5.18	125.09	119.40
1	A5	56	ARG	NH1-CZ-NH2	5.18	125.09	119.40
1	AX	56	ARG	NH1-CZ-NH2	5.18	125.09	119.40
1	Cg	84	SER	N-CA-CB	5.18	118.27	110.50
1	Cm	84	SER	N-CA-CB	5.18	118.26	110.50
1	Am	56	ARG	NH1-CZ-NH2	5.17	125.09	119.40
1	Av	56	ARG	NH1-CZ-NH2	5.17	125.09	119.40
1	CS	84	SER	N-CA-CB	5.17	118.26	110.50
1	AF	56	ARG	NH1-CZ-NH2	5.17	125.09	119.40
1	C7	84	SER	N-CA-CB	5.17	118.26	110.50
1	Cx	84	SER	N-CA-CB	5.17	118.25	110.50
1	A7	56	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	Af	82	TRP	CB-CG-CD1	-5.17	120.28	127.00
1	C6	84	SER	N-CA-CB	5.17	118.25	110.50
1	CB	84	SER	N-CA-CB	5.17	118.25	110.50
1	CZ	84	SER	N-CA-CB	5.17	118.25	110.50
1	Cc	84	SER	N-CA-CB	5.17	118.25	110.50
1	An	56	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	B4	83	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	CG	84	SER	N-CA-CB	5.17	118.25	110.50
1	AI	56	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	Aw	56	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	Cb	84	SER	N-CA-CB	5.17	118.25	110.50
1	Ao	82	TRP	CB-CG-CD1	-5.16	120.29	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Cl	84	SER	N-CA-CB	5.16	118.25	110.50
1	Co	84	SER	N-CA-CB	5.16	118.25	110.50
1	AG	56	ARG	NH1-CZ-NH2	5.16	125.08	119.40
1	C1	84	SER	N-CA-CB	5.16	118.24	110.50
1	C8	84	SER	N-CA-CB	5.16	118.24	110.50
1	CC	84	SER	N-CA-CB	5.16	118.24	110.50
1	CO	84	SER	N-CA-CB	5.16	118.24	110.50
1	A2	56	ARG	NH1-CZ-NH2	5.16	125.08	119.40
1	AM	56	ARG	NH1-CZ-NH2	5.16	125.08	119.40
1	Ah	82	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	Ai	56	ARG	NH1-CZ-NH2	5.16	125.08	119.40
1	Au	56	ARG	NH1-CZ-NH2	5.16	125.08	119.40
1	Ch	84	SER	N-CA-CB	5.16	118.24	110.50
1	A6	82	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	Cw	84	SER	N-CA-CB	5.16	118.24	110.50
1	C3	84	SER	N-CA-CB	5.16	118.24	110.50
1	Ab	56	ARG	NH1-CZ-NH2	5.16	125.07	119.40
1	Ai	82	TRP	CB-CG-CD1	-5.16	120.30	127.00
1	As	56	ARG	NH1-CZ-NH2	5.16	125.07	119.40
1	Cf	84	SER	N-CA-CB	5.16	118.23	110.50
1	Ci	84	SER	N-CA-CB	5.16	118.23	110.50
1	AU	56	ARG	NH1-CZ-NH2	5.15	125.07	119.40
1	Cr	84	SER	N-CA-CB	5.15	118.23	110.50
1	AA	82	TRP	CB-CG-CD1	-5.15	120.30	127.00
1	AD	82	TRP	CB-CG-CD1	-5.15	120.30	127.00
1	CI	84	SER	N-CA-CB	5.15	118.23	110.50
1	AL	56	ARG	NH1-CZ-NH2	5.15	125.07	119.40
1	AT	56	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	Ap	56	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	CJ	84	SER	N-CA-CB	5.15	118.22	110.50
1	CW	84	SER	N-CA-CB	5.15	118.23	110.50
1	Cs	84	SER	N-CA-CB	5.15	118.23	110.50
1	Ct	84	SER	N-CA-CB	5.15	118.22	110.50
1	A5	82	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	AS	56	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	As	82	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	Aw	82	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	A0	56	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	Av	82	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	Ac	82	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	Cu	84	SER	N-CA-CB	5.15	118.22	110.50
1	A8	82	TRP	CB-CG-CD1	-5.14	120.31	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ap	82	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	CF	84	SER	N-CA-CB	5.14	118.22	110.50
1	AO	56	ARG	NH1-CZ-NH2	5.14	125.06	119.40
1	AP	56	ARG	NH1-CZ-NH2	5.14	125.06	119.40
1	AT	82	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	AY	82	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	Cj	84	SER	N-CA-CB	5.14	118.22	110.50
1	A3	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	AK	56	ARG	NH1-CZ-NH2	5.14	125.06	119.40
1	Cn	84	SER	N-CA-CB	5.14	118.21	110.50
1	AW	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	Al	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	Aq	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	C4	84	SER	N-CA-CB	5.14	118.21	110.50
1	Ck	84	SER	N-CA-CB	5.14	118.21	110.50
1	AC	56	ARG	NH1-CZ-NH2	5.14	125.05	119.40
1	AM	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	Aa	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	Ar	82	TRP	CB-CG-CD1	-5.14	120.32	127.00
1	Ax	56	ARG	NH1-CZ-NH2	5.14	125.05	119.40
1	C5	84	SER	N-CA-CB	5.14	118.20	110.50
1	CD	84	SER	N-CA-CB	5.14	118.20	110.50
1	CH	84	SER	N-CA-CB	5.14	118.20	110.50
1	CN	84	SER	N-CA-CB	5.14	118.20	110.50
1	Cq	84	SER	N-CA-CB	5.14	118.21	110.50
1	A5	48	VAL	CB-CA-C	-5.13	101.64	111.40
1	Ae	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	Ax	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	CK	84	SER	N-CA-CB	5.13	118.20	110.50
1	CQ	84	SER	N-CA-CB	5.13	118.20	110.50
1	CT	84	SER	N-CA-CB	5.13	118.20	110.50
1	CY	84	SER	N-CA-CB	5.13	118.20	110.50
1	AL	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	AX	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	Ag	56	ARG	NH1-CZ-NH2	5.13	125.05	119.40
1	At	56	ARG	NH1-CZ-NH2	5.13	125.05	119.40
1	C9	84	SER	N-CA-CB	5.13	118.20	110.50
1	CU	84	SER	N-CA-CB	5.13	118.20	110.50
1	Ca	84	SER	N-CA-CB	5.13	118.20	110.50
1	AG	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	AK	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	AP	82	TRP	CB-CG-CD1	-5.13	120.33	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AZ	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	CP	84	SER	N-CA-CB	5.13	118.20	110.50
1	AQ	56	ARG	NH1-CZ-NH2	5.13	125.04	119.40
1	AK	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	AR	56	ARG	NH1-CZ-NH2	5.13	125.04	119.40
1	Af	56	ARG	NH1-CZ-NH2	5.13	125.04	119.40
1	AN	82	TRP	CB-CG-CD1	-5.13	120.34	127.00
1	AS	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	Ag	82	TRP	CB-CG-CD1	-5.13	120.33	127.00
1	C2	84	SER	N-CA-CB	5.13	118.19	110.50
1	CL	84	SER	N-CA-CB	5.13	118.19	110.50
1	Cd	84	SER	N-CA-CB	5.13	118.19	110.50
1	A2	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AI	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AE	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AQ	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AV	56	ARG	NH1-CZ-NH2	5.12	125.04	119.40
1	Cv	84	SER	N-CA-CB	5.12	118.19	110.50
1	AF	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AV	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	Am	48	VAL	CB-CA-C	-5.12	101.67	111.40
1	At	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	C0	84	SER	N-CA-CB	5.12	118.18	110.50
1	A1	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	An	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	AB	56	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	AJ	56	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	AO	82	TRP	CB-CG-CD1	-5.12	120.34	127.00
1	Aj	82	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	AI	48	VAL	CB-CA-C	-5.12	101.68	111.40
1	Ad	82	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	AK	48	VAL	CB-CA-C	-5.12	101.68	111.40
1	Aj	48	VAL	CB-CA-C	-5.12	101.68	111.40
1	Aq	56	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	CV	84	SER	N-CA-CB	5.12	118.17	110.50
1	A0	82	TRP	CB-CG-CD1	-5.11	120.35	127.00
1	AC	82	TRP	CB-CG-CD1	-5.11	120.35	127.00
1	A7	82	TRP	CB-CG-CD1	-5.11	120.35	127.00
1	AC	48	VAL	CB-CA-C	-5.11	101.69	111.40
1	Ah	56	ARG	NH1-CZ-NH2	5.11	125.02	119.40
1	AH	48	VAL	CB-CA-C	-5.11	101.69	111.40
1	Ae	48	VAL	CB-CA-C	-5.11	101.69	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aj	56	ARG	NH1-CZ-NH2	5.11	125.02	119.40
1	Au	82	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	A4	82	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	Ak	48	VAL	CB-CA-C	-5.11	101.70	111.40
1	AH	82	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	AG	48	VAL	CB-CA-C	-5.10	101.70	111.40
1	AT	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	Ao	56	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	Ar	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	Ad	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	Am	82	TRP	CB-CG-CD1	-5.10	120.37	127.00
1	AN	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	Au	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	A8	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	AD	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	Ax	48	VAL	CB-CA-C	-5.10	101.71	111.40
1	A2	48	VAL	CB-CA-C	-5.10	101.72	111.40
1	Ab	48	VAL	CB-CA-C	-5.10	101.72	111.40
1	AV	48	VAL	CB-CA-C	-5.09	101.72	111.40
1	Ab	82	TRP	CB-CG-CD1	-5.09	120.38	127.00
1	Ag	48	VAL	CB-CA-C	-5.09	101.72	111.40
1	Al	48	VAL	CB-CA-C	-5.09	101.72	111.40
1	Aw	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	A0	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	A1	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	AA	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	AE	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	AX	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	As	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	B6	83	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	AP	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	At	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	A9	82	TRP	CB-CG-CD1	-5.09	120.39	127.00
1	AQ	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	AY	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	AZ	48	VAL	CB-CA-C	-5.09	101.73	111.40
1	Ac	48	VAL	CB-CA-C	-5.09	101.74	111.40
1	A6	48	VAL	CB-CA-C	-5.08	101.74	111.40
1	A4	48	VAL	CB-CA-C	-5.08	101.74	111.40
1	A9	48	VAL	CB-CA-C	-5.08	101.74	111.40
1	BS	83	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	AB	48	VAL	CB-CA-C	-5.08	101.75	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AS	48	VAL	CB-CA-C	-5.08	101.75	111.40
1	AU	48	VAL	CB-CA-C	-5.08	101.75	111.40
1	A3	48	VAL	CB-CA-C	-5.08	101.75	111.40
1	A7	48	VAL	CB-CA-C	-5.08	101.75	111.40
1	Ai	48	VAL	CB-CA-C	-5.08	101.75	111.40
1	AF	48	VAL	CB-CA-C	-5.08	101.76	111.40
1	Aa	48	VAL	CB-CA-C	-5.08	101.76	111.40
1	AW	48	VAL	CB-CA-C	-5.07	101.76	111.40
1	AO	48	VAL	CB-CA-C	-5.07	101.77	111.40
1	Bg	83	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	Ao	48	VAL	CB-CA-C	-5.07	101.77	111.40
1	AM	48	VAL	CB-CA-C	-5.07	101.77	111.40
1	AR	48	VAL	CB-CA-C	-5.07	101.78	111.40
1	An	48	VAL	CB-CA-C	-5.06	101.78	111.40
1	Av	48	VAL	CB-CA-C	-5.06	101.78	111.40
1	Ap	48	VAL	CB-CA-C	-5.06	101.78	111.40
1	AL	48	VAL	CB-CA-C	-5.06	101.79	111.40
1	Ah	48	VAL	CB-CA-C	-5.06	101.79	111.40
1	Aq	48	VAL	CB-CA-C	-5.06	101.79	111.40
1	AJ	48	VAL	CB-CA-C	-5.05	101.81	111.40
1	Af	48	VAL	CB-CA-C	-5.04	101.81	111.40
1	CS	48	VAL	CB-CA-C	-5.04	101.81	111.40
1	CN	48	VAL	CB-CA-C	-5.03	101.84	111.40
1	Cf	48	VAL	CB-CA-C	-5.03	101.84	111.40
1	CP	82	TRP	CB-CG-CD1	-5.03	120.46	127.00
1	Cp	48	VAL	CB-CA-C	-5.03	101.84	111.40
1	B2	83	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	CC	48	VAL	CB-CA-C	-5.03	101.84	111.40
1	BM	83	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	CY	48	VAL	CB-CA-C	-5.03	101.85	111.40
1	C9	48	VAL	CB-CA-C	-5.03	101.85	111.40
1	CV	48	VAL	CB-CA-C	-5.03	101.85	111.40
1	CQ	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	C0	82	TRP	CB-CG-CD1	-5.02	120.47	127.00
1	CP	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	CW	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	Ca	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	Ck	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	Ct	48	VAL	CB-CA-C	-5.02	101.86	111.40
1	B1	83	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	Bq	83	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C6	48	VAL	CB-CA-C	-5.02	101.87	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BL	83	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	CH	48	VAL	CB-CA-C	-5.02	101.87	111.40
1	CI	48	VAL	CB-CA-C	-5.01	101.87	111.40
1	CL	48	VAL	CB-CA-C	-5.01	101.87	111.40
1	CT	48	VAL	CB-CA-C	-5.01	101.87	111.40
1	Cu	48	VAL	CB-CA-C	-5.01	101.87	111.40
1	C1	48	VAL	CB-CA-C	-5.01	101.88	111.40
1	CE	48	VAL	CB-CA-C	-5.01	101.88	111.40
1	CB	48	VAL	CB-CA-C	-5.01	101.89	111.40
1	CD	48	VAL	CB-CA-C	-5.01	101.89	111.40
1	CZ	48	VAL	CB-CA-C	-5.01	101.89	111.40
1	Bb	83	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	Br	83	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	Cq	48	VAL	CB-CA-C	-5.00	101.89	111.40
1	Cv	48	VAL	CB-CA-C	-5.00	101.89	111.40
1	Cx	48	VAL	CB-CA-C	-5.00	101.89	111.40
1	CF	82	TRP	CB-CG-CD1	-5.00	120.50	127.00
1	Cd	48	VAL	CB-CA-C	-5.00	101.89	111.40
1	C2	82	TRP	CB-CG-CD1	-5.00	120.50	127.00
1	C8	48	VAL	CB-CA-C	-5.00	101.90	111.40
1	CA	48	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	965	0	964	10	0
1	A1	965	0	964	9	0
1	A2	965	0	964	11	0
1	A3	965	0	964	10	0
1	A4	965	0	964	9	0
1	A5	965	0	964	9	0
1	A6	965	0	964	9	0
1	A7	965	0	964	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A8	965	0	964	10	0
1	A9	965	0	964	11	0
1	AA	965	0	964	13	0
1	AB	965	0	964	14	0
1	AC	965	0	964	10	0
1	AD	965	0	964	15	0
1	AE	965	0	964	13	0
1	AF	965	0	964	14	0
1	AG	965	0	964	14	0
1	AH	965	0	964	14	0
1	AI	965	0	964	13	0
1	AJ	965	0	964	15	0
1	AK	965	0	964	14	0
1	AL	965	0	964	14	0
1	AM	965	0	964	13	0
1	AN	965	0	964	14	0
1	AO	965	0	964	14	0
1	AP	965	0	964	15	0
1	AQ	965	0	964	12	0
1	AR	965	0	964	14	0
1	AS	965	0	964	13	0
1	AT	965	0	964	14	0
1	AU	965	0	964	15	0
1	AV	965	0	964	13	0
1	AW	965	0	964	14	0
1	AX	965	0	964	14	0
1	AY	965	0	964	10	0
1	AZ	965	0	964	10	0
1	Aa	965	0	964	0	0
1	Ab	965	0	964	0	0
1	Ac	965	0	964	0	0
1	Ad	965	0	964	0	0
1	Ae	965	0	964	0	0
1	Af	965	0	964	0	0
1	Ag	965	0	964	0	0
1	Ah	965	0	964	0	0
1	Ai	965	0	964	0	0
1	Aj	965	0	964	0	0
1	Ak	965	0	964	0	0
1	Al	965	0	964	0	0
1	Am	965	0	964	0	0
1	An	965	0	964	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ao	965	0	964	0	0
1	Ap	965	0	964	0	0
1	Aq	965	0	964	0	0
1	Ar	965	0	964	0	0
1	As	965	0	964	0	0
1	At	965	0	964	0	0
1	Au	965	0	964	0	0
1	Av	965	0	964	0	0
1	Aw	965	0	964	0	0
1	Ax	965	0	964	0	0
1	B0	965	0	964	9	0
1	B1	965	0	964	9	0
1	B2	965	0	964	9	0
1	B3	965	0	964	9	0
1	B4	965	0	964	9	0
1	B5	965	0	964	10	0
1	B6	965	0	964	9	0
1	B7	965	0	964	10	0
1	B8	965	0	964	9	0
1	B9	965	0	964	9	0
1	BA	965	0	964	15	0
1	BB	965	0	964	11	0
1	BC	965	0	964	16	0
1	BD	965	0	964	14	0
1	BE	965	0	964	14	0
1	BF	965	0	964	15	0
1	BG	965	0	964	13	0
1	BH	965	0	964	15	0
1	BI	965	0	964	15	0
1	BJ	965	0	964	14	0
1	BK	965	0	964	14	0
1	BL	965	0	964	16	0
1	BM	965	0	964	14	0
1	BN	965	0	964	14	0
1	BO	965	0	964	15	0
1	BP	965	0	964	15	0
1	BQ	965	0	964	14	0
1	BR	965	0	964	15	0
1	BS	965	0	964	12	0
1	BT	965	0	964	15	0
1	BU	965	0	964	14	0
1	BV	965	0	964	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BW	965	0	964	15	0
1	BX	965	0	964	14	0
1	BY	965	0	964	9	0
1	BZ	965	0	964	10	0
1	Ba	965	0	964	0	0
1	Bb	965	0	964	0	0
1	Bc	965	0	964	0	0
1	Bd	965	0	964	0	0
1	Be	965	0	964	0	0
1	Bf	965	0	964	0	0
1	Bg	965	0	964	0	0
1	Bh	965	0	964	0	0
1	Bi	965	0	964	0	0
1	Bj	965	0	964	0	0
1	Bk	965	0	964	0	0
1	Bl	965	0	964	0	0
1	Bm	965	0	964	0	0
1	Bn	965	0	964	0	0
1	Bo	965	0	964	0	0
1	Bp	965	0	964	0	0
1	Bq	965	0	964	0	0
1	Br	965	0	964	0	0
1	Bs	965	0	964	0	0
1	Bt	965	0	964	0	0
1	Bu	965	0	964	0	0
1	Bv	965	0	964	0	0
1	Bw	965	0	964	0	0
1	Bx	965	0	964	0	0
1	C0	965	0	964	7	0
1	C1	965	0	964	6	0
1	C2	965	0	964	6	0
1	C3	965	0	964	6	0
1	C4	965	0	964	6	0
1	C5	965	0	964	5	0
1	C6	965	0	964	7	0
1	C7	965	0	964	5	0
1	C8	965	0	964	6	0
1	C9	965	0	964	6	0
1	CA	965	0	964	8	0
1	CB	965	0	964	7	0
1	CC	965	0	964	7	0
1	CD	965	0	964	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CE	965	0	964	8	0
1	CF	965	0	964	8	0
1	CG	965	0	964	8	0
1	CH	965	0	964	8	0
1	CI	965	0	964	7	0
1	CJ	965	0	964	8	0
1	CK	965	0	964	7	0
1	CL	965	0	964	6	0
1	CM	965	0	964	7	0
1	CN	965	0	964	8	0
1	CO	965	0	964	8	0
1	CP	965	0	964	8	0
1	CQ	965	0	964	8	0
1	CR	965	0	964	7	0
1	CS	965	0	964	8	0
1	CT	965	0	964	8	0
1	CU	965	0	964	8	0
1	CV	965	0	964	8	0
1	CW	965	0	964	7	0
1	CX	965	0	964	8	0
1	CY	965	0	964	6	0
1	CZ	965	0	964	5	0
1	Ca	965	0	964	0	0
1	Cb	965	0	964	0	0
1	Cc	965	0	964	0	0
1	Cd	965	0	964	0	0
1	Ce	965	0	964	0	0
1	Cf	965	0	964	0	0
1	Cg	965	0	964	0	0
1	Ch	965	0	964	0	0
1	Ci	965	0	964	0	0
1	Cj	965	0	964	0	0
1	Ck	965	0	964	0	0
1	Cl	965	0	964	0	0
1	Cm	965	0	964	0	0
1	Cn	965	0	964	0	0
1	Co	965	0	964	0	0
1	Cp	965	0	964	0	0
1	Cq	965	0	964	0	0
1	Cr	965	0	964	0	0
1	Cs	965	0	964	0	0
1	Ct	965	0	964	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Cu	965	0	964	0	0
1	Cv	965	0	964	0	0
1	Cw	965	0	964	0	0
1	Cx	965	0	964	0	0
All	All	173700	0	173520	842	0

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 2.

All (842) 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:AN:128:ILE:HA	1:BJ:3:ASN:HD22	213.87	0.74
1:AV:128:ILE:HA	1:BR:3:ASN:HD22	1.53	0.74
1:AF:128:ILE:HA	1:BG:3:ASN:HD22	1.53	0.74
1:AX:128:ILE:HA	1:BY:3:ASN:HD22	1.53	0.74
1:AE:128:ILE:HA	1:BG:3:ASN:HD22	148.66	0.74
1:AX:128:ILE:HA	1:BT:3:ASN:HD22	182.74	0.74
1:AO:128:ILE:HA	1:BP:3:ASN:HD22	1.53	0.74
1:A6:128:ILE:HA	1:B9:3:ASN:HD22	1.53	0.74
1:AB:128:ILE:HA	1:BI:3:ASN:HD22	73.85	0.74
1:AP:128:ILE:HA	1:BL:3:ASN:HD22	188.49	0.74
1:AM:128:ILE:HA	1:BH:3:ASN:HD22	213.99	0.74
1:AM:128:ILE:HA	1:BN:3:ASN:HD22	1.53	0.74
1:A9:128:ILE:HA	1:B7:3:ASN:HD22	1.53	0.74
1:AT:128:ILE:HA	1:BU:3:ASN:HD22	1.53	0.73
1:AT:128:ILE:HA	1:BK:3:ASN:HD22	238.60	0.73
1:AF:128:ILE:HA	1:BO:3:ASN:HD22	182.74	0.73
1:AG:128:ILE:HA	1:BD:3:ASN:HD22	184.28	0.73
1:AJ:128:ILE:HA	1:B1:3:ASN:HD22	1.53	0.73
1:AV:128:ILE:HA	1:BK:3:ASN:HD22	212.51	0.73
1:AS:128:ILE:HA	1:BP:3:ASN:HD22	83.12	0.73
1:AK:128:ILE:HA	1:BL:3:ASN:HD22	1.53	0.73
1:AY:128:ILE:HA	1:BH:3:ASN:HD22	1.53	0.73
1:AZ:128:ILE:HA	1:BZ:3:ASN:HD22	1.53	0.73
1:AU:128:ILE:HA	1:B5:3:ASN:HD22	1.53	0.73
1:AD:128:ILE:HA	1:BW:3:ASN:HD22	182.52	0.73
1:A7:128:ILE:HA	1:BT:3:ASN:HD22	1.53	0.73
1:A8:128:ILE:HA	1:BN:3:ASN:HD22	145.47	0.73
1:AQ:128:ILE:HA	1:BS:3:ASN:HD22	1.53	0.73
1:AC:128:ILE:HA	1:BB:3:ASN:HD22	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A0:128:ILE:HA	1:BE:3:ASN:HD22	182.74	0.73
1:AL:128:ILE:HA	1:B2:3:ASN:HD22	1.53	0.73
1:AB:128:ILE:HA	1:BA:3:ASN:HD22	1.53	0.73
1:AR:128:ILE:HA	1:BX:3:ASN:HD22	130.79	0.73
1:AH:128:ILE:HA	1:BI:3:ASN:HD22	1.53	0.73
1:AW:128:ILE:HA	1:BU:3:ASN:HD22	54.33	0.73
1:AI:128:ILE:HA	1:BV:3:ASN:HD22	184.29	0.73
1:AK:128:ILE:HA	1:BM:3:ASN:HD22	101.19	0.73
1:AA:128:ILE:HA	1:B0:3:ASN:HD22	216.97	0.73
1:AD:128:ILE:HA	1:BC:3:ASN:HD22	1.53	0.73
1:A1:128:ILE:HA	1:BM:3:ASN:HD22	1.53	0.73
1:AA:128:ILE:HA	1:BE:3:ASN:HD22	1.53	0.73
1:A2:128:ILE:HA	1:BO:3:ASN:HD22	1.53	0.72
1:AR:128:ILE:HA	1:BF:3:ASN:HD22	1.53	0.72
1:AG:128:ILE:HA	1:BW:3:ASN:HD22	1.53	0.72
1:AW:128:ILE:HA	1:BV:3:ASN:HD22	1.53	0.72
1:AH:128:ILE:HA	1:B3:3:ASN:HD22	181.47	0.72
1:A4:128:ILE:HA	1:BX:3:ASN:HD22	1.53	0.72
1:AU:128:ILE:HA	1:BF:3:ASN:HD22	149.49	0.72
1:A3:128:ILE:HA	1:B8:3:ASN:HD22	1.53	0.72
1:AI:128:ILE:HA	1:BJ:3:ASN:HD22	1.53	0.72
1:AL:128:ILE:HA	1:BA:3:ASN:HD22	149.49	0.72
1:A5:128:ILE:HA	1:BQ:3:ASN:HD22	235.73	0.72
1:AN:128:ILE:HA	1:BC:3:ASN:HD22	148.66	0.71
1:AO:128:ILE:HA	1:B6:3:ASN:HD22	212.51	0.71
1:AJ:128:ILE:HA	1:BR:3:ASN:HD22	194.63	0.71
1:AS:128:ILE:HA	1:B4:3:ASN:HD22	1.53	0.71
1:AE:128:ILE:HA	1:BD:3:ASN:HD22	1.53	0.71
1:AP:128:ILE:HA	1:BQ:3:ASN:HD22	1.53	0.70
1:C6:10:VAL:HG12	1:C6:12:ASN:HB2	1.79	0.64
1:A9:97:THR:HG22	1:A9:99:SER:H	1.63	0.64
1:AV:97:THR:HG22	1:AV:99:SER:H	1.63	0.64
1:AW:97:THR:HG22	1:AW:99:SER:H	1.63	0.64
1:CF:10:VAL:HG12	1:CF:12:ASN:HB2	1.79	0.64
1:CS:10:VAL:HG12	1:CS:12:ASN:HB2	1.79	0.64
1:C2:10:VAL:HG12	1:C2:12:ASN:HB2	1.79	0.64
1:CG:10:VAL:HG12	1:CG:12:ASN:HB2	1.80	0.64
1:C8:10:VAL:HG12	1:C8:12:ASN:HB2	1.79	0.64
1:A8:97:THR:HG22	1:A8:99:SER:H	1.62	0.64
1:A0:97:THR:HG22	1:A0:99:SER:H	1.63	0.64
1:CH:10:VAL:HG12	1:CH:12:ASN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AN:97:THR:HG22	1:AN:99:SER:H	1.62	0.64
1:CL:10:VAL:HG12	1:CL:12:ASN:HB2	1.79	0.64
1:AI:97:THR:HG22	1:AI:99:SER:H	1.63	0.64
1:CE:10:VAL:HG12	1:CE:12:ASN:HB2	1.79	0.64
1:CU:10:VAL:HG12	1:CU:12:ASN:HB2	1.79	0.64
1:C4:10:VAL:HG12	1:C4:12:ASN:HB2	1.79	0.64
1:A1:97:THR:HG22	1:A1:99:SER:H	1.63	0.64
1:AB:97:THR:HG22	1:AB:99:SER:H	1.63	0.64
1:C9:10:VAL:HG12	1:C9:12:ASN:HB2	1.79	0.64
1:AT:97:THR:HG22	1:AT:99:SER:H	1.63	0.64
1:AR:97:THR:HG22	1:AR:99:SER:H	1.63	0.64
1:AD:97:THR:HG22	1:AD:99:SER:H	1.63	0.64
1:CA:10:VAL:HG12	1:CA:12:ASN:HB2	1.79	0.64
1:AX:97:THR:HG22	1:AX:99:SER:H	1.63	0.64
1:A6:97:THR:HG22	1:A6:99:SER:H	1.63	0.64
1:CM:10:VAL:HG12	1:CM:12:ASN:HB2	1.80	0.64
1:AJ:97:THR:HG22	1:AJ:99:SER:H	1.63	0.64
1:AS:97:THR:HG22	1:AS:99:SER:H	1.63	0.64
1:A2:97:THR:HG22	1:A2:99:SER:H	1.63	0.64
1:CQ:10:VAL:HG12	1:CQ:12:ASN:HB2	1.80	0.64
1:AE:97:THR:HG22	1:AE:99:SER:H	1.63	0.64
1:AF:97:THR:HG22	1:AF:99:SER:H	1.63	0.64
1:AO:97:THR:HG22	1:AO:99:SER:H	1.63	0.64
1:CX:10:VAL:HG12	1:CX:12:ASN:HB2	1.79	0.64
1:CN:10:VAL:HG12	1:CN:12:ASN:HB2	1.79	0.64
1:AC:97:THR:HG22	1:AC:99:SER:H	1.63	0.64
1:A5:97:THR:HG22	1:A5:99:SER:H	1.63	0.64
1:AG:97:THR:HG22	1:AG:99:SER:H	1.63	0.64
1:CW:10:VAL:HG12	1:CW:12:ASN:HB2	1.79	0.64
1:AL:97:THR:HG22	1:AL:99:SER:H	1.63	0.64
1:CY:10:VAL:HG12	1:CY:12:ASN:HB2	1.79	0.64
1:AM:97:THR:HG22	1:AM:99:SER:H	1.63	0.64
1:CO:10:VAL:HG12	1:CO:12:ASN:HB2	1.79	0.64
1:CC:10:VAL:HG12	1:CC:12:ASN:HB2	1.80	0.64
1:CV:10:VAL:HG12	1:CV:12:ASN:HB2	1.79	0.64
1:CP:10:VAL:HG12	1:CP:12:ASN:HB2	1.79	0.64
1:AU:97:THR:HG22	1:AU:99:SER:H	1.63	0.64
1:CK:10:VAL:HG12	1:CK:12:ASN:HB2	1.80	0.64
1:AY:97:THR:HG22	1:AY:99:SER:H	1.63	0.64
1:AA:97:THR:HG22	1:AA:99:SER:H	1.63	0.64
1:CR:10:VAL:HG12	1:CR:12:ASN:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CI:10:VAL:HG12	1:CI:12:ASN:HB2	1.80	0.63
1:C0:10:VAL:HG12	1:C0:12:ASN:HB2	1.79	0.63
1:C1:10:VAL:HG12	1:C1:12:ASN:HB2	1.79	0.63
1:AH:97:THR:HG22	1:AH:99:SER:H	1.63	0.63
1:CJ:10:VAL:HG12	1:CJ:12:ASN:HB2	1.79	0.63
1:AK:97:THR:HG22	1:AK:99:SER:H	1.63	0.63
1:CD:10:VAL:HG12	1:CD:12:ASN:HB2	1.79	0.63
1:C5:10:VAL:HG12	1:C5:12:ASN:HB2	1.79	0.63
1:CB:10:VAL:HG12	1:CB:12:ASN:HB2	1.79	0.63
1:A4:97:THR:HG22	1:A4:99:SER:H	1.63	0.63
1:AP:97:THR:HG22	1:AP:99:SER:H	1.63	0.63
1:AQ:97:THR:HG22	1:AQ:99:SER:H	1.63	0.63
1:C7:10:VAL:HG12	1:C7:12:ASN:HB2	1.79	0.62
1:A3:97:THR:HG22	1:A3:99:SER:H	1.63	0.62
1:AZ:97:THR:HG22	1:AZ:99:SER:H	1.63	0.62
1:CT:10:VAL:HG12	1:CT:12:ASN:HB2	1.79	0.62
1:A7:97:THR:HG22	1:A7:99:SER:H	1.63	0.62
1:CZ:10:VAL:HG12	1:CZ:12:ASN:HB2	1.80	0.61
1:C3:10:VAL:HG12	1:C3:12:ASN:HB2	1.80	0.61
1:BA:20:VAL:HG13	1:BA:32:TRP:HB3	1.84	0.60
1:BU:20:VAL:HG13	1:BU:32:TRP:HB3	1.83	0.60
1:BQ:20:VAL:HG13	1:BQ:32:TRP:HB3	1.84	0.60
1:BC:20:VAL:HG13	1:BC:32:TRP:HB3	1.83	0.60
1:BF:20:VAL:HG13	1:BF:32:TRP:HB3	1.83	0.60
1:BV:20:VAL:HG13	1:BV:32:TRP:HB3	1.83	0.60
1:BH:20:VAL:HG13	1:BH:32:TRP:HB3	1.83	0.60
1:BR:20:VAL:HG13	1:BR:32:TRP:HB3	1.83	0.60
1:BB:20:VAL:HG13	1:BB:32:TRP:HB3	1.84	0.60
1:BK:20:VAL:HG13	1:BK:32:TRP:HB3	1.83	0.60
1:BX:20:VAL:HG13	1:BX:32:TRP:HB3	1.83	0.60
1:BE:20:VAL:HG13	1:BE:32:TRP:HB3	1.83	0.60
1:BN:20:VAL:HG13	1:BN:32:TRP:HB3	1.83	0.60
1:B6:20:VAL:HG13	1:B6:32:TRP:HB3	1.83	0.60
1:B7:20:VAL:HG13	1:B7:32:TRP:HB3	1.83	0.60
1:BY:20:VAL:HG13	1:BY:32:TRP:HB3	1.84	0.60
1:BJ:20:VAL:HG13	1:BJ:32:TRP:HB3	1.83	0.60
1:B0:20:VAL:HG13	1:B0:32:TRP:HB3	1.84	0.60
1:B1:20:VAL:HG13	1:B1:32:TRP:HB3	1.84	0.60
1:BD:20:VAL:HG13	1:BD:32:TRP:HB3	1.84	0.60
1:BM:20:VAL:HG13	1:BM:32:TRP:HB3	1.84	0.60
1:BW:20:VAL:HG13	1:BW:32:TRP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:20:VAL:HG13	1:B5:32:TRP:HB3	1.83	0.60
1:BT:20:VAL:HG13	1:BT:32:TRP:HB3	1.84	0.60
1:BO:20:VAL:HG13	1:BO:32:TRP:HB3	1.84	0.60
1:BL:20:VAL:HG13	1:BL:32:TRP:HB3	1.84	0.59
1:B3:20:VAL:HG13	1:B3:32:TRP:HB3	1.83	0.59
1:BI:20:VAL:HG13	1:BI:32:TRP:HB3	1.83	0.59
1:BP:20:VAL:HG13	1:BP:32:TRP:HB3	1.84	0.59
1:BS:20:VAL:HG13	1:BS:32:TRP:HB3	1.84	0.59
1:BG:20:VAL:HG13	1:BG:32:TRP:HB3	1.84	0.59
1:B4:20:VAL:HG13	1:B4:32:TRP:HB3	1.84	0.59
1:BZ:20:VAL:HG13	1:BZ:32:TRP:HB3	1.83	0.59
1:B8:20:VAL:HG13	1:B8:32:TRP:HB3	1.83	0.58
1:B2:20:VAL:HG13	1:B2:32:TRP:HB3	1.84	0.58
1:B9:20:VAL:HG13	1:B9:32:TRP:HB3	1.83	0.58
1:AQ:129:TYR:OH	1:BS:1:ALA:HB3	2.06	0.56
1:AO:129:TYR:OH	1:BP:1:ALA:HB3	2.06	0.56
1:AF:129:TYR:OH	1:BO:1:ALA:HB3	192.89	0.56
1:AE:129:TYR:OH	1:BD:1:ALA:HB3	2.06	0.56
1:AU:129:TYR:OH	1:B5:1:ALA:HB3	2.06	0.56
1:A9:129:TYR:OH	1:B7:1:ALA:HB3	2.06	0.56
1:A3:129:TYR:OH	1:B8:1:ALA:HB3	2.06	0.56
1:AS:129:TYR:OH	1:BP:1:ALA:HB3	94.09	0.56
1:AT:129:TYR:OH	1:BK:1:ALA:HB3	242.79	0.56
1:AN:129:TYR:OH	1:BJ:1:ALA:HB3	221.26	0.56
1:AW:129:TYR:OH	1:BU:1:ALA:HB3	47.21	0.56
1:AD:129:TYR:OH	1:BW:1:ALA:HB3	192.20	0.56
1:A8:20:VAL:HG13	1:A8:32:TRP:HB3	1.88	0.56
1:AM:129:TYR:OH	1:BH:1:ALA:HB3	218.99	0.56
1:AC:129:TYR:OH	1:BB:1:ALA:HB3	2.06	0.56
1:AP:129:TYR:OH	1:BQ:1:ALA:HB3	2.06	0.56
1:AH:20:VAL:HG13	1:AH:32:TRP:HB3	1.88	0.56
1:AN:129:TYR:OH	1:BC:1:ALA:HB3	157.36	0.56
1:A4:129:TYR:OH	1:BX:1:ALA:HB3	2.06	0.56
1:AL:20:VAL:HG13	1:AL:32:TRP:HB3	1.88	0.56
1:AU:20:VAL:HG13	1:AU:32:TRP:HB3	1.88	0.56
1:AH:129:TYR:OH	1:B3:1:ALA:HB3	182.80	0.56
1:AB:129:TYR:OH	1:BA:1:ALA:HB3	2.06	0.56
1:AP:129:TYR:OH	1:BL:1:ALA:HB3	191.18	0.56
1:AX:129:TYR:OH	1:BT:1:ALA:HB3	192.89	0.56
1:A7:20:VAL:HG13	1:A7:32:TRP:HB3	1.88	0.56
1:AJ:129:TYR:OH	1:B1:1:ALA:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AG:129:TYR:OH	1:BD:1:ALA:HB3	195.81	0.56
1:AA:20:VAL:HG13	1:AA:32:TRP:HB3	1.88	0.56
1:AB:20:VAL:HG13	1:AB:32:TRP:HB3	1.88	0.56
1:CS:20:VAL:HG13	1:CS:32:TRP:HB3	1.89	0.56
1:AI:20:VAL:HG13	1:AI:32:TRP:HB3	1.88	0.56
1:AV:129:TYR:OH	1:BK:1:ALA:HB3	219.08	0.55
1:AI:129:TYR:OH	1:BV:1:ALA:HB3	195.81	0.55
1:AG:129:TYR:OH	1:BW:1:ALA:HB3	2.06	0.55
1:AU:129:TYR:OH	1:BF:1:ALA:HB3	157.27	0.55
1:AY:129:TYR:OH	1:BH:1:ALA:HB3	2.06	0.55
1:C6:20:VAL:HG13	1:C6:32:TRP:HB3	1.88	0.55
1:AK:20:VAL:HG13	1:AK:32:TRP:HB3	1.88	0.55
1:A2:20:VAL:HG13	1:A2:32:TRP:HB3	1.88	0.55
1:AW:20:VAL:HG13	1:AW:32:TRP:HB3	1.88	0.55
1:A3:20:VAL:HG13	1:A3:32:TRP:HB3	1.88	0.55
1:AA:129:TYR:OH	1:B0:1:ALA:HB3	222.55	0.55
1:A5:20:VAL:HG13	1:A5:32:TRP:HB3	1.88	0.55
1:AF:20:VAL:HG13	1:AF:32:TRP:HB3	1.88	0.55
1:CO:20:VAL:HG13	1:CO:32:TRP:HB3	1.89	0.55
1:AE:129:TYR:OH	1:BG:1:ALA:HB3	157.36	0.55
1:CR:20:VAL:HG13	1:CR:32:TRP:HB3	1.89	0.55
1:AG:20:VAL:HG13	1:AG:32:TRP:HB3	1.88	0.55
1:CK:20:VAL:HG13	1:CK:32:TRP:HB3	1.89	0.55
1:AR:20:VAL:HG13	1:AR:32:TRP:HB3	1.88	0.55
1:CN:20:VAL:HG13	1:CN:32:TRP:HB3	1.89	0.55
1:AT:129:TYR:OH	1:BU:1:ALA:HB3	2.06	0.55
1:AB:129:TYR:OH	1:BI:1:ALA:HB3	72.20	0.55
1:A7:129:TYR:OH	1:BT:1:ALA:HB3	2.06	0.55
1:AA:129:TYR:OH	1:BE:1:ALA:HB3	2.06	0.55
1:AJ:20:VAL:HG13	1:AJ:32:TRP:HB3	1.88	0.55
1:CY:20:VAL:HG13	1:CY:32:TRP:HB3	1.89	0.55
1:CQ:20:VAL:HG13	1:CQ:32:TRP:HB3	1.89	0.55
1:C0:20:VAL:HG13	1:C0:32:TRP:HB3	1.89	0.55
1:CC:20:VAL:HG13	1:CC:32:TRP:HB3	1.89	0.55
1:CD:20:VAL:HG13	1:CD:32:TRP:HB3	1.89	0.55
1:C3:20:VAL:HG13	1:C3:32:TRP:HB3	1.89	0.55
1:AD:129:TYR:OH	1:BC:1:ALA:HB3	2.06	0.55
1:AK:129:TYR:OH	1:BM:1:ALA:HB3	99.73	0.55
1:AL:129:TYR:OH	1:BA:1:ALA:HB3	157.27	0.55
1:A0:129:TYR:OH	1:BE:1:ALA:HB3	192.89	0.55
1:CX:20:VAL:HG13	1:CX:32:TRP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CP:20:VAL:HG13	1:CP:32:TRP:HB3	1.89	0.55
1:CH:20:VAL:HG13	1:CH:32:TRP:HB3	1.89	0.55
1:A6:20:VAL:HG13	1:A6:32:TRP:HB3	1.88	0.55
1:AZ:129:TYR:OH	1:BZ:1:ALA:HB3	2.06	0.55
1:CB:20:VAL:HG13	1:CB:32:TRP:HB3	1.89	0.55
1:CV:20:VAL:HG13	1:CV:32:TRP:HB3	1.89	0.55
1:AP:20:VAL:HG13	1:AP:32:TRP:HB3	1.88	0.55
1:AZ:20:VAL:HG13	1:AZ:32:TRP:HB3	1.88	0.55
1:AW:129:TYR:OH	1:BV:1:ALA:HB3	2.06	0.55
1:AR:129:TYR:OH	1:BF:1:ALA:HB3	2.06	0.55
1:A8:129:TYR:OH	1:BN:1:ALA:HB3	152.36	0.55
1:AM:129:TYR:OH	1:BN:1:ALA:HB3	2.06	0.55
1:A1:129:TYR:OH	1:BM:1:ALA:HB3	2.06	0.55
1:AL:129:TYR:OH	1:B2:1:ALA:HB3	2.06	0.55
1:CJ:20:VAL:HG13	1:CJ:32:TRP:HB3	1.89	0.55
1:AV:20:VAL:HG13	1:AV:32:TRP:HB3	1.88	0.55
1:CM:20:VAL:HG13	1:CM:32:TRP:HB3	1.89	0.55
1:AF:129:TYR:OH	1:BG:1:ALA:HB3	2.06	0.55
1:A5:129:TYR:OH	1:BQ:1:ALA:HB3	244.04	0.55
1:AK:129:TYR:OH	1:BL:1:ALA:HB3	2.06	0.55
1:AS:20:VAL:HG13	1:AS:32:TRP:HB3	1.88	0.55
1:CI:20:VAL:HG13	1:CI:32:TRP:HB3	1.89	0.55
1:AC:20:VAL:HG13	1:AC:32:TRP:HB3	1.88	0.55
1:AM:20:VAL:HG13	1:AM:32:TRP:HB3	1.88	0.55
1:AO:129:TYR:OH	1:B6:1:ALA:HB3	219.08	0.55
1:AH:129:TYR:OH	1:BI:1:ALA:HB3	2.06	0.55
1:AQ:20:VAL:HG13	1:AQ:32:TRP:HB3	1.88	0.55
1:AT:20:VAL:HG13	1:AT:32:TRP:HB3	1.88	0.55
1:CE:20:VAL:HG13	1:CE:32:TRP:HB3	1.89	0.55
1:AI:129:TYR:OH	1:BJ:1:ALA:HB3	2.06	0.55
1:A2:129:TYR:OH	1:BO:1:ALA:HB3	2.06	0.55
1:AX:129:TYR:OH	1:BY:1:ALA:HB3	2.06	0.55
1:CZ:20:VAL:HG13	1:CZ:32:TRP:HB3	1.89	0.55
1:AO:20:VAL:HG13	1:AO:32:TRP:HB3	1.88	0.55
1:AJ:129:TYR:OH	1:BR:1:ALA:HB3	206.01	0.55
1:AD:20:VAL:HG13	1:AD:32:TRP:HB3	1.88	0.55
1:AX:20:VAL:HG13	1:AX:32:TRP:HB3	1.88	0.55
1:AV:129:TYR:OH	1:BR:1:ALA:HB3	2.06	0.55
1:CW:20:VAL:HG13	1:CW:32:TRP:HB3	1.89	0.55
1:AE:20:VAL:HG13	1:AE:32:TRP:HB3	1.88	0.55
1:AS:129:TYR:OH	1:B4:1:ALA:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CG:20:VAL:HG13	1:CG:32:TRP:HB3	1.89	0.54
1:A6:129:TYR:OH	1:B9:1:ALA:HB3	2.06	0.54
1:CU:20:VAL:HG13	1:CU:32:TRP:HB3	1.89	0.54
1:A4:20:VAL:HG13	1:A4:32:TRP:HB3	1.88	0.54
1:AR:129:TYR:OH	1:BX:1:ALA:HB3	135.81	0.54
1:AN:20:VAL:HG13	1:AN:32:TRP:HB3	1.88	0.54
1:AY:20:VAL:HG13	1:AY:32:TRP:HB3	1.88	0.54
1:CL:20:VAL:HG13	1:CL:32:TRP:HB3	1.89	0.54
1:CF:20:VAL:HG13	1:CF:32:TRP:HB3	1.89	0.54
1:CA:20:VAL:HG13	1:CA:32:TRP:HB3	1.89	0.54
1:C1:20:VAL:HG13	1:C1:32:TRP:HB3	1.89	0.54
1:C2:20:VAL:HG13	1:C2:32:TRP:HB3	1.89	0.54
1:BO:105:VAL:O	1:BO:109:GLN:HG2	2.08	0.54
1:BJ:105:VAL:O	1:BJ:109:GLN:HG2	2.08	0.54
1:BF:105:VAL:O	1:BF:109:GLN:HG2	2.08	0.54
1:A0:20:VAL:HG13	1:A0:32:TRP:HB3	1.88	0.54
1:C7:20:VAL:HG13	1:C7:32:TRP:HB3	1.89	0.54
1:BQ:105:VAL:O	1:BQ:109:GLN:HG2	2.08	0.54
1:B7:105:VAL:O	1:B7:109:GLN:HG2	2.08	0.54
1:BA:105:VAL:O	1:BA:109:GLN:HG2	2.08	0.54
1:BT:105:VAL:O	1:BT:109:GLN:HG2	2.08	0.54
1:BM:105:VAL:O	1:BM:109:GLN:HG2	2.08	0.54
1:BC:105:VAL:O	1:BC:109:GLN:HG2	2.08	0.54
1:BV:105:VAL:O	1:BV:109:GLN:HG2	2.08	0.54
1:BU:105:VAL:O	1:BU:109:GLN:HG2	2.08	0.54
1:BE:105:VAL:O	1:BE:109:GLN:HG2	2.08	0.54
1:C5:20:VAL:HG13	1:C5:32:TRP:HB3	1.89	0.54
1:BI:105:VAL:O	1:BI:109:GLN:HG2	2.08	0.54
1:CT:20:VAL:HG13	1:CT:32:TRP:HB3	1.89	0.54
1:B0:105:VAL:O	1:B0:109:GLN:HG2	2.08	0.54
1:BK:105:VAL:O	1:BK:109:GLN:HG2	2.08	0.54
1:BL:105:VAL:O	1:BL:109:GLN:HG2	2.08	0.54
1:B3:105:VAL:O	1:B3:109:GLN:HG2	2.08	0.54
1:BX:105:VAL:O	1:BX:109:GLN:HG2	2.08	0.54
1:BY:105:VAL:O	1:BY:109:GLN:HG2	2.08	0.54
1:B8:105:VAL:O	1:B8:109:GLN:HG2	2.08	0.54
1:BB:105:VAL:O	1:BB:109:GLN:HG2	2.08	0.54
1:B5:105:VAL:O	1:B5:109:GLN:HG2	2.08	0.53
1:BG:105:VAL:O	1:BG:109:GLN:HG2	2.08	0.53
1:A9:20:VAL:HG13	1:A9:32:TRP:HB3	1.88	0.53
1:A1:20:VAL:HG13	1:A1:32:TRP:HB3	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C8:20:VAL:HG13	1:C8:32:TRP:HB3	1.89	0.53
1:C9:20:VAL:HG13	1:C9:32:TRP:HB3	1.89	0.53
1:B2:105:VAL:O	1:B2:109:GLN:HG2	2.08	0.53
1:BR:105:VAL:O	1:BR:109:GLN:HG2	2.08	0.53
1:BD:105:VAL:O	1:BD:109:GLN:HG2	2.08	0.53
1:C4:20:VAL:HG13	1:C4:32:TRP:HB3	1.89	0.53
1:BP:105:VAL:O	1:BP:109:GLN:HG2	2.08	0.53
1:BH:105:VAL:O	1:BH:109:GLN:HG2	2.08	0.53
1:B1:105:VAL:O	1:B1:109:GLN:HG2	2.08	0.53
1:BW:105:VAL:O	1:BW:109:GLN:HG2	2.08	0.53
1:B6:105:VAL:O	1:B6:109:GLN:HG2	2.08	0.53
1:BZ:105:VAL:O	1:BZ:109:GLN:HG2	2.08	0.53
1:BS:105:VAL:O	1:BS:109:GLN:HG2	2.08	0.53
1:BN:105:VAL:O	1:BN:109:GLN:HG2	2.08	0.53
1:A7:97:THR:HG22	1:A7:99:SER:N	2.25	0.52
1:B4:105:VAL:O	1:B4:109:GLN:HG2	2.08	0.52
1:AI:38:ARG:NH1	1:CU:125:ASN:O	168.34	0.52
1:AB:97:THR:HG22	1:AB:99:SER:N	2.25	0.52
1:A6:97:THR:HG22	1:A6:99:SER:N	2.25	0.52
1:AL:97:THR:HG22	1:AL:99:SER:N	2.25	0.52
1:A3:97:THR:HG22	1:A3:99:SER:N	2.25	0.52
1:AA:38:ARG:NH1	1:CF:125:ASN:O	2.43	0.52
1:AH:38:ARG:NH1	1:CG:125:ASN:O	2.43	0.52
1:AE:38:ARG:NH1	1:CP:125:ASN:O	2.43	0.52
1:AL:38:ARG:NH1	1:C9:125:ASN:O	225.25	0.52
1:AB:38:ARG:NH1	1:CH:125:ASN:O	88.15	0.52
1:AR:97:THR:HG22	1:AR:99:SER:N	2.25	0.52
1:AE:97:THR:HG22	1:AE:99:SER:N	2.25	0.52
1:AF:97:THR:HG22	1:AF:99:SER:N	2.25	0.52
1:AO:97:THR:HG22	1:AO:99:SER:N	2.25	0.52
1:AK:97:THR:HG22	1:AK:99:SER:N	2.25	0.52
1:AO:38:ARG:NH1	1:CN:125:ASN:O	2.43	0.52
1:AC:38:ARG:NH1	1:C3:125:ASN:O	203.68	0.52
1:AN:38:ARG:NH1	1:CL:125:ASN:O	147.39	0.52
1:AI:97:THR:HG22	1:AI:99:SER:N	2.25	0.52
1:AD:97:THR:HG22	1:AD:99:SER:N	2.25	0.52
1:AS:97:THR:HG22	1:AS:99:SER:N	2.25	0.52
1:AU:97:THR:HG22	1:AU:99:SER:N	2.25	0.52
1:A6:38:ARG:NH1	1:CA:125:ASN:O	196.48	0.52
1:AS:38:ARG:NH1	1:CT:125:ASN:O	2.43	0.52
1:AA:97:THR:HG22	1:AA:99:SER:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B9:105:VAL:O	1:B9:109:GLN:HG2	2.08	0.52
1:AN:97:THR:HG22	1:AN:99:SER:N	2.25	0.52
1:AT:97:THR:HG22	1:AT:99:SER:N	2.25	0.52
1:AJ:97:THR:HG22	1:AJ:99:SER:N	2.25	0.52
1:AY:97:THR:HG22	1:AY:99:SER:N	2.25	0.52
1:AM:38:ARG:NH1	1:CD:125:ASN:O	2.43	0.52
1:AC:38:ARG:NH1	1:CL:125:ASN:O	2.43	0.52
1:A3:38:ARG:NH1	1:C5:125:ASN:O	2.43	0.52
1:AW:97:THR:HG22	1:AW:99:SER:N	2.25	0.52
1:AQ:97:THR:HG22	1:AQ:99:SER:N	2.25	0.52
1:AZ:97:THR:HG22	1:AZ:99:SER:N	2.25	0.52
1:AE:38:ARG:NH1	1:CI:125:ASN:O	96.37	0.52
1:AG:38:ARG:NH1	1:CH:125:ASN:O	2.43	0.52
1:AK:38:ARG:NH1	1:CO:125:ASN:O	181.26	0.52
1:AZ:38:ARG:NH1	1:CS:125:ASN:O	211.93	0.52
1:AR:38:ARG:NH1	1:C0:125:ASN:O	204.64	0.52
1:AT:38:ARG:NH1	1:CS:125:ASN:O	2.43	0.52
1:AP:38:ARG:NH1	1:CE:125:ASN:O	2.43	0.52
1:AJ:38:ARG:NH1	1:CQ:125:ASN:O	182.20	0.52
1:AG:97:THR:HG22	1:AG:99:SER:N	2.25	0.51
1:A4:97:THR:HG22	1:A4:99:SER:N	2.25	0.51
1:AX:38:ARG:NH1	1:CW:125:ASN:O	2.43	0.51
1:A0:38:ARG:NH1	1:C2:125:ASN:O	2.43	0.51
1:A9:97:THR:HG22	1:A9:99:SER:N	2.25	0.51
1:AA:38:ARG:NH1	1:C8:125:ASN:O	199.71	0.51
1:AJ:38:ARG:NH1	1:CK:125:ASN:O	2.43	0.51
1:A4:38:ARG:NH1	1:C4:125:ASN:O	2.43	0.51
1:A0:97:THR:HG22	1:A0:99:SER:N	2.25	0.51
1:AX:97:THR:HG22	1:AX:99:SER:N	2.25	0.51
1:AM:97:THR:HG22	1:AM:99:SER:N	2.25	0.51
1:AB:38:ARG:NH1	1:CI:125:ASN:O	2.43	0.51
1:AD:38:ARG:NH1	1:CV:125:ASN:O	203.68	0.51
1:AP:38:ARG:NH1	1:CK:125:ASN:O	185.48	0.51
1:AC:97:THR:HG22	1:AC:99:SER:N	2.25	0.51
1:AW:38:ARG:NH1	1:CW:125:ASN:O	39.00	0.51
1:AF:38:ARG:NH1	1:CN:125:ASN:O	140.80	0.51
1:A8:38:ARG:NH1	1:CM:125:ASN:O	204.64	0.51
1:AY:38:ARG:NH1	1:CY:125:ASN:O	2.43	0.51
1:AL:38:ARG:NH1	1:CC:125:ASN:O	2.43	0.51
1:AO:38:ARG:NH1	1:C6:125:ASN:O	223.02	0.51
1:AT:38:ARG:NH1	1:CJ:125:ASN:O	224.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AV:97:THR:HG22	1:AV:99:SER:N	2.25	0.51
1:A8:97:THR:HG22	1:A8:99:SER:N	2.25	0.51
1:AH:97:THR:HG22	1:AH:99:SER:N	2.25	0.51
1:AV:38:ARG:NH1	1:CU:125:ASN:O	2.43	0.51
1:AX:38:ARG:NH1	1:CZ:125:ASN:O	58.39	0.51
1:AF:38:ARG:NH1	1:CA:125:ASN:O	2.43	0.51
1:AS:38:ARG:NH1	1:CR:125:ASN:O	60.32	0.51
1:AI:38:ARG:NH1	1:CB:125:ASN:O	2.43	0.51
1:AQ:38:ARG:NH1	1:CT:125:ASN:O	58.39	0.51
1:AQ:38:ARG:NH1	1:CR:125:ASN:O	2.43	0.51
1:AU:38:ARG:NH1	1:CV:125:ASN:O	2.43	0.51
1:AA:60:ILE:HB	1:AA:88:MET:HG3	1.93	0.51
1:A9:38:ARG:NH1	1:C7:125:ASN:O	2.43	0.51
1:AN:38:ARG:NH1	1:CO:125:ASN:O	2.43	0.51
1:AP:97:THR:HG22	1:AP:99:SER:N	2.25	0.51
1:AK:38:ARG:NH1	1:CJ:125:ASN:O	2.43	0.51
1:AW:60:ILE:HB	1:AW:88:MET:HG3	1.93	0.51
1:AK:60:ILE:HB	1:AK:88:MET:HG3	1.93	0.51
1:A8:60:ILE:HB	1:A8:88:MET:HG3	1.93	0.51
1:A1:97:THR:HG22	1:A1:99:SER:N	2.25	0.51
1:AW:38:ARG:NH1	1:CX:125:ASN:O	2.43	0.51
1:AG:38:ARG:NH1	1:CC:125:ASN:O	168.18	0.51
1:AG:60:ILE:HB	1:AG:88:MET:HG3	1.93	0.51
1:A1:38:ARG:NH1	1:C1:125:ASN:O	2.43	0.51
1:AQ:60:ILE:HB	1:AQ:88:MET:HG3	1.93	0.51
1:AL:60:ILE:HB	1:AL:88:MET:HG3	1.93	0.51
1:A7:60:ILE:HB	1:A7:88:MET:HG3	1.93	0.51
1:AB:60:ILE:HB	1:AB:88:MET:HG3	1.93	0.51
1:AT:60:ILE:HB	1:AT:88:MET:HG3	1.93	0.51
1:AU:60:ILE:HB	1:AU:88:MET:HG3	1.93	0.51
1:A0:60:ILE:HB	1:A0:88:MET:HG3	1.93	0.51
1:AX:60:ILE:HB	1:AX:88:MET:HG3	1.93	0.51
1:A2:97:THR:HG22	1:A2:99:SER:N	2.25	0.50
1:A2:38:ARG:NH1	1:CD:125:ASN:O	108.63	0.50
1:AM:38:ARG:NH1	1:CG:125:ASN:O	171.74	0.50
1:A5:38:ARG:NH1	1:CP:125:ASN:O	234.74	0.50
1:AH:60:ILE:HB	1:AH:88:MET:HG3	1.93	0.50
1:AI:60:ILE:HB	1:AI:88:MET:HG3	1.93	0.50
1:AR:60:ILE:HB	1:AR:88:MET:HG3	1.93	0.50
1:AS:60:ILE:HB	1:AS:88:MET:HG3	1.93	0.50
1:AN:60:ILE:HB	1:AN:88:MET:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:60:ILE:HB	1:AM:88:MET:HG3	1.93	0.50
1:AV:60:ILE:HB	1:AV:88:MET:HG3	1.93	0.50
1:A3:60:ILE:HB	1:A3:88:MET:HG3	1.93	0.50
1:AD:60:ILE:HB	1:AD:88:MET:HG3	1.93	0.50
1:AH:38:ARG:NH1	1:CF:125:ASN:O	88.15	0.50
1:AU:38:ARG:NH1	1:CE:125:ASN:O	140.80	0.50
1:A2:60:ILE:HB	1:A2:88:MET:HG3	1.93	0.50
1:AD:38:ARG:NH1	1:CM:125:ASN:O	2.43	0.50
1:AP:60:ILE:HB	1:AP:88:MET:HG3	1.93	0.50
1:A7:38:ARG:NH1	1:CB:125:ASN:O	225.25	0.50
1:A5:97:THR:HG22	1:A5:99:SER:N	2.25	0.50
1:AR:38:ARG:NH1	1:CQ:125:ASN:O	2.43	0.50
1:AZ:60:ILE:HB	1:AZ:88:MET:HG3	1.93	0.50
1:A9:60:ILE:HB	1:A9:88:MET:HG3	1.93	0.50
1:AF:60:ILE:HB	1:AF:88:MET:HG3	1.93	0.50
1:A5:60:ILE:HB	1:A5:88:MET:HG3	1.93	0.50
1:AW:3:ASN:O	1:BU:117:PRO:HB3	115.00	0.50
1:AG:3:ASN:O	1:BD:117:PRO:HB3	145.65	0.50
1:AS:3:ASN:O	1:B4:117:PRO:HB3	2.12	0.50
1:AL:3:ASN:O	1:BA:117:PRO:HB3	105.31	0.50
1:AV:38:ARG:NH1	1:CX:125:ASN:O	60.32	0.49
1:AJ:3:ASN:O	1:BR:117:PRO:HB3	193.09	0.49
1:AB:3:ASN:O	1:BI:117:PRO:HB3	80.08	0.49
1:AI:3:ASN:O	1:BJ:117:PRO:HB3	2.12	0.49
1:A5:3:ASN:O	1:BQ:117:PRO:HB3	238.91	0.49
1:AC:3:ASN:O	1:BB:117:PRO:HB3	2.12	0.49
1:A4:60:ILE:HB	1:A4:88:MET:HG3	1.93	0.49
1:AO:60:ILE:HB	1:AO:88:MET:HG3	1.93	0.49
1:A2:3:ASN:O	1:BO:117:PRO:HB3	2.12	0.49
1:AF:3:ASN:O	1:BO:117:PRO:HB3	166.16	0.49
1:AH:3:ASN:O	1:B3:117:PRO:HB3	224.60	0.49
1:AL:3:ASN:O	1:B2:117:PRO:HB3	2.12	0.49
1:AE:60:ILE:HB	1:AE:88:MET:HG3	1.93	0.49
1:AR:3:ASN:O	1:BX:117:PRO:HB3	144.81	0.49
1:A0:3:ASN:O	1:BE:117:PRO:HB3	166.16	0.49
1:A6:3:ASN:O	1:B9:117:PRO:HB3	2.12	0.49
1:AK:3:ASN:O	1:BM:117:PRO:HB3	124.30	0.49
1:AP:3:ASN:O	1:BQ:117:PRO:HB3	2.12	0.49
1:AA:3:ASN:O	1:B0:117:PRO:HB3	220.41	0.49
1:A3:3:ASN:O	1:B8:117:PRO:HB3	2.12	0.49
1:AE:3:ASN:O	1:BG:117:PRO:HB3	105.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AT:3:ASN:O	1:BU:117:PRO:HB3	2.12	0.49
1:AO:3:ASN:O	1:B6:117:PRO:HB3	235.45	0.49
1:A1:3:ASN:O	1:BM:117:PRO:HB3	2.12	0.49
1:AR:3:ASN:O	1:BF:117:PRO:HB3	2.12	0.49
1:AQ:3:ASN:O	1:BS:117:PRO:HB3	2.12	0.49
1:A6:60:ILE:HB	1:A6:88:MET:HG3	1.93	0.49
1:AX:3:ASN:O	1:BY:117:PRO:HB3	2.12	0.49
1:AJ:60:ILE:HB	1:AJ:88:MET:HG3	1.93	0.49
1:AG:3:ASN:O	1:BW:117:PRO:HB3	2.12	0.49
1:AT:3:ASN:O	1:BK:117:PRO:HB3	254.72	0.49
1:AO:3:ASN:O	1:BP:117:PRO:HB3	2.12	0.49
1:AB:3:ASN:O	1:BA:117:PRO:HB3	2.12	0.49
1:AH:3:ASN:O	1:BI:117:PRO:HB3	2.12	0.49
1:AK:3:ASN:O	1:BL:117:PRO:HB3	2.12	0.49
1:A9:3:ASN:O	1:B7:117:PRO:HB3	2.12	0.49
1:AJ:3:ASN:O	1:B1:117:PRO:HB3	2.12	0.49
1:AU:3:ASN:O	1:B5:117:PRO:HB3	2.12	0.49
1:A7:3:ASN:O	1:BT:117:PRO:HB3	2.13	0.49
1:AC:60:ILE:HB	1:AC:88:MET:HG3	1.93	0.49
1:AM:3:ASN:O	1:BH:117:PRO:HB3	220.36	0.49
1:AN:3:ASN:O	1:BC:117:PRO:HB3	105.22	0.49
1:AN:3:ASN:O	1:BJ:117:PRO:HB3	204.07	0.49
1:A4:3:ASN:O	1:BX:117:PRO:HB3	2.12	0.49
1:A1:60:ILE:HB	1:A1:88:MET:HG3	1.93	0.49
1:AD:3:ASN:O	1:BC:117:PRO:HB3	2.12	0.49
1:AV:3:ASN:O	1:BR:117:PRO:HB3	2.12	0.49
1:A8:3:ASN:O	1:BN:117:PRO:HB3	182.72	0.49
1:AV:3:ASN:O	1:BK:117:PRO:HB3	235.45	0.49
1:AW:3:ASN:O	1:BV:117:PRO:HB3	2.12	0.48
1:AY:60:ILE:HB	1:AY:88:MET:HG3	1.93	0.48
1:AI:3:ASN:O	1:BV:117:PRO:HB3	145.65	0.48
1:AS:3:ASN:O	1:BP:117:PRO:HB3	77.26	0.48
1:AU:3:ASN:O	1:BF:117:PRO:HB3	105.31	0.48
1:AY:3:ASN:O	1:BH:117:PRO:HB3	2.12	0.48
1:AD:3:ASN:O	1:BW:117:PRO:HB3	167.99	0.48
1:AF:3:ASN:O	1:BG:117:PRO:HB3	2.12	0.48
1:AP:3:ASN:O	1:BL:117:PRO:HB3	194.94	0.48
1:AZ:3:ASN:O	1:BZ:117:PRO:HB3	2.12	0.48
1:AE:3:ASN:O	1:BD:117:PRO:HB3	2.12	0.48
1:AX:3:ASN:O	1:BT:117:PRO:HB3	166.16	0.48
1:AM:3:ASN:O	1:BN:117:PRO:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A9:86:LEU:HD21	1:A9:88:MET:HE3	1.96	0.48
1:AA:3:ASN:O	1:BE:117:PRO:HB3	2.12	0.48
1:A1:105:VAL:O	1:A1:109:GLN:HG2	2.15	0.47
1:AL:105:VAL:O	1:AL:109:GLN:HG2	2.15	0.47
1:A6:105:VAL:O	1:A6:109:GLN:HG2	2.15	0.47
1:AR:105:VAL:O	1:AR:109:GLN:HG2	2.15	0.47
1:AJ:105:VAL:O	1:AJ:109:GLN:HG2	2.15	0.47
1:A9:105:VAL:O	1:A9:109:GLN:HG2	2.15	0.47
1:AT:105:VAL:O	1:AT:109:GLN:HG2	2.15	0.47
1:A3:105:VAL:O	1:A3:109:GLN:HG2	2.15	0.47
1:AX:105:VAL:O	1:AX:109:GLN:HG2	2.15	0.47
1:AN:105:VAL:O	1:AN:109:GLN:HG2	2.15	0.47
1:A7:105:VAL:O	1:A7:109:GLN:HG2	2.15	0.47
1:AV:105:VAL:O	1:AV:109:GLN:HG2	2.15	0.47
1:AF:105:VAL:O	1:AF:109:GLN:HG2	2.15	0.47
1:AO:105:VAL:O	1:AO:109:GLN:HG2	2.15	0.47
1:AG:105:VAL:O	1:AG:109:GLN:HG2	2.15	0.46
1:BK:38:ARG:NH1	1:BL:125:ASN:O	2.49	0.46
1:AI:105:VAL:O	1:AI:109:GLN:HG2	2.15	0.46
1:A8:105:VAL:O	1:A8:109:GLN:HG2	2.15	0.46
1:B1:125:ASN:O	1:BJ:38:ARG:NH1	2.49	0.46
1:AB:105:VAL:O	1:AB:109:GLN:HG2	2.15	0.46
1:BF:125:ASN:O	1:BV:38:ARG:NH1	33.41	0.46
1:BO:38:ARG:NH1	1:BP:125:ASN:O	2.49	0.46
1:B7:125:ASN:O	1:BA:38:ARG:NH1	239.89	0.46
1:AM:105:VAL:O	1:AM:109:GLN:HG2	2.15	0.46
1:A4:105:VAL:O	1:A4:109:GLN:HG2	2.15	0.46
1:BC:125:ASN:O	1:BN:38:ARG:NH1	101.67	0.46
1:BD:125:ASN:O	1:BE:38:ARG:NH1	2.49	0.46
1:BD:125:ASN:O	1:BH:38:ARG:NH1	139.46	0.46
1:BC:38:ARG:NH1	1:BI:125:ASN:O	119.19	0.46
1:BQ:38:ARG:NH1	1:BS:125:ASN:O	2.49	0.46
1:BH:125:ASN:O	1:BZ:38:ARG:NH1	2.49	0.46
1:B8:38:ARG:NH1	1:B9:125:ASN:O	2.49	0.46
1:BL:38:ARG:NH1	1:BM:125:ASN:O	97.13	0.46
1:B9:38:ARG:NH1	1:BT:125:ASN:O	2.49	0.46
1:BX:38:ARG:NH1	1:BY:125:ASN:O	2.49	0.46
1:BB:125:ASN:O	1:BC:38:ARG:NH1	2.49	0.46
1:AE:105:VAL:O	1:AE:109:GLN:HG2	2.15	0.46
1:AY:105:VAL:O	1:AY:109:GLN:HG2	2.15	0.46
1:AW:105:VAL:O	1:AW:109:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B0:38:ARG:NH1	1:BN:125:ASN:O	165.37	0.46
1:B5:38:ARG:NH1	1:B8:125:ASN:O	2.49	0.46
1:BK:38:ARG:NH1	1:BR:125:ASN:O	211.30	0.46
1:BR:125:ASN:O	1:BV:38:ARG:NH1	2.49	0.46
1:B5:125:ASN:O	1:BU:38:ARG:NH1	2.49	0.46
1:BK:125:ASN:O	1:BU:38:ARG:NH1	243.16	0.46
1:B3:125:ASN:O	1:BI:38:ARG:NH1	200.60	0.46
1:BU:125:ASN:O	1:BX:38:ARG:NH1	138.59	0.46
1:B4:38:ARG:NH1	1:BO:125:ASN:O	2.49	0.46
1:BG:38:ARG:NH1	1:BO:125:ASN:O	168.43	0.46
1:BG:38:ARG:NH1	1:BW:125:ASN:O	2.49	0.46
1:AZ:105:VAL:O	1:AZ:109:GLN:HG2	2.15	0.46
1:B6:125:ASN:O	1:BP:38:ARG:NH1	217.13	0.46
1:AC:105:VAL:O	1:AC:109:GLN:HG2	2.15	0.46
1:BL:125:ASN:O	1:BQ:38:ARG:NH1	212.11	0.46
1:BJ:125:ASN:O	1:BO:38:ARG:NH1	198.13	0.46
1:BP:125:ASN:O	1:BT:38:ARG:NH1	126.96	0.46
1:B2:38:ARG:NH1	1:BE:125:ASN:O	147.08	0.46
1:BA:38:ARG:NH1	1:BE:125:ASN:O	2.49	0.46
1:BB:125:ASN:O	1:BD:38:ARG:NH1	33.41	0.46
1:BA:125:ASN:O	1:BM:38:ARG:NH1	126.96	0.46
1:AH:105:VAL:O	1:AH:109:GLN:HG2	2.15	0.46
1:CN:60:ILE:HB	1:CN:88:MET:HG3	1.98	0.46
1:AS:105:VAL:O	1:AS:109:GLN:HG2	2.15	0.46
1:CJ:60:ILE:HB	1:CJ:88:MET:HG3	1.98	0.46
1:CS:60:ILE:HB	1:CS:88:MET:HG3	1.98	0.46
1:AP:105:VAL:O	1:AP:109:GLN:HG2	2.15	0.46
1:CG:60:ILE:HB	1:CG:88:MET:HG3	1.98	0.46
1:CH:60:ILE:HB	1:CH:88:MET:HG3	1.98	0.46
1:CQ:60:ILE:HB	1:CQ:88:MET:HG3	1.98	0.46
1:CK:60:ILE:HB	1:CK:88:MET:HG3	1.98	0.46
1:CV:20:VAL:HG13	1:CV:32:TRP:CB	2.46	0.46
1:CI:20:VAL:HG13	1:CI:32:TRP:CB	2.46	0.46
1:C5:20:VAL:HG13	1:C5:32:TRP:CB	2.46	0.46
1:BC:125:ASN:O	1:BD:38:ARG:NH1	2.49	0.46
1:B2:125:ASN:O	1:BL:38:ARG:NH1	2.49	0.46
1:CD:60:ILE:HB	1:CD:88:MET:HG3	1.98	0.46
1:CY:60:ILE:HB	1:CY:88:MET:HG3	1.98	0.46
1:AK:105:VAL:O	1:AK:109:GLN:HG2	2.15	0.46
1:AU:105:VAL:O	1:AU:109:GLN:HG2	2.15	0.46
1:CR:60:ILE:HB	1:CR:88:MET:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BF:38:ARG:NH1	1:BG:125:ASN:O	2.49	0.46
1:CT:60:ILE:HB	1:CT:88:MET:HG3	1.98	0.46
1:CU:60:ILE:HB	1:CU:88:MET:HG3	1.98	0.46
1:CS:20:VAL:HG13	1:CS:32:TRP:CB	2.46	0.46
1:CC:20:VAL:HG13	1:CC:32:TRP:CB	2.46	0.46
1:BP:38:ARG:NH1	1:BQ:125:ASN:O	2.49	0.46
1:CX:60:ILE:HB	1:CX:88:MET:HG3	1.98	0.46
1:AA:105:VAL:O	1:AA:109:GLN:HG2	2.15	0.46
1:A0:105:VAL:O	1:A0:109:GLN:HG2	2.15	0.46
1:CA:60:ILE:HB	1:CA:88:MET:HG3	1.98	0.46
1:CL:20:VAL:HG13	1:CL:32:TRP:CB	2.46	0.46
1:BF:125:ASN:O	1:BR:38:ARG:NH1	2.49	0.46
1:BJ:38:ARG:NH1	1:BV:125:ASN:O	147.57	0.46
1:BV:125:ASN:O	1:BW:38:ARG:NH1	2.49	0.46
1:C2:60:ILE:HB	1:C2:88:MET:HG3	1.98	0.46
1:C4:60:ILE:HB	1:C4:88:MET:HG3	1.98	0.46
1:B4:125:ASN:O	1:BS:38:ARG:NH1	2.49	0.46
1:BS:38:ARG:NH1	1:BX:125:ASN:O	180.13	0.46
1:C0:60:ILE:HB	1:C0:88:MET:HG3	1.98	0.46
1:CO:20:VAL:HG13	1:CO:32:TRP:CB	2.46	0.45
1:C0:20:VAL:HG13	1:C0:32:TRP:CB	2.46	0.45
1:CJ:20:VAL:HG13	1:CJ:32:TRP:CB	2.46	0.45
1:CM:20:VAL:HG13	1:CM:32:TRP:CB	2.46	0.45
1:CT:20:VAL:HG13	1:CT:32:TRP:CB	2.46	0.45
1:C8:20:VAL:HG13	1:C8:32:TRP:CB	2.46	0.45
1:BR:38:ARG:NH1	1:BS:125:ASN:O	79.44	0.45
1:BT:38:ARG:NH1	1:BU:125:ASN:O	2.49	0.45
1:BH:125:ASN:O	1:BN:38:ARG:NH1	225.15	0.45
1:BE:38:ARG:NH1	1:BW:125:ASN:O	127.09	0.45
1:B6:38:ARG:NH1	1:BX:125:ASN:O	2.49	0.45
1:CW:60:ILE:HB	1:CW:88:MET:HG3	1.98	0.45
1:B1:38:ARG:NH1	1:BZ:125:ASN:O	2.49	0.45
1:A2:105:VAL:O	1:A2:109:GLN:HG2	2.15	0.45
1:AD:105:VAL:O	1:AD:109:GLN:HG2	2.15	0.45
1:CQ:20:VAL:HG13	1:CQ:32:TRP:CB	2.46	0.45
1:CH:20:VAL:HG13	1:CH:32:TRP:CB	2.46	0.45
1:BH:38:ARG:NH1	1:BI:125:ASN:O	2.49	0.45
1:B0:125:ASN:O	1:BB:38:ARG:NH1	225.73	0.45
1:B7:38:ARG:NH1	1:BQ:125:ASN:O	225.15	0.45
1:A5:105:VAL:O	1:A5:109:GLN:HG2	2.15	0.45
1:CM:60:ILE:HB	1:CM:88:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:105:VAL:O	1:AQ:109:GLN:HG2	2.15	0.45
1:CI:60:ILE:HB	1:CI:88:MET:HG3	1.98	0.45
1:CZ:60:ILE:HB	1:CZ:88:MET:HG3	1.98	0.45
1:CN:20:VAL:HG13	1:CN:32:TRP:CB	2.46	0.45
1:BI:38:ARG:NH1	1:BJ:125:ASN:O	2.49	0.45
1:B3:38:ARG:NH1	1:BM:125:ASN:O	2.49	0.45
1:C5:60:ILE:HB	1:C5:88:MET:HG3	1.98	0.45
1:CL:60:ILE:HB	1:CL:88:MET:HG3	1.98	0.45
1:C6:20:VAL:HG13	1:C6:32:TRP:CB	2.46	0.45
1:CF:20:VAL:HG13	1:CF:32:TRP:CB	2.46	0.45
1:C4:20:VAL:HG13	1:C4:32:TRP:CB	2.46	0.45
1:BK:125:ASN:O	1:BW:38:ARG:NH1	212.11	0.45
1:BT:125:ASN:O	1:BY:38:ARG:NH1	168.43	0.45
1:BA:125:ASN:O	1:BB:38:ARG:NH1	2.49	0.45
1:BM:38:ARG:NH1	1:BN:125:ASN:O	2.49	0.45
1:CK:20:VAL:HG13	1:CK:32:TRP:CB	2.46	0.45
1:C3:20:VAL:HG13	1:C3:32:TRP:CB	2.46	0.45
1:CG:20:VAL:HG13	1:CG:32:TRP:CB	2.46	0.45
1:CA:20:VAL:HG13	1:CA:32:TRP:CB	2.46	0.45
1:C2:20:VAL:HG13	1:C2:32:TRP:CB	2.46	0.45
1:C3:60:ILE:HB	1:C3:88:MET:HG3	1.98	0.45
1:CV:60:ILE:HB	1:CV:88:MET:HG3	1.98	0.45
1:CP:60:ILE:HB	1:CP:88:MET:HG3	1.98	0.45
1:C6:60:ILE:HB	1:C6:88:MET:HG3	1.98	0.45
1:CY:20:VAL:HG13	1:CY:32:TRP:CB	2.46	0.45
1:CE:20:VAL:HG13	1:CE:32:TRP:CB	2.46	0.45
1:CW:20:VAL:HG13	1:CW:32:TRP:CB	2.46	0.45
1:CU:20:VAL:HG13	1:CU:32:TRP:CB	2.46	0.45
1:A7:86:LEU:HD21	1:A7:88:MET:HE3	1.98	0.45
1:C1:60:ILE:HB	1:C1:88:MET:HG3	1.98	0.45
1:CR:20:VAL:HG13	1:CR:32:TRP:CB	2.46	0.45
1:CB:20:VAL:HG13	1:CB:32:TRP:CB	2.46	0.45
1:CE:60:ILE:HB	1:CE:88:MET:HG3	1.98	0.45
1:C9:20:VAL:HG13	1:C9:32:TRP:CB	2.46	0.45
1:CF:60:ILE:HB	1:CF:88:MET:HG3	1.98	0.45
1:CX:20:VAL:HG13	1:CX:32:TRP:CB	2.46	0.45
1:C7:20:VAL:HG13	1:C7:32:TRP:CB	2.46	0.45
1:C7:60:ILE:HB	1:C7:88:MET:HG3	1.98	0.45
1:CP:20:VAL:HG13	1:CP:32:TRP:CB	2.46	0.45
1:CO:60:ILE:HB	1:CO:88:MET:HG3	1.98	0.45
1:C9:60:ILE:HB	1:C9:88:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CZ:20:VAL:HG13	1:CZ:32:TRP:CB	2.46	0.44
1:CB:60:ILE:HB	1:CB:88:MET:HG3	1.98	0.44
1:CC:60:ILE:HB	1:CC:88:MET:HG3	1.98	0.44
1:CD:20:VAL:HG13	1:CD:32:TRP:CB	2.46	0.44
1:C8:60:ILE:HB	1:C8:88:MET:HG3	1.98	0.44
1:CF:92:ILE:HA	1:CF:93:PRO:HD3	1.88	0.44
1:C1:20:VAL:HG13	1:C1:32:TRP:CB	2.46	0.44
1:CJ:92:ILE:HA	1:CJ:93:PRO:HD3	1.88	0.43
1:CE:92:ILE:HA	1:CE:93:PRO:HD3	1.88	0.43
1:AH:86:LEU:HD21	1:AH:88:MET:HE3	2.01	0.43
1:CU:92:ILE:HA	1:CU:93:PRO:HD3	1.88	0.43
1:A2:86:LEU:HD21	1:A2:88:MET:HE3	2.01	0.43
1:CN:92:ILE:HA	1:CN:93:PRO:HD3	1.88	0.43
1:CA:92:ILE:HA	1:CA:93:PRO:HD3	1.88	0.43
1:C6:92:ILE:HA	1:C6:93:PRO:HD3	1.88	0.43
1:CS:92:ILE:HA	1:CS:93:PRO:HD3	1.88	0.43
1:CO:92:ILE:HA	1:CO:93:PRO:HD3	1.88	0.42
1:CX:92:ILE:HA	1:CX:93:PRO:HD3	1.88	0.42
1:CG:92:ILE:HA	1:CG:93:PRO:HD3	1.88	0.42
1:BR:62:VAL:HB	1:BR:86:LEU:HB3	2.02	0.42
1:BE:62:VAL:HB	1:BE:86:LEU:HB3	2.02	0.42
1:C3:92:ILE:HA	1:C3:93:PRO:HD3	1.88	0.42
1:BL:62:VAL:HB	1:BL:86:LEU:HB3	2.02	0.42
1:AQ:86:LEU:HD21	1:AQ:88:MET:HE3	2.01	0.42
1:BZ:62:VAL:HB	1:BZ:86:LEU:HB3	2.02	0.42
1:BS:62:VAL:HB	1:BS:86:LEU:HB3	2.02	0.42
1:B9:62:VAL:HB	1:B9:86:LEU:HB3	2.02	0.42
1:BM:62:VAL:HB	1:BM:86:LEU:HB3	2.02	0.42
1:CQ:92:ILE:HA	1:CQ:93:PRO:HD3	1.88	0.42
1:B5:62:VAL:HB	1:B5:86:LEU:HB3	2.02	0.42
1:CC:92:ILE:HA	1:CC:93:PRO:HD3	1.88	0.42
1:BP:62:VAL:HB	1:BP:86:LEU:HB3	2.02	0.42
1:BI:62:VAL:HB	1:BI:86:LEU:HB3	2.02	0.42
1:BB:62:VAL:HB	1:BB:86:LEU:HB3	2.02	0.42
1:BC:62:VAL:HB	1:BC:86:LEU:HB3	2.02	0.42
1:B1:62:VAL:HB	1:B1:86:LEU:HB3	2.02	0.42
1:BX:62:VAL:HB	1:BX:86:LEU:HB3	2.02	0.42
1:BT:62:VAL:HB	1:BT:86:LEU:HB3	2.02	0.42
1:AD:86:LEU:HD21	1:AD:88:MET:HE3	2.14	0.42
1:BN:62:VAL:HB	1:BN:86:LEU:HB3	2.02	0.42
1:B7:62:VAL:HB	1:B7:86:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CH:92:ILE:HA	1:CH:93:PRO:HD3	1.88	0.42
1:B3:62:VAL:HB	1:B3:86:LEU:HB3	2.02	0.42
1:C0:92:ILE:HA	1:C0:93:PRO:HD3	1.88	0.42
1:BF:62:VAL:HB	1:BF:86:LEU:HB3	2.02	0.42
1:B6:62:VAL:HB	1:B6:86:LEU:HB3	2.02	0.42
1:BH:62:VAL:HB	1:BH:86:LEU:HB3	2.02	0.42
1:B0:62:VAL:HB	1:B0:86:LEU:HB3	2.02	0.42
1:BD:62:VAL:HB	1:BD:86:LEU:HB3	2.02	0.42
1:BR:33:ILE:HD12	1:BR:38:ARG:CZ	2.50	0.41
1:BG:33:ILE:HD12	1:BG:38:ARG:CZ	2.51	0.41
1:BB:33:ILE:HD12	1:BB:38:ARG:CZ	2.50	0.41
1:BS:33:ILE:HD12	1:BS:38:ARG:CZ	2.50	0.41
1:B2:62:VAL:HB	1:B2:86:LEU:HB3	2.02	0.41
1:AT:86:LEU:HD21	1:AT:88:MET:HE3	2.07	0.41
1:B4:62:VAL:HB	1:B4:86:LEU:HB3	2.02	0.41
1:A0:86:LEU:HD21	1:A0:88:MET:HE3	2.02	0.41
1:BV:33:ILE:HD12	1:BV:38:ARG:CZ	2.51	0.41
1:BE:33:ILE:HD12	1:BE:38:ARG:CZ	2.50	0.41
1:B5:33:ILE:HD12	1:B5:38:ARG:CZ	2.50	0.41
1:BP:33:ILE:HD12	1:BP:38:ARG:CZ	2.50	0.41
1:BO:62:VAL:HB	1:BO:86:LEU:HB3	2.02	0.41
1:BG:62:VAL:HB	1:BG:86:LEU:HB3	2.02	0.41
1:BJ:62:VAL:HB	1:BJ:86:LEU:HB3	2.02	0.41
1:BQ:33:ILE:HD12	1:BQ:38:ARG:CZ	2.51	0.41
1:BJ:33:ILE:HD12	1:BJ:38:ARG:CZ	2.50	0.41
1:BC:33:ILE:HD12	1:BC:38:ARG:CZ	2.50	0.41
1:BH:33:ILE:HD12	1:BH:38:ARG:CZ	2.51	0.41
1:B9:33:ILE:HD12	1:B9:38:ARG:CZ	2.51	0.41
1:BY:33:ILE:HD12	1:BY:38:ARG:CZ	2.50	0.41
1:B7:33:ILE:HD12	1:B7:38:ARG:CZ	2.51	0.41
1:BU:33:ILE:HD12	1:BU:38:ARG:CZ	2.50	0.41
1:BT:33:ILE:HD12	1:BT:38:ARG:CZ	2.51	0.41
1:BF:33:ILE:HD12	1:BF:38:ARG:CZ	2.51	0.41
1:B6:33:ILE:HD12	1:B6:38:ARG:CZ	2.51	0.41
1:BQ:62:VAL:HB	1:BQ:86:LEU:HB3	2.02	0.41
1:B4:33:ILE:HD12	1:B4:38:ARG:CZ	2.50	0.41
1:BZ:33:ILE:HD12	1:BZ:38:ARG:CZ	2.50	0.41
1:BL:33:ILE:HD12	1:BL:38:ARG:CZ	2.51	0.41
1:BU:62:VAL:HB	1:BU:86:LEU:HB3	2.02	0.41
1:B8:62:VAL:HB	1:B8:86:LEU:HB3	2.02	0.41
1:BK:62:VAL:HB	1:BK:86:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BW:33:ILE:HD12	1:BW:38:ARG:CZ	2.50	0.41
1:BO:33:ILE:HD12	1:BO:38:ARG:CZ	2.51	0.41
1:BX:33:ILE:HD12	1:BX:38:ARG:CZ	2.50	0.41
1:BA:33:ILE:HD12	1:BA:38:ARG:CZ	2.50	0.41
1:BD:33:ILE:HD12	1:BD:38:ARG:CZ	2.50	0.41
1:BW:62:VAL:HB	1:BW:86:LEU:HB3	2.02	0.41
1:CT:92:ILE:HA	1:CT:93:PRO:HD3	1.88	0.41
1:CH:104:ILE:HG22	1:CH:108:MET:CE	2.51	0.41
1:BA:62:VAL:HB	1:BA:86:LEU:HB3	2.02	0.41
1:BV:62:VAL:HB	1:BV:86:LEU:HB3	2.02	0.41
1:BK:33:ILE:HD12	1:BK:38:ARG:CZ	2.51	0.41
1:BN:33:ILE:HD12	1:BN:38:ARG:CZ	2.50	0.41
1:B3:33:ILE:HD12	1:B3:38:ARG:CZ	2.51	0.41
1:BM:33:ILE:HD12	1:BM:38:ARG:CZ	2.50	0.41
1:CV:104:ILE:HG22	1:CV:108:MET:CE	2.51	0.41
1:CE:104:ILE:HG22	1:CE:108:MET:CE	2.51	0.41
1:CQ:104:ILE:HG22	1:CQ:108:MET:CE	2.51	0.41
1:A3:86:LEU:HD21	1:A3:88:MET:HE3	2.03	0.41
1:AP:86:LEU:HD21	1:AP:88:MET:HE3	2.11	0.41
1:B2:33:ILE:HD12	1:B2:38:ARG:CZ	2.50	0.41
1:BI:33:ILE:HD12	1:BI:38:ARG:CZ	2.51	0.41
1:C2:104:ILE:HG22	1:C2:108:MET:CE	2.51	0.41
1:CD:104:ILE:HG22	1:CD:108:MET:CE	2.51	0.41
1:CO:104:ILE:HG22	1:CO:108:MET:CE	2.51	0.41
1:CG:104:ILE:HG22	1:CG:108:MET:CE	2.51	0.41
1:CP:104:ILE:HG22	1:CP:108:MET:CE	2.51	0.41
1:CJ:104:ILE:HG22	1:CJ:108:MET:CE	2.51	0.41
1:CS:104:ILE:HG22	1:CS:108:MET:CE	2.51	0.41
1:CM:104:ILE:HG22	1:CM:108:MET:CE	2.51	0.41
1:CN:104:ILE:HG22	1:CN:108:MET:CE	2.51	0.41
1:CF:104:ILE:HG22	1:CF:108:MET:CE	2.51	0.41
1:AL:86:LEU:HD22	1:BA:108:MET:HG2	122.47	0.41
1:CR:104:ILE:HG22	1:CR:108:MET:CE	2.51	0.41
1:A8:86:LEU:HD21	1:A8:88:MET:HE3	2.03	0.41
1:AF:86:LEU:HD21	1:AF:88:MET:HE3	2.03	0.41
1:CK:104:ILE:HG22	1:CK:108:MET:CE	2.51	0.41
1:CB:104:ILE:HG22	1:CB:108:MET:CE	2.51	0.41
1:AX:86:LEU:HD22	1:BT:108:MET:HG2	169.94	0.41
1:CX:104:ILE:HG22	1:CX:108:MET:CE	2.51	0.41
1:BY:62:VAL:HB	1:BY:86:LEU:HB3	2.02	0.41
1:AG:86:LEU:HD22	1:BW:108:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C8:104:ILE:HG22	1:C8:108:MET:CE	2.51	0.41
1:CA:104:ILE:HG22	1:CA:108:MET:CE	2.51	0.41
1:C9:104:ILE:HG22	1:C9:108:MET:CE	2.51	0.41
1:C1:104:ILE:HG22	1:C1:108:MET:CE	2.51	0.41
1:AN:86:LEU:HD22	1:BC:108:MET:HG2	122.57	0.40
1:A2:86:LEU:HD22	1:BO:108:MET:HG2	2.04	0.40
1:AK:86:LEU:HD22	1:BL:108:MET:HG2	2.03	0.40
1:AJ:86:LEU:HD22	1:BR:108:MET:HG2	189.17	0.40
1:B8:33:ILE:HD12	1:B8:38:ARG:CZ	2.50	0.40
1:B1:33:ILE:HD12	1:B1:38:ARG:CZ	2.51	0.40
1:CW:104:ILE:HG22	1:CW:108:MET:CE	2.51	0.40
1:CT:104:ILE:HG22	1:CT:108:MET:CE	2.51	0.40
1:CU:104:ILE:HG22	1:CU:108:MET:CE	2.51	0.40
1:AP:86:LEU:HD22	1:BL:108:MET:HG2	182.48	0.40
1:AJ:86:LEU:HD21	1:AJ:88:MET:HE3	2.03	0.40
1:AO:86:LEU:HD22	1:BP:108:MET:HG2	2.04	0.40
1:CI:104:ILE:HG22	1:CI:108:MET:CE	2.51	0.40
1:CP:92:ILE:HA	1:CP:93:PRO:HD3	1.88	0.40
1:C0:104:ILE:HG22	1:C0:108:MET:CE	2.51	0.40
1:A9:86:LEU:HD22	1:B7:108:MET:HG2	2.03	0.40
1:AY:86:LEU:HD22	1:BH:108:MET:HG2	2.03	0.40
1:CV:92:ILE:HA	1:CV:93:PRO:HD3	1.88	0.40
1:C6:104:ILE:HG22	1:C6:108:MET:CE	2.51	0.40
1:AU:86:LEU:HD22	1:B5:108:MET:HG2	2.03	0.40
1:AR:86:LEU:HD22	1:BF:108:MET:HG2	2.04	0.40
1:B0:33:ILE:HD12	1:B0:38:ARG:CZ	2.50	0.40
1:CY:104:ILE:HG22	1:CY:108:MET:CE	2.51	0.40
1:AB:86:LEU:HD22	1:BI:108:MET:HG2	65.59	0.40
1:AW:86:LEU:HD21	1:AW:88:MET:HE3	2.12	0.40
1:AQ:86:LEU:HD22	1:BS:108:MET:HG2	2.03	0.40
1:AD:86:LEU:HD22	1:BC:108:MET:HG2	2.04	0.40
1:AU:86:LEU:HD22	1:BF:108:MET:HG2	122.47	0.40
1:AZ:86:LEU:HD22	1:BZ:108:MET:HG2	2.04	0.40
1:C4:92:ILE:HA	1:C4:93:PRO:HD3	1.88	0.40

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	A0	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A1	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A2	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A3	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A4	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	A5	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A6	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A7	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A8	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	A9	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AA	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AB	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AC	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AD	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AE	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AF	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AG	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AH	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AI	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AJ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AK	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AL	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AM	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AN	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AO	127/129 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AP	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AQ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AR	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AS	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AT	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AU	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AX	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AY	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	AZ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Aa	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ab	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ac	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
1	Ad	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ae	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Af	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ag	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ah	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ai	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Aj	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ak	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Al	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Am	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	An	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ao	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ap	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Aq	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ar	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	As	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	At	127/129 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Au	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Av	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Aw	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ax	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	B0	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	B1	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	B2	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	B3	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	B4	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	B5	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	B6	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	B7	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	B8	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	B9	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BA	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BB	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BC	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BD	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BE	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BF	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BG	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BH	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BI	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BJ	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BK	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BL	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BM	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BN	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BO	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BP	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BQ	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BR	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BS	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BT	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BU	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BV	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BW	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BX	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BY	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	BZ	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Ba	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bb	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bc	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bd	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Be	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bf	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bg	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bh	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bi	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bj	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bk	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bl	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bm	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bn	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bo	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bp	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bq	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Br	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bs	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bt	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bu	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bv	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bw	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	Bx	127/129 (98%)	123 (97%)	3 (2%)	1 (1%)	24	69
1	C0	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C1	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C2	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C3	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C4	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C5	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C6	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C7	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C8	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	C9	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CA	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CB	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CC	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CD	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CE	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CF	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CG	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CH	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CI	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CJ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CK	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CL	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CM	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CN	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CO	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CP	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CQ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CR	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CS	127/129 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CT	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CU	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CW	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CX	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CY	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	CZ	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ca	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cb	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cc	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cd	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ce	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cf	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cg	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ch	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ci	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cj	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ck	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cl	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cm	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cn	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Co	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cp	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cq	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cr	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cs	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Ct	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cu	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cv	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cw	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
1	Cx	127/129 (98%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	22860/23220 (98%)	22138 (97%)	662 (3%)	60 (0%)	50	83

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B0	2	SER
1	B1	2	SER
1	B2	2	SER
1	B3	2	SER
1	B4	2	SER
1	B5	2	SER
1	B6	2	SER
1	B7	2	SER
1	B8	2	SER
1	B9	2	SER
1	BA	2	SER
1	BB	2	SER
1	BC	2	SER
1	BD	2	SER
1	BE	2	SER
1	BF	2	SER
1	BG	2	SER
1	BH	2	SER
1	BI	2	SER
1	BJ	2	SER
1	BK	2	SER
1	BL	2	SER
1	BM	2	SER
1	BN	2	SER
1	BO	2	SER
1	BP	2	SER
1	BQ	2	SER
1	BR	2	SER
1	BS	2	SER
1	BT	2	SER
1	BU	2	SER
1	BV	2	SER
1	BW	2	SER
1	BX	2	SER
1	BY	2	SER
1	BZ	2	SER
1	Ba	2	SER

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Mol	Chain	Res	Type
1	Bb	2	SER
1	Bc	2	SER
1	Bd	2	SER
1	Be	2	SER
1	Bf	2	SER
1	Bg	2	SER
1	Bh	2	SER
1	Bi	2	SER
1	Bj	2	SER
1	Bk	2	SER
1	Bl	2	SER
1	Bm	2	SER
1	Bn	2	SER
1	Bo	2	SER
1	Bp	2	SER
1	Bq	2	SER
1	Br	2	SER
1	Bs	2	SER
1	Bt	2	SER
1	Bu	2	SER
1	Bv	2	SER
1	Bw	2	SER
1	Bx	2	SER

### 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 PDB entries followed by that with respect to all EM entries.

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	A0	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	A1	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	A2	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	A3	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	A4	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	A5	106/106 (100%)	91 (86%)	15 (14%)	4	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A6	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	A7	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	A8	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	A9	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AA	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AB	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AC	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AD	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AE	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AF	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AG	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AH	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AI	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AJ	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AK	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AL	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AM	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AN	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AO	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AP	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AQ	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AR	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AS	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AT	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AU	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AV	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AW	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AX	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AY	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	AZ	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Aa	106/106 (100%)	91 (86%)	15 (14%)	4	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ab	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ac	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ad	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ae	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Af	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ag	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ah	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ai	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Aj	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ak	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Al	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Am	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	An	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ao	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ap	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Aq	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ar	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	As	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	At	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Au	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Av	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Aw	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	Ax	106/106 (100%)	91 (86%)	15 (14%)	4	26
1	B0	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	B1	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	B2	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	B3	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	B4	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	B5	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	B6	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	B7	106/106 (100%)	97 (92%)	9 (8%)	13	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B8	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	B9	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	BA	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BB	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	BC	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BD	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BE	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	BF	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BG	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	BH	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BI	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BJ	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	BK	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BL	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	BM	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BN	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BO	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	BP	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BQ	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BR	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BS	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	BT	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BU	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	BV	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BW	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BX	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	BY	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	BZ	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Ba	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bb	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Bc	106/106 (100%)	97 (92%)	9 (8%)	13	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bd	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Be	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Bf	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bg	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Bh	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Bi	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Bj	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Bk	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bl	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bm	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Bn	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bo	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bp	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bq	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Br	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Bs	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	Bt	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bu	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bv	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bw	106/106 (100%)	97 (92%)	9 (8%)	13	48
1	Bx	106/106 (100%)	96 (91%)	10 (9%)	11	42
1	C0	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	C1	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	C2	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	C3	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	C4	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	C5	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	C6	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	C7	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	C8	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	C9	106/106 (100%)	94 (89%)	12 (11%)	7	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CA	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CB	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CC	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CD	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CE	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CF	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CG	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CH	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CI	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CJ	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CK	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CL	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CM	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CN	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CO	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CP	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CQ	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CR	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CS	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CT	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CU	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CV	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CW	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CX	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CY	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	CZ	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Ca	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cb	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cc	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cd	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Ce	106/106 (100%)	94 (89%)	12 (11%)	7	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Cf	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cg	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Ch	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Ci	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cj	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Ck	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cl	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cm	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cn	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Co	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cp	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cq	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cr	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cs	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Ct	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cu	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cv	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cw	106/106 (100%)	94 (89%)	12 (11%)	7	33
1	Cx	106/106 (100%)	94 (89%)	12 (11%)	7	33
All	All	19080/19080 (100%)	16895 (88%)	2185 (12%)	11	32

All (2185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A0	2	SER
1	A0	4	PHE
1	A0	6	GLN
1	A0	8	VAL
1	A0	19	THR
1	A0	20	VAL
1	A0	25	PHE
1	A0	33	ILE
1	A0	48	VAL
1	A0	50	GLN
1	A0	52	SER

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Mol	Chain	Res	Type
1	A0	79	VAL
1	A0	109	GLN
1	A0	126	SER
1	A0	128	ILE
1	A1	2	SER
1	A1	4	PHE
1	A1	6	GLN
1	A1	8	VAL
1	A1	19	THR
1	A1	20	VAL
1	A1	25	PHE
1	A1	33	ILE
1	A1	48	VAL
1	A1	50	GLN
1	A1	52	SER
1	A1	79	VAL
1	A1	109	GLN
1	A1	126	SER
1	A1	128	ILE
1	A2	2	SER
1	A2	4	PHE
1	A2	6	GLN
1	A2	8	VAL
1	A2	19	THR
1	A2	20	VAL
1	A2	25	PHE
1	A2	33	ILE
1	A2	48	VAL
1	A2	50	GLN
1	A2	52	SER
1	A2	79	VAL
1	A2	109	GLN
1	A2	126	SER
1	A2	128	ILE
1	A3	2	SER
1	A3	4	PHE
1	A3	6	GLN
1	A3	8	VAL
1	A3	19	THR
1	A3	20	VAL
1	A3	25	PHE
1	A3	33	ILE

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Mol	Chain	Res	Type
1	A3	48	VAL
1	A3	50	GLN
1	A3	52	SER
1	A3	79	VAL
1	A3	109	GLN
1	A3	126	SER
1	A3	128	ILE
1	A4	2	SER
1	A4	4	PHE
1	A4	6	GLN
1	A4	8	VAL
1	A4	19	THR
1	A4	20	VAL
1	A4	25	PHE
1	A4	33	ILE
1	A4	48	VAL
1	A4	50	GLN
1	A4	52	SER
1	A4	79	VAL
1	A4	109	GLN
1	A4	126	SER
1	A4	128	ILE
1	A5	2	SER
1	A5	4	PHE
1	A5	6	GLN
1	A5	8	VAL
1	A5	19	THR
1	A5	20	VAL
1	A5	25	PHE
1	A5	33	ILE
1	A5	48	VAL
1	A5	50	GLN
1	A5	52	SER
1	A5	79	VAL
1	A5	109	GLN
1	A5	126	SER
1	A5	128	ILE
1	A6	2	SER
1	A6	4	PHE
1	A6	6	GLN
1	A6	8	VAL
1	A6	19	THR

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Mol	Chain	Res	Type
1	A6	20	VAL
1	A6	25	PHE
1	A6	33	ILE
1	A6	48	VAL
1	A6	50	GLN
1	A6	52	SER
1	A6	79	VAL
1	A6	109	GLN
1	A6	126	SER
1	A6	128	ILE
1	A7	2	SER
1	A7	4	PHE
1	A7	6	GLN
1	A7	8	VAL
1	A7	19	THR
1	A7	20	VAL
1	A7	25	PHE
1	A7	33	ILE
1	A7	48	VAL
1	A7	50	GLN
1	A7	52	SER
1	A7	79	VAL
1	A7	109	GLN
1	A7	126	SER
1	A7	128	ILE
1	A8	2	SER
1	A8	4	PHE
1	A8	6	GLN
1	A8	8	VAL
1	A8	19	THR
1	A8	20	VAL
1	A8	25	PHE
1	A8	33	ILE
1	A8	48	VAL
1	A8	50	GLN
1	A8	52	SER
1	A8	79	VAL
1	A8	109	GLN
1	A8	126	SER
1	A8	128	ILE
1	A9	2	SER
1	A9	4	PHE

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Mol	Chain	Res	Type
1	A9	6	GLN
1	A9	8	VAL
1	A9	19	THR
1	A9	20	VAL
1	A9	25	PHE
1	A9	33	ILE
1	A9	48	VAL
1	A9	50	GLN
1	A9	52	SER
1	A9	79	VAL
1	A9	109	GLN
1	A9	126	SER
1	A9	128	ILE
1	AA	2	SER
1	AA	4	PHE
1	AA	6	GLN
1	AA	8	VAL
1	AA	19	THR
1	AA	20	VAL
1	AA	25	PHE
1	AA	33	ILE
1	AA	48	VAL
1	AA	50	GLN
1	AA	52	SER
1	AA	79	VAL
1	AA	109	GLN
1	AA	126	SER
1	AA	128	ILE
1	AB	2	SER
1	AB	4	PHE
1	AB	6	GLN
1	AB	8	VAL
1	AB	19	THR
1	AB	20	VAL
1	AB	25	PHE
1	AB	33	ILE
1	AB	48	VAL
1	AB	50	GLN
1	AB	52	SER
1	AB	79	VAL
1	AB	109	GLN
1	AB	126	SER

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Mol	Chain	Res	Type
1	AB	128	ILE
1	AC	2	SER
1	AC	4	PHE
1	AC	6	GLN
1	AC	8	VAL
1	AC	19	THR
1	AC	20	VAL
1	AC	25	PHE
1	AC	33	ILE
1	AC	48	VAL
1	AC	50	GLN
1	AC	52	SER
1	AC	79	VAL
1	AC	109	GLN
1	AC	126	SER
1	AC	128	ILE
1	AD	2	SER
1	AD	4	PHE
1	AD	6	GLN
1	AD	8	VAL
1	AD	19	THR
1	AD	20	VAL
1	AD	25	PHE
1	AD	33	ILE
1	AD	48	VAL
1	AD	50	GLN
1	AD	52	SER
1	AD	79	VAL
1	AD	109	GLN
1	AD	126	SER
1	AD	128	ILE
1	AE	2	SER
1	AE	4	PHE
1	AE	6	GLN
1	AE	8	VAL
1	AE	19	THR
1	AE	20	VAL
1	AE	25	PHE
1	AE	33	ILE
1	AE	48	VAL
1	AE	50	GLN
1	AE	52	SER

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Mol	Chain	Res	Type
1	AE	79	VAL
1	AE	109	GLN
1	AE	126	SER
1	AE	128	ILE
1	AF	2	SER
1	AF	4	PHE
1	AF	6	GLN
1	AF	8	VAL
1	AF	19	THR
1	AF	20	VAL
1	AF	25	PHE
1	AF	33	ILE
1	AF	48	VAL
1	AF	50	GLN
1	AF	52	SER
1	AF	79	VAL
1	AF	109	GLN
1	AF	126	SER
1	AF	128	ILE
1	AG	2	SER
1	AG	4	PHE
1	AG	6	GLN
1	AG	8	VAL
1	AG	19	THR
1	AG	20	VAL
1	AG	25	PHE
1	AG	33	ILE
1	AG	48	VAL
1	AG	50	GLN
1	AG	52	SER
1	AG	79	VAL
1	AG	109	GLN
1	AG	126	SER
1	AG	128	ILE
1	AH	2	SER
1	AH	4	PHE
1	AH	6	GLN
1	AH	8	VAL
1	AH	19	THR
1	AH	20	VAL
1	AH	25	PHE
1	AH	33	ILE

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Mol	Chain	Res	Type
1	AH	48	VAL
1	AH	50	GLN
1	AH	52	SER
1	AH	79	VAL
1	AH	109	GLN
1	AH	126	SER
1	AH	128	ILE
1	AI	2	SER
1	AI	4	PHE
1	AI	6	GLN
1	AI	8	VAL
1	AI	19	THR
1	AI	20	VAL
1	AI	25	PHE
1	AI	33	ILE
1	AI	48	VAL
1	AI	50	GLN
1	AI	52	SER
1	AI	79	VAL
1	AI	109	GLN
1	AI	126	SER
1	AI	128	ILE
1	AJ	2	SER
1	AJ	4	PHE
1	AJ	6	GLN
1	AJ	8	VAL
1	AJ	19	THR
1	AJ	20	VAL
1	AJ	25	PHE
1	AJ	33	ILE
1	AJ	48	VAL
1	AJ	50	GLN
1	AJ	52	SER
1	AJ	79	VAL
1	AJ	109	GLN
1	AJ	126	SER
1	AJ	128	ILE
1	AK	2	SER
1	AK	4	PHE
1	AK	6	GLN
1	AK	8	VAL
1	AK	19	THR

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Mol	Chain	Res	Type
1	AK	20	VAL
1	AK	25	PHE
1	AK	33	ILE
1	AK	48	VAL
1	AK	50	GLN
1	AK	52	SER
1	AK	79	VAL
1	AK	109	GLN
1	AK	126	SER
1	AK	128	ILE
1	AL	2	SER
1	AL	4	PHE
1	AL	6	GLN
1	AL	8	VAL
1	AL	19	THR
1	AL	20	VAL
1	AL	25	PHE
1	AL	33	ILE
1	AL	48	VAL
1	AL	50	GLN
1	AL	52	SER
1	AL	79	VAL
1	AL	109	GLN
1	AL	126	SER
1	AL	128	ILE
1	AM	2	SER
1	AM	4	PHE
1	AM	6	GLN
1	AM	8	VAL
1	AM	19	THR
1	AM	20	VAL
1	AM	25	PHE
1	AM	33	ILE
1	AM	48	VAL
1	AM	50	GLN
1	AM	52	SER
1	AM	79	VAL
1	AM	109	GLN
1	AM	126	SER
1	AM	128	ILE
1	AN	2	SER
1	AN	4	PHE

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Mol	Chain	Res	Type
1	AN	6	GLN
1	AN	8	VAL
1	AN	19	THR
1	AN	20	VAL
1	AN	25	PHE
1	AN	33	ILE
1	AN	48	VAL
1	AN	50	GLN
1	AN	52	SER
1	AN	79	VAL
1	AN	109	GLN
1	AN	126	SER
1	AN	128	ILE
1	AO	2	SER
1	AO	4	PHE
1	AO	6	GLN
1	AO	8	VAL
1	AO	19	THR
1	AO	20	VAL
1	AO	25	PHE
1	AO	33	ILE
1	AO	48	VAL
1	AO	50	GLN
1	AO	52	SER
1	AO	79	VAL
1	AO	109	GLN
1	AO	126	SER
1	AO	128	ILE
1	AP	2	SER
1	AP	4	PHE
1	AP	6	GLN
1	AP	8	VAL
1	AP	19	THR
1	AP	20	VAL
1	AP	25	PHE
1	AP	33	ILE
1	AP	48	VAL
1	AP	50	GLN
1	AP	52	SER
1	AP	79	VAL
1	AP	109	GLN
1	AP	126	SER

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Mol	Chain	Res	Type
1	AP	128	ILE
1	AQ	2	SER
1	AQ	4	PHE
1	AQ	6	GLN
1	AQ	8	VAL
1	AQ	19	THR
1	AQ	20	VAL
1	AQ	25	PHE
1	AQ	33	ILE
1	AQ	48	VAL
1	AQ	50	GLN
1	AQ	52	SER
1	AQ	79	VAL
1	AQ	109	GLN
1	AQ	126	SER
1	AQ	128	ILE
1	AR	2	SER
1	AR	4	PHE
1	AR	6	GLN
1	AR	8	VAL
1	AR	19	THR
1	AR	20	VAL
1	AR	25	PHE
1	AR	33	ILE
1	AR	48	VAL
1	AR	50	GLN
1	AR	52	SER
1	AR	79	VAL
1	AR	109	GLN
1	AR	126	SER
1	AR	128	ILE
1	AS	2	SER
1	AS	4	PHE
1	AS	6	GLN
1	AS	8	VAL
1	AS	19	THR
1	AS	20	VAL
1	AS	25	PHE
1	AS	33	ILE
1	AS	48	VAL
1	AS	50	GLN
1	AS	52	SER

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Mol	Chain	Res	Type
1	AS	79	VAL
1	AS	109	GLN
1	AS	126	SER
1	AS	128	ILE
1	AT	2	SER
1	AT	4	PHE
1	AT	6	GLN
1	AT	8	VAL
1	AT	19	THR
1	AT	20	VAL
1	AT	25	PHE
1	AT	33	ILE
1	AT	48	VAL
1	AT	50	GLN
1	AT	52	SER
1	AT	79	VAL
1	AT	109	GLN
1	AT	126	SER
1	AT	128	ILE
1	AU	2	SER
1	AU	4	PHE
1	AU	6	GLN
1	AU	8	VAL
1	AU	19	THR
1	AU	20	VAL
1	AU	25	PHE
1	AU	33	ILE
1	AU	48	VAL
1	AU	50	GLN
1	AU	52	SER
1	AU	79	VAL
1	AU	109	GLN
1	AU	126	SER
1	AU	128	ILE
1	AV	2	SER
1	AV	4	PHE
1	AV	6	GLN
1	AV	8	VAL
1	AV	19	THR
1	AV	20	VAL
1	AV	25	PHE
1	AV	33	ILE

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Mol	Chain	Res	Type
1	AV	48	VAL
1	AV	50	GLN
1	AV	52	SER
1	AV	79	VAL
1	AV	109	GLN
1	AV	126	SER
1	AV	128	ILE
1	AW	2	SER
1	AW	4	PHE
1	AW	6	GLN
1	AW	8	VAL
1	AW	19	THR
1	AW	20	VAL
1	AW	25	PHE
1	AW	33	ILE
1	AW	48	VAL
1	AW	50	GLN
1	AW	52	SER
1	AW	79	VAL
1	AW	109	GLN
1	AW	126	SER
1	AW	128	ILE
1	AX	2	SER
1	AX	4	PHE
1	AX	6	GLN
1	AX	8	VAL
1	AX	19	THR
1	AX	20	VAL
1	AX	25	PHE
1	AX	33	ILE
1	AX	48	VAL
1	AX	50	GLN
1	AX	52	SER
1	AX	79	VAL
1	AX	109	GLN
1	AX	126	SER
1	AX	128	ILE
1	AY	2	SER
1	AY	4	PHE
1	AY	6	GLN
1	AY	8	VAL
1	AY	19	THR

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Mol	Chain	Res	Type
1	AY	20	VAL
1	AY	25	PHE
1	AY	33	ILE
1	AY	48	VAL
1	AY	50	GLN
1	AY	52	SER
1	AY	79	VAL
1	AY	109	GLN
1	AY	126	SER
1	AY	128	ILE
1	AZ	2	SER
1	AZ	4	PHE
1	AZ	6	GLN
1	AZ	8	VAL
1	AZ	19	THR
1	AZ	20	VAL
1	AZ	25	PHE
1	AZ	33	ILE
1	AZ	48	VAL
1	AZ	50	GLN
1	AZ	52	SER
1	AZ	79	VAL
1	AZ	109	GLN
1	AZ	126	SER
1	AZ	128	ILE
1	Aa	2	SER
1	Aa	4	PHE
1	Aa	6	GLN
1	Aa	8	VAL
1	Aa	19	THR
1	Aa	20	VAL
1	Aa	25	PHE
1	Aa	33	ILE
1	Aa	48	VAL
1	Aa	50	GLN
1	Aa	52	SER
1	Aa	79	VAL
1	Aa	109	GLN
1	Aa	126	SER
1	Aa	128	ILE
1	Ab	2	SER
1	Ab	4	PHE

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Mol	Chain	Res	Type
1	Ab	6	GLN
1	Ab	8	VAL
1	Ab	19	THR
1	Ab	20	VAL
1	Ab	25	PHE
1	Ab	33	ILE
1	Ab	48	VAL
1	Ab	50	GLN
1	Ab	52	SER
1	Ab	79	VAL
1	Ab	109	GLN
1	Ab	126	SER
1	Ab	128	ILE
1	Ac	2	SER
1	Ac	4	PHE
1	Ac	6	GLN
1	Ac	8	VAL
1	Ac	19	THR
1	Ac	20	VAL
1	Ac	25	PHE
1	Ac	33	ILE
1	Ac	48	VAL
1	Ac	50	GLN
1	Ac	52	SER
1	Ac	79	VAL
1	Ac	109	GLN
1	Ac	126	SER
1	Ac	128	ILE
1	Ad	2	SER
1	Ad	4	PHE
1	Ad	6	GLN
1	Ad	8	VAL
1	Ad	19	THR
1	Ad	20	VAL
1	Ad	25	PHE
1	Ad	33	ILE
1	Ad	48	VAL
1	Ad	50	GLN
1	Ad	52	SER
1	Ad	79	VAL
1	Ad	109	GLN
1	Ad	126	SER

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Mol	Chain	Res	Type
1	Ad	128	ILE
1	Ae	2	SER
1	Ae	4	PHE
1	Ae	6	GLN
1	Ae	8	VAL
1	Ae	19	THR
1	Ae	20	VAL
1	Ae	25	PHE
1	Ae	33	ILE
1	Ae	48	VAL
1	Ae	50	GLN
1	Ae	52	SER
1	Ae	79	VAL
1	Ae	109	GLN
1	Ae	126	SER
1	Ae	128	ILE
1	Af	2	SER
1	Af	4	PHE
1	Af	6	GLN
1	Af	8	VAL
1	Af	19	THR
1	Af	20	VAL
1	Af	25	PHE
1	Af	33	ILE
1	Af	48	VAL
1	Af	50	GLN
1	Af	52	SER
1	Af	79	VAL
1	Af	109	GLN
1	Af	126	SER
1	Af	128	ILE
1	Ag	2	SER
1	Ag	4	PHE
1	Ag	6	GLN
1	Ag	8	VAL
1	Ag	19	THR
1	Ag	20	VAL
1	Ag	25	PHE
1	Ag	33	ILE
1	Ag	48	VAL
1	Ag	50	GLN
1	Ag	52	SER

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Mol	Chain	Res	Type
1	Ag	79	VAL
1	Ag	109	GLN
1	Ag	126	SER
1	Ag	128	ILE
1	Ah	2	SER
1	Ah	4	PHE
1	Ah	6	GLN
1	Ah	8	VAL
1	Ah	19	THR
1	Ah	20	VAL
1	Ah	25	PHE
1	Ah	33	ILE
1	Ah	48	VAL
1	Ah	50	GLN
1	Ah	52	SER
1	Ah	79	VAL
1	Ah	109	GLN
1	Ah	126	SER
1	Ah	128	ILE
1	Ai	2	SER
1	Ai	4	PHE
1	Ai	6	GLN
1	Ai	8	VAL
1	Ai	19	THR
1	Ai	20	VAL
1	Ai	25	PHE
1	Ai	33	ILE
1	Ai	48	VAL
1	Ai	50	GLN
1	Ai	52	SER
1	Ai	79	VAL
1	Ai	109	GLN
1	Ai	126	SER
1	Ai	128	ILE
1	Aj	2	SER
1	Aj	4	PHE
1	Aj	6	GLN
1	Aj	8	VAL
1	Aj	19	THR
1	Aj	20	VAL
1	Aj	25	PHE
1	Aj	33	ILE

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Mol	Chain	Res	Type
1	Aj	48	VAL
1	Aj	50	GLN
1	Aj	52	SER
1	Aj	79	VAL
1	Aj	109	GLN
1	Aj	126	SER
1	Aj	128	ILE
1	Ak	2	SER
1	Ak	4	PHE
1	Ak	6	GLN
1	Ak	8	VAL
1	Ak	19	THR
1	Ak	20	VAL
1	Ak	25	PHE
1	Ak	33	ILE
1	Ak	48	VAL
1	Ak	50	GLN
1	Ak	52	SER
1	Ak	79	VAL
1	Ak	109	GLN
1	Ak	126	SER
1	Ak	128	ILE
1	Al	2	SER
1	Al	4	PHE
1	Al	6	GLN
1	Al	8	VAL
1	Al	19	THR
1	Al	20	VAL
1	Al	25	PHE
1	Al	33	ILE
1	Al	48	VAL
1	Al	50	GLN
1	Al	52	SER
1	Al	79	VAL
1	Al	109	GLN
1	Al	126	SER
1	Al	128	ILE
1	Am	2	SER
1	Am	4	PHE
1	Am	6	GLN
1	Am	8	VAL
1	Am	19	THR

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Mol	Chain	Res	Type
1	Am	20	VAL
1	Am	25	PHE
1	Am	33	ILE
1	Am	48	VAL
1	Am	50	GLN
1	Am	52	SER
1	Am	79	VAL
1	Am	109	GLN
1	Am	126	SER
1	Am	128	ILE
1	An	2	SER
1	An	4	PHE
1	An	6	GLN
1	An	8	VAL
1	An	19	THR
1	An	20	VAL
1	An	25	PHE
1	An	33	ILE
1	An	48	VAL
1	An	50	GLN
1	An	52	SER
1	An	79	VAL
1	An	109	GLN
1	An	126	SER
1	An	128	ILE
1	Ao	2	SER
1	Ao	4	PHE
1	Ao	6	GLN
1	Ao	8	VAL
1	Ao	19	THR
1	Ao	20	VAL
1	Ao	25	PHE
1	Ao	33	ILE
1	Ao	48	VAL
1	Ao	50	GLN
1	Ao	52	SER
1	Ao	79	VAL
1	Ao	109	GLN
1	Ao	126	SER
1	Ao	128	ILE
1	Ap	2	SER
1	Ap	4	PHE

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Mol	Chain	Res	Type
1	Ap	6	GLN
1	Ap	8	VAL
1	Ap	19	THR
1	Ap	20	VAL
1	Ap	25	PHE
1	Ap	33	ILE
1	Ap	48	VAL
1	Ap	50	GLN
1	Ap	52	SER
1	Ap	79	VAL
1	Ap	109	GLN
1	Ap	126	SER
1	Ap	128	ILE
1	Aq	2	SER
1	Aq	4	PHE
1	Aq	6	GLN
1	Aq	8	VAL
1	Aq	19	THR
1	Aq	20	VAL
1	Aq	25	PHE
1	Aq	33	ILE
1	Aq	48	VAL
1	Aq	50	GLN
1	Aq	52	SER
1	Aq	79	VAL
1	Aq	109	GLN
1	Aq	126	SER
1	Aq	128	ILE
1	Ar	2	SER
1	Ar	4	PHE
1	Ar	6	GLN
1	Ar	8	VAL
1	Ar	19	THR
1	Ar	20	VAL
1	Ar	25	PHE
1	Ar	33	ILE
1	Ar	48	VAL
1	Ar	50	GLN
1	Ar	52	SER
1	Ar	79	VAL
1	Ar	109	GLN
1	Ar	126	SER

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Mol	Chain	Res	Type
1	Ar	128	ILE
1	As	2	SER
1	As	4	PHE
1	As	6	GLN
1	As	8	VAL
1	As	19	THR
1	As	20	VAL
1	As	25	PHE
1	As	33	ILE
1	As	48	VAL
1	As	50	GLN
1	As	52	SER
1	As	79	VAL
1	As	109	GLN
1	As	126	SER
1	As	128	ILE
1	At	2	SER
1	At	4	PHE
1	At	6	GLN
1	At	8	VAL
1	At	19	THR
1	At	20	VAL
1	At	25	PHE
1	At	33	ILE
1	At	48	VAL
1	At	50	GLN
1	At	52	SER
1	At	79	VAL
1	At	109	GLN
1	At	126	SER
1	At	128	ILE
1	Au	2	SER
1	Au	4	PHE
1	Au	6	GLN
1	Au	8	VAL
1	Au	19	THR
1	Au	20	VAL
1	Au	25	PHE
1	Au	33	ILE
1	Au	48	VAL
1	Au	50	GLN
1	Au	52	SER

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Mol	Chain	Res	Type
1	Au	79	VAL
1	Au	109	GLN
1	Au	126	SER
1	Au	128	ILE
1	Av	2	SER
1	Av	4	PHE
1	Av	6	GLN
1	Av	8	VAL
1	Av	19	THR
1	Av	20	VAL
1	Av	25	PHE
1	Av	33	ILE
1	Av	48	VAL
1	Av	50	GLN
1	Av	52	SER
1	Av	79	VAL
1	Av	109	GLN
1	Av	126	SER
1	Av	128	ILE
1	Aw	2	SER
1	Aw	4	PHE
1	Aw	6	GLN
1	Aw	8	VAL
1	Aw	19	THR
1	Aw	20	VAL
1	Aw	25	PHE
1	Aw	33	ILE
1	Aw	48	VAL
1	Aw	50	GLN
1	Aw	52	SER
1	Aw	79	VAL
1	Aw	109	GLN
1	Aw	126	SER
1	Aw	128	ILE
1	Ax	2	SER
1	Ax	4	PHE
1	Ax	6	GLN
1	Ax	8	VAL
1	Ax	19	THR
1	Ax	20	VAL
1	Ax	25	PHE
1	Ax	33	ILE

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Mol	Chain	Res	Type
1	Ax	48	VAL
1	Ax	50	GLN
1	Ax	52	SER
1	Ax	79	VAL
1	Ax	109	GLN
1	Ax	126	SER
1	Ax	128	ILE
1	B0	20	VAL
1	B0	33	ILE
1	B0	35	SER
1	B0	38	ARG
1	B0	48	VAL
1	B0	54	GLN
1	B0	77	LEU
1	B0	103	LEU
1	B0	109	GLN
1	B1	20	VAL
1	B1	33	ILE
1	B1	35	SER
1	B1	38	ARG
1	B1	48	VAL
1	B1	54	GLN
1	B1	77	LEU
1	B1	103	LEU
1	B1	109	GLN
1	B2	20	VAL
1	B2	33	ILE
1	B2	35	SER
1	B2	38	ARG
1	B2	48	VAL
1	B2	54	GLN
1	B2	77	LEU
1	B2	103	LEU
1	B2	109	GLN
1	B3	20	VAL
1	B3	33	ILE
1	B3	35	SER
1	B3	38	ARG
1	B3	48	VAL
1	B3	54	GLN
1	B3	77	LEU
1	B3	103	LEU

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Mol	Chain	Res	Type
1	B3	109	GLN
1	B4	4	PHE
1	B4	20	VAL
1	B4	33	ILE
1	B4	35	SER
1	B4	38	ARG
1	B4	48	VAL
1	B4	54	GLN
1	B4	77	LEU
1	B4	103	LEU
1	B4	109	GLN
1	B5	4	PHE
1	B5	20	VAL
1	B5	33	ILE
1	B5	35	SER
1	B5	38	ARG
1	B5	48	VAL
1	B5	54	GLN
1	B5	77	LEU
1	B5	103	LEU
1	B5	109	GLN
1	B6	20	VAL
1	B6	33	ILE
1	B6	35	SER
1	B6	38	ARG
1	B6	48	VAL
1	B6	54	GLN
1	B6	77	LEU
1	B6	103	LEU
1	B6	109	GLN
1	B7	20	VAL
1	B7	33	ILE
1	B7	35	SER
1	B7	38	ARG
1	B7	48	VAL
1	B7	54	GLN
1	B7	77	LEU
1	B7	103	LEU
1	B7	109	GLN
1	B8	4	PHE
1	B8	20	VAL
1	B8	33	ILE

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Mol	Chain	Res	Type
1	B8	35	SER
1	B8	38	ARG
1	B8	48	VAL
1	B8	54	GLN
1	B8	77	LEU
1	B8	103	LEU
1	B8	109	GLN
1	B9	4	PHE
1	B9	20	VAL
1	B9	33	ILE
1	B9	35	SER
1	B9	38	ARG
1	B9	48	VAL
1	B9	54	GLN
1	B9	77	LEU
1	B9	103	LEU
1	B9	109	GLN
1	BA	20	VAL
1	BA	33	ILE
1	BA	35	SER
1	BA	38	ARG
1	BA	48	VAL
1	BA	54	GLN
1	BA	77	LEU
1	BA	103	LEU
1	BA	109	GLN
1	BB	4	PHE
1	BB	20	VAL
1	BB	33	ILE
1	BB	35	SER
1	BB	38	ARG
1	BB	48	VAL
1	BB	54	GLN
1	BB	77	LEU
1	BB	103	LEU
1	BB	109	GLN
1	BC	20	VAL
1	BC	33	ILE
1	BC	35	SER
1	BC	38	ARG
1	BC	48	VAL
1	BC	54	GLN

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Mol	Chain	Res	Type
1	BC	77	LEU
1	BC	103	LEU
1	BC	109	GLN
1	BD	20	VAL
1	BD	33	ILE
1	BD	35	SER
1	BD	38	ARG
1	BD	48	VAL
1	BD	54	GLN
1	BD	77	LEU
1	BD	103	LEU
1	BD	109	GLN
1	BE	4	PHE
1	BE	20	VAL
1	BE	33	ILE
1	BE	35	SER
1	BE	38	ARG
1	BE	48	VAL
1	BE	54	GLN
1	BE	77	LEU
1	BE	103	LEU
1	BE	109	GLN
1	BF	20	VAL
1	BF	33	ILE
1	BF	35	SER
1	BF	38	ARG
1	BF	48	VAL
1	BF	54	GLN
1	BF	77	LEU
1	BF	103	LEU
1	BF	109	GLN
1	BG	4	PHE
1	BG	20	VAL
1	BG	33	ILE
1	BG	35	SER
1	BG	38	ARG
1	BG	48	VAL
1	BG	54	GLN
1	BG	77	LEU
1	BG	103	LEU
1	BG	109	GLN
1	BH	20	VAL

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Mol	Chain	Res	Type
1	BH	33	ILE
1	BH	35	SER
1	BH	38	ARG
1	BH	48	VAL
1	BH	54	GLN
1	BH	77	LEU
1	BH	103	LEU
1	BH	109	GLN
1	BI	20	VAL
1	BI	33	ILE
1	BI	35	SER
1	BI	38	ARG
1	BI	48	VAL
1	BI	54	GLN
1	BI	77	LEU
1	BI	103	LEU
1	BI	109	GLN
1	BJ	4	PHE
1	BJ	20	VAL
1	BJ	33	ILE
1	BJ	35	SER
1	BJ	38	ARG
1	BJ	48	VAL
1	BJ	54	GLN
1	BJ	77	LEU
1	BJ	103	LEU
1	BJ	109	GLN
1	BK	20	VAL
1	BK	33	ILE
1	BK	35	SER
1	BK	38	ARG
1	BK	48	VAL
1	BK	54	GLN
1	BK	77	LEU
1	BK	103	LEU
1	BK	109	GLN
1	BL	4	PHE
1	BL	20	VAL
1	BL	33	ILE
1	BL	35	SER
1	BL	38	ARG
1	BL	48	VAL

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Mol	Chain	Res	Type
1	BL	54	GLN
1	BL	77	LEU
1	BL	103	LEU
1	BL	109	GLN
1	BM	20	VAL
1	BM	33	ILE
1	BM	35	SER
1	BM	38	ARG
1	BM	48	VAL
1	BM	54	GLN
1	BM	77	LEU
1	BM	103	LEU
1	BM	109	GLN
1	BN	20	VAL
1	BN	33	ILE
1	BN	35	SER
1	BN	38	ARG
1	BN	48	VAL
1	BN	54	GLN
1	BN	77	LEU
1	BN	103	LEU
1	BN	109	GLN
1	BO	4	PHE
1	BO	20	VAL
1	BO	33	ILE
1	BO	35	SER
1	BO	38	ARG
1	BO	48	VAL
1	BO	54	GLN
1	BO	77	LEU
1	BO	103	LEU
1	BO	109	GLN
1	BP	20	VAL
1	BP	33	ILE
1	BP	35	SER
1	BP	38	ARG
1	BP	48	VAL
1	BP	54	GLN
1	BP	77	LEU
1	BP	103	LEU
1	BP	109	GLN
1	BQ	20	VAL

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Mol	Chain	Res	Type
1	BQ	33	ILE
1	BQ	35	SER
1	BQ	38	ARG
1	BQ	48	VAL
1	BQ	54	GLN
1	BQ	77	LEU
1	BQ	103	LEU
1	BQ	109	GLN
1	BR	20	VAL
1	BR	33	ILE
1	BR	35	SER
1	BR	38	ARG
1	BR	48	VAL
1	BR	54	GLN
1	BR	77	LEU
1	BR	103	LEU
1	BR	109	GLN
1	BS	4	PHE
1	BS	20	VAL
1	BS	33	ILE
1	BS	35	SER
1	BS	38	ARG
1	BS	48	VAL
1	BS	54	GLN
1	BS	77	LEU
1	BS	103	LEU
1	BS	109	GLN
1	BT	20	VAL
1	BT	33	ILE
1	BT	35	SER
1	BT	38	ARG
1	BT	48	VAL
1	BT	54	GLN
1	BT	77	LEU
1	BT	103	LEU
1	BT	109	GLN
1	BU	4	PHE
1	BU	20	VAL
1	BU	33	ILE
1	BU	35	SER
1	BU	38	ARG
1	BU	48	VAL

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Mol	Chain	Res	Type
1	BU	54	GLN
1	BU	77	LEU
1	BU	103	LEU
1	BU	109	GLN
1	BV	20	VAL
1	BV	33	ILE
1	BV	35	SER
1	BV	38	ARG
1	BV	48	VAL
1	BV	54	GLN
1	BV	77	LEU
1	BV	103	LEU
1	BV	109	GLN
1	BW	20	VAL
1	BW	33	ILE
1	BW	35	SER
1	BW	38	ARG
1	BW	48	VAL
1	BW	54	GLN
1	BW	77	LEU
1	BW	103	LEU
1	BW	109	GLN
1	BX	4	PHE
1	BX	20	VAL
1	BX	33	ILE
1	BX	35	SER
1	BX	38	ARG
1	BX	48	VAL
1	BX	54	GLN
1	BX	77	LEU
1	BX	103	LEU
1	BX	109	GLN
1	BY	20	VAL
1	BY	33	ILE
1	BY	35	SER
1	BY	38	ARG
1	BY	48	VAL
1	BY	54	GLN
1	BY	77	LEU
1	BY	103	LEU
1	BY	109	GLN
1	BZ	20	VAL

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Mol	Chain	Res	Type
1	BZ	33	ILE
1	BZ	35	SER
1	BZ	38	ARG
1	BZ	48	VAL
1	BZ	54	GLN
1	BZ	77	LEU
1	BZ	103	LEU
1	BZ	109	GLN
1	Ba	20	VAL
1	Ba	33	ILE
1	Ba	35	SER
1	Ba	38	ARG
1	Ba	48	VAL
1	Ba	54	GLN
1	Ba	77	LEU
1	Ba	103	LEU
1	Ba	109	GLN
1	Bb	4	PHE
1	Bb	20	VAL
1	Bb	33	ILE
1	Bb	35	SER
1	Bb	38	ARG
1	Bb	48	VAL
1	Bb	54	GLN
1	Bb	77	LEU
1	Bb	103	LEU
1	Bb	109	GLN
1	Bc	20	VAL
1	Bc	33	ILE
1	Bc	35	SER
1	Bc	38	ARG
1	Bc	48	VAL
1	Bc	54	GLN
1	Bc	77	LEU
1	Bc	103	LEU
1	Bc	109	GLN
1	Bd	4	PHE
1	Bd	20	VAL
1	Bd	33	ILE
1	Bd	35	SER
1	Bd	38	ARG
1	Bd	48	VAL

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Mol	Chain	Res	Type
1	Bd	54	GLN
1	Bd	77	LEU
1	Bd	103	LEU
1	Bd	109	GLN
1	Be	4	PHE
1	Be	20	VAL
1	Be	33	ILE
1	Be	35	SER
1	Be	38	ARG
1	Be	48	VAL
1	Be	54	GLN
1	Be	77	LEU
1	Be	103	LEU
1	Be	109	GLN
1	Bf	20	VAL
1	Bf	33	ILE
1	Bf	35	SER
1	Bf	38	ARG
1	Bf	48	VAL
1	Bf	54	GLN
1	Bf	77	LEU
1	Bf	103	LEU
1	Bf	109	GLN
1	Bg	4	PHE
1	Bg	20	VAL
1	Bg	33	ILE
1	Bg	35	SER
1	Bg	38	ARG
1	Bg	48	VAL
1	Bg	54	GLN
1	Bg	77	LEU
1	Bg	103	LEU
1	Bg	109	GLN
1	Bh	4	PHE
1	Bh	20	VAL
1	Bh	33	ILE
1	Bh	35	SER
1	Bh	38	ARG
1	Bh	48	VAL
1	Bh	54	GLN
1	Bh	77	LEU
1	Bh	103	LEU

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Mol	Chain	Res	Type
1	Bh	109	GLN
1	Bi	4	PHE
1	Bi	20	VAL
1	Bi	33	ILE
1	Bi	35	SER
1	Bi	38	ARG
1	Bi	48	VAL
1	Bi	54	GLN
1	Bi	77	LEU
1	Bi	103	LEU
1	Bi	109	GLN
1	Bj	4	PHE
1	Bj	20	VAL
1	Bj	33	ILE
1	Bj	35	SER
1	Bj	38	ARG
1	Bj	48	VAL
1	Bj	54	GLN
1	Bj	77	LEU
1	Bj	103	LEU
1	Bj	109	GLN
1	Bk	20	VAL
1	Bk	33	ILE
1	Bk	35	SER
1	Bk	38	ARG
1	Bk	48	VAL
1	Bk	54	GLN
1	Bk	77	LEU
1	Bk	103	LEU
1	Bk	109	GLN
1	Bl	20	VAL
1	Bl	33	ILE
1	Bl	35	SER
1	Bl	38	ARG
1	Bl	48	VAL
1	Bl	54	GLN
1	Bl	77	LEU
1	Bl	103	LEU
1	Bl	109	GLN
1	Bm	4	PHE
1	Bm	20	VAL
1	Bm	33	ILE

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Mol	Chain	Res	Type
1	Bm	35	SER
1	Bm	38	ARG
1	Bm	48	VAL
1	Bm	54	GLN
1	Bm	77	LEU
1	Bm	103	LEU
1	Bm	109	GLN
1	Bn	20	VAL
1	Bn	33	ILE
1	Bn	35	SER
1	Bn	38	ARG
1	Bn	48	VAL
1	Bn	54	GLN
1	Bn	77	LEU
1	Bn	103	LEU
1	Bn	109	GLN
1	Bo	20	VAL
1	Bo	33	ILE
1	Bo	35	SER
1	Bo	38	ARG
1	Bo	48	VAL
1	Bo	54	GLN
1	Bo	77	LEU
1	Bo	103	LEU
1	Bo	109	GLN
1	Bp	20	VAL
1	Bp	33	ILE
1	Bp	35	SER
1	Bp	38	ARG
1	Bp	48	VAL
1	Bp	54	GLN
1	Bp	77	LEU
1	Bp	103	LEU
1	Bp	109	GLN
1	Bq	4	PHE
1	Bq	20	VAL
1	Bq	33	ILE
1	Bq	35	SER
1	Bq	38	ARG
1	Bq	48	VAL
1	Bq	54	GLN
1	Bq	77	LEU

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Mol	Chain	Res	Type
1	Bq	103	LEU
1	Bq	109	GLN
1	Br	4	PHE
1	Br	20	VAL
1	Br	33	ILE
1	Br	35	SER
1	Br	38	ARG
1	Br	48	VAL
1	Br	54	GLN
1	Br	77	LEU
1	Br	103	LEU
1	Br	109	GLN
1	Bs	4	PHE
1	Bs	20	VAL
1	Bs	33	ILE
1	Bs	35	SER
1	Bs	38	ARG
1	Bs	48	VAL
1	Bs	54	GLN
1	Bs	77	LEU
1	Bs	103	LEU
1	Bs	109	GLN
1	Bt	20	VAL
1	Bt	33	ILE
1	Bt	35	SER
1	Bt	38	ARG
1	Bt	48	VAL
1	Bt	54	GLN
1	Bt	77	LEU
1	Bt	103	LEU
1	Bt	109	GLN
1	Bu	20	VAL
1	Bu	33	ILE
1	Bu	35	SER
1	Bu	38	ARG
1	Bu	48	VAL
1	Bu	54	GLN
1	Bu	77	LEU
1	Bu	103	LEU
1	Bu	109	GLN
1	Bv	20	VAL
1	Bv	33	ILE

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Mol	Chain	Res	Type
1	Bv	35	SER
1	Bv	38	ARG
1	Bv	48	VAL
1	Bv	54	GLN
1	Bv	77	LEU
1	Bv	103	LEU
1	Bv	109	GLN
1	Bw	20	VAL
1	Bw	33	ILE
1	Bw	35	SER
1	Bw	38	ARG
1	Bw	48	VAL
1	Bw	54	GLN
1	Bw	77	LEU
1	Bw	103	LEU
1	Bw	109	GLN
1	Bx	4	PHE
1	Bx	20	VAL
1	Bx	33	ILE
1	Bx	35	SER
1	Bx	38	ARG
1	Bx	48	VAL
1	Bx	54	GLN
1	Bx	77	LEU
1	Bx	103	LEU
1	Bx	109	GLN
1	C0	11	ASP
1	C0	20	VAL
1	C0	23	SER
1	C0	37	SER
1	C0	38	ARG
1	C0	49	ARG
1	C0	66	LYS
1	C0	76	GLU
1	C0	84	SER
1	C0	87	ASN
1	C0	109	GLN
1	C0	114	ASP
1	C1	11	ASP
1	C1	20	VAL
1	C1	23	SER
1	C1	37	SER

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Mol	Chain	Res	Type
1	C1	38	ARG
1	C1	49	ARG
1	C1	66	LYS
1	C1	76	GLU
1	C1	84	SER
1	C1	87	ASN
1	C1	109	GLN
1	C1	114	ASP
1	C2	11	ASP
1	C2	20	VAL
1	C2	23	SER
1	C2	37	SER
1	C2	38	ARG
1	C2	49	ARG
1	C2	66	LYS
1	C2	76	GLU
1	C2	84	SER
1	C2	87	ASN
1	C2	109	GLN
1	C2	114	ASP
1	C3	11	ASP
1	C3	20	VAL
1	C3	23	SER
1	C3	37	SER
1	C3	38	ARG
1	C3	49	ARG
1	C3	66	LYS
1	C3	76	GLU
1	C3	84	SER
1	C3	87	ASN
1	C3	109	GLN
1	C3	114	ASP
1	C4	11	ASP
1	C4	20	VAL
1	C4	23	SER
1	C4	37	SER
1	C4	38	ARG
1	C4	49	ARG
1	C4	66	LYS
1	C4	76	GLU
1	C4	84	SER
1	C4	87	ASN

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Mol	Chain	Res	Type
1	C4	109	GLN
1	C4	114	ASP
1	C5	11	ASP
1	C5	20	VAL
1	C5	23	SER
1	C5	37	SER
1	C5	38	ARG
1	C5	49	ARG
1	C5	66	LYS
1	C5	76	GLU
1	C5	84	SER
1	C5	87	ASN
1	C5	109	GLN
1	C5	114	ASP
1	C6	11	ASP
1	C6	20	VAL
1	C6	23	SER
1	C6	37	SER
1	C6	38	ARG
1	C6	49	ARG
1	C6	66	LYS
1	C6	76	GLU
1	C6	84	SER
1	C6	87	ASN
1	C6	109	GLN
1	C6	114	ASP
1	C7	11	ASP
1	C7	20	VAL
1	C7	23	SER
1	C7	37	SER
1	C7	38	ARG
1	C7	49	ARG
1	C7	66	LYS
1	C7	76	GLU
1	C7	84	SER
1	C7	87	ASN
1	C7	109	GLN
1	C7	114	ASP
1	C8	11	ASP
1	C8	20	VAL
1	C8	23	SER
1	C8	37	SER

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Mol	Chain	Res	Type
1	C8	38	ARG
1	C8	49	ARG
1	C8	66	LYS
1	C8	76	GLU
1	C8	84	SER
1	C8	87	ASN
1	C8	109	GLN
1	C8	114	ASP
1	C9	11	ASP
1	C9	20	VAL
1	C9	23	SER
1	C9	37	SER
1	C9	38	ARG
1	C9	49	ARG
1	C9	66	LYS
1	C9	76	GLU
1	C9	84	SER
1	C9	87	ASN
1	C9	109	GLN
1	C9	114	ASP
1	CA	11	ASP
1	CA	20	VAL
1	CA	23	SER
1	CA	37	SER
1	CA	38	ARG
1	CA	49	ARG
1	CA	66	LYS
1	CA	76	GLU
1	CA	84	SER
1	CA	87	ASN
1	CA	109	GLN
1	CA	114	ASP
1	CB	11	ASP
1	CB	20	VAL
1	CB	23	SER
1	CB	37	SER
1	CB	38	ARG
1	CB	49	ARG
1	CB	66	LYS
1	CB	76	GLU
1	CB	84	SER
1	CB	87	ASN

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Mol	Chain	Res	Type
1	CB	109	GLN
1	CB	114	ASP
1	CC	11	ASP
1	CC	20	VAL
1	CC	23	SER
1	CC	37	SER
1	CC	38	ARG
1	CC	49	ARG
1	CC	66	LYS
1	CC	76	GLU
1	CC	84	SER
1	CC	87	ASN
1	CC	109	GLN
1	CC	114	ASP
1	CD	11	ASP
1	CD	20	VAL
1	CD	23	SER
1	CD	37	SER
1	CD	38	ARG
1	CD	49	ARG
1	CD	66	LYS
1	CD	76	GLU
1	CD	84	SER
1	CD	87	ASN
1	CD	109	GLN
1	CD	114	ASP
1	CE	11	ASP
1	CE	20	VAL
1	CE	23	SER
1	CE	37	SER
1	CE	38	ARG
1	CE	49	ARG
1	CE	66	LYS
1	CE	76	GLU
1	CE	84	SER
1	CE	87	ASN
1	CE	109	GLN
1	CE	114	ASP
1	CF	11	ASP
1	CF	20	VAL
1	CF	23	SER
1	CF	37	SER

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Mol	Chain	Res	Type
1	CF	38	ARG
1	CF	49	ARG
1	CF	66	LYS
1	CF	76	GLU
1	CF	84	SER
1	CF	87	ASN
1	CF	109	GLN
1	CF	114	ASP
1	CG	11	ASP
1	CG	20	VAL
1	CG	23	SER
1	CG	37	SER
1	CG	38	ARG
1	CG	49	ARG
1	CG	66	LYS
1	CG	76	GLU
1	CG	84	SER
1	CG	87	ASN
1	CG	109	GLN
1	CG	114	ASP
1	CH	11	ASP
1	CH	20	VAL
1	CH	23	SER
1	CH	37	SER
1	CH	38	ARG
1	CH	49	ARG
1	CH	66	LYS
1	CH	76	GLU
1	CH	84	SER
1	CH	87	ASN
1	CH	109	GLN
1	CH	114	ASP
1	CI	11	ASP
1	CI	20	VAL
1	CI	23	SER
1	CI	37	SER
1	CI	38	ARG
1	CI	49	ARG
1	CI	66	LYS
1	CI	76	GLU
1	CI	84	SER
1	CI	87	ASN

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Mol	Chain	Res	Type
1	CI	109	GLN
1	CI	114	ASP
1	CJ	11	ASP
1	CJ	20	VAL
1	CJ	23	SER
1	CJ	37	SER
1	CJ	38	ARG
1	CJ	49	ARG
1	CJ	66	LYS
1	CJ	76	GLU
1	CJ	84	SER
1	CJ	87	ASN
1	CJ	109	GLN
1	CJ	114	ASP
1	CK	11	ASP
1	CK	20	VAL
1	CK	23	SER
1	CK	37	SER
1	CK	38	ARG
1	CK	49	ARG
1	CK	66	LYS
1	CK	76	GLU
1	CK	84	SER
1	CK	87	ASN
1	CK	109	GLN
1	CK	114	ASP
1	CL	11	ASP
1	CL	20	VAL
1	CL	23	SER
1	CL	37	SER
1	CL	38	ARG
1	CL	49	ARG
1	CL	66	LYS
1	CL	76	GLU
1	CL	84	SER
1	CL	87	ASN
1	CL	109	GLN
1	CL	114	ASP
1	CM	11	ASP
1	CM	20	VAL
1	CM	23	SER
1	CM	37	SER

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Mol	Chain	Res	Type
1	CM	38	ARG
1	CM	49	ARG
1	CM	66	LYS
1	CM	76	GLU
1	CM	84	SER
1	CM	87	ASN
1	CM	109	GLN
1	CM	114	ASP
1	CN	11	ASP
1	CN	20	VAL
1	CN	23	SER
1	CN	37	SER
1	CN	38	ARG
1	CN	49	ARG
1	CN	66	LYS
1	CN	76	GLU
1	CN	84	SER
1	CN	87	ASN
1	CN	109	GLN
1	CN	114	ASP
1	CO	11	ASP
1	CO	20	VAL
1	CO	23	SER
1	CO	37	SER
1	CO	38	ARG
1	CO	49	ARG
1	CO	66	LYS
1	CO	76	GLU
1	CO	84	SER
1	CO	87	ASN
1	CO	109	GLN
1	CO	114	ASP
1	CP	11	ASP
1	CP	20	VAL
1	CP	23	SER
1	CP	37	SER
1	CP	38	ARG
1	CP	49	ARG
1	CP	66	LYS
1	CP	76	GLU
1	CP	84	SER
1	CP	87	ASN

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Mol	Chain	Res	Type
1	CP	109	GLN
1	CP	114	ASP
1	CQ	11	ASP
1	CQ	20	VAL
1	CQ	23	SER
1	CQ	37	SER
1	CQ	38	ARG
1	CQ	49	ARG
1	CQ	66	LYS
1	CQ	76	GLU
1	CQ	84	SER
1	CQ	87	ASN
1	CQ	109	GLN
1	CQ	114	ASP
1	CR	11	ASP
1	CR	20	VAL
1	CR	23	SER
1	CR	37	SER
1	CR	38	ARG
1	CR	49	ARG
1	CR	66	LYS
1	CR	76	GLU
1	CR	84	SER
1	CR	87	ASN
1	CR	109	GLN
1	CR	114	ASP
1	CS	11	ASP
1	CS	20	VAL
1	CS	23	SER
1	CS	37	SER
1	CS	38	ARG
1	CS	49	ARG
1	CS	66	LYS
1	CS	76	GLU
1	CS	84	SER
1	CS	87	ASN
1	CS	109	GLN
1	CS	114	ASP
1	CT	11	ASP
1	CT	20	VAL
1	CT	23	SER
1	CT	37	SER

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Mol	Chain	Res	Type
1	CT	38	ARG
1	CT	49	ARG
1	CT	66	LYS
1	CT	76	GLU
1	CT	84	SER
1	CT	87	ASN
1	CT	109	GLN
1	CT	114	ASP
1	CU	11	ASP
1	CU	20	VAL
1	CU	23	SER
1	CU	37	SER
1	CU	38	ARG
1	CU	49	ARG
1	CU	66	LYS
1	CU	76	GLU
1	CU	84	SER
1	CU	87	ASN
1	CU	109	GLN
1	CU	114	ASP
1	CV	11	ASP
1	CV	20	VAL
1	CV	23	SER
1	CV	37	SER
1	CV	38	ARG
1	CV	49	ARG
1	CV	66	LYS
1	CV	76	GLU
1	CV	84	SER
1	CV	87	ASN
1	CV	109	GLN
1	CV	114	ASP
1	CW	11	ASP
1	CW	20	VAL
1	CW	23	SER
1	CW	37	SER
1	CW	38	ARG
1	CW	49	ARG
1	CW	66	LYS
1	CW	76	GLU
1	CW	84	SER
1	CW	87	ASN

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Mol	Chain	Res	Type
1	CW	109	GLN
1	CW	114	ASP
1	CX	11	ASP
1	CX	20	VAL
1	CX	23	SER
1	CX	37	SER
1	CX	38	ARG
1	CX	49	ARG
1	CX	66	LYS
1	CX	76	GLU
1	CX	84	SER
1	CX	87	ASN
1	CX	109	GLN
1	CX	114	ASP
1	CY	11	ASP
1	CY	20	VAL
1	CY	23	SER
1	CY	37	SER
1	CY	38	ARG
1	CY	49	ARG
1	CY	66	LYS
1	CY	76	GLU
1	CY	84	SER
1	CY	87	ASN
1	CY	109	GLN
1	CY	114	ASP
1	CZ	11	ASP
1	CZ	20	VAL
1	CZ	23	SER
1	CZ	37	SER
1	CZ	38	ARG
1	CZ	49	ARG
1	CZ	66	LYS
1	CZ	76	GLU
1	CZ	84	SER
1	CZ	87	ASN
1	CZ	109	GLN
1	CZ	114	ASP
1	Ca	11	ASP
1	Ca	20	VAL
1	Ca	23	SER
1	Ca	37	SER

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Mol	Chain	Res	Type
1	Ca	38	ARG
1	Ca	49	ARG
1	Ca	66	LYS
1	Ca	76	GLU
1	Ca	84	SER
1	Ca	87	ASN
1	Ca	109	GLN
1	Ca	114	ASP
1	Cb	11	ASP
1	Cb	20	VAL
1	Cb	23	SER
1	Cb	37	SER
1	Cb	38	ARG
1	Cb	49	ARG
1	Cb	66	LYS
1	Cb	76	GLU
1	Cb	84	SER
1	Cb	87	ASN
1	Cb	109	GLN
1	Cb	114	ASP
1	Cc	11	ASP
1	Cc	20	VAL
1	Cc	23	SER
1	Cc	37	SER
1	Cc	38	ARG
1	Cc	49	ARG
1	Cc	66	LYS
1	Cc	76	GLU
1	Cc	84	SER
1	Cc	87	ASN
1	Cc	109	GLN
1	Cc	114	ASP
1	Cd	11	ASP
1	Cd	20	VAL
1	Cd	23	SER
1	Cd	37	SER
1	Cd	38	ARG
1	Cd	49	ARG
1	Cd	66	LYS
1	Cd	76	GLU
1	Cd	84	SER
1	Cd	87	ASN

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Mol	Chain	Res	Type
1	Cd	109	GLN
1	Cd	114	ASP
1	Ce	11	ASP
1	Ce	20	VAL
1	Ce	23	SER
1	Ce	37	SER
1	Ce	38	ARG
1	Ce	49	ARG
1	Ce	66	LYS
1	Ce	76	GLU
1	Ce	84	SER
1	Ce	87	ASN
1	Ce	109	GLN
1	Ce	114	ASP
1	Cf	11	ASP
1	Cf	20	VAL
1	Cf	23	SER
1	Cf	37	SER
1	Cf	38	ARG
1	Cf	49	ARG
1	Cf	66	LYS
1	Cf	76	GLU
1	Cf	84	SER
1	Cf	87	ASN
1	Cf	109	GLN
1	Cf	114	ASP
1	Cg	11	ASP
1	Cg	20	VAL
1	Cg	23	SER
1	Cg	37	SER
1	Cg	38	ARG
1	Cg	49	ARG
1	Cg	66	LYS
1	Cg	76	GLU
1	Cg	84	SER
1	Cg	87	ASN
1	Cg	109	GLN
1	Cg	114	ASP
1	Ch	11	ASP
1	Ch	20	VAL
1	Ch	23	SER
1	Ch	37	SER

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Mol	Chain	Res	Type
1	Ch	38	ARG
1	Ch	49	ARG
1	Ch	66	LYS
1	Ch	76	GLU
1	Ch	84	SER
1	Ch	87	ASN
1	Ch	109	GLN
1	Ch	114	ASP
1	Ci	11	ASP
1	Ci	20	VAL
1	Ci	23	SER
1	Ci	37	SER
1	Ci	38	ARG
1	Ci	49	ARG
1	Ci	66	LYS
1	Ci	76	GLU
1	Ci	84	SER
1	Ci	87	ASN
1	Ci	109	GLN
1	Ci	114	ASP
1	Cj	11	ASP
1	Cj	20	VAL
1	Cj	23	SER
1	Cj	37	SER
1	Cj	38	ARG
1	Cj	49	ARG
1	Cj	66	LYS
1	Cj	76	GLU
1	Cj	84	SER
1	Cj	87	ASN
1	Cj	109	GLN
1	Cj	114	ASP
1	Ck	11	ASP
1	Ck	20	VAL
1	Ck	23	SER
1	Ck	37	SER
1	Ck	38	ARG
1	Ck	49	ARG
1	Ck	66	LYS
1	Ck	76	GLU
1	Ck	84	SER
1	Ck	87	ASN

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Mol	Chain	Res	Type
1	Ck	109	GLN
1	Ck	114	ASP
1	Cl	11	ASP
1	Cl	20	VAL
1	Cl	23	SER
1	Cl	37	SER
1	Cl	38	ARG
1	Cl	49	ARG
1	Cl	66	LYS
1	Cl	76	GLU
1	Cl	84	SER
1	Cl	87	ASN
1	Cl	109	GLN
1	Cl	114	ASP
1	Cm	11	ASP
1	Cm	20	VAL
1	Cm	23	SER
1	Cm	37	SER
1	Cm	38	ARG
1	Cm	49	ARG
1	Cm	66	LYS
1	Cm	76	GLU
1	Cm	84	SER
1	Cm	87	ASN
1	Cm	109	GLN
1	Cm	114	ASP
1	Cn	11	ASP
1	Cn	20	VAL
1	Cn	23	SER
1	Cn	37	SER
1	Cn	38	ARG
1	Cn	49	ARG
1	Cn	66	LYS
1	Cn	76	GLU
1	Cn	84	SER
1	Cn	87	ASN
1	Cn	109	GLN
1	Cn	114	ASP
1	Co	11	ASP
1	Co	20	VAL
1	Co	23	SER
1	Co	37	SER

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Mol	Chain	Res	Type
1	Co	38	ARG
1	Co	49	ARG
1	Co	66	LYS
1	Co	76	GLU
1	Co	84	SER
1	Co	87	ASN
1	Co	109	GLN
1	Co	114	ASP
1	Cp	11	ASP
1	Cp	20	VAL
1	Cp	23	SER
1	Cp	37	SER
1	Cp	38	ARG
1	Cp	49	ARG
1	Cp	66	LYS
1	Cp	76	GLU
1	Cp	84	SER
1	Cp	87	ASN
1	Cp	109	GLN
1	Cp	114	ASP
1	Cq	11	ASP
1	Cq	20	VAL
1	Cq	23	SER
1	Cq	37	SER
1	Cq	38	ARG
1	Cq	49	ARG
1	Cq	66	LYS
1	Cq	76	GLU
1	Cq	84	SER
1	Cq	87	ASN
1	Cq	109	GLN
1	Cq	114	ASP
1	Cr	11	ASP
1	Cr	20	VAL
1	Cr	23	SER
1	Cr	37	SER
1	Cr	38	ARG
1	Cr	49	ARG
1	Cr	66	LYS
1	Cr	76	GLU
1	Cr	84	SER
1	Cr	87	ASN

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Mol	Chain	Res	Type
1	Cr	109	GLN
1	Cr	114	ASP
1	Cs	11	ASP
1	Cs	20	VAL
1	Cs	23	SER
1	Cs	37	SER
1	Cs	38	ARG
1	Cs	49	ARG
1	Cs	66	LYS
1	Cs	76	GLU
1	Cs	84	SER
1	Cs	87	ASN
1	Cs	109	GLN
1	Cs	114	ASP
1	Ct	11	ASP
1	Ct	20	VAL
1	Ct	23	SER
1	Ct	37	SER
1	Ct	38	ARG
1	Ct	49	ARG
1	Ct	66	LYS
1	Ct	76	GLU
1	Ct	84	SER
1	Ct	87	ASN
1	Ct	109	GLN
1	Ct	114	ASP
1	Cu	11	ASP
1	Cu	20	VAL
1	Cu	23	SER
1	Cu	37	SER
1	Cu	38	ARG
1	Cu	49	ARG
1	Cu	66	LYS
1	Cu	76	GLU
1	Cu	84	SER
1	Cu	87	ASN
1	Cu	109	GLN
1	Cu	114	ASP
1	Cv	11	ASP
1	Cv	20	VAL
1	Cv	23	SER
1	Cv	37	SER

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Mol	Chain	Res	Type
1	Cv	38	ARG
1	Cv	49	ARG
1	Cv	66	LYS
1	Cv	76	GLU
1	Cv	84	SER
1	Cv	87	ASN
1	Cv	109	GLN
1	Cv	114	ASP
1	Cw	11	ASP
1	Cw	20	VAL
1	Cw	23	SER
1	Cw	37	SER
1	Cw	38	ARG
1	Cw	49	ARG
1	Cw	66	LYS
1	Cw	76	GLU
1	Cw	84	SER
1	Cw	87	ASN
1	Cw	109	GLN
1	Cw	114	ASP
1	Cx	11	ASP
1	Cx	20	VAL
1	Cx	23	SER
1	Cx	37	SER
1	Cx	38	ARG
1	Cx	49	ARG
1	Cx	66	LYS
1	Cx	76	GLU
1	Cx	84	SER
1	Cx	87	ASN
1	Cx	109	GLN
1	Cx	114	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (229) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	40	GLN
1	A0	109	GLN
1	A1	40	GLN
1	A1	109	GLN
1	A2	40	GLN
1	A2	109	GLN

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Mol	Chain	Res	Type
1	A3	40	GLN
1	A3	109	GLN
1	A4	40	GLN
1	A4	109	GLN
1	A5	40	GLN
1	A5	109	GLN
1	A6	40	GLN
1	A6	109	GLN
1	A7	40	GLN
1	A7	109	GLN
1	A8	40	GLN
1	A8	109	GLN
1	A9	40	GLN
1	A9	109	GLN
1	AA	40	GLN
1	AA	109	GLN
1	AB	40	GLN
1	AB	109	GLN
1	AC	40	GLN
1	AC	109	GLN
1	AD	40	GLN
1	AD	109	GLN
1	AE	40	GLN
1	AE	109	GLN
1	AF	40	GLN
1	AG	40	GLN
1	AG	109	GLN
1	AH	40	GLN
1	AI	40	GLN
1	AI	109	GLN
1	AJ	40	GLN
1	AJ	109	GLN
1	AK	40	GLN
1	AL	40	GLN
1	AL	109	GLN
1	AM	40	GLN
1	AM	109	GLN
1	AN	40	GLN
1	AN	109	GLN
1	AO	40	GLN
1	AO	109	GLN
1	AP	40	GLN

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Mol	Chain	Res	Type
1	AP	109	GLN
1	AQ	40	GLN
1	AR	40	GLN
1	AR	109	GLN
1	AS	40	GLN
1	AS	109	GLN
1	AT	40	GLN
1	AT	109	GLN
1	AU	109	GLN
1	AV	40	GLN
1	AV	109	GLN
1	AW	40	GLN
1	AW	109	GLN
1	AX	40	GLN
1	AY	40	GLN
1	AY	109	GLN
1	AZ	40	GLN
1	Aa	40	GLN
1	Aa	109	GLN
1	Ab	40	GLN
1	Ac	40	GLN
1	Ac	109	GLN
1	Ad	40	GLN
1	Ad	109	GLN
1	Ae	40	GLN
1	Ae	109	GLN
1	Af	40	GLN
1	Af	109	GLN
1	Ag	40	GLN
1	Ag	109	GLN
1	Ah	40	GLN
1	Ah	109	GLN
1	Ai	40	GLN
1	Ai	109	GLN
1	Aj	40	GLN
1	Aj	109	GLN
1	Ak	40	GLN
1	Ak	109	GLN
1	Al	40	GLN
1	Al	109	GLN
1	Am	40	GLN
1	Am	109	GLN

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Mol	Chain	Res	Type
1	An	40	GLN
1	An	109	GLN
1	Ao	40	GLN
1	Ap	40	GLN
1	Ap	109	GLN
1	Aq	40	GLN
1	Ar	40	GLN
1	Ar	109	GLN
1	As	40	GLN
1	As	109	GLN
1	At	40	GLN
1	At	109	GLN
1	Au	40	GLN
1	Av	40	GLN
1	Av	109	GLN
1	Aw	40	GLN
1	Aw	109	GLN
1	Ax	40	GLN
1	Ax	109	GLN
1	B0	3	ASN
1	B0	36	ASN
1	B1	3	ASN
1	B1	36	ASN
1	B2	3	ASN
1	B2	36	ASN
1	B3	3	ASN
1	B3	36	ASN
1	B4	3	ASN
1	B4	36	ASN
1	B5	3	ASN
1	B5	36	ASN
1	B6	3	ASN
1	B6	36	ASN
1	B7	3	ASN
1	B7	36	ASN
1	B8	3	ASN
1	B8	36	ASN
1	B9	3	ASN
1	B9	36	ASN
1	BA	3	ASN
1	BA	36	ASN
1	BB	3	ASN

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Mol	Chain	Res	Type
1	BB	36	ASN
1	BC	3	ASN
1	BC	36	ASN
1	BD	3	ASN
1	BD	36	ASN
1	BE	3	ASN
1	BE	36	ASN
1	BF	3	ASN
1	BF	36	ASN
1	BG	3	ASN
1	BG	36	ASN
1	BH	3	ASN
1	BH	36	ASN
1	BI	3	ASN
1	BI	36	ASN
1	BJ	3	ASN
1	BJ	36	ASN
1	BK	3	ASN
1	BK	36	ASN
1	BL	3	ASN
1	BL	36	ASN
1	BM	3	ASN
1	BM	36	ASN
1	BN	3	ASN
1	BN	36	ASN
1	BO	3	ASN
1	BO	36	ASN
1	BP	3	ASN
1	BP	36	ASN
1	BQ	3	ASN
1	BQ	36	ASN
1	BR	3	ASN
1	BR	36	ASN
1	BS	3	ASN
1	BS	36	ASN
1	BT	3	ASN
1	BT	36	ASN
1	BU	3	ASN
1	BU	36	ASN
1	BV	3	ASN
1	BV	36	ASN
1	BW	3	ASN

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Mol	Chain	Res	Type
1	BW	36	ASN
1	BX	3	ASN
1	BX	36	ASN
1	BY	3	ASN
1	BY	36	ASN
1	BZ	3	ASN
1	BZ	36	ASN
1	Ba	3	ASN
1	Ba	36	ASN
1	Bb	3	ASN
1	Bb	36	ASN
1	Bc	3	ASN
1	Bc	36	ASN
1	Bd	3	ASN
1	Bd	36	ASN
1	Be	3	ASN
1	Be	36	ASN
1	Bf	3	ASN
1	Bf	36	ASN
1	Bg	3	ASN
1	Bg	36	ASN
1	Bh	3	ASN
1	Bh	36	ASN
1	Bi	3	ASN
1	Bi	36	ASN
1	Bj	3	ASN
1	Bj	36	ASN
1	Bk	3	ASN
1	Bk	36	ASN
1	Bl	3	ASN
1	Bl	36	ASN
1	Bm	3	ASN
1	Bm	36	ASN
1	Bn	3	ASN
1	Bn	36	ASN
1	Bo	3	ASN
1	Bo	36	ASN
1	Bp	3	ASN
1	Bp	36	ASN
1	Bq	3	ASN
1	Bq	36	ASN
1	Br	3	ASN

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Mol	Chain	Res	Type
1	Br	36	ASN
1	Bs	3	ASN
1	Bs	36	ASN
1	Bt	3	ASN
1	Bt	36	ASN
1	Bu	3	ASN
1	Bu	36	ASN
1	Bv	3	ASN
1	Bv	36	ASN
1	Bw	3	ASN
1	Bw	36	ASN
1	Bx	3	ASN
1	Bx	36	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.