



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:06 am GMT

PDB ID : 4P3Q
Title : Room-temperature WT DHFR, time-averaged ensemble
Authors : Keedy, D.A.; van den Bedem, H.; Fraser, J.S.
Deposited on : 2014-03-10
Resolution : 1.35 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

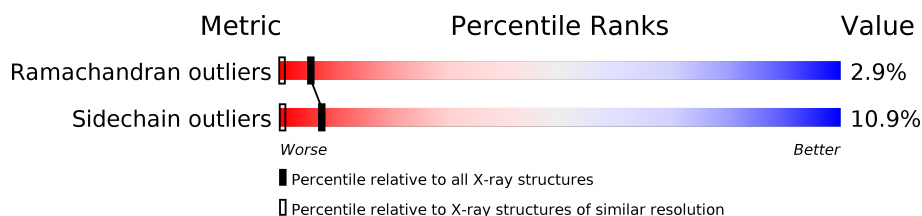
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	110173	1048 (1.38-1.34)
Sidechain outliers	110143	1048 (1.38-1.34)












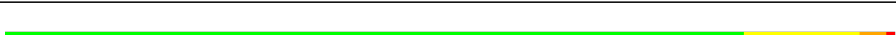


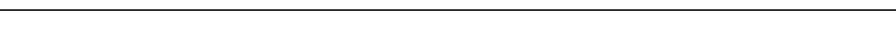
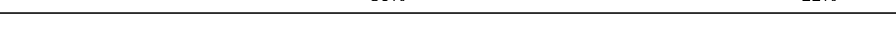

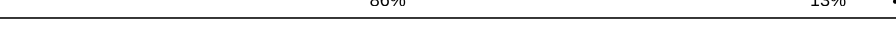







The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	159	 87% 11% .
1	10-A	159	 89% 8% ..
1	100-A	159	 87% 11% .
1	101-A	159	 92% 6% .
1	102-A	159	 90% 9% ..
1	103-A	159	 87% 10% .
1	104-A	159	 89% 9% .
1	105-A	159	 87% 9% ..
1	106-A	159	 82% 16% .


























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Mol	Chain	Length	Quality of chain
1	107-A	159	 83% 13% .
1	108-A	159	 84% 14% ..
1	109-A	159	 84% 14% ..
1	11-A	159	 87% 9% ..
1	110-A	159	 85% 12% .
1	111-A	159	 85% 13% ..
1	112-A	159	 85% 13% ..
1	113-A	159	 81% 14% . .
1	114-A	159	 82% 12% 5% .
1	115-A	159	 80% 15% . .
1	116-A	159	 83% 13% . .
1	117-A	159	 83% 13% . .
1	118-A	159	 84% 13% . .
1	119-A	159	 87% 12% .
1	12-A	159	 86% 11% .
1	120-A	159	 91% 8% .
1	121-A	159	 86% 13% .
1	122-A	159	 86% 11% .
1	123-A	159	 87% 11% .
1	124-A	159	 87% 13% .
1	125-A	159	 87% 12% .
1	126-A	159	 90% 9% .
1	127-A	159	 90% 9% .
1	128-A	159	 88% 11% .
1	129-A	159	 92% 7% .


























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Mol	Chain	Length	Quality of chain
1	13-A	159	 91% 8% .
1	130-A	159	 92% 6% .
1	131-A	159	 86% 13% .
1	132-A	159	 89% 8% ..
1	133-A	159	 90% 8% ..
1	134-A	159	 89% 9% .
1	135-A	159	 92% 7% ..
1	136-A	159	 86% 11% ..
1	137-A	159	 87% 8% ..
1	138-A	159	 85% 11% ..
1	139-A	159	 87% 11% ..
1	14-A	159	 87% 11% ..
1	140-A	159	 88% 9% ..
1	141-A	159	 86% 11% ..
1	142-A	159	 84% 13% ..
1	143-A	159	 87% 9% ..
1	144-A	159	 80% 15% ..
1	145-A	159	 84% 13% ..
1	146-A	159	 84% 13% ..
1	147-A	159	 87% 11% ..
1	148-A	159	 86% 11% ..
1	149-A	159	 87% 11% .
1	15-A	159	 87% 11% .
1	150-A	159	 84% 14% .
1	151-A	159	 85% 13% .


























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Mol	Chain	Length	Quality of chain
1	152-A	159	 90% 9% .
1	153-A	159	 87% 9% . .
1	154-A	159	 88% 8% .
1	155-A	159	 86% 11% .
1	156-A	159	 81% 17% .
1	157-A	159	 77% 20% .
1	158-A	159	 86% 10% . .
1	159-A	159	 84% 9% 6% .
1	16-A	159	 86% 12% . .
1	160-A	159	 86% 12% . .
1	161-A	159	 86% 10% . .
1	162-A	159	 86% 10% . .
1	163-A	159	 86% 12% .
1	164-A	159	 86% 9% . .
1	165-A	159	 87% 11% . .
1	166-A	159	 88% 10% . .
1	167-A	159	 82% 13% . .
1	17-A	159	 87% 11% . .
1	18-A	159	 90% 9% .
1	19-A	159	 89% 10% . .
1	2-A	159	 89% 9% .
1	20-A	159	 86% 13% .
1	21-A	159	 88% 11% .
1	22-A	159	 89% 9% .
1	23-A	159	 88% 9% .















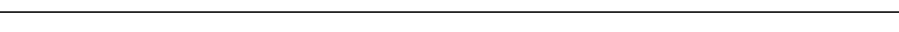

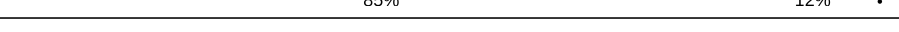

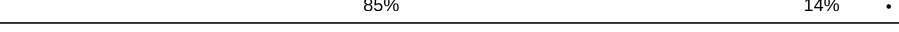






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Mol	Chain	Length	Quality of chain
1	24-A	159	 87% 11% .
1	25-A	159	 84% 14% .
1	26-A	159	 87% 12% ..
1	27-A	159	 85% 13% .
1	28-A	159	 84% 11% . .
1	29-A	159	 81% 16% . .
1	3-A	159	 88% 10% ..
1	30-A	159	 81% 14% 5%
1	31-A	159	 83% 11% 6%
1	32-A	159	 79% 16% . .
1	33-A	159	 83% 9% 6% .
1	34-A	159	 79% 17% .
1	35-A	159	 84% 12% . .
1	36-A	159	 83% 13% . .
1	37-A	159	 82% 15% .
1	38-A	159	 82% 15% .
1	39-A	159	 81% 16% .
1	4-A	159	 84% 14% ..
1	40-A	159	 84% 12% . .
1	41-A	159	 84% 13% . .
1	42-A	159	 86% 11% . .
1	43-A	159	 87% 11% ..
1	44-A	159	 87% 11% .
1	45-A	159	 84% 13% .
1	46-A	159	 86% 13% .















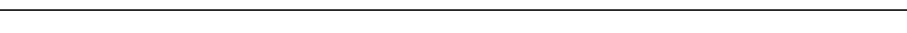




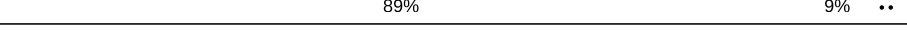





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Mol	Chain	Length	Quality of chain
1	47-A	159	 86% 11% ..
1	48-A	159	 90% 7% ..
1	49-A	159	 87% 10% ..
1	5-A	159	 91% 6% ..
1	50-A	159	 84% 12% ..
1	51-A	159	 86% 11% ..
1	52-A	159	 85% 12% ..
1	53-A	159	 86% 9% ..
1	54-A	159	 87% 12% .
1	55-A	159	 87% 12% .
1	56-A	159	 87% 9% .
1	57-A	159	 87% 10% ..
1	58-A	159	 89% 10% .
1	59-A	159	 92% 6% .
1	6-A	159	 84% 13% .
1	60-A	159	 85% 12% .
1	61-A	159	 86% 11% ..
1	62-A	159	 85% 14% .
1	63-A	159	 89% 11%
1	64-A	159	 91% 8% .
1	65-A	159	 87% 12% .
1	66-A	159	 87% 9% ..
1	67-A	159	 89% 8% .
1	68-A	159	 89% 8% ..
1	69-A	159	 87% 9% ..

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Mol	Chain	Length	Quality of chain
1	7-A	159	 82% 15% ..
1	70-A	159	 87% 10% ..
1	71-A	159	 87% 9% .
1	72-A	159	 84% 13% ..
1	73-A	159	 87% 9% ..
1	74-A	159	 86% 11% ..
1	75-A	159	 88% 10% .
1	76-A	159	 85% 14% .
1	77-A	159	 90% 9% .
1	78-A	159	 84% 14% .
1	79-A	159	 87% 10% ..
1	8-A	159	 84% 12% ..
1	80-A	159	 84% 12% ..
1	81-A	159	 88% 8% ..
1	82-A	159	 87% 10% ..
1	83-A	159	 87% 11% ..
1	84-A	159	 91% 8% .
1	85-A	159	 86% 12% .
1	86-A	159	 89% 9% ..
1	87-A	159	 91% 6% .
1	88-A	159	 87% 12% .
1	89-A	159	 87% 11% .
1	9-A	159	 87% 9% ..
1	90-A	159	 87% 10% .
1	91-A	159	 89% 9% .

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Mol	Chain	Length	Quality of chain
1	92-A	159	 88% 10% •
1	93-A	159	 89% 9% •
1	94-A	159	 84% 15% •
1	95-A	159	 84% 14% ••
1	96-A	159	 87% 10% •
1	97-A	159	 86% 11% •
1	98-A	159	 86% 13% •
1	99-A	159	 86% 14% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 451154 atoms, of which 211088 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	1-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	2-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	3-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	4-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	5-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	6-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	7-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	8-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	9-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	10-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	11-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	12-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	13-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	14-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	15-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				
1	16-A	159	Total	C	H	N	O	S		0	0	0
			2491	805	1223	217	239	7				

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	18-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	19-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	20-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	21-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	22-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	23-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	24-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	25-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	26-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	27-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	28-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	29-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	30-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	31-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	32-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	33-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	34-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	35-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	36-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	37-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	39-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	40-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	41-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	42-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	43-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	44-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	45-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	46-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	47-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	48-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	49-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	50-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	51-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	52-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	53-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	54-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	55-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	56-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	57-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	58-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	60-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	61-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	62-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	63-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	64-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	65-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	66-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	67-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	68-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	69-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	70-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	71-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	72-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	73-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	74-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	75-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	76-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	77-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	78-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	79-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	80-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	81-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	82-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	83-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	84-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	85-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	86-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	87-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	88-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	89-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	90-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	91-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	92-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	93-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	94-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	95-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	96-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	97-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	98-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	99-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	100-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	101-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	102-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	103-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	104-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	105-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	106-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	107-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	108-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	109-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	110-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	111-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	112-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	113-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	114-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	115-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	116-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	117-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	118-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	119-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	120-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	121-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	122-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	123-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	124-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	125-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	126-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	127-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	128-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	129-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	130-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	131-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	132-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	133-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	134-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	135-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	136-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	137-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	138-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	139-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	140-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	141-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	142-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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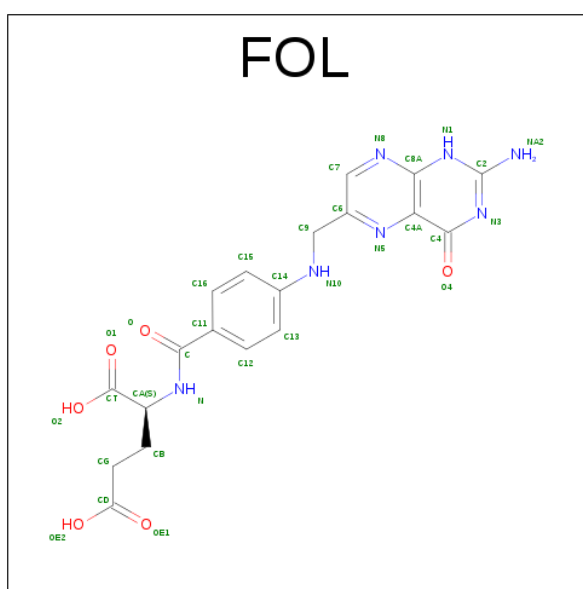
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	143-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	144-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	145-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	146-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	147-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	148-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	149-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	150-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	151-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	152-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	153-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	154-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	155-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	156-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	157-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	158-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	159-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	160-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	161-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	162-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	163-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	164-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	165-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	166-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	167-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: C₁₉H₁₉N₇O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	2-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	3-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	4-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	5-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	6-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	7-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	8-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	9-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	10-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	11-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	12-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	13-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	14-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	15-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	16-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	17-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	18-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	19-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	20-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	21-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	22-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	23-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	24-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	25-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	26-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	27-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	28-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	29-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	30-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	31-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	32-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	33-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	34-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	35-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	36-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	37-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	38-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	39-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	40-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	41-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	42-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	43-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	44-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	45-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	46-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	47-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	48-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	49-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	50-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	51-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	52-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	53-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	54-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	55-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	56-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	57-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	58-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	59-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	60-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	61-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	62-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	63-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	64-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	65-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	66-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	67-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	68-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	69-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	70-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	71-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	72-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	73-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	74-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	75-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	76-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	77-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	78-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	79-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	80-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	81-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	82-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	83-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	84-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	85-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	86-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	87-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	88-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	89-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	90-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	91-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	92-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	93-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	94-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	95-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	96-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	97-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	98-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	99-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	100-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	101-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	102-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	103-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	104-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	105-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	106-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	107-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	108-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	109-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	110-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	111-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	112-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	113-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	114-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	115-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	116-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	117-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	118-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	119-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	120-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	121-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	122-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	123-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	124-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	125-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	126-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	127-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	128-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	129-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	130-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	131-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	132-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	133-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	134-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	135-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	136-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	137-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	138-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	139-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	140-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	141-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	142-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	143-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	144-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	145-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	146-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	147-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	148-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	149-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	150-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	151-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	152-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	153-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	154-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	155-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	156-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	157-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	158-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	159-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	160-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	161-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	162-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	163-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	164-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	165-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	166-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	167-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	122-A	2	Total	Ca	0	0
			2	2		
3	110-A	2	Total	Ca	0	0
			2	2		
3	37-A	2	Total	Ca	0	0
			2	2		
3	80-A	2	Total	Ca	0	0
			2	2		
3	94-A	2	Total	Ca	0	0
			2	2		
3	167-A	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	162-A	2	Total 2	Ca 2	0	0
3	60-A	2	Total 2	Ca 2	0	0
3	148-A	2	Total 2	Ca 2	0	0
3	123-A	2	Total 2	Ca 2	0	0
3	44-A	2	Total 2	Ca 2	0	0
3	150-A	2	Total 2	Ca 2	0	0
3	128-A	2	Total 2	Ca 2	0	0
3	135-A	2	Total 2	Ca 2	0	0
3	50-A	2	Total 2	Ca 2	0	0
3	138-A	2	Total 2	Ca 2	0	0
3	104-A	2	Total 2	Ca 2	0	0
3	12-A	2	Total 2	Ca 2	0	0
3	114-A	2	Total 2	Ca 2	0	0
3	19-A	2	Total 2	Ca 2	0	0
3	165-A	2	Total 2	Ca 2	0	0
3	73-A	2	Total 2	Ca 2	0	0
3	1-A	2	Total 2	Ca 2	0	0
3	53-A	2	Total 2	Ca 2	0	0
3	143-A	2	Total 2	Ca 2	0	0
3	25-A	2	Total 2	Ca 2	0	0
3	131-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	32-A	2	Total 2	Ca 2	0	0
3	93-A	2	Total 2	Ca 2	0	0
3	77-A	2	Total 2	Ca 2	0	0
3	161-A	2	Total 2	Ca 2	0	0
3	58-A	2	Total 2	Ca 2	0	0
3	130-A	2	Total 2	Ca 2	0	0
3	57-A	2	Total 2	Ca 2	0	0
3	29-A	2	Total 2	Ca 2	0	0
3	101-A	2	Total 2	Ca 2	0	0
3	3-A	2	Total 2	Ca 2	0	0
3	11-A	2	Total 2	Ca 2	0	0
3	84-A	2	Total 2	Ca 2	0	0
3	98-A	2	Total 2	Ca 2	0	0
3	144-A	2	Total 2	Ca 2	0	0
3	127-A	2	Total 2	Ca 2	0	0
3	154-A	2	Total 2	Ca 2	0	0
3	108-A	2	Total 2	Ca 2	0	0
3	16-A	2	Total 2	Ca 2	0	0
3	65-A	2	Total 2	Ca 2	0	0
3	117-A	2	Total 2	Ca 2	0	0
3	41-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	5-A	2	Total 2	Ca 2	0	0
3	8-A	2	Total 2	Ca 2	0	0
3	21-A	2	Total 2	Ca 2	0	0
3	109-A	2	Total 2	Ca 2	0	0
3	102-A	2	Total 2	Ca 2	0	0
3	113-A	2	Total 2	Ca 2	0	0
3	36-A	2	Total 2	Ca 2	0	0
3	81-A	2	Total 2	Ca 2	0	0
3	160-A	2	Total 2	Ca 2	0	0
3	97-A	2	Total 2	Ca 2	0	0
3	61-A	2	Total 2	Ca 2	0	0
3	149-A	2	Total 2	Ca 2	0	0
3	48-A	2	Total 2	Ca 2	0	0
3	124-A	2	Total 2	Ca 2	0	0
3	45-A	2	Total 2	Ca 2	0	0
3	153-A	2	Total 2	Ca 2	0	0
3	129-A	2	Total 2	Ca 2	0	0
3	134-A	2	Total 2	Ca 2	0	0
3	35-A	2	Total 2	Ca 2	0	0
3	105-A	2	Total 2	Ca 2	0	0
3	7-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	15-A	2	Total 2	Ca 2	0	0
3	88-A	2	Total 2	Ca 2	0	0
3	18-A	2	Total 2	Ca 2	0	0
3	72-A	2	Total 2	Ca 2	0	0
3	159-A	2	Total 2	Ca 2	0	0
3	52-A	2	Total 2	Ca 2	0	0
3	140-A	2	Total 2	Ca 2	0	0
3	26-A	2	Total 2	Ca 2	0	0
3	120-A	2	Total 2	Ca 2	0	0
3	118-A	2	Total 2	Ca 2	0	0
3	89-A	2	Total 2	Ca 2	0	0
3	31-A	2	Total 2	Ca 2	0	0
3	82-A	2	Total 2	Ca 2	0	0
3	92-A	2	Total 2	Ca 2	0	0
3	76-A	2	Total 2	Ca 2	0	0
3	46-A	2	Total 2	Ca 2	0	0
3	137-A	2	Total 2	Ca 2	0	0
3	56-A	2	Total 2	Ca 2	0	0
3	106-A	2	Total 2	Ca 2	0	0
3	10-A	2	Total 2	Ca 2	0	0
3	85-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	145-A	2	Total 2	Ca 2	0	0
3	157-A	2	Total 2	Ca 2	0	0
3	39-A	2	Total 2	Ca 2	0	0
3	133-A	2	Total 2	Ca 2	0	0
3	91-A	2	Total 2	Ca 2	0	0
3	66-A	2	Total 2	Ca 2	0	0
3	79-A	2	Total 2	Ca 2	0	0
3	55-A	2	Total 2	Ca 2	0	0
3	22-A	2	Total 2	Ca 2	0	0
3	103-A	2	Total 2	Ca 2	0	0
3	112-A	2	Total 2	Ca 2	0	0
3	86-A	2	Total 2	Ca 2	0	0
3	96-A	2	Total 2	Ca 2	0	0
3	62-A	2	Total 2	Ca 2	0	0
3	146-A	2	Total 2	Ca 2	0	0
3	49-A	2	Total 2	Ca 2	0	0
3	125-A	2	Total 2	Ca 2	0	0
3	42-A	2	Total 2	Ca 2	0	0
3	152-A	2	Total 2	Ca 2	0	0
3	119-A	2	Total 2	Ca 2	0	0
3	34-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	14-A	2	Total 2	Ca 2	0	0
3	63-A	2	Total 2	Ca 2	0	0
3	68-A	2	Total 2	Ca 2	0	0
3	71-A	2	Total 2	Ca 2	0	0
3	158-A	2	Total 2	Ca 2	0	0
3	141-A	2	Total 2	Ca 2	0	0
3	27-A	2	Total 2	Ca 2	0	0
3	163-A	2	Total 2	Ca 2	0	0
3	121-A	2	Total 2	Ca 2	0	0
3	111-A	2	Total 2	Ca 2	0	0
3	30-A	2	Total 2	Ca 2	0	0
3	83-A	2	Total 2	Ca 2	0	0
3	95-A	2	Total 2	Ca 2	0	0
3	2-A	2	Total 2	Ca 2	0	0
3	9-A	2	Total 2	Ca 2	0	0
3	75-A	2	Total 2	Ca 2	0	0
3	47-A	2	Total 2	Ca 2	0	0
3	151-A	2	Total 2	Ca 2	0	0
3	136-A	2	Total 2	Ca 2	0	0
3	51-A	2	Total 2	Ca 2	0	0
3	139-A	2	Total 2	Ca 2	0	0

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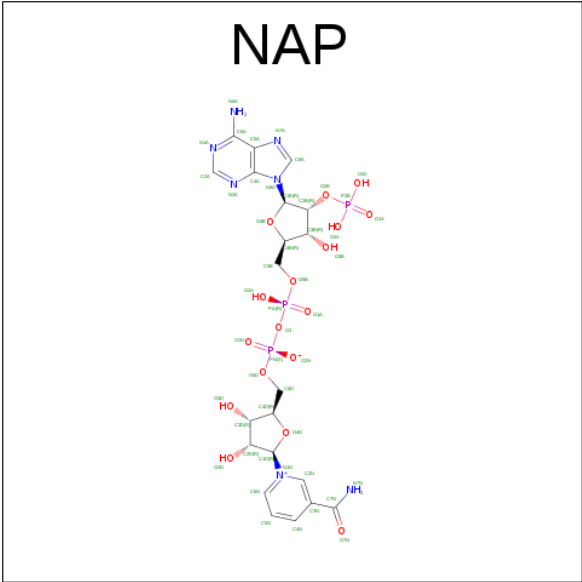
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	107-A	2	Total 2	Ca 2	0	0
3	13-A	2	Total 2	Ca 2	0	0
3	115-A	2	Total 2	Ca 2	0	0
3	74-A	2	Total 2	Ca 2	0	0
3	142-A	2	Total 2	Ca 2	0	0
3	24-A	2	Total 2	Ca 2	0	0
3	156-A	2	Total 2	Ca 2	0	0
3	4-A	2	Total 2	Ca 2	0	0
3	38-A	2	Total 2	Ca 2	0	0
3	132-A	2	Total 2	Ca 2	0	0
3	33-A	2	Total 2	Ca 2	0	0
3	116-A	2	Total 2	Ca 2	0	0
3	164-A	2	Total 2	Ca 2	0	0
3	90-A	2	Total 2	Ca 2	0	0
3	67-A	2	Total 2	Ca 2	0	0
3	166-A	2	Total 2	Ca 2	0	0
3	78-A	2	Total 2	Ca 2	0	0
3	59-A	2	Total 2	Ca 2	0	0
3	54-A	2	Total 2	Ca 2	0	0
3	23-A	2	Total 2	Ca 2	0	0
3	28-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	100-A	2	Total 2	Ca 2	0	0
3	87-A	2	Total 2	Ca 2	0	0
3	99-A	2	Total 2	Ca 2	0	0
3	6-A	2	Total 2	Ca 2	0	0
3	147-A	2	Total 2	Ca 2	0	0
3	126-A	2	Total 2	Ca 2	0	0
3	43-A	2	Total 2	Ca 2	0	0
3	155-A	2	Total 2	Ca 2	0	0
3	17-A	2	Total 2	Ca 2	0	0
3	64-A	2	Total 2	Ca 2	0	0
3	69-A	2	Total 2	Ca 2	0	0
3	70-A	2	Total 2	Ca 2	0	0
3	40-A	2	Total 2	Ca 2	0	0
3	20-A	2	Total 2	Ca 2	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	1-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	2-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	3-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	4-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	5-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	6-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	7-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	8-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	9-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	10-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	11-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	12-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	13-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	14-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	15-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	16-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	17-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	18-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	19-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	20-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	21-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	22-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	23-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	24-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	25-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	26-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	27-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	28-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	29-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	30-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	31-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	32-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	33-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	34-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	35-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	36-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	37-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	38-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	39-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	40-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	41-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	42-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	43-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	44-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	45-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	46-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	47-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	48-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	49-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	50-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	51-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	52-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	53-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	54-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	55-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	56-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	57-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	58-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	59-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	60-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	61-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	62-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	63-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	64-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	65-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	66-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	67-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	68-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	69-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	70-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	71-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	72-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	73-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	74-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	75-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	76-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	77-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	78-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	79-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	80-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	81-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	82-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	83-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	84-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	85-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	86-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	87-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	88-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	89-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	90-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	91-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	92-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	93-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	94-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	95-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	96-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	97-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	98-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	99-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	100-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	101-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	102-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	103-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	104-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	105-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	106-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	107-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	108-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	109-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	110-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	111-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	112-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	113-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	114-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	115-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	116-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	117-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	118-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	119-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	120-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	121-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	122-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	123-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	124-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	125-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	126-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	127-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	128-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	129-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	130-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	131-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	132-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	133-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	134-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	135-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	136-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	137-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	138-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	139-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	140-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	141-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	142-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	143-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	144-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	145-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	146-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	147-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	148-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	149-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	150-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	151-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	152-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	153-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	154-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	155-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	156-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	157-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	158-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	159-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	160-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	161-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	162-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	163-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	164-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	165-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	166-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	167-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	83	Total	O	0	0
			83	83		
5	2-A	83	Total	O	0	0
			83	83		
5	3-A	79	Total	O	0	0
			79	79		
5	4-A	68	Total	O	0	0
			68	68		
5	5-A	75	Total	O	0	0
			75	75		
5	6-A	80	Total	O	0	0
			80	80		
5	7-A	99	Total	O	0	0
			99	99		
5	8-A	89	Total	O	0	0
			89	89		
5	9-A	79	Total	O	0	0
			79	79		
5	10-A	79	Total	O	0	0
			79	79		
5	11-A	82	Total	O	0	0
			82	82		
5	12-A	88	Total	O	0	0
			88	88		
5	13-A	89	Total	O	0	0
			89	89		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	14-A	96	Total 96	O 96	0	0
5	15-A	96	Total 96	O 96	0	0
5	16-A	94	Total 94	O 94	0	0
5	17-A	84	Total 84	O 84	0	0
5	18-A	89	Total 89	O 89	0	0
5	19-A	80	Total 80	O 80	0	0
5	20-A	73	Total 73	O 73	0	0
5	21-A	92	Total 92	O 92	0	0
5	22-A	91	Total 91	O 91	0	0
5	23-A	94	Total 94	O 94	0	0
5	24-A	95	Total 95	O 95	0	0
5	25-A	76	Total 76	O 76	0	0
5	26-A	83	Total 83	O 83	0	0
5	27-A	81	Total 81	O 81	0	0
5	28-A	81	Total 81	O 81	0	0
5	29-A	83	Total 83	O 83	0	0
5	30-A	84	Total 84	O 84	0	0
5	31-A	86	Total 86	O 86	0	0
5	32-A	85	Total 85	O 85	0	0
5	33-A	86	Total 86	O 86	0	0
5	34-A	93	Total 93	O 93	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	35-A	93	Total 93	O 93	0	0
5	36-A	77	Total 77	O 77	0	0
5	37-A	82	Total 82	O 82	0	0
5	38-A	87	Total 87	O 87	0	0
5	39-A	93	Total 93	O 93	0	0
5	40-A	84	Total 84	O 84	0	0
5	41-A	82	Total 82	O 82	0	0
5	42-A	83	Total 83	O 83	0	0
5	43-A	95	Total 95	O 95	0	0
5	44-A	100	Total 100	O 100	0	0
5	45-A	93	Total 93	O 93	0	0
5	46-A	92	Total 92	O 92	0	0
5	47-A	98	Total 98	O 98	0	0
5	48-A	92	Total 92	O 92	0	0
5	49-A	89	Total 89	O 89	0	0
5	50-A	78	Total 78	O 78	0	0
5	51-A	68	Total 68	O 68	0	0
5	52-A	77	Total 77	O 77	0	0
5	53-A	87	Total 87	O 87	0	0
5	54-A	92	Total 92	O 92	0	0
5	55-A	92	Total 92	O 92	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	56-A	82	Total	O	0	0
			82	82		
5	57-A	86	Total	O	0	0
			86	86		
5	58-A	89	Total	O	0	0
			89	89		
5	59-A	96	Total	O	0	0
			96	96		
5	60-A	96	Total	O	0	0
			96	96		
5	61-A	98	Total	O	0	0
			98	98		
5	62-A	100	Total	O	0	0
			100	100		
5	63-A	97	Total	O	0	0
			97	97		
5	64-A	87	Total	O	0	0
			87	87		
5	65-A	83	Total	O	0	0
			83	83		
5	66-A	77	Total	O	0	0
			77	77		
5	67-A	78	Total	O	0	0
			78	78		
5	68-A	79	Total	O	0	0
			79	79		
5	69-A	79	Total	O	0	0
			79	79		
5	70-A	85	Total	O	0	0
			85	85		
5	71-A	91	Total	O	0	0
			91	91		
5	72-A	101	Total	O	0	0
			101	101		
5	73-A	94	Total	O	0	0
			94	94		
5	74-A	85	Total	O	0	0
			85	85		
5	75-A	92	Total	O	0	0
			92	92		
5	76-A	82	Total	O	0	0
			82	82		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	77-A	85	Total 85	O 85	0	0
5	78-A	84	Total 84	O 84	0	0
5	79-A	86	Total 86	O 86	0	0
5	80-A	85	Total 85	O 85	0	0
5	81-A	92	Total 92	O 92	0	0
5	82-A	91	Total 91	O 91	0	0
5	83-A	98	Total 98	O 98	0	0
5	84-A	94	Total 94	O 94	0	0
5	85-A	94	Total 94	O 94	0	0
5	86-A	88	Total 88	O 88	0	0
5	87-A	84	Total 84	O 84	0	0
5	88-A	82	Total 82	O 82	0	0
5	89-A	92	Total 92	O 92	0	0
5	90-A	98	Total 98	O 98	0	0
5	91-A	75	Total 75	O 75	0	0
5	92-A	77	Total 77	O 77	0	0
5	93-A	78	Total 78	O 78	0	0
5	94-A	92	Total 92	O 92	0	0
5	95-A	101	Total 101	O 101	0	0
5	96-A	106	Total 106	O 106	0	0
5	97-A	94	Total 94	O 94	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	98-A	86	Total 86	O 86	0	0
5	99-A	87	Total 87	O 87	0	0
5	100-A	80	Total 80	O 80	0	0
5	101-A	76	Total 76	O 76	0	0
5	102-A	80	Total 80	O 80	0	0
5	103-A	89	Total 89	O 89	0	0
5	104-A	88	Total 88	O 88	0	0
5	105-A	97	Total 97	O 97	0	0
5	106-A	85	Total 85	O 85	0	0
5	107-A	87	Total 87	O 87	0	0
5	108-A	93	Total 93	O 93	0	0
5	109-A	82	Total 82	O 82	0	0
5	110-A	82	Total 82	O 82	0	0
5	111-A	75	Total 75	O 75	0	0
5	112-A	85	Total 85	O 85	0	0
5	113-A	97	Total 97	O 97	0	0
5	114-A	98	Total 98	O 98	0	0
5	115-A	86	Total 86	O 86	0	0
5	116-A	89	Total 89	O 89	0	0
5	117-A	85	Total 85	O 85	0	0
5	118-A	89	Total 89	O 89	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	119-A	88	Total	O	0	0
			88	88		
5	120-A	95	Total	O	0	0
			95	95		
5	121-A	93	Total	O	0	0
			93	93		
5	122-A	90	Total	O	0	0
			90	90		
5	123-A	82	Total	O	0	0
			82	82		
5	124-A	81	Total	O	0	0
			81	81		
5	125-A	84	Total	O	0	0
			84	84		
5	126-A	101	Total	O	0	0
			101	101		
5	127-A	96	Total	O	0	0
			96	96		
5	128-A	90	Total	O	0	0
			90	90		
5	129-A	89	Total	O	0	0
			89	89		
5	130-A	81	Total	O	0	0
			81	81		
5	131-A	75	Total	O	0	0
			75	75		
5	132-A	87	Total	O	0	0
			87	87		
5	133-A	96	Total	O	0	0
			96	96		
5	134-A	89	Total	O	0	0
			89	89		
5	135-A	89	Total	O	0	0
			89	89		
5	136-A	87	Total	O	0	0
			87	87		
5	137-A	88	Total	O	0	0
			88	88		
5	138-A	88	Total	O	0	0
			88	88		
5	139-A	96	Total	O	0	0
			96	96		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	140-A	88	Total 88	O 88	0	0
5	141-A	80	Total 80	O 80	0	0
5	142-A	80	Total 80	O 80	0	0
5	143-A	83	Total 83	O 83	0	0
5	144-A	84	Total 84	O 84	0	0
5	145-A	99	Total 99	O 99	0	0
5	146-A	101	Total 101	O 101	0	0
5	147-A	105	Total 105	O 105	0	0
5	148-A	103	Total 103	O 103	0	0
5	149-A	86	Total 86	O 86	0	0
5	150-A	94	Total 94	O 94	0	0
5	151-A	92	Total 92	O 92	0	0
5	152-A	89	Total 89	O 89	0	0
5	153-A	99	Total 99	O 99	0	0
5	154-A	98	Total 98	O 98	0	0
5	155-A	78	Total 78	O 78	0	0
5	156-A	79	Total 79	O 79	0	0
5	157-A	80	Total 80	O 80	0	0
5	158-A	78	Total 78	O 78	0	0
5	159-A	82	Total 82	O 82	0	0
5	160-A	82	Total 82	O 82	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	161-A	86	Total 86	O 86	0	0
5	162-A	84	Total 84	O 84	0	0
5	163-A	91	Total 91	O 91	0	0
5	164-A	92	Total 92	O 92	0	0
5	165-A	90	Total 90	O 90	0	0
5	166-A	81	Total 81	O 81	0	0
5	167-A	89	Total 89	O 89	0	0

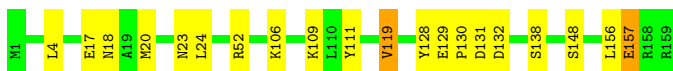
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

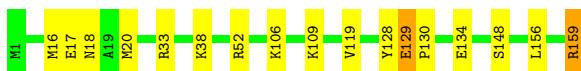
- Molecule 1: Dihydrofolate reductase

Chain 1-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 2-A:  89% 9% .




- Molecule 1: Dihydrofolate reductase

Chain 3-A:  88% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 4-A:  84% 14% ..




- Molecule 1: Dihydrofolate reductase

Chain 5-A:  91% 6% ..




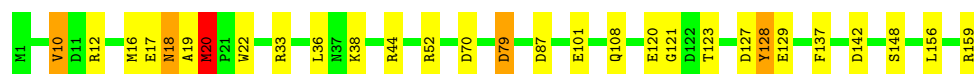
- Molecule 1: Dihydrofolate reductase

Chain 6-A:  84% 13%




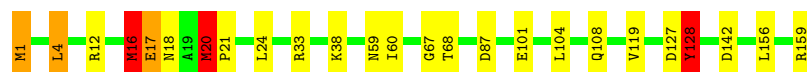
- Molecule 1: Dihydrofolate reductase

Chain 7-A:  82% 15%




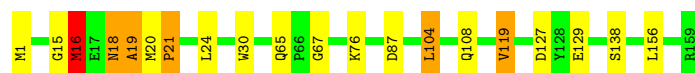
- Molecule 1: Dihydrofolate reductase

Chain 8-A:  84% 12%



- Molecule 1: Dihydrofolate reductase

Chain 9-A:  87% 9%



- Molecule 1: Dihydrofolate reductase

Chain 10-A:  89% 8%



- Molecule 1: Dihydrofolate reductase

Chain 11-A:  87% 9%



- Molecule 1: Dihydrofolate reductase

Chain 12-A:  86% 11%



- Molecule 1: Dihydrofolate reductase

Chain 13-A:  91% 8%



- Molecule 1: Dihydrofolate reductase

Chain 14-A: 87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 15-A: 87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 16-A: 86% 12% ..



- Molecule 1: Dihydrofolate reductase

Chain 17-A: 87% 11% ..



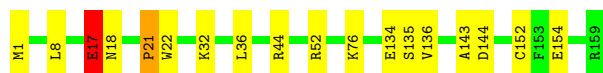
- Molecule 1: Dihydrofolate reductase

Chain 18-A: 90% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 19-A: 89% 10% ..

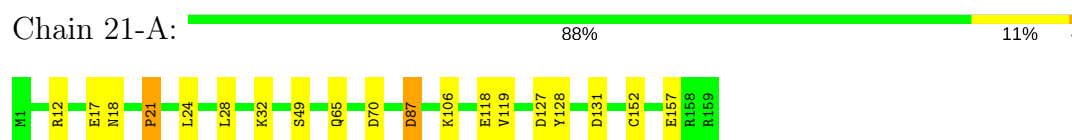


- Molecule 1: Dihydrofolate reductase

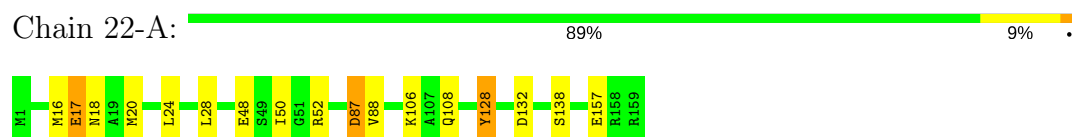
Chain 20-A: 86% 13% .



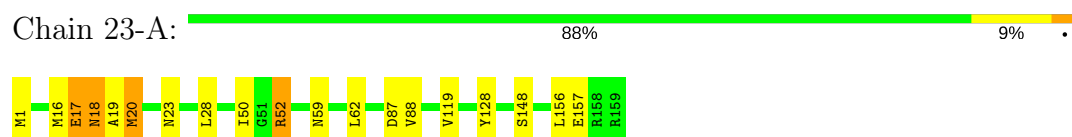
- Molecule 1: Dihydrofolate reductase



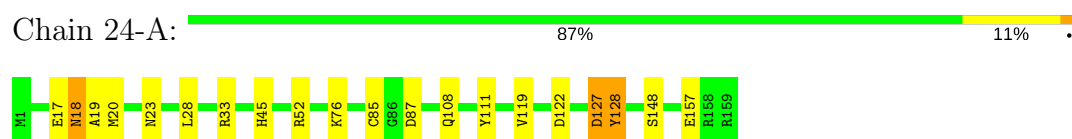
- Molecule 1: Dihydrofolate reductase



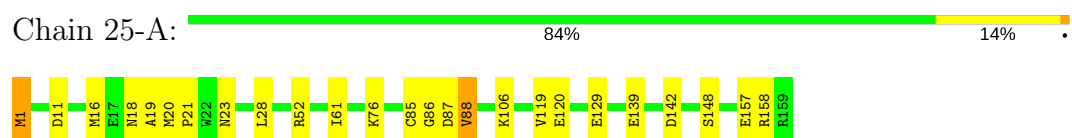
- Molecule 1: Dihydrofolate reductase



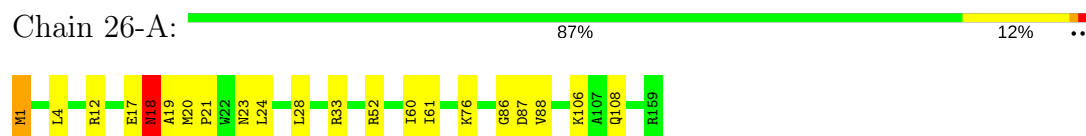
- Molecule 1: Dihydrofolate reductase



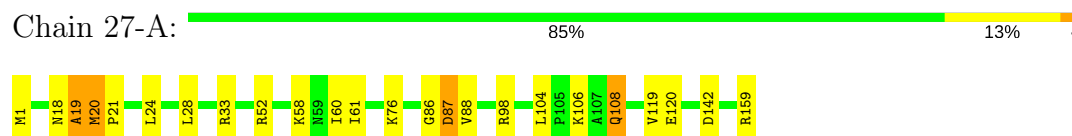
- Molecule 1: Dihydrofolate reductase




- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase




- Molecule 1: Dihydrofolate reductase

Chain 28-A:  84% 11% . .




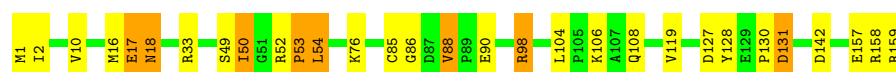
- Molecule 1: Dihydrofolate reductase

Chain 29-A:  81% 16% . .




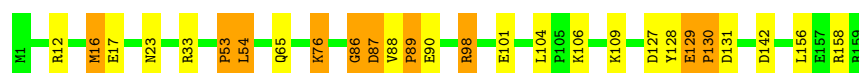
- Molecule 1: Dihydrofolate reductase

Chain 30-A:  81% 14% 5%




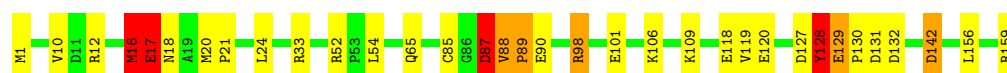
- Molecule 1: Dihydrofolate reductase

Chain 31-A:  83% 11% 6%




- Molecule 1: Dihydrofolate reductase

Chain 32-A:  79% 16% . .




- Molecule 1: Dihydrofolate reductase

Chain 33-A:  83% 9% 6% .




- Molecule 1: Dihydrofolate reductase

Chain 34-A:  79% 17% .



- Molecule 1: Dihydrofolate reductase

Chain 35-A:  84% 12% . .



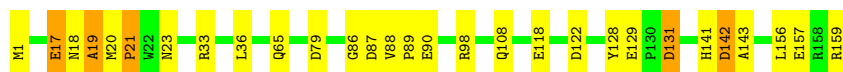
- Molecule 1: Dihydrofolate reductase

Chain 36-A: 83% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 37-A: 82% 15% .



- Molecule 1: Dihydrofolate reductase

Chain 38-A: 82% 15% .



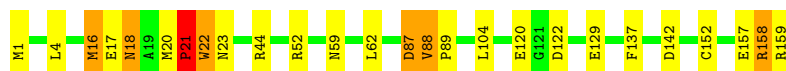
- Molecule 1: Dihydrofolate reductase

Chain 39-A: 81% 16% .



- Molecule 1: Dihydrofolate reductase

Chain 40-A: 84% 12% ..



- Molecule 1: Dihydrofolate reductase

Chain 41-A: 84% 13% ..




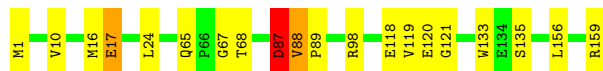
- Molecule 1: Dihydrofolate reductase

Chain 42-A: 86% 11% ..



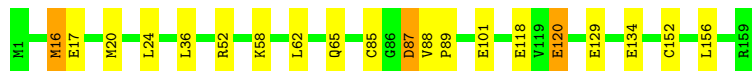
- Molecule 1: Dihydrofolate reductase

Chain 43-A:  87% 11% ..



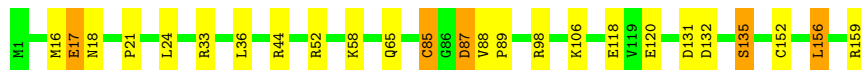
- Molecule 1: Dihydrofolate reductase

Chain 44-A:  87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 45-A:  84% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 46-A:  86% 13% .



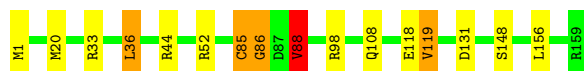
- Molecule 1: Dihydrofolate reductase

Chain 47-A:  86% 11% ..




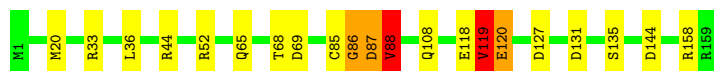
- Molecule 1: Dihydrofolate reductase

Chain 48-A:  90% 7% ..




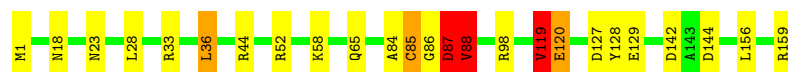
- Molecule 1: Dihydrofolate reductase

Chain 49-A:  87% 10% ..



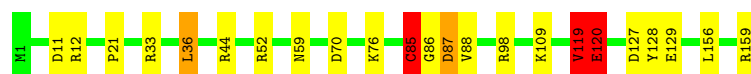
- Molecule 1: Dihydrofolate reductase

Chain 50-A:  84% 12% ..




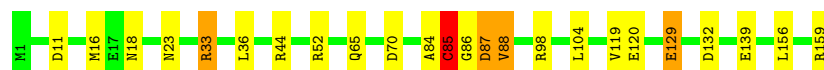
- Molecule 1: Dihydrofolate reductase

Chain 51-A:  86% 11% ..



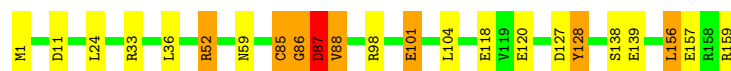
- Molecule 1: Dihydrofolate reductase

Chain 52-A:  85% 12% ..



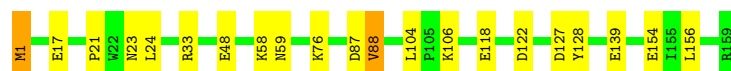
- Molecule 1: Dihydrofolate reductase

Chain 53-A:  86% 9% ..



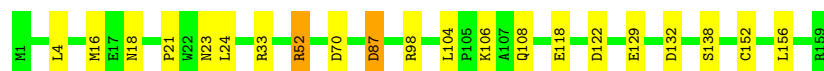
- Molecule 1: Dihydrofolate reductase

Chain 54-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 55-A:  87% 12% .



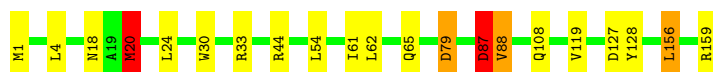
- Molecule 1: Dihydrofolate reductase

Chain 56-A:  87% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 57-A:  87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 58-A:  89% 10%




- Molecule 1: Dihydrofolate reductase

Chain 59-A:  92% 6%



- Molecule 1: Dihydrofolate reductase

Chain 60-A:  85% 12%




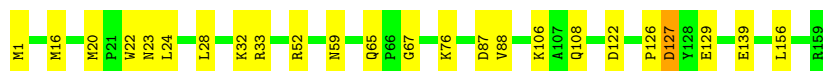
- Molecule 1: Dihydrofolate reductase

Chain 61-A:  86% 11%



- Molecule 1: Dihydrofolate reductase

Chain 62-A:  85% 14%



- Molecule 1: Dihydrofolate reductase

Chain 63-A:  89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 64-A:  91% 8%



- Molecule 1: Dihydrofolate reductase

Chain 65-A:  87% 12%



- Molecule 1: Dihydrofolate reductase

Chain 66-A:  87% 9%



- Molecule 1: Dihydrofolate reductase

Chain 67-A:  89% 8%



- Molecule 1: Dihydrofolate reductase

Chain 68-A:  89% 8%



- Molecule 1: Dihydrofolate reductase

Chain 69-A:  87% 9%



- Molecule 1: Dihydrofolate reductase

Chain 70-A:  87% 10%




- Molecule 1: Dihydrofolate reductase

Chain 71-A:  87% 9%



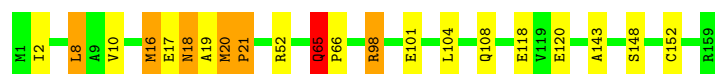
- Molecule 1: Dihydrofolate reductase

Chain 72-A:  84% 13% . .



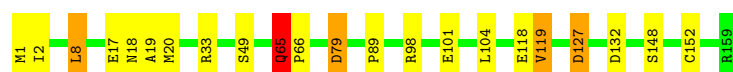
- Molecule 1: Dihydrofolate reductase

Chain 73-A:  87% 9% . .



- Molecule 1: Dihydrofolate reductase

Chain 74-A:  86% 11% . .




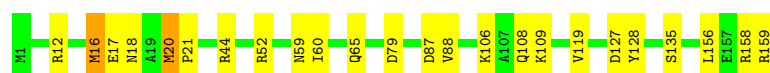
- Molecule 1: Dihydrofolate reductase

Chain 75-A:  88% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 76-A:  85% 14% .




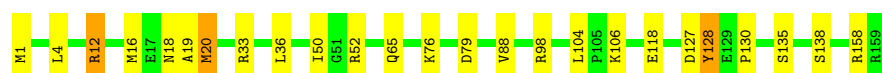
- Molecule 1: Dihydrofolate reductase

Chain 77-A:  90% 9% .




- Molecule 1: Dihydrofolate reductase

Chain 78-A:  84% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 79-A:  87% 10% . .



- Molecule 1: Dihydrofolate reductase

Chain 80-A: 84% 12% ..



- Molecule 1: Dihydrofolate reductase

Chain 81-A: 88% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 82-A: 87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 83-A: 87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 84-A: 91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 85-A: 86% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 86-A: 89% 9% ..



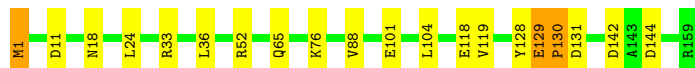
● Molecule 1: Dihydrofolate reductase

Chain 87-A:  91% 6% .

● Molecule 1: Dihydrofolate reductase

Chain 88-A:  87% 12% .

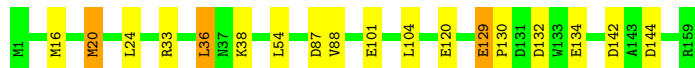
● Molecule 1: Dihydrofolate reductase

Chain 89-A:  87% 11% .

● Molecule 1: Dihydrofolate reductase

Chain 90-A:  87% 10% .

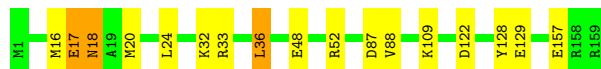
● Molecule 1: Dihydrofolate reductase

Chain 91-A:  89% 9% .


● Molecule 1: Dihydrofolate reductase

Chain 92-A:  88% 10% .

● Molecule 1: Dihydrofolate reductase

Chain 93-A:  89% 9% .

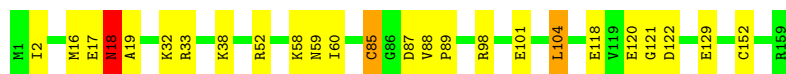
● Molecule 1: Dihydrofolate reductase

Chain 94-A:  84% 15% .



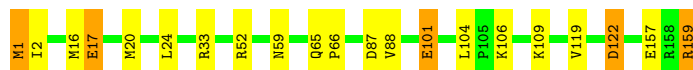
- Molecule 1: Dihydrofolate reductase

Chain 95-A:  84% 14% ..




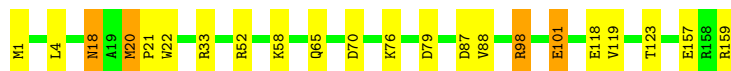
- Molecule 1: Dihydrofolate reductase

Chain 96-A:  87% 10% .




- Molecule 1: Dihydrofolate reductase

Chain 97-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 98-A:  86% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 99-A:  86% 14% .



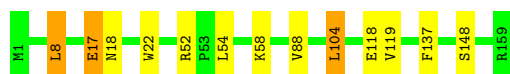
- Molecule 1: Dihydrofolate reductase

Chain 100-A:  87% 11% .



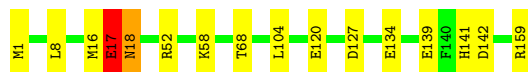
- Molecule 1: Dihydrofolate reductase

Chain 101-A:  92% 6% .



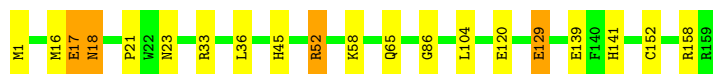
- Molecule 1: Dihydrofolate reductase

Chain 102-A: 90% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 103-A: 87% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 104-A: 89% 9% .



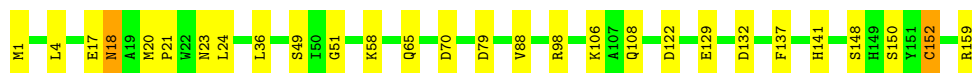
- Molecule 1: Dihydrofolate reductase

Chain 105-A: 87% 9% ..



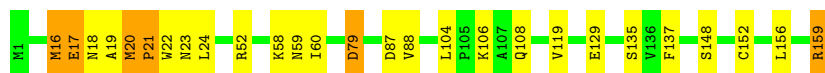
- Molecule 1: Dihydrofolate reductase

Chain 106-A: 82% 16% .



- Molecule 1: Dihydrofolate reductase

Chain 107-A: 83% 13% .

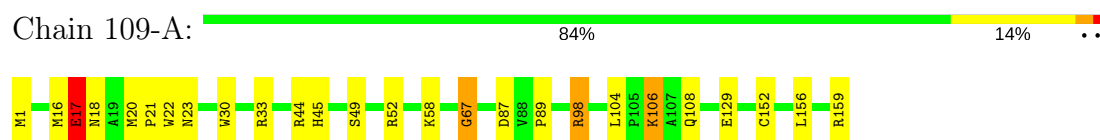


- Molecule 1: Dihydrofolate reductase

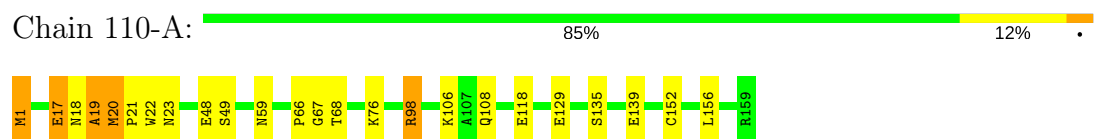
Chain 108-A: 84% 14% ..



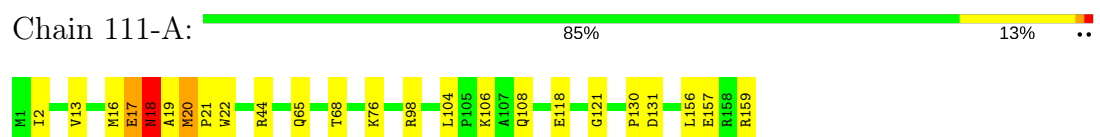
● Molecule 1: Dihydrofolate reductase



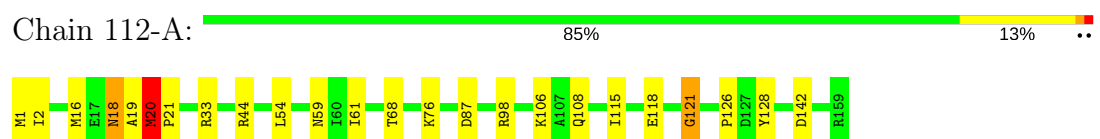
● Molecule 1: Dihydrofolate reductase



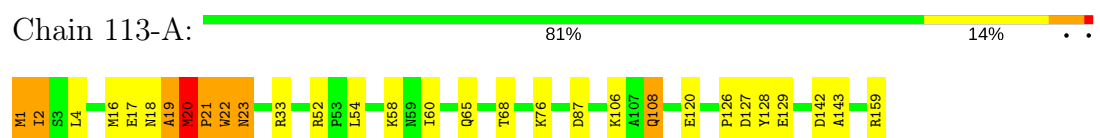
● Molecule 1: Dihydrofolate reductase



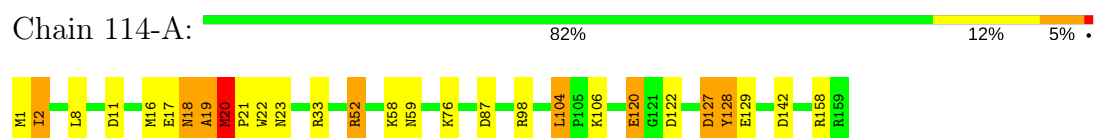
● Molecule 1: Dihydrofolate reductase



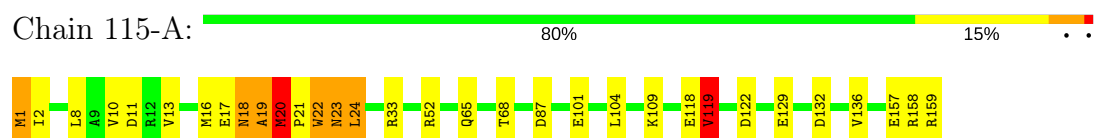
● Molecule 1: Dihydrofolate reductase




● Molecule 1: Dihydrofolate reductase



● Molecule 1: Dihydrofolate reductase




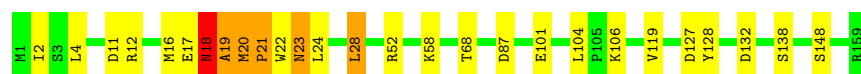
● Molecule 1: Dihydrofolate reductase

Chain 116-A:  83% 13% . .




- Molecule 1: Dihydrofolate reductase

Chain 117-A:  83% 13% . .



- Molecule 1: Dihydrofolate reductase

Chain 118-A:  84% 13% . .



- Molecule 1: Dihydrofolate reductase

Chain 119-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 120-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 121-A:  86% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 122-A:  86% 11% .



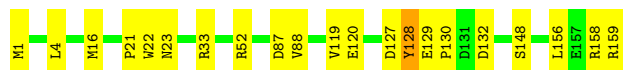
- Molecule 1: Dihydrofolate reductase

Chain 123-A:  87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 124-A: 87% 13%



- Molecule 1: Dihydrofolate reductase

Chain 125-A: 87% 12%



- Molecule 1: Dihydrofolate reductase

Chain 126-A: 90% 9%



- Molecule 1: Dihydrofolate reductase

Chain 127-A: 90% 9%



- Molecule 1: Dihydrofolate reductase

Chain 128-A: 88% 11%



- Molecule 1: Dihydrofolate reductase

Chain 129-A: 92% 7%

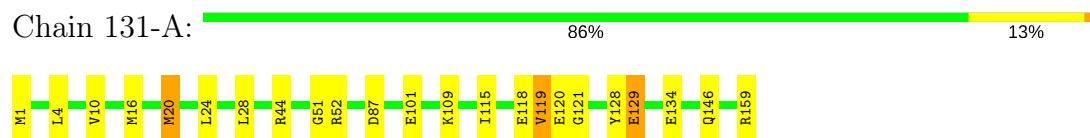


- Molecule 1: Dihydrofolate reductase

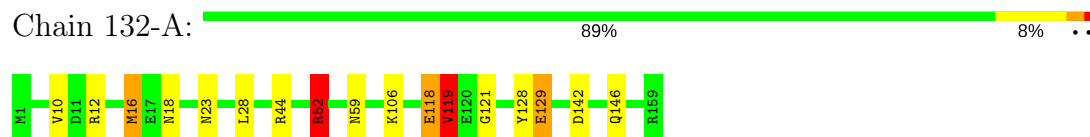
Chain 130-A: 92% 6%



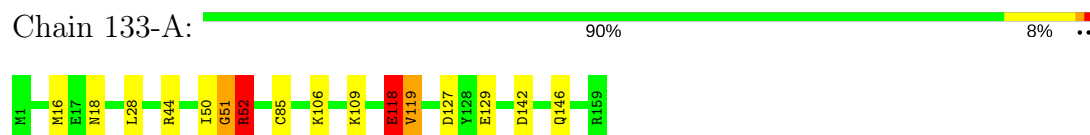
● Molecule 1: Dihydrofolate reductase



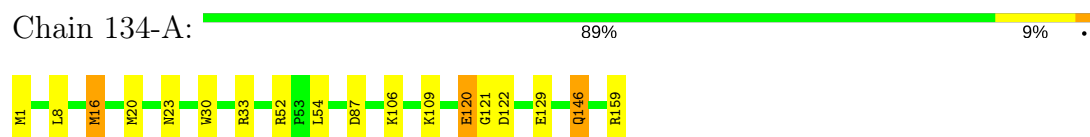
● Molecule 1: Dihydrofolate reductase



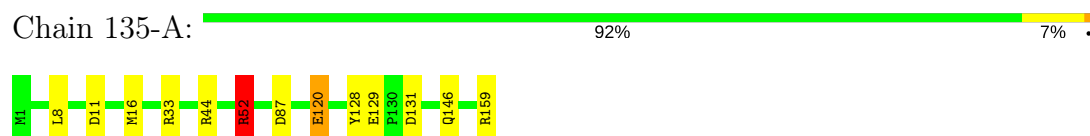
● Molecule 1: Dihydrofolate reductase



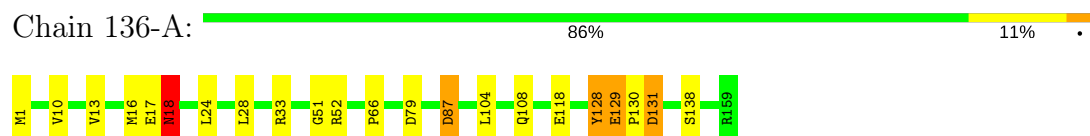
● Molecule 1: Dihydrofolate reductase



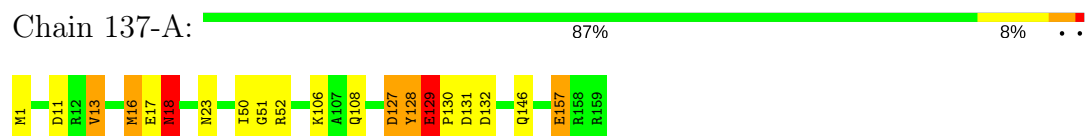
● Molecule 1: Dihydrofolate reductase



● Molecule 1: Dihydrofolate reductase



● Molecule 1: Dihydrofolate reductase



● Molecule 1: Dihydrofolate reductase

Chain 138-A:  85% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 139-A:  87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 140-A:  88% 9% ..




- Molecule 1: Dihydrofolate reductase

Chain 141-A:  86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 142-A:  84% 13% ..




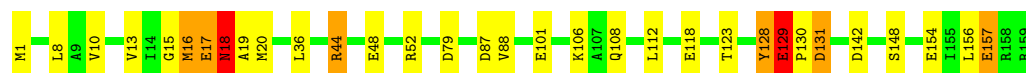
- Molecule 1: Dihydrofolate reductase

Chain 143-A:  87% 9% ..




- Molecule 1: Dihydrofolate reductase

Chain 144-A:  80% 15% ..



- Molecule 1: Dihydrofolate reductase

Chain 145-A:  84% 13% ..



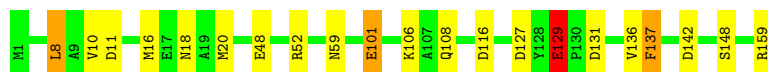
- Molecule 1: Dihydrofolate reductase

Chain 146-A: 84% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 147-A: 87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 148-A: 86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 149-A: 87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 150-A: 84% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 151-A: 85% 13% .

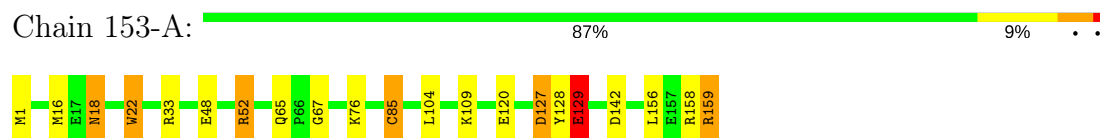


- Molecule 1: Dihydrofolate reductase

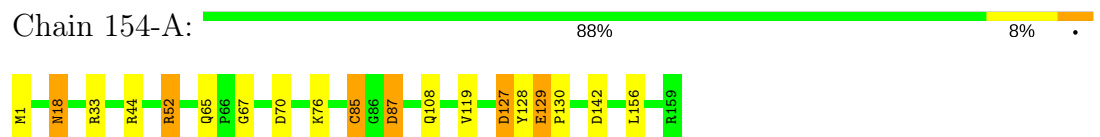
Chain 152-A: 90% 9% .



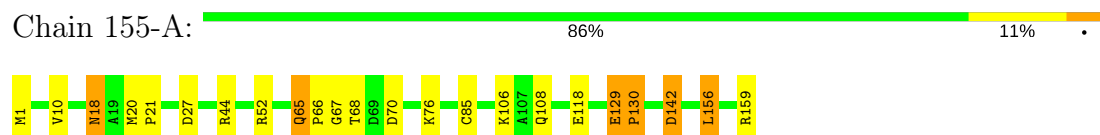
- Molecule 1: Dihydrofolate reductase



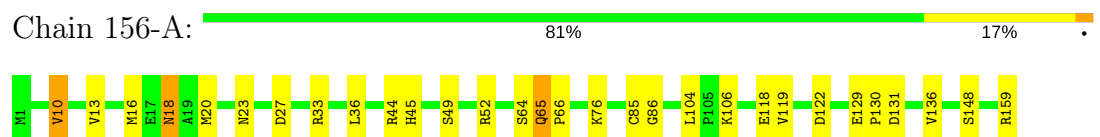
- Molecule 1: Dihydrofolate reductase



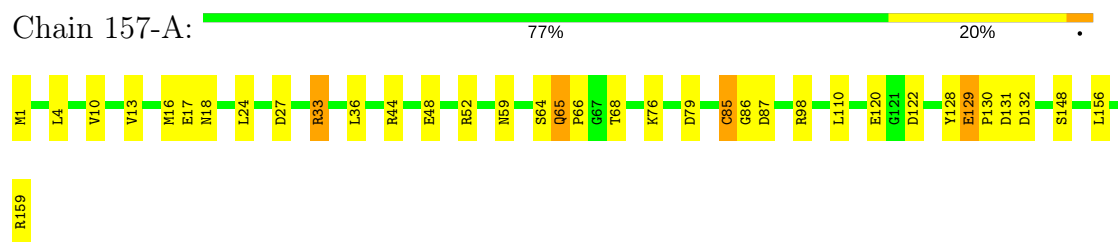
- Molecule 1: Dihydrofolate reductase



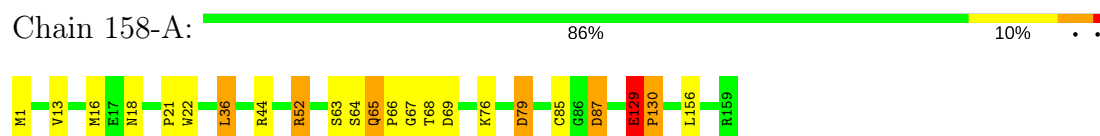
- Molecule 1: Dihydrofolate reductase



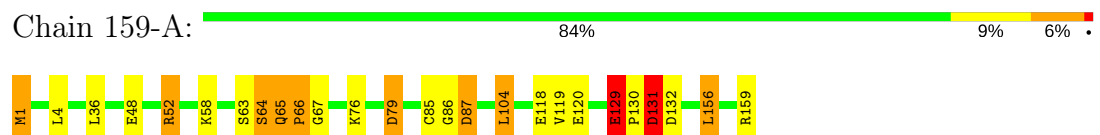
- Molecule 1: Dihydrofolate reductase



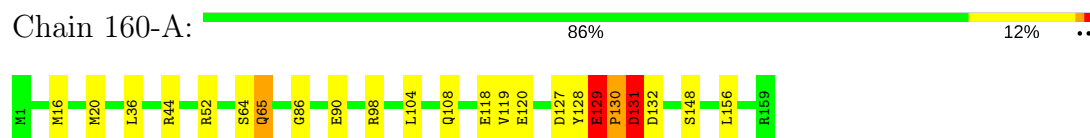
- Molecule 1: Dihydrofolate reductase



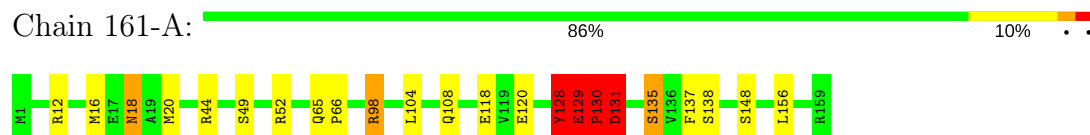
- Molecule 1: Dihydrofolate reductase



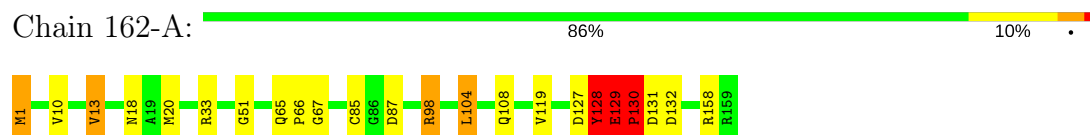
- Molecule 1: Dihydrofolate reductase



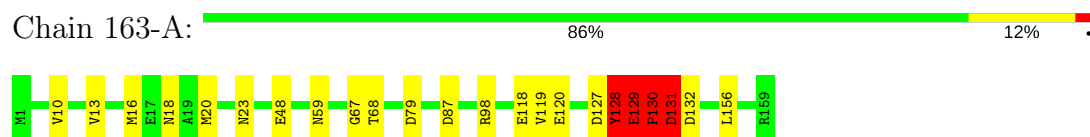
- Molecule 1: Dihydrofolate reductase



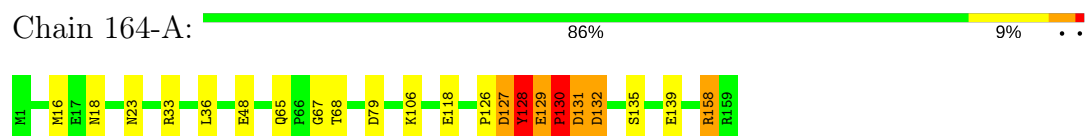
- Molecule 1: Dihydrofolate reductase



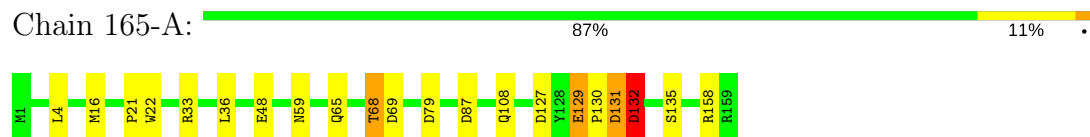
- Molecule 1: Dihydrofolate reductase



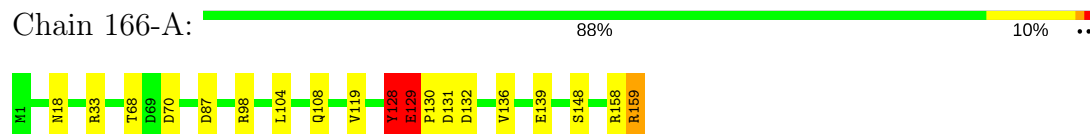
- Molecule 1: Dihydrofolate reductase




- Molecule 1: Dihydrofolate reductase

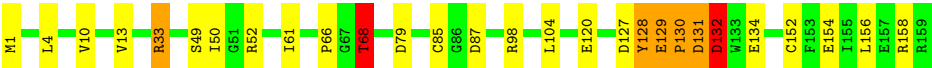


- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase

Chain 167-A:  82% 13% . .



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	34.32Å 45.51Å 98.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.34 – 1.35	Depositor
% Data completeness (in resolution range)	91.6 (41.34-1.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 1.35Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.8.4_1496)	Depositor
R, R_{free}	0.118 , 0.153	Depositor
Wilson B-factor (Å ²)	11.3	Xtriage
Anisotropy	0.174	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	451154	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FOL, CA, NAP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1-A	0.70	0/1302	0.91	3/1770 (0.2%)
1	2-A	0.71	0/1302	0.91	2/1770 (0.1%)
1	3-A	0.70	0/1302	1.01	4/1770 (0.2%)
1	4-A	0.76	2/1302 (0.2%)	0.97	5/1770 (0.3%)
1	5-A	0.73	0/1302	1.03	3/1770 (0.2%)
1	6-A	0.91	4/1302 (0.3%)	1.03	6/1770 (0.3%)
1	7-A	0.94	6/1302 (0.5%)	1.09	8/1770 (0.5%)
1	8-A	0.86	5/1302 (0.4%)	1.14	11/1770 (0.6%)
1	9-A	0.82	0/1302	1.00	6/1770 (0.3%)
1	10-A	0.66	0/1302	0.87	2/1770 (0.1%)
1	11-A	0.73	1/1302 (0.1%)	0.94	4/1770 (0.2%)
1	12-A	0.73	1/1302 (0.1%)	0.98	3/1770 (0.2%)
1	13-A	0.67	1/1302 (0.1%)	0.91	2/1770 (0.1%)
1	14-A	0.78	1/1302 (0.1%)	0.92	2/1770 (0.1%)
1	15-A	0.76	0/1302	0.94	1/1770 (0.1%)
1	16-A	0.72	0/1302	0.99	5/1770 (0.3%)
1	17-A	0.75	3/1302 (0.2%)	0.94	2/1770 (0.1%)
1	18-A	0.74	1/1302 (0.1%)	0.91	1/1770 (0.1%)
1	19-A	0.73	2/1302 (0.2%)	0.90	1/1770 (0.1%)
1	20-A	0.76	2/1302 (0.2%)	0.93	7/1770 (0.4%)
1	21-A	0.76	2/1302 (0.2%)	0.97	5/1770 (0.3%)
1	22-A	0.71	0/1302	0.99	4/1770 (0.2%)
1	23-A	0.75	0/1302	0.95	4/1770 (0.2%)
1	24-A	0.71	0/1302	0.95	3/1770 (0.2%)
1	25-A	0.72	0/1302	0.93	2/1770 (0.1%)
1	26-A	0.78	0/1302	0.95	4/1770 (0.2%)
1	27-A	0.78	0/1302	0.98	5/1770 (0.3%)
1	28-A	0.80	1/1302 (0.1%)	1.04	5/1770 (0.3%)
1	29-A	0.86	4/1302 (0.3%)	1.01	4/1770 (0.2%)
1	30-A	0.85	1/1302 (0.1%)	1.18	8/1770 (0.5%)
1	31-A	0.91	3/1302 (0.2%)	1.17	9/1770 (0.5%)
1	32-A	0.99	4/1302 (0.3%)	1.15	13/1770 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	33-A	0.91	2/1302 (0.2%)	1.15	10/1770 (0.6%)
1	34-A	0.95	5/1302 (0.4%)	1.09	10/1770 (0.6%)
1	35-A	0.88	3/1302 (0.2%)	1.08	7/1770 (0.4%)
1	36-A	0.86	3/1302 (0.2%)	1.08	8/1770 (0.5%)
1	37-A	0.82	2/1302 (0.2%)	1.06	6/1770 (0.3%)
1	38-A	0.81	1/1302 (0.1%)	1.02	9/1770 (0.5%)
1	39-A	0.79	3/1302 (0.2%)	1.09	10/1770 (0.6%)
1	40-A	0.81	1/1302 (0.1%)	1.07	10/1770 (0.6%)
1	41-A	0.71	0/1302	1.09	7/1770 (0.4%)
1	42-A	0.73	0/1302	1.04	10/1770 (0.6%)
1	43-A	0.74	1/1302 (0.1%)	1.03	8/1770 (0.5%)
1	44-A	0.74	1/1302 (0.1%)	0.94	3/1770 (0.2%)
1	45-A	0.71	1/1302 (0.1%)	0.94	4/1770 (0.2%)
1	46-A	0.76	2/1302 (0.2%)	1.00	4/1770 (0.2%)
1	47-A	0.76	1/1302 (0.1%)	1.03	7/1770 (0.4%)
1	48-A	0.71	0/1302	0.96	4/1770 (0.2%)
1	49-A	0.77	3/1302 (0.2%)	0.96	6/1770 (0.3%)
1	50-A	0.76	1/1302 (0.1%)	1.06	5/1770 (0.3%)
1	51-A	0.79	3/1302 (0.2%)	1.01	4/1770 (0.2%)
1	52-A	0.79	3/1302 (0.2%)	1.10	8/1770 (0.5%)
1	53-A	0.74	1/1302 (0.1%)	1.04	8/1770 (0.5%)
1	54-A	0.71	1/1302 (0.1%)	0.92	2/1770 (0.1%)
1	55-A	0.74	1/1302 (0.1%)	0.96	3/1770 (0.2%)
1	56-A	0.90	5/1302 (0.4%)	1.09	7/1770 (0.4%)
1	57-A	0.80	2/1302 (0.2%)	1.11	12/1770 (0.7%)
1	58-A	0.93	1/1302 (0.1%)	1.09	10/1770 (0.6%)
1	59-A	0.86	2/1302 (0.2%)	0.99	5/1770 (0.3%)
1	60-A	0.73	1/1302 (0.1%)	0.94	6/1770 (0.3%)
1	61-A	0.70	1/1302 (0.1%)	0.94	5/1770 (0.3%)
1	62-A	0.71	0/1302	0.93	3/1770 (0.2%)
1	63-A	0.73	0/1302	1.00	4/1770 (0.2%)
1	64-A	0.67	0/1302	0.88	1/1770 (0.1%)
1	65-A	0.68	0/1302	1.05	10/1770 (0.6%)
1	66-A	0.74	1/1302 (0.1%)	1.01	6/1770 (0.3%)
1	67-A	0.78	1/1302 (0.1%)	0.95	3/1770 (0.2%)
1	68-A	0.77	1/1302 (0.1%)	1.10	12/1770 (0.7%)
1	69-A	0.81	1/1302 (0.1%)	1.04	10/1770 (0.6%)
1	70-A	1.04	4/1302 (0.3%)	1.00	5/1770 (0.3%)
1	71-A	0.95	4/1302 (0.3%)	1.01	7/1770 (0.4%)
1	72-A	0.74	1/1302 (0.1%)	1.00	4/1770 (0.2%)
1	73-A	0.73	2/1302 (0.2%)	0.98	7/1770 (0.4%)
1	74-A	0.79	2/1302 (0.2%)	1.00	5/1770 (0.3%)
1	75-A	0.79	3/1302 (0.2%)	0.96	3/1770 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	76-A	0.73	0/1302	0.96	5/1770 (0.3%)
1	77-A	0.72	0/1302	0.88	4/1770 (0.2%)
1	78-A	0.72	1/1302 (0.1%)	0.97	4/1770 (0.2%)
1	79-A	0.72	0/1302	1.05	9/1770 (0.5%)
1	80-A	0.79	3/1302 (0.2%)	1.05	7/1770 (0.4%)
1	81-A	0.86	4/1302 (0.3%)	1.09	9/1770 (0.5%)
1	82-A	0.84	3/1302 (0.2%)	1.07	6/1770 (0.3%)
1	83-A	0.91	4/1302 (0.3%)	1.10	10/1770 (0.6%)
1	84-A	0.83	1/1302 (0.1%)	1.09	6/1770 (0.3%)
1	85-A	0.71	1/1302 (0.1%)	0.96	5/1770 (0.3%)
1	86-A	0.78	1/1302 (0.1%)	1.00	3/1770 (0.2%)
1	87-A	0.74	1/1302 (0.1%)	0.95	5/1770 (0.3%)
1	88-A	0.74	2/1302 (0.2%)	0.98	3/1770 (0.2%)
1	89-A	0.74	2/1302 (0.2%)	0.97	3/1770 (0.2%)
1	90-A	0.71	1/1302 (0.1%)	0.99	4/1770 (0.2%)
1	91-A	0.76	0/1302	1.04	4/1770 (0.2%)
1	92-A	0.77	2/1302 (0.2%)	1.03	4/1770 (0.2%)
1	93-A	0.74	0/1302	1.00	4/1770 (0.2%)
1	94-A	0.73	2/1302 (0.2%)	0.94	3/1770 (0.2%)
1	95-A	0.84	6/1302 (0.5%)	0.95	2/1770 (0.1%)
1	96-A	0.76	1/1302 (0.1%)	0.99	4/1770 (0.2%)
1	97-A	0.72	2/1302 (0.2%)	0.98	6/1770 (0.3%)
1	98-A	0.71	1/1302 (0.1%)	1.00	7/1770 (0.4%)
1	99-A	0.69	2/1302 (0.2%)	0.99	8/1770 (0.5%)
1	100-A	0.66	0/1302	0.95	5/1770 (0.3%)
1	101-A	0.76	1/1302 (0.1%)	0.90	3/1770 (0.2%)
1	102-A	0.73	1/1302 (0.1%)	0.90	2/1770 (0.1%)
1	103-A	0.71	0/1302	0.96	5/1770 (0.3%)
1	104-A	0.83	4/1302 (0.3%)	1.05	4/1770 (0.2%)
1	105-A	0.88	4/1302 (0.3%)	1.04	5/1770 (0.3%)
1	106-A	0.85	3/1302 (0.2%)	1.10	7/1770 (0.4%)
1	107-A	0.86	2/1302 (0.2%)	1.07	7/1770 (0.4%)
1	108-A	1.05	1/1302 (0.1%)	1.14	4/1770 (0.2%)
1	109-A	0.84	3/1302 (0.2%)	1.21	12/1770 (0.7%)
1	110-A	0.77	2/1302 (0.2%)	1.11	4/1770 (0.2%)
1	111-A	0.74	1/1302 (0.1%)	1.12	7/1770 (0.4%)
1	112-A	0.78	0/1302	1.02	4/1770 (0.2%)
1	113-A	0.80	2/1302 (0.2%)	1.08	6/1770 (0.3%)
1	114-A	0.78	1/1302 (0.1%)	1.08	10/1770 (0.6%)
1	115-A	0.81	3/1302 (0.2%)	1.08	11/1770 (0.6%)
1	116-A	0.87	5/1302 (0.4%)	1.02	5/1770 (0.3%)
1	117-A	0.82	2/1302 (0.2%)	1.05	8/1770 (0.5%)
1	118-A	0.80	2/1302 (0.2%)	0.98	3/1770 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	119-A	0.74	0/1302	0.90	3/1770 (0.2%)
1	120-A	0.74	1/1302 (0.1%)	0.99	7/1770 (0.4%)
1	121-A	0.79	1/1302 (0.1%)	1.01	5/1770 (0.3%)
1	122-A	0.76	2/1302 (0.2%)	1.04	6/1770 (0.3%)
1	123-A	0.72	0/1302	0.93	2/1770 (0.1%)
1	124-A	0.71	0/1302	0.93	0/1770
1	125-A	0.74	1/1302 (0.1%)	0.93	2/1770 (0.1%)
1	126-A	0.67	0/1302	0.91	4/1770 (0.2%)
1	127-A	0.71	2/1302 (0.2%)	0.97	4/1770 (0.2%)
1	128-A	0.74	1/1302 (0.1%)	0.89	1/1770 (0.1%)
1	129-A	0.78	2/1302 (0.2%)	0.87	3/1770 (0.2%)
1	130-A	0.68	0/1302	0.96	5/1770 (0.3%)
1	131-A	0.85	2/1302 (0.2%)	1.09	9/1770 (0.5%)
1	132-A	0.77	2/1302 (0.2%)	1.02	7/1770 (0.4%)
1	133-A	0.85	3/1302 (0.2%)	1.02	3/1770 (0.2%)
1	134-A	0.84	2/1302 (0.2%)	1.01	3/1770 (0.2%)
1	135-A	0.71	0/1302	0.91	3/1770 (0.2%)
1	136-A	0.71	1/1302 (0.1%)	0.99	7/1770 (0.4%)
1	137-A	0.71	1/1302 (0.1%)	0.99	7/1770 (0.4%)
1	138-A	0.75	3/1302 (0.2%)	1.01	5/1770 (0.3%)
1	139-A	0.75	0/1302	0.99	5/1770 (0.3%)
1	140-A	0.78	1/1302 (0.1%)	0.97	5/1770 (0.3%)
1	141-A	0.85	3/1302 (0.2%)	0.97	4/1770 (0.2%)
1	142-A	0.77	3/1302 (0.2%)	1.00	6/1770 (0.3%)
1	143-A	0.82	1/1302 (0.1%)	1.00	6/1770 (0.3%)
1	144-A	0.93	7/1302 (0.5%)	1.10	11/1770 (0.6%)
1	145-A	0.74	1/1302 (0.1%)	1.02	6/1770 (0.3%)
1	146-A	0.84	3/1302 (0.2%)	1.04	7/1770 (0.4%)
1	147-A	0.80	1/1302 (0.1%)	1.00	5/1770 (0.3%)
1	148-A	0.74	1/1302 (0.1%)	1.06	6/1770 (0.3%)
1	149-A	0.83	3/1302 (0.2%)	1.03	5/1770 (0.3%)
1	150-A	0.69	1/1302 (0.1%)	0.94	2/1770 (0.1%)
1	151-A	0.76	1/1302 (0.1%)	1.06	9/1770 (0.5%)
1	152-A	0.79	3/1302 (0.2%)	0.99	5/1770 (0.3%)
1	153-A	0.75	2/1302 (0.2%)	0.95	4/1770 (0.2%)
1	154-A	0.76	1/1302 (0.1%)	1.03	8/1770 (0.5%)
1	155-A	0.79	1/1302 (0.1%)	1.12	11/1770 (0.6%)
1	156-A	0.86	5/1302 (0.4%)	1.02	4/1770 (0.2%)
1	157-A	0.99	7/1302 (0.5%)	1.20	11/1770 (0.6%)
1	158-A	0.91	1/1302 (0.1%)	1.14	10/1770 (0.6%)
1	159-A	1.03	11/1302 (0.8%)	1.15	11/1770 (0.6%)
1	160-A	0.78	0/1302	1.02	6/1770 (0.3%)
1	161-A	0.80	1/1302 (0.1%)	1.04	6/1770 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	162-A	0.86	6/1302 (0.5%)	1.00	6/1770 (0.3%)
1	163-A	0.78	2/1302 (0.2%)	0.96	4/1770 (0.2%)
1	164-A	0.76	1/1302 (0.1%)	0.96	4/1770 (0.2%)
1	165-A	0.74	1/1302 (0.1%)	0.97	5/1770 (0.3%)
1	166-A	0.77	1/1302 (0.1%)	1.00	8/1770 (0.5%)
1	167-A	0.76	2/1302 (0.2%)	1.01	7/1770 (0.4%)
All	All	0.79	287/217434 (0.1%)	1.01	932/295590 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	2-A	0	1
1	3-A	0	1
1	4-A	0	3
1	5-A	0	3
1	6-A	0	2
1	7-A	0	5
1	8-A	0	4
1	9-A	0	5
1	10-A	0	5
1	11-A	0	2
1	12-A	0	3
1	13-A	0	3
1	14-A	0	3
1	15-A	0	1
1	16-A	0	3
1	17-A	0	4
1	18-A	0	2
1	19-A	0	2
1	20-A	0	2
1	21-A	0	2
1	22-A	0	1
1	23-A	0	3
1	24-A	0	2
1	25-A	0	3
1	26-A	0	3
1	27-A	0	1
1	28-A	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	29-A	0	1
1	30-A	0	1
1	31-A	0	2
1	32-A	0	4
1	33-A	0	6
1	34-A	0	3
1	35-A	0	2
1	36-A	0	4
1	37-A	0	2
1	38-A	0	2
1	39-A	0	1
1	40-A	0	2
1	41-A	0	4
1	42-A	0	2
1	43-A	0	1
1	44-A	0	2
1	45-A	0	2
1	46-A	0	3
1	47-A	0	1
1	48-A	0	2
1	49-A	0	4
1	50-A	0	4
1	51-A	0	3
1	52-A	0	4
1	53-A	0	4
1	57-A	0	1
1	61-A	0	1
1	62-A	0	1
1	63-A	0	1
1	66-A	0	3
1	67-A	0	1
1	68-A	0	2
1	69-A	0	1
1	70-A	0	1
1	71-A	0	2
1	72-A	0	4
1	73-A	0	2
1	74-A	0	1
1	75-A	0	1
1	78-A	0	1
1	79-A	0	2
1	80-A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	81-A	0	2
1	82-A	0	1
1	83-A	0	1
1	84-A	0	1
1	85-A	0	1
1	86-A	0	2
1	88-A	0	1
1	89-A	0	2
1	90-A	0	2
1	91-A	0	1
1	94-A	0	1
1	95-A	0	1
1	97-A	0	1
1	98-A	0	1
1	99-A	0	1
1	100-A	0	1
1	102-A	0	1
1	104-A	0	2
1	105-A	0	4
1	107-A	0	3
1	108-A	0	2
1	109-A	0	2
1	110-A	0	2
1	111-A	0	2
1	112-A	0	2
1	113-A	0	5
1	114-A	0	4
1	115-A	0	3
1	116-A	0	3
1	117-A	0	4
1	122-A	0	3
1	124-A	0	1
1	126-A	0	1
1	127-A	0	1
1	130-A	0	1
1	131-A	0	2
1	132-A	0	3
1	133-A	0	3
1	134-A	0	1
1	136-A	0	2
1	137-A	0	2
1	138-A	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	139-A	0	1
1	140-A	0	2
1	141-A	0	1
1	143-A	0	2
1	144-A	0	2
1	145-A	0	4
1	146-A	0	4
1	147-A	0	1
1	149-A	0	2
1	150-A	0	2
1	151-A	0	2
1	152-A	0	2
1	154-A	0	1
1	155-A	0	2
1	156-A	0	1
1	157-A	0	3
1	158-A	0	2
1	159-A	0	5
1	160-A	0	3
1	161-A	0	3
1	162-A	0	5
1	163-A	0	5
1	164-A	0	5
1	165-A	0	1
1	166-A	0	2
1	167-A	0	1
All	All	0	312

All (287) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	70-A	152	CYS	CB-SG	24.25	2.23	1.82
1	108-A	152	CYS	CB-SG	21.03	2.18	1.82
1	71-A	152	CYS	CB-SG	18.24	2.13	1.82
1	58-A	152	CYS	CB-SG	16.08	2.09	1.82
1	129-A	152	CYS	CB-SG	13.95	2.06	1.82
1	149-A	85	CYS	CB-SG	12.27	2.03	1.82
1	107-A	152	CYS	CB-SG	12.07	2.02	1.82
1	152-A	152	CYS	CB-SG	11.46	2.01	1.82
1	95-A	152	CYS	CB-SG	10.51	2.00	1.82
1	67-A	152	CYS	CB-SG	10.29	1.99	1.82
1	106-A	152	CYS	CB-SG	10.15	1.99	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-A	152	CYS	CB-SG	10.09	1.99	1.82
1	32-A	17	GLU	CB-CG	9.95	1.71	1.52
1	141-A	152	CYS	CB-SG	-9.49	1.66	1.82
1	34-A	158	ARG	CG-CD	9.26	1.75	1.51
1	146-A	17	GLU	CB-CG	9.14	1.69	1.52
1	104-A	139	GLU	CB-CG	9.05	1.69	1.52
1	51-A	85	CYS	CB-SG	-8.80	1.67	1.82
1	159-A	64	SER	CA-CB	8.52	1.65	1.52
1	66-A	157	GLU	CG-CD	8.51	1.64	1.51
1	144-A	10	VAL	CA-CB	8.40	1.72	1.54
1	69-A	88	VAL	CB-CG2	-8.36	1.35	1.52
1	50-A	85	CYS	CB-SG	-8.35	1.68	1.82
1	97-A	101	GLU	CB-CG	8.35	1.68	1.52
1	162-A	13	VAL	CB-CG1	-8.34	1.35	1.52
1	96-A	101	GLU	CB-CG	8.14	1.67	1.52
1	56-A	98	ARG	CG-CD	-8.12	1.31	1.51
1	156-A	118	GLU	CB-CG	8.10	1.67	1.52
1	70-A	22	TRP	CB-CG	8.09	1.64	1.50
1	159-A	129	GLU	CD-OE2	8.09	1.34	1.25
1	105-A	17	GLU	CB-CG	8.04	1.67	1.52
1	89-A	88	VAL	CB-CG2	-7.97	1.36	1.52
1	6-A	10	VAL	CB-CG2	-7.95	1.36	1.52
1	52-A	85	CYS	CB-SG	-7.94	1.68	1.82
1	14-A	118	GLU	CB-CG	7.91	1.67	1.52
1	87-A	88	VAL	CB-CG2	-7.88	1.36	1.52
1	75-A	152	CYS	CB-SG	-7.84	1.69	1.82
1	144-A	16	MET	N-CA	7.80	1.61	1.46
1	78-A	20	MET	CG-SD	7.70	2.01	1.81
1	159-A	48	GLU	CB-CG	7.67	1.66	1.52
1	29-A	120	GLU	CB-CG	7.65	1.66	1.52
1	95-A	101	GLU	CB-CG	7.61	1.66	1.52
1	116-A	152	CYS	CB-SG	7.55	1.95	1.82
1	74-A	101	GLU	CB-CG	7.52	1.66	1.52
1	106-A	18	ASN	N-CA	-7.45	1.31	1.46
1	116-A	85	CYS	CB-SG	-7.43	1.69	1.82
1	164-A	48	GLU	CB-CG	7.43	1.66	1.52
1	138-A	157	GLU	CB-CG	7.39	1.66	1.52
1	144-A	154	GLU	CB-CG	7.39	1.66	1.52
1	29-A	120	GLU	CG-CD	7.30	1.62	1.51
1	33-A	158	ARG	CG-CD	7.29	1.70	1.51
1	21-A	21	PRO	CA-C	7.22	1.67	1.52
1	59-A	58	LYS	CE-NZ	-7.22	1.31	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	32-A	101	GLU	CB-CG	-7.21	1.38	1.52
1	40-A	152	CYS	CB-SG	7.19	1.94	1.82
1	8-A	101	GLU	CB-CG	-7.17	1.38	1.52
1	131-A	120	GLU	CB-CG	7.06	1.65	1.52
1	35-A	129	GLU	CB-CG	7.04	1.65	1.52
1	56-A	88	VAL	CB-CG1	-6.98	1.38	1.52
1	116-A	18	ASN	CB-CG	-6.97	1.35	1.51
1	83-A	88	VAL	CB-CG2	-6.90	1.38	1.52
1	105-A	88	VAL	CB-CG2	-6.90	1.38	1.52
1	162-A	129	GLU	CB-CG	6.84	1.65	1.52
1	104-A	139	GLU	CG-CD	6.84	1.62	1.51
1	20-A	17	GLU	CG-CD	-6.83	1.41	1.51
1	115-A	118	GLU	CB-CG	6.83	1.65	1.52
1	159-A	64	SER	CB-OG	-6.79	1.33	1.42
1	34-A	158	ARG	CD-NE	6.78	1.57	1.46
1	18-A	139	GLU	CB-CG	6.75	1.65	1.52
1	161-A	118	GLU	CB-CG	6.70	1.64	1.52
1	158-A	85	CYS	CB-SG	6.70	1.93	1.82
1	46-A	152	CYS	CB-SG	6.63	1.93	1.82
1	104-A	88	VAL	CB-CG2	-6.63	1.39	1.52
1	113-A	16	MET	CB-CG	6.63	1.72	1.51
1	138-A	129	GLU	CD-OE1	-6.61	1.18	1.25
1	159-A	48	GLU	CG-CD	6.59	1.61	1.51
1	133-A	85	CYS	CB-SG	-6.58	1.71	1.82
1	29-A	38	LYS	CE-NZ	-6.57	1.32	1.49
1	159-A	129	GLU	CG-CD	6.55	1.61	1.51
1	82-A	119	VAL	CB-CG1	-6.54	1.39	1.52
1	131-A	120	GLU	CG-CD	6.54	1.61	1.51
1	98-A	101	GLU	CG-CD	6.53	1.61	1.51
1	153-A	85	CYS	CB-SG	-6.53	1.71	1.82
1	105-A	17	GLU	CG-CD	6.51	1.61	1.51
1	80-A	128	TYR	CD1-CE1	6.50	1.49	1.39
1	36-A	129	GLU	CB-CG	6.50	1.64	1.52
1	116-A	9	ALA	CA-CB	-6.48	1.38	1.52
1	39-A	157	GLU	CB-CG	6.47	1.64	1.52
1	30-A	85	CYS	CB-SG	-6.46	1.71	1.82
1	159-A	58	LYS	CE-NZ	6.45	1.65	1.49
1	17-A	101	GLU	CB-CG	6.44	1.64	1.52
1	136-A	108	GLN	CB-CG	6.43	1.70	1.52
1	142-A	152	CYS	CB-SG	6.38	1.93	1.82
1	71-A	22	TRP	CB-CG	6.35	1.61	1.50
1	155-A	142	ASP	CB-CG	-6.32	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	142-A	120	GLU	CB-CG	6.31	1.64	1.52
1	162-A	119	VAL	CB-CG2	-6.29	1.39	1.52
1	92-A	10	VAL	CB-CG1	-6.28	1.39	1.52
1	36-A	20	MET	N-CA	6.28	1.58	1.46
1	144-A	15	GLY	CA-C	6.27	1.61	1.51
1	159-A	129	GLU	CD-OE1	6.25	1.32	1.25
1	4-A	154	GLU	CB-CG	6.24	1.64	1.52
1	81-A	85	CYS	CB-SG	-6.22	1.71	1.82
1	95-A	88	VAL	CB-CG1	-6.21	1.39	1.52
1	88-A	152	CYS	CB-SG	6.21	1.92	1.82
1	149-A	101	GLU	CB-CG	6.20	1.64	1.52
1	31-A	101	GLU	CB-CG	6.16	1.63	1.52
1	110-A	19	ALA	CA-CB	6.16	1.65	1.52
1	157-A	48	GLU	CB-CG	6.16	1.63	1.52
1	31-A	76	LYS	CE-NZ	6.15	1.64	1.49
1	159-A	131	ASP	CB-CG	6.13	1.64	1.51
1	145-A	13	VAL	CB-CG2	-6.12	1.40	1.52
1	109-A	17	GLU	CG-CD	6.12	1.61	1.51
1	115-A	101	GLU	CB-CG	6.12	1.63	1.52
1	95-A	38	LYS	CE-NZ	6.10	1.64	1.49
1	156-A	159	ARG	CG-CD	6.09	1.67	1.51
1	162-A	85	CYS	CB-SG	-6.07	1.72	1.82
1	7-A	128	TYR	CB-CG	-6.05	1.42	1.51
1	149-A	101	GLU	CG-CD	6.04	1.61	1.51
1	32-A	142	ASP	CB-CG	6.04	1.64	1.51
1	156-A	118	GLU	CG-CD	6.02	1.60	1.51
1	6-A	101	GLU	CB-CG	-6.02	1.40	1.52
1	57-A	79	ASP	CB-CG	6.02	1.64	1.51
1	61-A	88	VAL	CB-CG2	-6.01	1.40	1.52
1	33-A	89	PRO	CA-CB	-5.96	1.41	1.53
1	167-A	85	CYS	CB-SG	-5.96	1.72	1.81
1	109-A	106	LYS	CB-CG	5.96	1.68	1.52
1	144-A	157	GLU	CB-CG	-5.95	1.40	1.52
1	92-A	129	GLU	CB-CG	5.93	1.63	1.52
1	57-A	159	ARG	CG-CD	5.92	1.66	1.51
1	32-A	159	ARG	CG-CD	5.92	1.66	1.51
1	117-A	101	GLU	CB-CG	5.91	1.63	1.52
1	6-A	159	ARG	CG-CD	5.91	1.66	1.51
1	165-A	108	GLN	CG-CD	5.90	1.64	1.51
1	95-A	101	GLU	CG-CD	5.89	1.60	1.51
1	121-A	98	ARG	CG-CD	5.89	1.66	1.51
1	157-A	48	GLU	CG-CD	5.88	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	38-A	108	GLN	CB-CG	-5.87	1.36	1.52
1	118-A	157	GLU	CB-CG	5.87	1.63	1.52
1	157-A	44	ARG	CG-CD	5.86	1.66	1.51
1	37-A	157	GLU	CB-CG	5.85	1.63	1.52
1	60-A	98	ARG	CG-CD	5.84	1.66	1.51
1	144-A	101	GLU	CB-CG	5.84	1.63	1.52
1	36-A	108	GLN	CB-CG	5.83	1.68	1.52
1	56-A	154	GLU	CD-OE2	5.83	1.32	1.25
1	115-A	18	ASN	CB-CG	-5.83	1.37	1.51
1	73-A	152	CYS	CB-SG	-5.82	1.72	1.81
1	20-A	120	GLU	CB-CG	5.82	1.63	1.52
1	43-A	133	TRP	CB-CG	-5.82	1.39	1.50
1	157-A	129	GLU	CG-CD	-5.80	1.43	1.51
1	109-A	17	GLU	CB-CG	5.80	1.63	1.52
1	157-A	85	CYS	CB-SG	-5.80	1.72	1.81
1	97-A	101	GLU	CG-CD	5.78	1.60	1.51
1	81-A	101	GLU	CB-CG	-5.77	1.41	1.52
1	86-A	85	CYS	CB-SG	-5.76	1.72	1.81
1	166-A	132	ASP	CA-C	5.76	1.68	1.52
1	80-A	126	PRO	CA-C	5.75	1.64	1.52
1	162-A	10	VAL	CB-CG2	-5.75	1.40	1.52
1	39-A	19	ALA	CA-CB	-5.74	1.40	1.52
1	54-A	118	GLU	CB-CG	5.73	1.63	1.52
1	19-A	152	CYS	CB-SG	-5.72	1.72	1.81
1	55-A	129	GLU	CG-CD	5.72	1.60	1.51
1	163-A	129	GLU	CG-CD	5.72	1.60	1.51
1	157-A	48	GLU	CD-OE2	5.71	1.31	1.25
1	11-A	17	GLU	CB-CG	5.70	1.62	1.52
1	52-A	129	GLU	CB-CG	5.69	1.62	1.52
1	99-A	120	GLU	CB-CG	5.69	1.62	1.52
1	59-A	20	MET	CB-CG	5.68	1.69	1.51
1	28-A	18	ASN	C-O	-5.66	1.12	1.23
1	7-A	10	VAL	CB-CG2	-5.65	1.41	1.52
1	71-A	154	GLU	CG-CD	5.65	1.60	1.51
1	101-A	88	VAL	CB-CG2	-5.64	1.41	1.52
1	49-A	119	VAL	CB-CG2	-5.64	1.41	1.52
1	138-A	157	GLU	CG-CD	5.62	1.60	1.51
1	74-A	79	ASP	CB-CG	5.60	1.63	1.51
1	122-A	98	ARG	CG-CD	5.60	1.66	1.51
1	47-A	16	MET	CB-CG	5.59	1.69	1.51
1	71-A	154	GLU	CB-CG	5.58	1.62	1.52
1	125-A	118	GLU	CB-CG	5.58	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	35-A	106	LYS	CD-CE	5.57	1.65	1.51
1	94-A	101	GLU	CB-CG	5.57	1.62	1.52
1	114-A	20	MET	CB-CG	5.56	1.69	1.51
1	7-A	79	ASP	CB-CG	5.55	1.63	1.51
1	99-A	120	GLU	CG-CD	5.54	1.60	1.51
1	81-A	101	GLU	CG-CD	-5.54	1.43	1.51
1	4-A	157	GLU	CB-CG	-5.53	1.41	1.52
1	107-A	159	ARG	CG-CD	-5.51	1.38	1.51
1	90-A	134	GLU	CB-CG	5.51	1.62	1.52
1	12-A	120	GLU	CG-CD	5.51	1.60	1.51
1	133-A	119	VAL	N-CA	5.51	1.57	1.46
1	133-A	118	GLU	CB-CG	-5.51	1.41	1.52
1	148-A	128	TYR	CD2-CE2	-5.50	1.31	1.39
1	105-A	129	GLU	CB-CG	-5.49	1.41	1.52
1	83-A	85	CYS	CB-SG	-5.47	1.72	1.81
1	51-A	119	VAL	CA-CB	5.46	1.66	1.54
1	83-A	152	CYS	CB-SG	-5.46	1.73	1.81
1	111-A	18	ASN	CB-CG	5.46	1.63	1.51
1	44-A	152	CYS	CB-SG	5.46	1.91	1.82
1	34-A	18	ASN	CA-C	5.46	1.67	1.52
1	73-A	101	GLU	CG-CD	5.46	1.60	1.51
1	132-A	119	VAL	CB-CG1	5.45	1.64	1.52
1	134-A	120	GLU	CG-CD	-5.45	1.43	1.51
1	147-A	101	GLU	CB-CG	5.44	1.62	1.52
1	159-A	85	CYS	CB-SG	-5.44	1.73	1.81
1	152-A	128	TYR	CD1-CE1	-5.42	1.31	1.39
1	81-A	129	GLU	CG-CD	5.42	1.60	1.51
1	132-A	129	GLU	CB-CG	5.42	1.62	1.52
1	17-A	139	GLU	CG-CD	5.40	1.60	1.51
1	52-A	44	ARG	CG-CD	5.40	1.65	1.51
1	152-A	129	GLU	CD-OE1	-5.39	1.19	1.25
1	146-A	17	GLU	CG-CD	5.38	1.60	1.51
1	7-A	120	GLU	CG-CD	5.37	1.60	1.51
1	34-A	22	TRP	CA-CB	5.36	1.65	1.53
1	122-A	18	ASN	CB-CG	5.35	1.63	1.51
1	7-A	101	GLU	CB-CG	-5.35	1.42	1.52
1	31-A	89	PRO	CA-C	-5.34	1.42	1.52
1	116-A	118	GLU	CB-CG	5.33	1.62	1.52
1	72-A	157	GLU	CB-CG	-5.33	1.42	1.52
1	84-A	98	ARG	CG-CD	5.32	1.65	1.51
1	53-A	101	GLU	CB-CG	-5.32	1.42	1.52
1	70-A	21	PRO	CA-C	5.32	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	19-A	17	GLU	CG-CD	-5.31	1.44	1.51
1	141-A	129	GLU	CG-CD	5.27	1.59	1.51
1	8-A	68	THR	CB-CG2	-5.26	1.34	1.52
1	106-A	20	MET	CB-CG	5.24	1.68	1.51
1	102-A	139	GLU	CG-CD	-5.24	1.44	1.51
1	49-A	108	GLN	CG-CD	5.24	1.63	1.51
1	8-A	17	GLU	N-CA	5.23	1.56	1.46
1	82-A	88	VAL	CB-CG2	-5.23	1.41	1.52
1	94-A	101	GLU	CG-CD	5.23	1.59	1.51
1	13-A	120	GLU	CB-CG	5.23	1.62	1.52
1	156-A	85	CYS	CA-CB	-5.22	1.42	1.53
1	17-A	152	CYS	CB-SG	5.21	1.91	1.82
1	8-A	16	MET	CG-SD	-5.21	1.67	1.81
1	157-A	52	ARG	CZ-NH2	5.21	1.39	1.33
1	75-A	101	GLU	CG-CD	-5.20	1.44	1.51
1	153-A	129	GLU	CD-OE2	-5.20	1.20	1.25
1	39-A	157	GLU	CG-CD	5.19	1.59	1.51
1	85-A	98	ARG	CG-CD	5.19	1.65	1.51
1	95-A	98	ARG	CB-CG	-5.18	1.38	1.52
1	29-A	20	MET	CG-SD	5.18	1.94	1.81
1	146-A	154	GLU	CB-CG	-5.18	1.42	1.52
1	34-A	89	PRO	C-O	5.18	1.33	1.23
1	163-A	48	GLU	CG-CD	5.18	1.59	1.51
1	143-A	157	GLU	CB-CG	-5.17	1.42	1.52
1	151-A	129	GLU	CG-CD	5.17	1.59	1.51
1	49-A	88	VAL	CA-CB	5.17	1.65	1.54
1	80-A	118	GLU	CB-CG	5.17	1.61	1.52
1	118-A	118	GLU	CB-CG	5.17	1.61	1.52
1	140-A	146	GLN	CB-CG	5.17	1.66	1.52
1	75-A	16	MET	CB-CG	5.17	1.67	1.51
1	159-A	131	ASP	CA-C	5.16	1.66	1.52
1	142-A	129	GLU	CG-CD	5.16	1.59	1.51
1	88-A	10	VAL	CB-CG2	-5.15	1.42	1.52
1	127-A	159	ARG	CG-CD	-5.15	1.39	1.51
1	144-A	131	ASP	CB-CG	5.15	1.62	1.51
1	45-A	152	CYS	CB-SG	-5.14	1.73	1.81
1	127-A	158	ARG	CG-CD	-5.14	1.39	1.51
1	167-A	152	CYS	CB-SG	5.14	1.91	1.82
1	117-A	119	VAL	CB-CG1	-5.14	1.42	1.52
1	137-A	157	GLU	CD-OE2	5.14	1.31	1.25
1	7-A	159	ARG	CG-CD	5.13	1.64	1.51
1	156-A	10	VAL	CB-CG1	-5.12	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	83-A	130	PRO	CA-C	5.11	1.63	1.52
1	134-A	146	GLN	CB-CG	-5.11	1.38	1.52
1	110-A	48	GLU	CG-CD	5.10	1.59	1.51
1	21-A	118	GLU	CG-CD	5.10	1.59	1.51
1	129-A	154	GLU	CB-CG	-5.10	1.42	1.52
1	120-A	16	MET	CB-CG	5.09	1.67	1.51
1	104-A	108	GLN	CB-CG	5.08	1.66	1.52
1	154-A	119	VAL	CA-CB	5.08	1.65	1.54
1	56-A	154	GLU	CG-CD	5.08	1.59	1.51
1	8-A	108	GLN	CB-CG	5.08	1.66	1.52
1	37-A	129	GLU	CG-CD	5.07	1.59	1.51
1	46-A	16	MET	CB-CG	5.07	1.67	1.51
1	141-A	19	ALA	CA-C	5.07	1.66	1.52
1	35-A	89	PRO	CA-C	5.06	1.62	1.52
1	150-A	10	VAL	CB-CG2	-5.04	1.42	1.52
1	82-A	128	TYR	N-CA	5.04	1.56	1.46
1	162-A	129	GLU	CD-OE2	-5.04	1.20	1.25
1	70-A	152	CYS	CA-CB	5.04	1.65	1.53
1	89-A	142	ASP	CB-CG	5.02	1.62	1.51
1	113-A	108	GLN	CG-CD	5.01	1.62	1.51
1	68-A	20	MET	N-CA	5.01	1.56	1.46
1	56-A	133	TRP	CB-CG	-5.01	1.41	1.50
1	51-A	159	ARG	CG-CD	5.00	1.64	1.51
1	128-A	108	GLN	CB-CG	5.00	1.66	1.52

All (932) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	110-A	98	ARG	NE-CZ-NH1	16.84	128.72	120.30
1	84-A	36	LEU	CA-CB-CG	16.15	152.45	115.30
1	109-A	98	ARG	NE-CZ-NH2	-15.74	112.43	120.30
1	109-A	98	ARG	NE-CZ-NH1	15.70	128.15	120.30
1	68-A	20	MET	C-N-CD	-14.29	89.16	120.60
1	113-A	20	MET	C-N-CD	-14.14	89.50	120.60
1	8-A	20	MET	C-N-CD	-13.50	90.90	120.60
1	108-A	152	CYS	CA-CB-SG	13.44	138.19	114.00
1	111-A	18	ASN	N-CA-C	-13.42	74.76	111.00
1	30-A	159	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	5-A	129	GLU	C-N-CD	-13.17	91.63	120.60
1	30-A	159	ARG	NE-CZ-NH1	12.99	126.80	120.30
1	66-A	20	MET	CG-SD-CE	12.93	120.89	100.20
1	36-A	88	VAL	C-N-CD	-12.89	92.23	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	104-A	152	CYS	CA-CB-SG	12.23	136.01	114.00
1	158-A	85	CYS	CA-CB-SG	-12.21	92.03	114.00
1	47-A	156	LEU	CA-CB-CG	12.16	143.26	115.30
1	106-A	20	MET	CG-SD-CE	12.13	119.61	100.20
1	110-A	98	ARG	NE-CZ-NH2	-12.11	114.25	120.30
1	107-A	159	ARG	NE-CZ-NH1	12.01	126.30	120.30
1	127-A	158	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	41-A	88	VAL	C-N-CD	-11.70	94.87	120.60
1	52-A	85	CYS	CA-CB-SG	-11.70	92.95	114.00
1	148-A	129	GLU	C-N-CD	-11.22	95.92	120.60
1	154-A	85	CYS	CA-CB-SG	10.86	133.55	114.00
1	8-A	16	MET	CG-SD-CE	10.75	117.40	100.20
1	81-A	12	ARG	NE-CZ-NH2	-10.53	115.04	120.30
1	65-A	98	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	155-A	129	GLU	C-N-CD	10.29	150.01	128.40
1	50-A	85	CYS	CA-CB-SG	-10.27	95.51	114.00
1	4-A	129	GLU	C-N-CD	-10.24	98.06	120.60
1	95-A	85	CYS	CA-CB-SG	-10.24	95.56	114.00
1	59-A	16	MET	CA-CB-CG	10.22	130.68	113.30
1	46-A	152	CYS	CA-CB-SG	10.21	132.38	114.00
1	70-A	20	MET	C-N-CD	-10.15	98.27	120.60
1	41-A	158	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	114-A	20	MET	C-N-CD	-10.10	98.39	120.60
1	32-A	12	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	109-A	20	MET	C-N-CD	-10.05	98.49	120.60
1	65-A	98	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	91-A	36	LEU	CA-CB-CG	10.01	138.32	115.30
1	53-A	86	GLY	N-CA-C	-9.92	88.29	113.10
1	127-A	158	ARG	NE-CZ-NH2	-9.81	115.39	120.30
1	149-A	129	GLU	C-N-CD	-9.75	99.16	120.60
1	58-A	104	LEU	CB-CG-CD1	9.69	127.47	111.00
1	52-A	86	GLY	N-CA-C	-9.64	88.99	113.10
1	16-A	129	GLU	C-N-CD	-9.63	99.41	120.60
1	153-A	85	CYS	CA-CB-SG	-9.59	96.73	114.00
1	3-A	129	GLU	C-N-CD	-9.53	99.64	120.60
1	63-A	28	LEU	CA-CB-CG	9.41	136.93	115.30
1	50-A	88	VAL	N-CA-C	9.36	136.28	111.00
1	90-A	129	GLU	C-N-CD	9.36	148.06	128.40
1	152-A	129	GLU	C-N-CD	9.37	148.07	128.40
1	144-A	44	ARG	NE-CZ-NH1	9.35	124.97	120.30
1	148-A	12	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	46-A	156	LEU	CA-CB-CG	9.33	136.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	66-A	98	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	98-A	20	MET	CG-SD-CE	9.32	115.12	100.20
1	39-A	16	MET	CG-SD-CE	-9.31	85.30	100.20
1	23-A	20	MET	N-CA-C	-9.31	85.87	111.00
1	53-A	52	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	122-A	20	MET	CG-SD-CE	9.29	115.06	100.20
1	69-A	20	MET	C-N-CD	-9.27	100.20	120.60
1	159-A	79	ASP	CB-CG-OD2	9.25	126.62	118.30
1	56-A	98	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	83-A	98	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	167-A	132	ASP	CB-CG-OD2	9.18	126.56	118.30
1	161-A	20	MET	CG-SD-CE	-9.14	85.58	100.20
1	120-A	20	MET	CG-SD-CE	-9.08	85.68	100.20
1	22-A	20	MET	CG-SD-CE	-9.07	85.68	100.20
1	54-A	88	VAL	CB-CA-C	9.05	128.60	111.40
1	55-A	52	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	86-A	36	LEU	CB-CG-CD1	8.99	126.28	111.00
1	103-A	52	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	95-A	104	LEU	CB-CG-CD1	8.97	126.25	111.00
1	136-A	131	ASP	CB-CG-OD2	-8.95	110.24	118.30
1	155-A	85	CYS	CA-CB-SG	8.93	130.08	114.00
1	144-A	131	ASP	CB-CG-OD2	8.85	126.27	118.30
1	69-A	98	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	87-A	36	LEU	CB-CG-CD1	8.82	126.00	111.00
1	42-A	88	VAL	C-N-CD	-8.81	101.21	120.60
1	107-A	159	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	115-A	20	MET	C-N-CD	-8.75	101.35	120.60
1	117-A	20	MET	C-N-CD	-8.75	101.36	120.60
1	157-A	79	ASP	CB-CG-OD2	-8.75	110.43	118.30
1	57-A	159	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	99-A	98	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	65-A	12	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	78-A	20	MET	CG-SD-CE	8.65	114.03	100.20
1	79-A	20	MET	CG-SD-CE	8.64	114.02	100.20
1	159-A	159	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	79-A	104	LEU	CB-CG-CD1	8.62	125.65	111.00
1	94-A	20	MET	CG-SD-CE	-8.59	86.46	100.20
1	112-A	121	GLY	N-CA-C	8.56	134.50	113.10
1	109-A	159	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	56-A	79	ASP	CB-CG-OD2	8.52	125.97	118.30
1	148-A	130	PRO	N-CA-C	-8.51	89.97	112.10
1	156-A	85	CYS	CA-CB-SG	-8.49	98.72	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	50-A	159	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	99-A	159	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	144-A	129	GLU	N-CA-C	8.37	133.59	111.00
1	118-A	20	MET	CA-CB-CG	8.35	127.49	113.30
1	120-A	98	ARG	NE-CZ-NH2	8.33	124.47	120.30
1	61-A	156	LEU	CA-CB-CG	8.33	134.45	115.30
1	58-A	20	MET	CG-SD-CE	-8.30	86.92	100.20
1	114-A	98	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	80-A	127	ASP	CB-CG-OD1	8.26	125.73	118.30
1	8-A	20	MET	C-N-CA	8.24	156.59	122.00
1	21-A	152	CYS	CA-CB-SG	-8.24	99.17	114.00
1	41-A	156	LEU	CA-CB-CG	8.20	134.16	115.30
1	15-A	11	ASP	CB-CG-OD1	8.20	125.68	118.30
1	131-A	119	VAL	N-CA-C	8.19	133.11	111.00
1	155-A	44	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	166-A	129	GLU	C-N-CD	-8.11	102.76	120.60
1	23-A	20	MET	CA-CB-CG	8.05	126.99	113.30
1	121-A	20	MET	CA-CB-CG	8.05	126.98	113.30
1	109-A	159	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	146-A	142	ASP	CB-CG-OD2	8.01	125.50	118.30
1	151-A	52	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	115-A	22	TRP	N-CA-C	7.99	132.57	111.00
1	79-A	127	ASP	CB-CG-OD2	7.97	125.47	118.30
1	120-A	158	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	157-A	86	GLY	N-CA-C	7.93	132.94	113.10
1	66-A	98	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	40-A	17	GLU	CB-CA-C	7.90	126.19	110.40
1	30-A	98	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	59-A	20	MET	CG-SD-CE	-7.87	87.61	100.20
1	5-A	20	MET	CG-SD-CE	7.86	112.78	100.20
1	83-A	98	ARG	NE-CZ-NH1	-7.85	116.37	120.30
1	131-A	4	LEU	CB-CG-CD2	7.84	124.33	111.00
1	51-A	85	CYS	CA-CB-SG	-7.84	99.89	114.00
1	107-A	152	CYS	CA-CB-SG	7.84	128.11	114.00
1	47-A	36	LEU	CA-CB-CG	7.83	133.31	115.30
1	73-A	16	MET	CB-CG-SD	7.82	135.86	112.40
1	83-A	36	LEU	CA-CB-CG	7.79	133.22	115.30
1	109-A	1	MET	CG-SD-CE	7.79	112.66	100.20
1	31-A	158	ARG	CG-CD-NE	-7.77	95.48	111.80
1	132-A	44	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	99-A	159	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	165-A	132	ASP	CB-CG-OD1	7.74	125.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	37-A	86	GLY	N-CA-C	-7.73	93.77	113.10
1	58-A	156	LEU	CA-CB-CG	7.73	133.08	115.30
1	33-A	158	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	14-A	104	LEU	CB-CG-CD2	7.69	124.07	111.00
1	63-A	1	MET	CA-CB-CG	7.68	126.36	113.30
1	50-A	87	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	111-A	159	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	145-A	112	LEU	CB-CG-CD1	-7.63	98.03	111.00
1	83-A	128	TYR	CA-CB-CG	7.57	127.78	113.40
1	84-A	36	LEU	CB-CG-CD1	-7.56	98.14	111.00
1	88-A	129	GLU	C-N-CD	7.56	144.28	128.40
1	30-A	98	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	157-A	33	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	46-A	17	GLU	N-CA-C	-7.53	90.66	111.00
1	31-A	127	ASP	N-CA-CB	7.53	124.16	110.60
1	166-A	132	ASP	N-CA-C	7.53	131.33	111.00
1	114-A	104	LEU	CB-CG-CD2	7.52	123.78	111.00
1	71-A	20	MET	C-N-CD	-7.51	104.08	120.60
1	47-A	79	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	36-A	122	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	91-A	20	MET	CG-SD-CE	7.49	112.17	100.20
1	122-A	121	GLY	N-CA-C	7.48	131.80	113.10
1	90-A	1	MET	CB-CA-C	7.47	125.33	110.40
1	85-A	128	TYR	CB-CA-C	7.46	125.33	110.40
1	16-A	159	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	122-A	129	GLU	C-N-CD	7.42	143.98	128.40
1	32-A	12	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	162-A	104	LEU	CB-CG-CD1	7.39	123.57	111.00
1	157-A	85	CYS	CA-CB-SG	-7.39	100.70	114.00
1	96-A	20	MET	CG-SD-CE	-7.38	88.40	100.20
1	31-A	98	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	162-A	1	MET	CG-SD-CE	7.35	111.95	100.20
1	98-A	98	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	145-A	129	GLU	N-CA-C	7.34	130.82	111.00
1	154-A	156	LEU	CA-CB-CG	7.34	132.18	115.30
1	7-A	44	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	50-A	36	LEU	CA-CB-CG	7.33	132.16	115.30
1	146-A	17	GLU	CB-CA-C	7.32	125.05	110.40
1	55-A	52	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	128-A	92	MET	CB-CG-SD	-7.31	90.46	112.40
1	99-A	98	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	7-A	12	ARG	NE-CZ-NH2	-7.31	116.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	65-A	12	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	121-A	121	GLY	N-CA-C	7.29	131.32	113.10
1	40-A	21	PRO	N-CA-C	7.28	131.04	112.10
1	77-A	52	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	49-A	36	LEU	CA-CB-CG	7.27	132.02	115.30
1	60-A	158	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	75-A	152	CYS	CA-CB-SG	-7.26	100.93	114.00
1	33-A	128	TYR	CA-CB-CG	7.26	127.19	113.40
1	97-A	159	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	80-A	128	TYR	CB-CG-CD1	7.25	125.35	121.00
1	154-A	129	GLU	C-N-CD	7.24	143.60	128.40
1	158-A	156	LEU	CA-CB-CG	7.23	131.93	115.30
1	161-A	131	ASP	CB-CG-OD1	7.23	124.81	118.30
1	142-A	18	ASN	N-CA-C	7.22	130.49	111.00
1	8-A	12	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	9-A	21	PRO	N-CA-C	7.21	130.85	112.10
1	53-A	156	LEU	CA-CB-CG	7.21	131.88	115.30
1	93-A	18	ASN	CB-CA-C	7.19	124.77	110.40
1	57-A	87	ASP	CB-CG-OD1	-7.17	111.84	118.30
1	148-A	1	MET	CG-SD-CE	7.17	111.67	100.20
1	39-A	158	ARG	NE-CZ-NH2	7.17	123.88	120.30
1	113-A	159	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	4-A	44	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	83-A	142	ASP	CB-CG-OD2	7.14	124.73	118.30
1	98-A	98	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	12-A	17	GLU	N-CA-C	7.09	130.15	111.00
1	82-A	127	ASP	CB-CG-OD1	7.08	124.67	118.30
1	147-A	8	LEU	CB-CG-CD1	-7.08	98.97	111.00
1	65-A	20	MET	CG-SD-CE	7.05	111.49	100.20
1	130-A	119	VAL	CA-CB-CG2	7.03	121.45	110.90
1	6-A	156	LEU	CA-CB-CG	7.03	131.47	115.30
1	57-A	4	LEU	CB-CG-CD2	7.02	122.94	111.00
1	67-A	20	MET	N-CA-C	7.00	129.89	111.00
1	63-A	98	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	59-A	20	MET	CA-CB-CG	6.99	125.19	113.30
1	68-A	20	MET	C-N-CA	6.99	151.35	122.00
1	39-A	98	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	36-A	119	VAL	N-CA-C	6.97	129.82	111.00
1	136-A	13	VAL	CB-CA-C	-6.96	98.17	111.40
1	20-A	108	GLN	CA-CB-CG	6.96	128.72	113.40
1	7-A	12	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	43-A	87	ASP	N-CA-C	6.94	129.74	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	80-A	128	TYR	CA-CB-CG	6.94	126.58	113.40
1	90-A	36	LEU	CA-CB-CG	6.93	131.23	115.30
1	52-A	52	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	82-A	158	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	74-A	98	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	154-A	44	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	114-A	20	MET	CB-CG-SD	6.86	132.98	112.40
1	158-A	36	LEU	CB-CG-CD2	6.85	122.65	111.00
1	146-A	142	ASP	CB-CG-OD1	-6.85	112.14	118.30
1	136-A	131	ASP	CB-CG-OD1	6.85	124.46	118.30
1	115-A	18	ASN	N-CA-C	6.84	129.47	111.00
1	144-A	156	LEU	CA-CB-CG	6.83	131.01	115.30
1	137-A	16	MET	CB-CG-SD	6.83	132.89	112.40
1	68-A	127	ASP	CB-CG-OD2	6.81	124.43	118.30
1	51-A	86	GLY	N-CA-C	-6.81	96.07	113.10
1	45-A	85	CYS	CA-CB-SG	-6.80	101.76	114.00
1	32-A	132	ASP	CB-CG-OD1	6.79	124.42	118.30
1	81-A	104	LEU	CB-CG-CD1	-6.79	99.46	111.00
1	100-A	98	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	7-A	44	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	12-A	119	VAL	CB-CA-C	-6.77	98.54	111.40
1	34-A	79	ASP	CB-CG-OD2	6.76	124.39	118.30
1	138-A	12	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	52-A	156	LEU	CA-CB-CG	6.76	130.86	115.30
1	47-A	85	CYS	CA-CB-SG	-6.76	101.84	114.00
1	70-A	20	MET	C-N-CA	6.75	150.35	122.00
1	143-A	129	GLU	C-N-CD	6.75	142.56	128.40
1	117-A	12	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	159-A	104	LEU	CB-CG-CD1	6.74	122.47	111.00
1	126-A	127	ASP	CB-CG-OD1	6.74	124.37	118.30
1	97-A	159	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	154-A	52	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	154-A	52	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	158-A	52	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	143-A	18	ASN	N-CA-C	6.71	129.12	111.00
1	70-A	152	CYS	CB-CA-C	6.71	123.81	110.40
1	57-A	156	LEU	CA-CB-CG	6.70	130.70	115.30
1	34-A	44	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	97-A	20	MET	CB-CG-SD	6.69	132.46	112.40
1	155-A	44	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	159-A	1	MET	CG-SD-CE	-6.68	89.51	100.20
1	70-A	20	MET	N-CA-C	6.67	129.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	33-A	128	TYR	N-CA-CB	-6.67	98.59	110.60
1	32-A	16	MET	CB-CG-SD	6.66	132.37	112.40
1	131-A	1	MET	CG-SD-CE	6.66	110.85	100.20
1	126-A	20	MET	CG-SD-CE	6.66	110.85	100.20
1	122-A	156	LEU	CA-CB-CG	6.65	130.59	115.30
1	74-A	8	LEU	CA-CB-CG	6.64	130.58	115.30
1	33-A	87	ASP	N-CA-C	6.64	128.93	111.00
1	33-A	12	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	11-A	21	PRO	N-CA-C	6.64	129.35	112.10
1	52-A	36	LEU	CB-CA-C	6.63	122.80	110.20
1	151-A	159	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	138-A	16	MET	CB-CG-SD	6.62	132.26	112.40
1	34-A	142	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	37-A	159	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	137-A	1	MET	CG-SD-CE	6.61	110.78	100.20
1	80-A	104	LEU	CB-CG-CD1	6.61	122.23	111.00
1	16-A	18	ASN	N-CA-C	6.58	128.78	111.00
1	37-A	19	ALA	N-CA-C	6.58	128.76	111.00
1	39-A	122	ASP	CB-CG-OD1	6.58	124.22	118.30
1	129-A	159	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	42-A	87	ASP	CB-CG-OD1	6.57	124.22	118.30
1	43-A	98	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	93-A	20	MET	N-CA-C	-6.56	93.29	111.00
1	132-A	119	VAL	N-CA-C	6.55	128.69	111.00
1	146-A	16	MET	CA-CB-CG	6.55	124.44	113.30
1	32-A	156	LEU	CA-CB-CG	6.55	130.36	115.30
1	32-A	87	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	121-A	20	MET	CB-CA-C	6.54	123.49	110.40
1	42-A	98	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	57-A	20	MET	CG-SD-CE	6.54	110.67	100.20
1	16-A	38	LYS	CD-CE-NZ	-6.54	96.67	111.70
1	112-A	33	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	110-A	1	MET	C-N-CA	-6.53	105.39	121.70
1	105-A	18	ASN	N-CA-C	-6.52	93.39	111.00
1	24-A	111	TYR	CA-CB-CG	-6.51	101.02	113.40
1	29-A	17	GLU	N-CA-C	-6.51	93.42	111.00
1	160-A	64	SER	N-CA-C	-6.50	93.46	111.00
1	106-A	70	ASP	CB-CG-OD1	6.49	124.14	118.30
1	74-A	79	ASP	CB-CG-OD1	6.48	124.13	118.30
1	160-A	129	GLU	C-N-CD	-6.47	106.38	120.60
1	32-A	85	CYS	CA-CB-SG	-6.46	102.37	114.00
1	144-A	128	TYR	CA-CB-CG	6.46	125.67	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	143-A	20	MET	CA-CB-CG	6.44	124.25	113.30
1	87-A	1	MET	CB-CG-SD	6.43	131.68	112.40
1	116-A	20	MET	N-CA-C	-6.42	93.67	111.00
1	162-A	130	PRO	CA-N-CD	-6.42	102.52	111.50
1	106-A	20	MET	CA-CB-CG	6.41	124.20	113.30
1	49-A	87	ASP	N-CA-C	6.41	128.31	111.00
1	66-A	157	GLU	OE1-CD-OE2	-6.40	115.62	123.30
1	155-A	129	GLU	C-N-CA	-6.40	95.12	122.00
1	80-A	126	PRO	N-CA-C	6.39	128.72	112.10
1	57-A	119	VAL	CB-CA-C	-6.38	99.28	111.40
1	105-A	20	MET	C-N-CD	6.38	141.80	128.40
1	109-A	152	CYS	CA-CB-SG	6.38	125.48	114.00
1	9-A	20	MET	C-N-CD	-6.38	106.58	120.60
1	79-A	119	VAL	CB-CA-C	-6.37	99.30	111.40
1	113-A	20	MET	C-N-CA	6.37	148.75	122.00
1	142-A	152	CYS	CA-CB-SG	6.37	125.46	114.00
1	115-A	11	ASP	CB-CG-OD1	6.37	124.03	118.30
1	70-A	152	CYS	CA-CB-SG	6.36	125.45	114.00
1	69-A	16	MET	CB-CG-SD	6.34	131.43	112.40
1	38-A	12	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	33-A	129	GLU	N-CA-C	6.32	128.06	111.00
1	9-A	104	LEU	CB-CG-CD1	6.31	121.72	111.00
1	41-A	19	ALA	N-CA-C	6.30	128.02	111.00
1	104-A	18	ASN	N-CA-C	-6.30	93.98	111.00
1	132-A	118	GLU	N-CA-C	6.30	128.02	111.00
1	165-A	16	MET	CG-SD-CE	6.30	110.28	100.20
1	98-A	87	ASP	CB-CG-OD1	6.30	123.97	118.30
1	141-A	19	ALA	N-CA-C	6.30	128.00	111.00
1	30-A	16	MET	CG-SD-CE	6.29	110.26	100.20
1	146-A	131	ASP	CB-CG-OD1	-6.28	112.64	118.30
1	68-A	79	ASP	CB-CG-OD1	6.27	123.94	118.30
1	150-A	136	VAL	N-CA-C	-6.27	94.08	111.00
1	23-A	20	MET	CB-CG-SD	6.27	131.20	112.40
1	9-A	119	VAL	CB-CA-C	-6.26	99.50	111.40
1	30-A	127	ASP	CB-CG-OD1	-6.26	112.66	118.30
1	40-A	22	TRP	N-CA-C	-6.26	94.11	111.00
1	47-A	87	ASP	CB-CG-OD2	6.26	123.93	118.30
1	82-A	142	ASP	CB-CG-OD2	6.26	123.93	118.30
1	135-A	120	GLU	CB-CA-C	6.26	122.91	110.40
1	35-A	127	ASP	N-CA-C	-6.25	94.12	111.00
1	157-A	98	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	159-A	4	LEU	CB-CG-CD2	6.25	121.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	60-A	127	ASP	CB-CG-OD1	6.25	123.92	118.30
1	140-A	1	MET	CG-SD-CE	-6.24	90.21	100.20
1	31-A	12	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	42-A	87	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	162-A	104	LEU	CB-CG-CD2	-6.24	100.40	111.00
1	72-A	88	VAL	CG1-CB-CG2	6.22	120.86	110.90
1	134-A	159	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	75-A	1	MET	CA-CB-CG	6.22	123.87	113.30
1	39-A	158	ARG	CG-CD-NE	6.21	124.85	111.80
1	138-A	12	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	67-A	87	ASP	CB-CG-OD2	6.21	123.89	118.30
1	132-A	44	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	115-A	119	VAL	CB-CA-C	-6.21	99.61	111.40
1	33-A	131	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	6-A	44	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	21-A	12	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	35-A	18	ASN	CB-CA-C	6.19	122.78	110.40
1	145-A	1	MET	CG-SD-CE	-6.19	90.30	100.20
1	68-A	52	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	31-A	53	PRO	N-CA-C	6.19	128.19	112.10
1	107-A	20	MET	CB-CG-SD	6.19	130.96	112.40
1	20-A	159	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	71-A	16	MET	N-CA-C	-6.18	94.31	111.00
1	125-A	16	MET	CA-CB-CG	6.18	123.81	113.30
1	8-A	4	LEU	CB-CG-CD1	-6.18	100.50	111.00
1	158-A	44	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	134-A	159	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	138-A	16	MET	CG-SD-CE	6.17	110.07	100.20
1	86-A	104	LEU	CB-CG-CD2	-6.16	100.52	111.00
1	109-A	17	GLU	N-CA-CB	6.16	121.69	110.60
1	153-A	127	ASP	N-CA-C	6.16	127.64	111.00
1	68-A	1	MET	CB-CA-C	6.16	122.72	110.40
1	136-A	18	ASN	CB-CA-C	-6.15	98.10	110.40
1	56-A	87	ASP	CB-CG-OD1	6.15	123.83	118.30
1	159-A	156	LEU	CA-CB-CG	6.14	129.42	115.30
1	76-A	16	MET	CG-SD-CE	6.13	110.01	100.20
1	56-A	4	LEU	CB-CG-CD2	6.13	121.42	111.00
1	53-A	87	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	151-A	129	GLU	C-N-CD	6.13	141.27	128.40
1	117-A	19	ALA	N-CA-C	6.13	127.54	111.00
1	21-A	152	CYS	CB-CA-C	-6.12	98.16	110.40
1	131-A	1	MET	CA-CB-CG	6.11	123.69	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	156-A	86	GLY	N-CA-C	6.11	128.38	113.10
1	38-A	88	VAL	C-N-CD	-6.11	107.17	120.60
1	93-A	129	GLU	CA-CB-CG	-6.11	99.96	113.40
1	135-A	52	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	40-A	159	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	166-A	128	TYR	CA-CB-CG	6.10	124.98	113.40
1	17-A	79	ASP	CB-CG-OD1	6.10	123.79	118.30
1	65-A	4	LEU	CB-CG-CD2	6.09	121.36	111.00
1	136-A	52	ARG	CB-CG-CD	6.09	127.44	111.60
1	147-A	159	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	60-A	158	ARG	CG-CD-NE	-6.09	99.01	111.80
1	166-A	159	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	58-A	33	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	89-A	142	ASP	CB-CG-OD2	6.09	123.78	118.30
1	86-A	159	ARG	CG-CD-NE	-6.08	99.02	111.80
1	87-A	104	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	75-A	101	GLU	OE1-CD-OE2	6.08	130.60	123.30
1	158-A	79	ASP	CB-CG-OD2	6.08	123.77	118.30
1	56-A	156	LEU	CB-CG-CD1	-6.08	100.67	111.00
1	12-A	119	VAL	N-CA-C	6.07	127.40	111.00
1	155-A	156	LEU	CB-CG-CD2	6.07	121.32	111.00
1	99-A	132	ASP	CB-CG-OD2	6.07	123.76	118.30
1	127-A	134	GLU	CA-CB-CG	6.07	126.75	113.40
1	108-A	4	LEU	CB-CG-CD2	6.07	121.31	111.00
1	16-A	159	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	28-A	20	MET	N-CA-C	6.06	127.37	111.00
1	126-A	20	MET	CB-CG-SD	-6.06	94.21	112.40
1	28-A	32	LYS	CD-CE-NZ	6.05	125.62	111.70
1	48-A	85	CYS	N-CA-C	6.05	127.34	111.00
1	82-A	159	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	20-A	36	LEU	CB-CG-CD1	6.04	121.27	111.00
1	125-A	20	MET	N-CA-C	-6.03	94.72	111.00
1	103-A	33	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	144-A	15	GLY	CA-C-O	-6.03	109.76	120.60
1	21-A	12	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	39-A	52	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	103-A	52	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	68-A	127	ASP	CB-CA-C	6.01	122.43	110.40
1	79-A	127	ASP	N-CA-C	6.01	127.24	111.00
1	79-A	127	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	103-A	129	GLU	CA-CB-CG	6.01	126.61	113.40
1	73-A	98	ARG	NE-CZ-NH1	6.00	123.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	40-A	16	MET	CG-SD-CE	5.99	109.78	100.20
1	134-A	16	MET	CB-CG-SD	5.99	130.37	112.40
1	165-A	127	ASP	N-CA-C	-5.99	94.84	111.00
1	32-A	98	ARG	CG-CD-NE	5.98	124.36	111.80
1	76-A	44	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	79-A	129	GLU	C-N-CA	-5.98	96.88	122.00
1	156-A	16	MET	CG-SD-CE	5.98	109.77	100.20
1	96-A	122	ASP	N-CA-CB	-5.98	99.84	110.60
1	35-A	104	LEU	CB-CG-CD2	5.97	121.16	111.00
1	39-A	104	LEU	CB-CG-CD2	5.97	121.15	111.00
1	152-A	159	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	10-A	156	LEU	CA-CB-CG	5.97	129.03	115.30
1	119-A	1	MET	CG-SD-CE	-5.97	90.65	100.20
1	11-A	156	LEU	CA-CB-CG	5.96	129.02	115.30
1	10-A	119	VAL	CB-CA-C	-5.96	100.08	111.40
1	131-A	20	MET	CB-CA-C	5.96	122.31	110.40
1	47-A	85	CYS	N-CA-C	5.96	127.08	111.00
1	45-A	156	LEU	CA-CB-CG	5.95	128.99	115.30
1	122-A	98	ARG	CG-CD-NE	5.95	124.30	111.80
1	27-A	108	GLN	CA-CB-CG	5.95	126.49	113.40
1	32-A	109	LYS	CD-CE-NZ	5.95	125.38	111.70
1	142-A	4	LEU	CB-CG-CD2	5.95	121.11	111.00
1	109-A	156	LEU	CA-CB-CG	5.94	128.97	115.30
1	159-A	132	ASP	N-CA-C	5.94	127.04	111.00
1	41-A	159	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	29-A	38	LYS	CD-CE-NZ	-5.94	98.04	111.70
1	149-A	44	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	85-A	16	MET	CG-SD-CE	-5.94	90.70	100.20
1	114-A	52	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	25-A	61	ILE	CG1-CB-CG2	-5.93	98.36	111.40
1	38-A	142	ASP	CB-CG-OD1	5.91	123.62	118.30
1	92-A	4	LEU	CB-CG-CD2	5.91	121.05	111.00
1	131-A	20	MET	CB-CG-SD	-5.91	94.69	112.40
1	2-A	159	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	133-A	44	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	130-A	119	VAL	N-CA-C	5.89	126.92	111.00
1	131-A	20	MET	CA-CB-CG	5.89	123.31	113.30
1	31-A	16	MET	CA-CB-CG	5.89	123.31	113.30
1	108-A	1	MET	CG-SD-CE	5.88	109.61	100.20
1	48-A	88	VAL	C-N-CD	5.88	140.75	128.40
1	52-A	36	LEU	CB-CG-CD1	-5.88	101.01	111.00
1	68-A	16	MET	CG-SD-CE	5.88	109.61	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	84-A	98	ARG	CA-CB-CG	5.88	126.33	113.40
1	109-A	44	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	61-A	159	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	136-A	24	LEU	CB-CG-CD1	5.88	120.99	111.00
1	106-A	152	CYS	CA-CB-SG	5.88	124.58	114.00
1	147-A	8	LEU	CB-CG-CD2	5.87	120.99	111.00
1	159-A	79	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	82-A	159	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	114-A	129	GLU	C-N-CA	-5.86	97.38	122.00
1	31-A	130	PRO	CA-C-O	-5.85	106.15	120.20
1	40-A	4	LEU	CB-CG-CD2	5.85	120.95	111.00
1	69-A	17	GLU	CB-CA-C	5.85	122.09	110.40
1	119-A	16	MET	CA-CB-CG	5.84	123.22	113.30
1	83-A	4	LEU	CB-CG-CD2	5.84	120.92	111.00
1	101-A	104	LEU	CB-CG-CD2	5.83	120.91	111.00
1	107-A	79	ASP	CB-CG-OD1	5.82	123.54	118.30
1	8-A	159	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	130-A	119	VAL	CB-CA-C	-5.82	100.35	111.40
1	81-A	4	LEU	CB-CG-CD2	5.82	120.89	111.00
1	89-A	36	LEU	CA-CB-CG	5.81	128.67	115.30
1	43-A	159	ARG	NE-CZ-NH2	5.81	123.20	120.30
1	160-A	131	ASP	CB-CG-OD1	5.81	123.53	118.30
1	6-A	44	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	8-A	12	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	117-A	28	LEU	CB-CG-CD1	-5.80	101.15	111.00
1	119-A	24	LEU	CB-CG-CD1	-5.80	101.15	111.00
1	164-A	158	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	32-A	129	GLU	C-N-CD	-5.79	107.86	120.60
1	109-A	44	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	65-A	70	ASP	CB-CG-OD1	5.79	123.51	118.30
1	166-A	131	ASP	C-N-CA	5.79	136.17	121.70
1	139-A	159	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	60-A	156	LEU	CA-CB-CG	5.78	128.60	115.30
1	41-A	159	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	92-A	36	LEU	CA-CB-CG	5.77	128.58	115.30
1	3-A	128	TYR	CB-CG-CD2	5.77	124.46	121.00
1	26-A	61	ILE	CG1-CB-CG2	-5.77	98.70	111.40
1	32-A	159	ARG	CB-CG-CD	5.77	126.59	111.60
1	107-A	20	MET	CG-SD-CE	-5.77	90.97	100.20
1	45-A	135	SER	CB-CA-C	-5.77	99.15	110.10
1	118-A	22	TRP	N-CA-C	5.77	126.57	111.00
1	120-A	58	LYS	CD-CE-NZ	5.77	124.96	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	113-A	129	GLU	C-N-CD	5.76	140.50	128.40
1	117-A	22	TRP	N-CA-C	5.76	126.56	111.00
1	137-A	127	ASP	CB-CG-OD1	5.76	123.48	118.30
1	34-A	158	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	116-A	20	MET	CB-CA-C	5.76	121.91	110.40
1	106-A	18	ASN	N-CA-C	-5.75	95.47	111.00
1	148-A	28	LEU	CA-CB-CG	-5.75	102.08	115.30
1	9-A	16	MET	CA-CB-CG	5.74	123.06	113.30
1	44-A	85	CYS	N-CA-C	5.74	126.51	111.00
1	144-A	44	ARG	CG-CD-NE	5.74	123.86	111.80
1	49-A	131	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	115-A	104	LEU	CB-CG-CD2	5.74	120.75	111.00
1	131-A	159	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	51-A	36	LEU	CB-CG-CD1	-5.74	101.25	111.00
1	55-A	87	ASP	N-CA-C	-5.74	95.51	111.00
1	115-A	24	LEU	CA-CB-CG	5.74	128.49	115.30
1	160-A	132	ASP	CB-CG-OD1	5.73	123.46	118.30
1	69-A	159	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	117-A	12	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	41-A	22	TRP	N-CA-C	-5.72	95.55	111.00
1	157-A	110	LEU	CA-CB-CG	5.72	128.45	115.30
1	157-A	36	LEU	CB-CG-CD2	5.72	120.72	111.00
1	152-A	129	GLU	C-N-CA	-5.71	98.01	122.00
1	42-A	158	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	40-A	158	ARG	CG-CD-NE	5.70	123.77	111.80
1	147-A	16	MET	CG-SD-CE	5.70	109.32	100.20
1	105-A	20	MET	CG-SD-CE	-5.69	91.09	100.20
1	149-A	86	GLY	N-CA-C	5.69	127.33	113.10
1	162-A	98	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	39-A	17	GLU	CB-CA-C	5.68	121.77	110.40
1	58-A	131	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	140-A	131	ASP	CB-CG-OD1	5.68	123.42	118.30
1	141-A	44	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	144-A	16	MET	N-CA-CB	5.68	120.82	110.60
1	165-A	69	ASP	N-CA-C	-5.68	95.66	111.00
1	87-A	126	PRO	N-CA-C	5.68	126.86	112.10
1	136-A	87	ASP	CB-CA-C	5.68	121.75	110.40
1	38-A	12	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	46-A	16	MET	N-CA-CB	5.67	120.81	110.60
1	132-A	52	ARG	N-CA-C	-5.67	95.68	111.00
1	71-A	152	CYS	CA-CB-SG	5.67	124.21	114.00
1	157-A	85	CYS	N-CA-C	5.67	126.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	18-A	4	LEU	CB-CG-CD2	5.67	120.64	111.00
1	114-A	20	MET	CA-CB-CG	5.67	122.94	113.30
1	27-A	61	ILE	CG1-CB-CG2	-5.66	98.94	111.40
1	13-A	98	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	61-A	20	MET	CB-CG-SD	-5.66	95.43	112.40
1	83-A	159	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	154-A	87	ASP	CB-CA-C	5.65	121.70	110.40
1	161-A	12	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	5-A	129	GLU	C-N-CA	5.65	145.73	122.00
1	35-A	19	ALA	N-CA-C	5.65	126.25	111.00
1	26-A	4	LEU	CB-CG-CD2	5.65	120.60	111.00
1	69-A	22	TRP	CA-CB-CG	5.65	124.43	113.70
1	14-A	131	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	78-A	16	MET	CG-SD-CE	5.64	109.23	100.20
1	29-A	50	ILE	N-CA-CB	5.64	123.78	110.80
1	113-A	16	MET	CB-CG-SD	5.64	129.32	112.40
1	167-A	129	GLU	C-N-CD	-5.64	108.19	120.60
1	143-A	44	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	52-A	33	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	65-A	98	ARG	CD-NE-CZ	5.64	131.49	123.60
1	84-A	129	GLU	C-N-CD	5.64	140.24	128.40
1	161-A	98	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	77-A	33	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	49-A	88	VAL	N-CA-CB	5.63	123.89	111.50
1	146-A	20	MET	C-N-CD	-5.63	108.21	120.60
1	28-A	159	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	84-A	128	TYR	CA-CB-CG	5.62	124.09	113.40
1	149-A	130	PRO	N-CA-C	-5.62	97.47	112.10
1	152-A	85	CYS	N-CA-CB	5.62	120.72	110.60
1	73-A	20	MET	C-N-CD	-5.62	108.23	120.60
1	71-A	1	MET	CG-SD-CE	5.62	109.19	100.20
1	45-A	131	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	100-A	159	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	167-A	156	LEU	CA-CB-CG	-5.62	102.38	115.30
1	108-A	16	MET	CA-CB-CG	5.62	122.85	113.30
1	111-A	104	LEU	CB-CG-CD2	5.62	120.55	111.00
1	31-A	130	PRO	O-C-N	5.61	131.68	122.70
1	53-A	36	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	111-A	159	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	164-A	131	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	20-A	4	LEU	CB-CG-CD2	-5.61	101.47	111.00
1	91-A	38	LYS	CD-CE-NZ	5.61	124.60	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	166-A	98	ARG	CG-CD-NE	5.61	123.58	111.80
1	61-A	129	GLU	C-N-CD	-5.61	108.27	120.60
1	59-A	52	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	158-A	129	GLU	N-CA-CB	5.60	120.68	110.60
1	73-A	101	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	138-A	11	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	81-A	33	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	33-A	158	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	166-A	158	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	115-A	20	MET	N-CA-C	-5.59	95.90	111.00
1	2-A	159	ARG	CG-CD-NE	5.59	123.54	111.80
1	58-A	156	LEU	CB-CG-CD1	5.59	120.50	111.00
1	137-A	18	ASN	CB-CA-C	-5.59	99.22	110.40
1	62-A	16	MET	CB-CG-SD	-5.59	95.64	112.40
1	87-A	4	LEU	CB-CG-CD2	-5.58	101.50	111.00
1	112-A	33	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	57-A	127	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	157-A	98	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	105-A	1	MET	CB-CG-SD	-5.57	95.68	112.40
1	40-A	142	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	73-A	65	GLN	C-N-CD	-5.57	108.35	120.60
1	114-A	98	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	167-A	4	LEU	CB-CG-CD2	5.57	120.46	111.00
1	1-A	132	ASP	CB-CG-OD2	5.57	123.31	118.30
1	42-A	98	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	3-A	128	TYR	CA-CB-CG	5.56	123.96	113.40
1	57-A	44	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	7-A	121	GLY	N-CA-C	5.55	126.98	113.10
1	37-A	131	ASP	CB-CG-OD1	5.55	123.30	118.30
1	163-A	129	GLU	N-CA-C	-5.55	96.01	111.00
1	106-A	98	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	159-A	52	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	62-A	106	LYS	CB-CA-C	5.55	121.49	110.40
1	159-A	64	SER	N-CA-C	5.54	125.97	111.00
1	94-A	104	LEU	CB-CG-CD1	5.54	120.42	111.00
1	98-A	159	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	143-A	16	MET	N-CA-C	5.54	125.95	111.00
1	48-A	36	LEU	CA-CB-CG	5.53	128.03	115.30
1	33-A	119	VAL	N-CA-C	5.53	125.93	111.00
1	160-A	44	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	43-A	88	VAL	C-N-CD	-5.52	108.45	120.60
1	146-A	16	MET	CB-CA-C	5.52	121.44	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	63-A	16	MET	CA-CB-CG	5.52	122.69	113.30
1	166-A	159	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	44-A	152	CYS	CA-CB-SG	5.52	123.93	114.00
1	79-A	12	ARG	CA-CB-CG	5.51	125.53	113.40
1	81-A	158	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	139-A	152	CYS	CA-CB-SG	-5.51	104.08	114.00
1	155-A	85	CYS	N-CA-CB	5.51	120.52	110.60
1	34-A	44	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	133-A	119	VAL	CB-CA-C	-5.51	100.94	111.40
1	109-A	16	MET	C-N-CA	-5.50	107.94	121.70
1	158-A	85	CYS	N-CA-CB	-5.50	100.69	110.60
1	51-A	12	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	65-A	33	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	4-A	44	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	29-A	20	MET	CB-CG-SD	5.50	128.90	112.40
1	162-A	130	PRO	N-CA-C	5.50	126.40	112.10
1	9-A	21	PRO	CA-N-CD	-5.50	103.80	111.50
1	151-A	85	CYS	CB-CA-C	5.50	121.39	110.40
1	42-A	4	LEU	CB-CG-CD2	5.49	120.33	111.00
1	42-A	33	ARG	CB-CA-C	5.49	121.38	110.40
1	60-A	98	ARG	CG-CD-NE	5.49	123.33	111.80
1	139-A	129	GLU	N-CA-C	5.49	125.83	111.00
1	165-A	132	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	137-A	13	VAL	CB-CA-C	-5.49	100.97	111.40
1	144-A	20	MET	CB-CG-SD	-5.49	95.94	112.40
1	8-A	33	ARG	CB-CG-CD	5.49	125.86	111.60
1	77-A	28	LEU	CA-CB-CG	-5.49	102.69	115.30
1	59-A	87	ASP	CB-CG-OD1	-5.48	113.36	118.30
1	137-A	13	VAL	N-CA-CB	5.48	123.56	111.50
1	68-A	52	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	57-A	159	ARG	CD-NE-CZ	5.48	131.27	123.60
1	68-A	33	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	140-A	1	MET	CB-CG-SD	5.48	128.83	112.40
1	71-A	22	TRP	N-CA-CB	5.48	120.46	110.60
1	27-A	20	MET	N-CA-C	5.47	125.78	111.00
1	93-A	36	LEU	CB-CG-CD1	5.47	120.30	111.00
1	114-A	16	MET	CG-SD-CE	5.47	108.96	100.20
1	111-A	44	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	120-A	16	MET	CB-CG-SD	5.46	128.78	112.40
1	85-A	101	GLU	CB-CA-C	-5.45	99.49	110.40
1	129-A	152	CYS	CA-CB-SG	5.45	123.81	114.00
1	44-A	20	MET	CG-SD-CE	5.44	108.91	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	164-A	158	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	91-A	33	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	97-A	22	TRP	N-CA-C	-5.44	96.32	111.00
1	71-A	67	GLY	N-CA-C	5.43	126.69	113.10
1	151-A	33	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	157-A	159	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	123-A	1	MET	CG-SD-CE	-5.43	91.51	100.20
1	88-A	129	GLU	C-N-CA	-5.43	99.21	122.00
1	99-A	12	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	30-A	1	MET	CA-CB-CG	5.42	122.52	113.30
1	83-A	127	ASP	CB-CG-OD2	5.42	123.18	118.30
1	99-A	1	MET	CG-SD-CE	5.42	108.87	100.20
1	161-A	12	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	163-A	128	TYR	N-CA-C	-5.42	96.37	111.00
1	71-A	154	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	17-A	1	MET	CG-SD-CE	-5.41	91.54	100.20
1	34-A	12	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	36-A	79	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	105-A	152	CYS	N-CA-CB	-5.41	100.87	110.60
1	36-A	79	ASP	CB-CG-OD1	5.40	123.16	118.30
1	54-A	1	MET	CG-SD-CE	-5.40	91.56	100.20
1	3-A	156	LEU	CA-CB-CG	5.40	127.71	115.30
1	34-A	85	CYS	N-CA-C	5.39	125.56	111.00
1	161-A	135	SER	CB-CA-C	-5.39	99.86	110.10
1	142-A	120	GLU	CB-CA-C	5.38	121.17	110.40
1	112-A	44	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	155-A	85	CYS	CB-CA-C	-5.38	99.64	110.40
1	35-A	132	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	130-A	44	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	114-A	127	ASP	N-CA-C	5.38	125.52	111.00
1	11-A	16	MET	CA-CB-CG	5.37	122.43	113.30
1	145-A	132	ASP	CB-CG-OD2	5.37	123.14	118.30
1	107-A	16	MET	C-N-CA	-5.37	108.28	121.70
1	69-A	20	MET	C-N-CA	5.37	144.54	122.00
1	8-A	128	TYR	CA-CB-CG	5.37	123.60	113.40
1	81-A	127	ASP	CB-CG-OD1	5.37	123.13	118.30
1	85-A	44	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	38-A	142	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	65-A	119	VAL	N-CA-C	-5.37	96.51	111.00
1	40-A	20	MET	CG-SD-CE	5.36	108.78	100.20
1	49-A	88	VAL	CA-CB-CG2	5.36	118.94	110.90
1	144-A	128	TYR	C-N-CA	5.36	135.10	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	116-A	12	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	147-A	20	MET	CG-SD-CE	-5.35	91.64	100.20
1	149-A	159	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	48-A	88	VAL	N-CA-C	-5.34	96.58	111.00
1	32-A	88	VAL	C-N-CD	5.34	139.61	128.40
1	8-A	142	ASP	CB-CG-OD1	5.34	123.10	118.30
1	106-A	20	MET	N-CA-C	5.34	125.41	111.00
1	122-A	12	ARG	CG-CD-NE	-5.34	100.59	111.80
1	7-A	79	ASP	CB-CA-C	5.33	121.06	110.40
1	72-A	79	ASP	CB-CG-OD1	5.33	123.10	118.30
1	163-A	79	ASP	CB-CG-OD1	5.33	123.10	118.30
1	56-A	20	MET	CG-SD-CE	5.33	108.73	100.20
1	132-A	12	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	81-A	131	ASP	N-CA-C	5.33	125.39	111.00
1	1-A	157	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	73-A	98	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	120-A	20	MET	CA-CB-CG	5.33	122.36	113.30
1	35-A	106	LYS	CD-CE-NZ	5.33	123.95	111.70
1	13-A	104	LEU	CB-CG-CD2	5.32	120.05	111.00
1	34-A	16	MET	CB-CG-SD	5.32	128.37	112.40
1	163-A	129	GLU	OE1-CD-OE2	-5.32	116.92	123.30
1	164-A	132	ASP	N-CA-C	5.32	125.36	111.00
1	155-A	1	MET	CG-SD-CE	-5.31	91.70	100.20
1	111-A	2	ILE	N-CA-C	-5.31	96.65	111.00
1	39-A	52	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	129-A	20	MET	CA-CB-CG	5.31	122.33	113.30
1	132-A	16	MET	CG-SD-CE	-5.31	91.70	100.20
1	77-A	52	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	151-A	52	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	26-A	12	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	167-A	68	THR	N-CA-C	5.30	125.31	111.00
1	154-A	127	ASP	N-CA-C	5.29	125.30	111.00
1	22-A	17	GLU	CB-CA-C	5.29	120.98	110.40
1	6-A	52	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	155-A	118	GLU	CB-CA-C	-5.29	99.82	110.40
1	43-A	87	ASP	CB-CA-C	-5.28	99.83	110.40
1	78-A	98	ARG	CG-CD-NE	5.28	122.90	111.80
1	42-A	158	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	103-A	16	MET	N-CA-C	-5.28	96.74	111.00
1	158-A	52	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	66-A	118	GLU	N-CA-C	-5.27	96.77	111.00
1	85-A	159	ARG	CG-CD-NE	-5.27	100.73	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	35-A	142	ASP	CB-CG-OD1	5.27	123.04	118.30
1	121-A	20	MET	CG-SD-CE	-5.27	91.77	100.20
1	84-A	104	LEU	CB-CG-CD1	5.27	119.95	111.00
1	57-A	79	ASP	CB-CG-OD2	5.26	123.04	118.30
1	117-A	18	ASN	N-CA-C	-5.26	96.79	111.00
1	144-A	18	ASN	CB-CA-C	-5.26	99.87	110.40
1	152-A	136	VAL	CB-CA-C	5.26	121.40	111.40
1	116-A	17	GLU	N-CA-C	-5.26	96.79	111.00
1	43-A	133	TRP	CB-CA-C	-5.26	99.88	110.40
1	58-A	79	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	101-A	54	LEU	CA-CB-CG	5.26	127.39	115.30
1	118-A	16	MET	CA-CB-CG	5.26	122.24	113.30
1	38-A	11	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	27-A	20	MET	CB-CG-SD	5.25	128.16	112.40
1	74-A	19	ALA	N-CA-C	-5.25	96.83	111.00
1	158-A	63	SER	CB-CA-C	-5.25	100.13	110.10
1	167-A	33	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	38-A	44	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	66-A	98	ARG	CG-CD-NE	5.25	122.82	111.80
1	53-A	159	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	97-A	98	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	21-A	131	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	142-A	131	ASP	N-CA-C	5.24	125.15	111.00
1	53-A	98	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	57-A	159	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	97-A	1	MET	N-CA-C	-5.23	96.87	111.00
1	25-A	87	ASP	N-CA-C	-5.23	96.88	111.00
1	92-A	44	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	79-A	131	ASP	CB-CG-OD1	5.23	123.00	118.30
1	26-A	12	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	64-A	127	ASP	CB-CG-OD2	5.22	123.00	118.30
1	43-A	1	MET	CG-SD-CE	5.22	108.55	100.20
1	53-A	128	TYR	CA-CB-CG	5.22	123.31	113.40
1	150-A	137	PHE	N-CA-C	5.22	125.09	111.00
1	7-A	129	GLU	OE1-CD-OE2	5.21	129.56	123.30
1	90-A	129	GLU	N-CA-C	5.21	125.08	111.00
1	89-A	119	VAL	N-CA-C	5.21	125.08	111.00
1	62-A	32	LYS	CD-CE-NZ	5.21	123.69	111.70
1	67-A	152	CYS	CA-CB-SG	5.21	123.38	114.00
1	7-A	79	ASP	N-CA-CB	-5.21	101.23	110.60
1	43-A	1	MET	CA-CB-CG	5.21	122.15	113.30
1	36-A	20	MET	N-CA-C	5.21	125.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	24-A	17	GLU	CB-CA-C	5.20	120.80	110.40
1	76-A	16	MET	CA-CB-CG	5.20	122.14	113.30
1	4-A	17	GLU	N-CA-C	-5.20	96.96	111.00
1	61-A	62	LEU	CA-CB-CG	5.20	127.26	115.30
1	126-A	4	LEU	CB-CG-CD2	5.20	119.84	111.00
1	60-A	98	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	104-A	52	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	36-A	69	ASP	N-CA-C	-5.19	96.98	111.00
1	127-A	33	ARG	CG-CD-NE	5.19	122.70	111.80
1	88-A	142	ASP	CB-CA-C	-5.19	100.03	110.40
1	94-A	1	MET	CA-CB-CG	5.18	122.11	113.30
1	143-A	86	GLY	N-CA-C	-5.18	100.15	113.10
1	80-A	109	LYS	CD-CE-NZ	5.18	123.61	111.70
1	123-A	128	TYR	CA-CB-CG	5.18	123.24	113.40
1	56-A	133	TRP	CB-CA-C	-5.17	100.06	110.40
1	28-A	52	ARG	CA-CB-CG	5.17	124.77	113.40
1	34-A	142	ASP	CB-CG-OD1	5.17	122.95	118.30
1	47-A	88	VAL	C-N-CD	5.17	139.25	128.40
1	38-A	127	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	101-A	8	LEU	CA-CB-CG	5.16	127.17	115.30
1	153-A	52	ARG	CG-CD-NE	5.16	122.62	111.80
1	6-A	152	CYS	CA-CB-SG	5.15	123.28	114.00
1	160-A	131	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	20-A	44	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	78-A	12	ARG	CA-CB-CG	5.15	124.73	113.40
1	11-A	156	LEU	CB-CG-CD1	5.15	119.75	111.00
1	76-A	127	ASP	N-CA-CB	-5.15	101.34	110.60
1	142-A	42	MET	CG-SD-CE	5.15	108.44	100.20
1	157-A	33	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	81-A	127	ASP	N-CA-C	5.15	124.89	111.00
1	68-A	20	MET	N-CA-C	5.14	124.89	111.00
1	100-A	44	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	30-A	131	ASP	CB-CG-OD1	5.14	122.93	118.30
1	81-A	104	LEU	CB-CG-CD2	5.14	119.74	111.00
1	49-A	120	GLU	CB-CA-C	-5.14	100.12	110.40
1	20-A	20	MET	CA-CB-CG	5.14	122.03	113.30
1	22-A	132	ASP	CB-CG-OD2	5.14	122.92	118.30
1	69-A	17	GLU	CA-CB-CG	5.14	124.70	113.40
1	151-A	85	CYS	CA-CB-SG	-5.14	104.75	114.00
1	156-A	44	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	145-A	112	LEU	CB-CG-CD2	5.13	119.73	111.00
1	28-A	19	ALA	C-N-CA	5.13	134.53	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	99-A	12	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	133-A	127	ASP	N-CA-C	5.13	124.85	111.00
1	58-A	152	CYS	CA-CB-SG	5.13	123.23	114.00
1	159-A	52	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	68-A	21	PRO	N-CA-C	5.12	125.42	112.10
1	115-A	129	GLU	N-CA-CB	5.12	119.82	110.60
1	69-A	135	SER	CB-CA-C	-5.12	100.37	110.10
1	104-A	108	GLN	CA-CB-CG	5.12	124.66	113.40
1	145-A	8	LEU	CA-CB-CG	5.12	127.08	115.30
1	153-A	159	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	42-A	1	MET	CA-CB-CG	5.12	122.00	113.30
1	83-A	2	ILE	CA-CB-CG1	-5.12	101.28	111.00
1	72-A	156	LEU	CA-CB-CG	5.11	127.06	115.30
1	20-A	20	MET	CG-SD-CE	5.11	108.38	100.20
1	1-A	131	ASP	CB-CG-OD1	5.11	122.90	118.30
1	120-A	98	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	141-A	36	LEU	CB-CG-CD2	-5.11	102.31	111.00
1	141-A	131	ASP	N-CA-C	5.11	124.79	111.00
1	73-A	8	LEU	CA-CB-CG	5.11	127.05	115.30
1	80-A	125	PHE	C-N-CD	-5.11	109.37	120.60
1	58-A	131	ASP	CB-CG-OD1	5.10	122.89	118.30
1	37-A	20	MET	N-CA-C	5.10	124.78	111.00
1	131-A	44	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	151-A	129	GLU	C-N-CA	-5.10	100.57	122.00
1	39-A	44	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	76-A	20	MET	CG-SD-CE	-5.10	92.04	100.20
1	4-A	52	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	52-A	159	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	102-A	159	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	100-A	159	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	155-A	159	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	116-A	16	MET	N-CA-C	5.09	124.74	111.00
1	83-A	11	ASP	CB-CG-OD1	5.09	122.88	118.30
1	117-A	4	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	69-A	50	ILE	CB-CA-C	-5.08	101.43	111.60
1	92-A	128	TYR	CB-CA-C	5.08	120.57	110.40
1	151-A	4	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	111-A	18	ASN	CB-CA-C	5.08	120.56	110.40
1	113-A	21	PRO	CA-N-CD	-5.08	104.39	111.50
1	137-A	128	TYR	CB-CA-C	5.08	120.55	110.40
1	100-A	104	LEU	CB-CG-CD2	5.07	119.62	111.00
1	135-A	131	ASP	CB-CG-OD1	5.07	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8-A	1	MET	CG-SD-CE	-5.06	92.10	100.20
1	24-A	127	ASP	N-CA-C	-5.06	97.34	111.00
1	27-A	19	ALA	C-N-CA	5.06	134.35	121.70
1	37-A	159	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	38-A	44	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	82-A	36	LEU	CB-CG-CD2	-5.06	102.40	111.00
1	96-A	159	ARG	CG-CD-NE	5.05	122.41	111.80
1	23-A	52	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	32-A	128	TYR	N-CA-C	5.05	124.63	111.00
1	139-A	159	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	139-A	36	LEU	CA-CB-CG	5.05	126.91	115.30
1	148-A	159	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	74-A	127	ASP	CB-CG-OD2	5.04	122.84	118.30
1	98-A	4	LEU	CB-CG-CD2	5.04	119.57	111.00
1	33-A	44	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	140-A	132	ASP	CB-CG-OD2	5.04	122.83	118.30
1	167-A	132	ASP	N-CA-C	5.04	124.59	111.00
1	98-A	98	ARG	CB-CA-C	-5.03	100.34	110.40
1	140-A	44	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	34-A	50	ILE	CG1-CB-CG2	-5.03	100.34	111.40
1	22-A	128	TYR	CA-CB-CG	5.03	122.95	113.40
1	115-A	1	MET	CB-CG-SD	-5.03	97.33	112.40
1	31-A	12	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	121-A	20	MET	N-CA-CB	-5.02	101.56	110.60
1	130-A	12	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	6-A	128	TYR	CB-CA-C	-5.02	100.35	110.40
1	110-A	98	ARG	CD-NE-CZ	5.02	130.63	123.60
1	96-A	1	MET	CA-CB-CG	5.02	121.83	113.30
1	72-A	98	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	19-A	44	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	36-A	88	VAL	C-N-CA	5.01	143.04	122.00
1	57-A	44	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	115-A	159	ARG	CG-CD-NE	-5.01	101.28	111.80
1	102-A	159	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	40-A	44	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	58-A	12	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (312) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	128	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	10-A	119	VAL	Peptide
1	10-A	17	GLU	Peptide
1	10-A	20	MET	Peptide
1	10-A	21	PRO	Peptide
1	10-A	67	GLY	Peptide
1	100-A	18	ASN	Peptide
1	102-A	17	GLU	Peptide
1	104-A	128	TYR	Peptide
1	104-A	16	MET	Peptide
1	105-A	128	TYR	Peptide
1	105-A	129	GLU	Peptide
1	105-A	17	GLU	Peptide
1	105-A	18	ASN	Peptide
1	107-A	17	GLU	Peptide
1	107-A	19	ALA	Peptide
1	107-A	22	TRP	Peptide
1	108-A	1	MET	Peptide
1	108-A	18	ASN	Peptide
1	109-A	17	GLU	Peptide
1	109-A	67	GLY	Peptide
1	11-A	119	VAL	Peptide
1	11-A	16	MET	Peptide
1	110-A	17	GLU	Peptide
1	110-A	67	GLY	Peptide
1	111-A	17	GLU	Peptide
1	111-A	20	MET	Peptide
1	112-A	1	MET	Peptide
1	112-A	20	MET	Peptide
1	113-A	1	MET	Peptide
1	113-A	17	GLU	Peptide
1	113-A	19	ALA	Peptide
1	113-A	20	MET	Peptide
1	113-A	22	TRP	Peptide
1	114-A	128	TYR	Peptide
1	114-A	17	GLU	Peptide
1	114-A	19	ALA	Peptide
1	114-A	20	MET	Peptide
1	115-A	17	GLU	Peptide
1	115-A	19	ALA	Peptide
1	115-A	20	MET	Peptide
1	116-A	121	GLY	Peptide
1	116-A	19	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	116-A	22	TRP	Peptide
1	117-A	17	GLU	Peptide
1	117-A	18	ASN	Mainchain,Peptide
1	117-A	21	PRO	Peptide
1	12-A	119	VAL	Peptide
1	12-A	16	MET	Peptide
1	12-A	21	PRO	Peptide
1	122-A	127	ASP	Peptide
1	122-A	129	GLU	Peptide
1	122-A	130	PRO	Peptide
1	124-A	128	TYR	Peptide
1	126-A	22	TRP	Peptide
1	127-A	120	GLU	Peptide
1	13-A	16	MET	Peptide
1	13-A	17	GLU	Peptide
1	13-A	21	PRO	Peptide
1	130-A	67	GLY	Peptide
1	131-A	118	GLU	Peptide
1	131-A	128	TYR	Peptide
1	132-A	118	GLU	Peptide
1	132-A	119	VAL	Peptide
1	132-A	52	ARG	Peptide
1	133-A	118	GLU	Peptide
1	133-A	51	GLY	Peptide
1	133-A	52	ARG	Peptide
1	134-A	52	ARG	Peptide
1	136-A	18	ASN	Peptide
1	136-A	51	GLY	Peptide
1	137-A	129	GLU	Peptide
1	137-A	18	ASN	Peptide
1	138-A	10	VAL	Peptide
1	138-A	129	GLU	Peptide
1	138-A	20	MET	Peptide
1	139-A	18	ASN	Peptide
1	14-A	17	GLU	Peptide
1	14-A	19	ALA	Peptide
1	14-A	21	PRO	Peptide
1	140-A	131	ASP	Peptide
1	140-A	18	ASN	Peptide
1	141-A	18	ASN	Peptide
1	143-A	129	GLU	Peptide
1	143-A	18	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	144-A	129	GLU	Peptide
1	144-A	18	ASN	Peptide
1	145-A	128	TYR	Peptide
1	145-A	129	GLU	Peptide
1	145-A	130	PRO	Peptide
1	145-A	18	ASN	Peptide
1	146-A	128	TYR	Peptide
1	146-A	130	PRO	Peptide
1	146-A	20	MET	Peptide
1	146-A	21	PRO	Peptide
1	147-A	129	GLU	Peptide
1	149-A	20	MET	Peptide
1	149-A	85	CYS	Peptide
1	15-A	128	TYR	Peptide
1	150-A	129	GLU	Peptide
1	150-A	83	ALA	Peptide
1	151-A	129	GLU	Peptide
1	151-A	130	PRO	Peptide
1	152-A	129	GLU	Peptide
1	152-A	130	PRO	Peptide
1	154-A	129	GLU	Peptide
1	155-A	129	GLU	Peptide
1	155-A	130	PRO	Peptide
1	156-A	129	GLU	Peptide
1	157-A	128	TYR	Peptide
1	157-A	65	GLN	Peptide
1	157-A	85	CYS	Peptide
1	158-A	130	PRO	Peptide
1	158-A	67	GLY	Peptide
1	159-A	1	MET	Peptide
1	159-A	129	GLU	Peptide
1	159-A	131	ASP	Peptide
1	159-A	63	SER	Peptide
1	159-A	86	GLY	Peptide
1	16-A	128	TYR	Peptide
1	16-A	16	MET	Peptide
1	16-A	18	ASN	Peptide
1	160-A	129	GLU	Peptide
1	160-A	131	ASP	Peptide
1	160-A	86	GLY	Peptide
1	161-A	128	TYR	Peptide
1	161-A	129	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	161-A	130	PRO	Peptide
1	162-A	127	ASP	Peptide
1	162-A	128	TYR	Peptide
1	162-A	130	PRO	Peptide
1	162-A	51	GLY	Peptide
1	162-A	67	GLY	Peptide
1	163-A	127	ASP	Peptide
1	163-A	128	TYR	Peptide
1	163-A	130	PRO	Peptide
1	163-A	131	ASP	Peptide
1	163-A	67	GLY	Peptide
1	164-A	126	PRO	Peptide
1	164-A	127	ASP	Peptide
1	164-A	128	TYR	Peptide
1	164-A	130	PRO	Peptide
1	164-A	67	GLY	Peptide
1	165-A	129	GLU	Peptide
1	166-A	128	TYR	Peptide
1	166-A	129	GLU	Peptide
1	167-A	128	TYR	Peptide
1	17-A	16	MET	Peptide
1	17-A	17	GLU	Peptide
1	17-A	18	ASN	Peptide
1	17-A	20	MET	Peptide
1	18-A	16	MET	Peptide
1	18-A	17	GLU	Peptide
1	19-A	17	GLU	Peptide
1	19-A	21	PRO	Peptide
1	2-A	20	MET	Peptide
1	20-A	16	MET	Peptide
1	20-A	87	ASP	Peptide
1	21-A	17	GLU	Peptide
1	21-A	87	ASP	Peptide
1	22-A	87	ASP	Peptide
1	23-A	17	GLU	Peptide
1	23-A	18	ASN	Peptide
1	23-A	87	ASP	Peptide
1	24-A	128	TYR	Peptide
1	24-A	18	ASN	Peptide
1	25-A	1	MET	Peptide
1	25-A	18	ASN	Peptide
1	25-A	86	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	26-A	1	MET	Peptide
1	26-A	18	ASN	Peptide
1	26-A	86	GLY	Peptide
1	27-A	86	GLY	Peptide
1	28-A	129	GLU	Peptide
1	28-A	20	MET	Peptide
1	28-A	86	GLY	Peptide
1	29-A	16	MET	Peptide
1	3-A	129	GLU	Peptide
1	30-A	86	GLY	Peptide
1	31-A	86	GLY	Peptide
1	31-A	89	PRO	Peptide
1	32-A	16	MET	Peptide
1	32-A	18	ASN	Peptide
1	32-A	87	ASP	Peptide
1	32-A	89	PRO	Peptide
1	33-A	118	GLU	Peptide
1	33-A	127	ASP	Peptide
1	33-A	141	HIS	Peptide
1	33-A	18	ASN	Peptide
1	33-A	22	TRP	Peptide
1	33-A	88	VAL	Peptide
1	34-A	128	TYR	Peptide
1	34-A	86	GLY	Peptide
1	34-A	88	VAL	Peptide
1	35-A	19	ALA	Peptide
1	35-A	88	VAL	Peptide
1	36-A	23	ASN	Peptide
1	36-A	67	GLY	Peptide
1	36-A	87	ASP	Peptide
1	36-A	88	VAL	Peptide
1	37-A	141	HIS	Peptide
1	37-A	87	ASP	Peptide
1	38-A	19	ALA	Peptide
1	38-A	87	ASP	Peptide
1	39-A	87	ASP	Peptide
1	4-A	127	ASP	Peptide
1	4-A	129	GLU	Peptide
1	4-A	86	GLY	Peptide
1	40-A	18	ASN	Peptide
1	40-A	87	ASP	Peptide
1	41-A	121	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	41-A	16	MET	Peptide
1	41-A	86	GLY	Peptide
1	41-A	88	VAL	Peptide
1	42-A	16	MET	Peptide
1	42-A	86	GLY	Peptide
1	43-A	16	MET	Peptide
1	44-A	16	MET	Peptide
1	44-A	87	ASP	Peptide
1	45-A	17	GLU	Peptide
1	45-A	87	ASP	Peptide
1	46-A	121	GLY	Peptide
1	46-A	86	GLY	Peptide
1	46-A	87	ASP	Peptide
1	47-A	88	VAL	Peptide
1	48-A	86	GLY	Peptide
1	48-A	88	VAL	Peptide
1	49-A	119	VAL	Peptide
1	49-A	86	GLY	Peptide
1	49-A	87	ASP	Peptide
1	49-A	88	VAL	Peptide
1	5-A	129	GLU	Peptide
1	5-A	17	GLU	Peptide
1	5-A	18	ASN	Peptide
1	50-A	119	VAL	Peptide
1	50-A	84	ALA	Peptide
1	50-A	86	GLY	Peptide
1	50-A	87	ASP	Peptide
1	51-A	120	GLU	Peptide
1	51-A	85	CYS	Peptide
1	51-A	87	ASP	Peptide
1	52-A	120	GLU	Peptide
1	52-A	84	ALA	Peptide
1	52-A	85	CYS	Peptide
1	52-A	87	ASP	Peptide
1	53-A	120	GLU	Peptide
1	53-A	85	CYS	Peptide
1	53-A	86	GLY	Peptide
1	53-A	87	ASP	Peptide
1	57-A	20	MET	Peptide
1	6-A	16	MET	Peptide
1	6-A	17	GLU	Peptide
1	61-A	129	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	62-A	126	PRO	Peptide
1	63-A	20	MET	Peptide
1	66-A	128	TYR	Peptide
1	66-A	20	MET	Peptide
1	66-A	87	ASP	Peptide
1	67-A	87	ASP	Peptide
1	68-A	20	MET	Peptide
1	68-A	21	PRO	Peptide
1	69-A	20	MET	Peptide
1	7-A	127	ASP	Peptide
1	7-A	16	MET	Peptide
1	7-A	18	ASN	Peptide
1	7-A	19	ALA	Peptide
1	7-A	20	MET	Peptide
1	70-A	20	MET	Peptide
1	71-A	20	MET	Peptide
1	71-A	21	PRO	Peptide
1	72-A	17	GLU	Peptide
1	72-A	18	ASN	Peptide
1	72-A	21	PRO	Peptide
1	72-A	65	GLN	Peptide
1	73-A	19	ALA	Peptide
1	73-A	65	GLN	Peptide
1	74-A	65	GLN	Peptide
1	75-A	128	TYR	Peptide
1	78-A	127	ASP	Peptide
1	79-A	126	PRO	Peptide
1	79-A	127	ASP	Peptide
1	8-A	119	VAL	Peptide
1	8-A	127	ASP	Peptide
1	8-A	16	MET	Peptide
1	8-A	20	MET	Peptide
1	80-A	126	PRO	Peptide
1	80-A	127	ASP	Peptide
1	81-A	127	ASP	Peptide
1	81-A	129	GLU	Peptide
1	82-A	129	GLU	Peptide
1	83-A	129	GLU	Peptide
1	84-A	130	PRO	Peptide
1	85-A	130	PRO	Peptide
1	86-A	127	ASP	Peptide
1	86-A	130	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	88-A	129	GLU	Peptide
1	89-A	1	MET	Peptide
1	89-A	129	GLU	Peptide
1	9-A	119	VAL	Peptide
1	9-A	15	GLY	Peptide
1	9-A	18	ASN	Peptide
1	9-A	19	ALA	Peptide
1	9-A	67	GLY	Peptide
1	90-A	128	TYR	Peptide
1	90-A	129	GLU	Peptide
1	91-A	129	GLU	Peptide
1	94-A	18	ASN	Peptide
1	95-A	18	ASN	Peptide
1	97-A	18	ASN	Peptide
1	98-A	18	ASN	Peptide
1	99-A	18	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1268	1223	1223	0	0
1	2-A	1268	1223	1223	0	0
1	3-A	1268	1223	1223	0	0
1	4-A	1268	1223	1223	0	0
1	5-A	1268	1223	1223	0	0
1	6-A	1268	1223	1223	0	0
1	7-A	1268	1223	1223	0	0
1	8-A	1268	1223	1223	0	0
1	9-A	1268	1223	1223	0	0
1	10-A	1268	1223	1223	0	0
1	11-A	1268	1223	1223	0	0
1	12-A	1268	1223	1222	0	0
1	13-A	1268	1223	1223	0	0
1	14-A	1268	1223	1223	0	0
1	15-A	1268	1223	1223	0	0
1	16-A	1268	1223	1223	0	0
1	17-A	1268	1223	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	18-A	1268	1223	1223	0	0
1	19-A	1268	1223	1223	0	0
1	20-A	1268	1223	1223	0	0
1	21-A	1268	1223	1223	0	0
1	22-A	1268	1223	1223	0	0
1	23-A	1268	1223	1223	0	0
1	24-A	1268	1223	1223	0	0
1	25-A	1268	1223	1223	0	0
1	26-A	1268	1223	1223	0	0
1	27-A	1268	1223	1222	0	0
1	28-A	1268	1223	1223	0	0
1	29-A	1268	1223	1223	0	0
1	30-A	1268	1223	1222	0	0
1	31-A	1268	1223	1223	0	0
1	32-A	1268	1223	1223	0	0
1	33-A	1268	1223	1223	0	0
1	34-A	1268	1223	1223	0	0
1	35-A	1268	1223	1223	0	0
1	36-A	1268	1223	1223	0	0
1	37-A	1268	1223	1223	0	0
1	38-A	1268	1223	1223	0	0
1	39-A	1268	1223	1223	0	0
1	40-A	1268	1223	1223	0	0
1	41-A	1268	1223	1223	0	0
1	42-A	1268	1223	1223	0	0
1	43-A	1268	1223	1223	0	0
1	44-A	1268	1223	1223	0	0
1	45-A	1268	1223	1223	0	0
1	46-A	1268	1223	1223	0	0
1	47-A	1268	1223	1223	0	0
1	48-A	1268	1223	1223	0	0
1	49-A	1268	1223	1223	0	0
1	50-A	1268	1223	1223	0	0
1	51-A	1268	1223	1223	0	0
1	52-A	1268	1223	1223	0	0
1	53-A	1268	1223	1223	0	0
1	54-A	1268	1223	1223	0	0
1	55-A	1268	1223	1222	0	0
1	56-A	1268	1223	1223	0	0
1	57-A	1268	1223	1222	0	0
1	58-A	1268	1223	1223	0	0
1	59-A	1268	1223	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	60-A	1268	1223	1223	0	0
1	61-A	1268	1223	1223	0	0
1	62-A	1268	1223	1223	0	0
1	63-A	1268	1223	1223	0	0
1	64-A	1268	1223	1223	0	0
1	65-A	1268	1223	1223	0	0
1	66-A	1268	1223	1223	0	0
1	67-A	1268	1223	1223	0	0
1	68-A	1268	1223	1223	0	0
1	69-A	1268	1223	1223	0	0
1	70-A	1268	1223	1223	0	0
1	71-A	1268	1223	1223	0	0
1	72-A	1268	1223	1223	0	0
1	73-A	1268	1223	1223	0	0
1	74-A	1268	1223	1223	0	0
1	75-A	1268	1223	1223	0	0
1	76-A	1268	1223	1222	0	0
1	77-A	1268	1223	1223	0	0
1	78-A	1268	1223	1223	0	0
1	79-A	1268	1223	1222	0	0
1	80-A	1268	1223	1223	0	0
1	81-A	1268	1223	1223	0	0
1	82-A	1268	1223	1223	0	0
1	83-A	1268	1223	1223	0	0
1	84-A	1268	1223	1223	0	0
1	85-A	1268	1223	1223	0	0
1	86-A	1268	1223	1222	0	0
1	87-A	1268	1223	1223	0	0
1	88-A	1268	1223	1223	0	0
1	89-A	1268	1223	1222	0	0
1	90-A	1268	1223	1223	0	0
1	91-A	1268	1223	1223	0	0
1	92-A	1268	1223	1223	0	0
1	93-A	1268	1223	1223	0	0
1	94-A	1268	1223	1223	0	0
1	95-A	1268	1223	1223	0	0
1	96-A	1268	1223	1223	0	0
1	97-A	1268	1223	1223	0	0
1	98-A	1268	1223	1223	0	0
1	99-A	1268	1223	1223	0	0
1	100-A	1268	1223	1223	0	0
1	101-A	1268	1223	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	102-A	1268	1223	1223	0	0
1	103-A	1268	1223	1223	0	0
1	104-A	1268	1223	1223	0	0
1	105-A	1268	1223	1223	0	0
1	106-A	1268	1223	1223	0	0
1	107-A	1268	1223	1223	0	0
1	108-A	1268	1223	1223	0	0
1	109-A	1268	1223	1223	0	0
1	110-A	1268	1223	1223	0	0
1	111-A	1268	1223	1223	0	0
1	112-A	1268	1223	1223	0	0
1	113-A	1268	1223	1223	0	0
1	114-A	1268	1223	1223	0	0
1	115-A	1268	1223	1223	0	0
1	116-A	1268	1223	1223	0	0
1	117-A	1268	1223	1223	0	0
1	118-A	1268	1223	1223	0	0
1	119-A	1268	1223	1222	0	0
1	120-A	1268	1223	1222	0	0
1	121-A	1268	1223	1223	0	0
1	122-A	1268	1223	1223	0	0
1	123-A	1268	1223	1223	0	0
1	124-A	1268	1223	1223	0	0
1	125-A	1268	1223	1223	0	0
1	126-A	1268	1223	1223	0	0
1	127-A	1268	1223	1223	0	0
1	128-A	1268	1223	1223	0	0
1	129-A	1268	1223	1223	0	0
1	130-A	1268	1223	1223	0	0
1	131-A	1268	1223	1223	0	0
1	132-A	1268	1223	1223	0	0
1	133-A	1268	1223	1223	0	0
1	134-A	1268	1223	1223	0	0
1	135-A	1268	1223	1223	0	0
1	136-A	1268	1223	1223	0	0
1	137-A	1268	1223	1223	0	0
1	138-A	1268	1223	1223	0	0
1	139-A	1268	1223	1223	0	0
1	140-A	1268	1223	1223	0	0
1	141-A	1268	1223	1222	0	0
1	142-A	1268	1223	1223	0	0
1	143-A	1268	1223	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	144-A	1268	1223	1223	0	0
1	145-A	1268	1223	1223	0	0
1	146-A	1268	1223	1223	0	0
1	147-A	1268	1223	1222	0	0
1	148-A	1268	1223	1223	0	0
1	149-A	1268	1223	1222	0	0
1	150-A	1268	1223	1223	0	0
1	151-A	1268	1223	1223	0	0
1	152-A	1268	1223	1223	0	0
1	153-A	1268	1223	1222	0	0
1	154-A	1268	1223	1222	0	0
1	155-A	1268	1223	1223	0	0
1	156-A	1268	1223	1223	0	0
1	157-A	1268	1223	1223	0	0
1	158-A	1268	1223	1223	0	0
1	159-A	1268	1223	1223	0	0
1	160-A	1268	1223	1223	0	0
1	161-A	1268	1223	1222	0	0
1	162-A	1268	1223	1222	0	0
1	163-A	1268	1223	1223	0	0
1	164-A	1268	1223	1223	0	0
1	165-A	1268	1223	1223	0	0
1	166-A	1268	1223	1223	0	0
1	167-A	1268	1223	1223	0	0
2	1-A	32	17	17	0	0
2	2-A	32	17	17	0	0
2	3-A	32	17	17	0	0
2	4-A	32	17	17	0	0
2	5-A	32	17	17	0	0
2	6-A	32	17	17	0	0
2	7-A	32	17	17	0	0
2	8-A	32	17	17	0	0
2	9-A	32	17	17	0	0
2	10-A	32	17	17	0	0
2	11-A	32	17	17	0	0
2	12-A	32	17	17	0	0
2	13-A	32	17	17	0	0
2	14-A	32	17	17	0	0
2	15-A	32	17	17	0	0
2	16-A	32	17	17	0	0
2	17-A	32	17	17	0	0
2	18-A	32	17	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	19-A	32	17	17	0	0
2	20-A	32	17	17	0	0
2	21-A	32	17	17	0	0
2	22-A	32	17	17	0	0
2	23-A	32	17	17	0	0
2	24-A	32	17	17	0	0
2	25-A	32	17	17	0	0
2	26-A	32	17	17	0	0
2	27-A	32	17	17	0	0
2	28-A	32	17	17	0	0
2	29-A	32	17	17	0	0
2	30-A	32	17	17	0	0
2	31-A	32	17	17	0	0
2	32-A	32	17	17	0	0
2	33-A	32	17	17	0	0
2	34-A	32	17	17	0	0
2	35-A	32	17	17	0	0
2	36-A	32	17	17	0	0
2	37-A	32	17	17	0	0
2	38-A	32	17	17	0	0
2	39-A	32	17	17	0	0
2	40-A	32	17	17	0	0
2	41-A	32	17	17	0	0
2	42-A	32	17	17	0	0
2	43-A	32	17	17	0	0
2	44-A	32	17	17	0	0
2	45-A	32	17	17	0	0
2	46-A	32	17	17	0	0
2	47-A	32	17	17	0	0
2	48-A	32	17	17	0	0
2	49-A	32	17	17	0	0
2	50-A	32	17	17	0	0
2	51-A	32	17	17	0	0
2	52-A	32	17	17	0	0
2	53-A	32	17	17	0	0
2	54-A	32	17	17	0	0
2	55-A	32	17	17	0	0
2	56-A	32	17	17	0	0
2	57-A	32	17	17	0	0
2	58-A	32	17	17	0	0
2	59-A	32	17	17	0	0
2	60-A	32	17	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	61-A	32	17	17	0	0
2	62-A	32	17	17	0	0
2	63-A	32	17	17	0	0
2	64-A	32	17	17	0	0
2	65-A	32	17	17	0	0
2	66-A	32	17	17	0	0
2	67-A	32	17	17	0	0
2	68-A	32	17	17	0	0
2	69-A	32	17	17	0	0
2	70-A	32	17	17	0	0
2	71-A	32	17	17	0	0
2	72-A	32	17	17	0	0
2	73-A	32	17	17	0	0
2	74-A	32	17	17	0	0
2	75-A	32	17	17	0	0
2	76-A	32	17	17	0	0
2	77-A	32	17	17	0	0
2	78-A	32	17	17	0	0
2	79-A	32	17	17	0	0
2	80-A	32	17	17	0	0
2	81-A	32	17	17	0	0
2	82-A	32	17	17	0	0
2	83-A	32	17	17	0	0
2	84-A	32	17	17	0	0
2	85-A	32	17	17	0	0
2	86-A	32	17	17	0	0
2	87-A	32	17	17	0	0
2	88-A	32	17	17	0	0
2	89-A	32	17	17	0	0
2	90-A	32	17	17	0	0
2	91-A	32	17	17	0	0
2	92-A	32	17	17	0	0
2	93-A	32	17	17	0	0
2	94-A	32	17	17	0	0
2	95-A	32	17	17	0	0
2	96-A	32	17	17	0	0
2	97-A	32	17	17	0	0
2	98-A	32	17	17	0	0
2	99-A	32	17	17	0	0
2	100-A	32	17	17	0	0
2	101-A	32	17	17	0	0
2	102-A	32	17	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	103-A	32	17	17	0	0
2	104-A	32	17	17	0	0
2	105-A	32	17	17	0	0
2	106-A	32	17	17	0	0
2	107-A	32	17	17	0	0
2	108-A	32	17	17	0	0
2	109-A	32	17	17	0	0
2	110-A	32	17	17	0	0
2	111-A	32	17	17	0	0
2	112-A	32	17	17	0	0
2	113-A	32	17	17	0	0
2	114-A	32	17	17	0	0
2	115-A	32	17	17	0	0
2	116-A	32	17	17	0	0
2	117-A	32	17	17	0	0
2	118-A	32	17	17	0	0
2	119-A	32	17	17	0	0
2	120-A	32	17	17	0	0
2	121-A	32	17	17	0	0
2	122-A	32	17	17	0	0
2	123-A	32	17	17	0	0
2	124-A	32	17	17	0	0
2	125-A	32	17	17	0	0
2	126-A	32	17	17	0	0
2	127-A	32	17	17	0	0
2	128-A	32	17	17	0	0
2	129-A	32	17	17	0	0
2	130-A	32	17	17	0	0
2	131-A	32	17	17	0	0
2	132-A	32	17	17	0	0
2	133-A	32	17	17	0	0
2	134-A	32	17	17	0	0
2	135-A	32	17	17	0	0
2	136-A	32	17	17	0	0
2	137-A	32	17	17	0	0
2	138-A	32	17	17	0	0
2	139-A	32	17	17	0	0
2	140-A	32	17	17	0	0
2	141-A	32	17	17	0	0
2	142-A	32	17	17	0	0
2	143-A	32	17	17	0	0
2	144-A	32	17	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	145-A	32	17	17	0	0
2	146-A	32	17	17	0	0
2	147-A	32	17	17	0	0
2	148-A	32	17	17	0	0
2	149-A	32	17	17	0	0
2	150-A	32	17	17	0	0
2	151-A	32	17	17	0	0
2	152-A	32	17	17	0	0
2	153-A	32	17	17	0	0
2	154-A	32	17	17	0	0
2	155-A	32	17	17	0	0
2	156-A	32	17	17	0	0
2	157-A	32	17	17	0	0
2	158-A	32	17	17	0	0
2	159-A	32	17	17	0	0
2	160-A	32	17	17	0	0
2	161-A	32	17	17	0	0
2	162-A	32	17	17	0	0
2	163-A	32	17	17	0	0
2	164-A	32	17	17	0	0
2	165-A	32	17	17	0	0
2	166-A	32	17	17	0	0
2	167-A	32	17	17	0	0
3	1-A	2	0	0	0	0
3	2-A	2	0	0	0	0
3	3-A	2	0	0	0	0
3	4-A	2	0	0	0	0
3	5-A	2	0	0	0	0
3	6-A	2	0	0	0	0
3	7-A	2	0	0	0	0
3	8-A	2	0	0	0	0
3	9-A	2	0	0	0	0
3	10-A	2	0	0	0	0
3	11-A	2	0	0	0	0
3	12-A	2	0	0	0	0
3	13-A	2	0	0	0	0
3	14-A	2	0	0	0	0
3	15-A	2	0	0	0	0
3	16-A	2	0	0	0	0
3	17-A	2	0	0	0	0
3	18-A	2	0	0	0	0
3	19-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	20-A	2	0	0	0	0
3	21-A	2	0	0	0	0
3	22-A	2	0	0	0	0
3	23-A	2	0	0	0	0
3	24-A	2	0	0	0	0
3	25-A	2	0	0	0	0
3	26-A	2	0	0	0	0
3	27-A	2	0	0	0	0
3	28-A	2	0	0	0	0
3	29-A	2	0	0	0	0
3	30-A	2	0	0	0	0
3	31-A	2	0	0	0	0
3	32-A	2	0	0	0	0
3	33-A	2	0	0	0	0
3	34-A	2	0	0	0	0
3	35-A	2	0	0	0	0
3	36-A	2	0	0	0	0
3	37-A	2	0	0	0	0
3	38-A	2	0	0	0	0
3	39-A	2	0	0	0	0
3	40-A	2	0	0	0	0
3	41-A	2	0	0	0	0
3	42-A	2	0	0	0	0
3	43-A	2	0	0	0	0
3	44-A	2	0	0	0	0
3	45-A	2	0	0	0	0
3	46-A	2	0	0	0	0
3	47-A	2	0	0	0	0
3	48-A	2	0	0	0	0
3	49-A	2	0	0	0	0
3	50-A	2	0	0	0	0
3	51-A	2	0	0	0	0
3	52-A	2	0	0	0	0
3	53-A	2	0	0	0	0
3	54-A	2	0	0	0	0
3	55-A	2	0	0	0	0
3	56-A	2	0	0	0	0
3	57-A	2	0	0	0	0
3	58-A	2	0	0	0	0
3	59-A	2	0	0	0	0
3	60-A	2	0	0	0	0
3	61-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	62-A	2	0	0	0	0
3	63-A	2	0	0	0	0
3	64-A	2	0	0	0	0
3	65-A	2	0	0	0	0
3	66-A	2	0	0	0	0
3	67-A	2	0	0	0	0
3	68-A	2	0	0	0	0
3	69-A	2	0	0	0	0
3	70-A	2	0	0	0	0
3	71-A	2	0	0	0	0
3	72-A	2	0	0	0	0
3	73-A	2	0	0	0	0
3	74-A	2	0	0	0	0
3	75-A	2	0	0	0	0
3	76-A	2	0	0	0	0
3	77-A	2	0	0	0	0
3	78-A	2	0	0	0	0
3	79-A	2	0	0	0	0
3	80-A	2	0	0	0	0
3	81-A	2	0	0	0	0
3	82-A	2	0	0	0	0
3	83-A	2	0	0	0	0
3	84-A	2	0	0	0	0
3	85-A	2	0	0	0	0
3	86-A	2	0	0	0	0
3	87-A	2	0	0	0	0
3	88-A	2	0	0	0	0
3	89-A	2	0	0	0	0
3	90-A	2	0	0	0	0
3	91-A	2	0	0	0	0
3	92-A	2	0	0	0	0
3	93-A	2	0	0	0	0
3	94-A	2	0	0	0	0
3	95-A	2	0	0	0	0
3	96-A	2	0	0	0	0
3	97-A	2	0	0	0	0
3	98-A	2	0	0	0	0
3	99-A	2	0	0	0	0
3	100-A	2	0	0	0	0
3	101-A	2	0	0	0	0
3	102-A	2	0	0	0	0
3	103-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	104-A	2	0	0	0	0
3	105-A	2	0	0	0	0
3	106-A	2	0	0	0	0
3	107-A	2	0	0	0	0
3	108-A	2	0	0	0	0
3	109-A	2	0	0	0	0
3	110-A	2	0	0	0	0
3	111-A	2	0	0	0	0
3	112-A	2	0	0	0	0
3	113-A	2	0	0	0	0
3	114-A	2	0	0	0	0
3	115-A	2	0	0	0	0
3	116-A	2	0	0	0	0
3	117-A	2	0	0	0	0
3	118-A	2	0	0	0	0
3	119-A	2	0	0	0	0
3	120-A	2	0	0	0	0
3	121-A	2	0	0	0	0
3	122-A	2	0	0	0	0
3	123-A	2	0	0	0	0
3	124-A	2	0	0	0	0
3	125-A	2	0	0	0	0
3	126-A	2	0	0	0	0
3	127-A	2	0	0	0	0
3	128-A	2	0	0	0	0
3	129-A	2	0	0	0	0
3	130-A	2	0	0	0	0
3	131-A	2	0	0	0	0
3	132-A	2	0	0	0	0
3	133-A	2	0	0	0	0
3	134-A	2	0	0	0	0
3	135-A	2	0	0	0	0
3	136-A	2	0	0	0	0
3	137-A	2	0	0	0	0
3	138-A	2	0	0	0	0
3	139-A	2	0	0	0	0
3	140-A	2	0	0	0	0
3	141-A	2	0	0	0	0
3	142-A	2	0	0	0	0
3	143-A	2	0	0	0	0
3	144-A	2	0	0	0	0
3	145-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	146-A	2	0	0	0	0
3	147-A	2	0	0	0	0
3	148-A	2	0	0	0	0
3	149-A	2	0	0	0	0
3	150-A	2	0	0	0	0
3	151-A	2	0	0	0	0
3	152-A	2	0	0	0	0
3	153-A	2	0	0	0	0
3	154-A	2	0	0	0	0
3	155-A	2	0	0	0	0
3	156-A	2	0	0	0	0
3	157-A	2	0	0	0	0
3	158-A	2	0	0	0	0
3	159-A	2	0	0	0	0
3	160-A	2	0	0	0	0
3	161-A	2	0	0	0	0
3	162-A	2	0	0	0	0
3	163-A	2	0	0	0	0
3	164-A	2	0	0	0	0
3	165-A	2	0	0	0	0
3	166-A	2	0	0	0	0
3	167-A	2	0	0	0	0
4	1-A	48	24	24	0	0
4	2-A	48	24	24	0	0
4	3-A	48	24	24	0	0
4	4-A	48	24	24	0	0
4	5-A	48	24	24	0	0
4	6-A	48	24	24	0	0
4	7-A	48	24	24	0	0
4	8-A	48	24	24	0	0
4	9-A	48	24	24	0	0
4	10-A	48	24	24	0	0
4	11-A	48	24	24	0	0
4	12-A	48	24	24	0	0
4	13-A	48	24	24	0	0
4	14-A	48	24	24	0	0
4	15-A	48	24	24	0	0
4	16-A	48	24	24	0	0
4	17-A	48	24	24	0	0
4	18-A	48	24	24	0	0
4	19-A	48	24	24	0	0
4	20-A	48	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	21-A	48	24	24	0	0
4	22-A	48	24	24	0	0
4	23-A	48	24	24	0	0
4	24-A	48	24	24	0	0
4	25-A	48	24	24	0	0
4	26-A	48	24	24	0	0
4	27-A	48	24	24	0	0
4	28-A	48	24	24	0	0
4	29-A	48	24	24	0	0
4	30-A	48	24	24	0	0
4	31-A	48	24	24	0	0
4	32-A	48	24	24	0	0
4	33-A	48	24	24	0	0
4	34-A	48	24	24	0	0
4	35-A	48	24	24	0	0
4	36-A	48	24	24	0	0
4	37-A	48	24	24	0	0
4	38-A	48	24	24	0	0
4	39-A	48	24	24	0	0
4	40-A	48	24	24	0	0
4	41-A	48	24	24	0	0
4	42-A	48	24	24	0	0
4	43-A	48	24	24	0	0
4	44-A	48	24	24	0	0
4	45-A	48	24	24	0	0
4	46-A	48	24	24	0	0
4	47-A	48	24	24	0	0
4	48-A	48	24	24	0	0
4	49-A	48	24	24	0	0
4	50-A	48	24	24	0	0
4	51-A	48	24	24	0	0
4	52-A	48	24	24	0	0
4	53-A	48	24	24	0	0
4	54-A	48	24	24	0	0
4	55-A	48	24	24	0	0
4	56-A	48	24	24	0	0
4	57-A	48	24	24	0	0
4	58-A	48	24	24	0	0
4	59-A	48	24	24	0	0
4	60-A	48	24	24	0	0
4	61-A	48	24	24	0	0
4	62-A	48	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	63-A	48	24	24	0	0
4	64-A	48	24	24	0	0
4	65-A	48	24	24	0	0
4	66-A	48	24	24	0	0
4	67-A	48	24	24	0	0
4	68-A	48	24	24	0	0
4	69-A	48	24	24	0	0
4	70-A	48	24	24	0	0
4	71-A	48	24	24	0	0
4	72-A	48	24	24	0	0
4	73-A	48	24	24	0	0
4	74-A	48	24	24	0	0
4	75-A	48	24	24	0	0
4	76-A	48	24	24	0	0
4	77-A	48	24	24	0	0
4	78-A	48	24	24	0	0
4	79-A	48	24	24	0	0
4	80-A	48	24	24	0	0
4	81-A	48	24	24	0	0
4	82-A	48	24	24	0	0
4	83-A	48	24	24	0	0
4	84-A	48	24	24	0	0
4	85-A	48	24	24	0	0
4	86-A	48	24	24	0	0
4	87-A	48	24	24	0	0
4	88-A	48	24	24	0	0
4	89-A	48	24	24	0	0
4	90-A	48	24	24	0	0
4	91-A	48	24	24	0	0
4	92-A	48	24	24	0	0
4	93-A	48	24	24	0	0
4	94-A	48	24	24	0	0
4	95-A	48	24	24	0	0
4	96-A	48	24	24	0	0
4	97-A	48	24	24	0	0
4	98-A	48	24	24	0	0
4	99-A	48	24	24	0	0
4	100-A	48	24	24	0	0
4	101-A	48	24	24	0	0
4	102-A	48	24	24	0	0
4	103-A	48	24	24	0	0
4	104-A	48	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	105-A	48	24	24	0	0
4	106-A	48	24	24	0	0
4	107-A	48	24	24	0	0
4	108-A	48	24	24	0	0
4	109-A	48	24	24	0	0
4	110-A	48	24	24	0	0
4	111-A	48	24	24	0	0
4	112-A	48	24	24	0	0
4	113-A	48	24	24	0	0
4	114-A	48	24	24	0	0
4	115-A	48	24	24	0	0
4	116-A	48	24	24	0	0
4	117-A	48	24	24	0	0
4	118-A	48	24	24	0	0
4	119-A	48	24	24	0	0
4	120-A	48	24	24	0	0
4	121-A	48	24	24	0	0
4	122-A	48	24	24	0	0
4	123-A	48	24	24	0	0
4	124-A	48	24	24	0	0
4	125-A	48	24	24	0	0
4	126-A	48	24	24	0	0
4	127-A	48	24	24	0	0
4	128-A	48	24	24	0	0
4	129-A	48	24	24	0	0
4	130-A	48	24	24	0	0
4	131-A	48	24	24	0	0
4	132-A	48	24	24	0	0
4	133-A	48	24	24	0	0
4	134-A	48	24	24	0	0
4	135-A	48	24	24	0	0
4	136-A	48	24	24	0	0
4	137-A	48	24	24	0	0
4	138-A	48	24	24	0	0
4	139-A	48	24	24	0	0
4	140-A	48	24	24	0	0
4	141-A	48	24	24	0	0
4	142-A	48	24	24	0	0
4	143-A	48	24	24	0	0
4	144-A	48	24	24	0	0
4	145-A	48	24	24	0	0
4	146-A	48	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	147-A	48	24	24	0	0
4	148-A	48	24	24	0	0
4	149-A	48	24	24	0	0
4	150-A	48	24	24	0	0
4	151-A	48	24	24	0	0
4	152-A	48	24	24	0	0
4	153-A	48	24	24	0	0
4	154-A	48	24	24	0	0
4	155-A	48	24	24	0	0
4	156-A	48	24	24	0	0
4	157-A	48	24	24	0	0
4	158-A	48	24	24	0	0
4	159-A	48	24	24	0	0
4	160-A	48	24	24	0	0
4	161-A	48	24	24	0	0
4	162-A	48	24	24	0	0
4	163-A	48	24	24	0	0
4	164-A	48	24	24	0	0
4	165-A	48	24	24	0	0
4	166-A	48	24	24	0	0
4	167-A	48	24	24	0	0
5	1-A	83	0	0	0	0
5	2-A	83	0	0	0	0
5	3-A	79	0	0	0	0
5	4-A	68	0	0	0	0
5	5-A	75	0	0	0	0
5	6-A	80	0	0	0	0
5	7-A	99	0	0	0	0
5	8-A	89	0	0	0	0
5	9-A	79	0	0	0	0
5	10-A	79	0	0	0	0
5	11-A	82	0	0	0	0
5	12-A	88	0	0	0	0
5	13-A	89	0	0	0	0
5	14-A	96	0	0	0	0
5	15-A	96	0	0	0	0
5	16-A	94	0	0	0	0
5	17-A	84	0	0	0	0
5	18-A	89	0	0	0	0
5	19-A	80	0	0	0	0
5	20-A	73	0	0	0	0
5	21-A	92	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	22-A	91	0	0	0	0
5	23-A	94	0	0	0	0
5	24-A	95	0	0	0	0
5	25-A	76	0	0	0	0
5	26-A	83	0	0	0	0
5	27-A	81	0	0	0	0
5	28-A	81	0	0	0	0
5	29-A	83	0	0	0	0
5	30-A	84	0	0	0	0
5	31-A	86	0	0	0	0
5	32-A	85	0	0	0	0
5	33-A	86	0	0	0	0
5	34-A	93	0	0	0	0
5	35-A	93	0	0	0	0
5	36-A	77	0	0	0	0
5	37-A	82	0	0	0	0
5	38-A	87	0	0	0	0
5	39-A	93	0	0	0	0
5	40-A	84	0	0	0	0
5	41-A	82	0	0	0	0
5	42-A	83	0	0	0	0
5	43-A	95	0	0	0	0
5	44-A	100	0	0	0	0
5	45-A	93	0	0	0	0
5	46-A	92	0	0	0	0
5	47-A	98	0	0	0	0
5	48-A	92	0	0	0	0
5	49-A	89	0	0	0	0
5	50-A	78	0	0	0	0
5	51-A	68	0	0	0	0
5	52-A	77	0	0	0	0
5	53-A	87	0	0	0	0
5	54-A	92	0	0	0	0
5	55-A	92	0	0	0	0
5	56-A	82	0	0	0	0
5	57-A	86	0	0	0	0
5	58-A	89	0	0	0	0
5	59-A	96	0	0	0	0
5	60-A	96	0	0	0	0
5	61-A	98	0	0	0	0
5	62-A	100	0	0	0	0
5	63-A	97	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	64-A	87	0	0	0	0
5	65-A	83	0	0	0	0
5	66-A	77	0	0	0	0
5	67-A	78	0	0	0	0
5	68-A	79	0	0	0	0
5	69-A	79	0	0	0	0
5	70-A	85	0	0	0	0
5	71-A	91	0	0	0	0
5	72-A	101	0	0	0	0
5	73-A	94	0	0	0	0
5	74-A	85	0	0	0	0
5	75-A	92	0	0	0	0
5	76-A	82	0	0	0	0
5	77-A	85	0	0	0	0
5	78-A	84	0	0	0	0
5	79-A	86	0	0	0	0
5	80-A	85	0	0	0	0
5	81-A	92	0	0	0	0
5	82-A	91	0	0	0	0
5	83-A	98	0	0	0	0
5	84-A	94	0	0	0	0
5	85-A	94	0	0	0	0
5	86-A	88	0	0	0	0
5	87-A	84	0	0	0	0
5	88-A	82	0	0	0	0
5	89-A	92	0	0	0	0
5	90-A	98	0	0	0	0
5	91-A	75	0	0	0	0
5	92-A	77	0	0	0	0
5	93-A	78	0	0	0	0
5	94-A	92	0	0	0	0
5	95-A	101	0	0	0	0
5	96-A	106	0	0	0	0
5	97-A	94	0	0	0	0
5	98-A	86	0	0	0	0
5	99-A	87	0	0	0	0
5	100-A	80	0	0	0	0
5	101-A	76	0	0	0	0
5	102-A	80	0	0	0	0
5	103-A	89	0	0	0	0
5	104-A	88	0	0	0	0
5	105-A	97	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	106-A	85	0	0	0	0
5	107-A	87	0	0	0	0
5	108-A	93	0	0	0	0
5	109-A	82	0	0	0	0
5	110-A	82	0	0	0	0
5	111-A	75	0	0	0	0
5	112-A	85	0	0	0	0
5	113-A	97	0	0	0	0
5	114-A	98	0	0	0	0
5	115-A	86	0	0	0	0
5	116-A	89	0	0	0	0
5	117-A	85	0	0	0	0
5	118-A	89	0	0	0	0
5	119-A	88	0	0	0	0
5	120-A	95	0	0	0	0
5	121-A	93	0	0	0	0
5	122-A	90	0	0	0	0
5	123-A	82	0	0	0	0
5	124-A	81	0	0	0	0
5	125-A	84	0	0	0	0
5	126-A	101	0	0	0	0
5	127-A	96	0	0	0	0
5	128-A	90	0	0	0	0
5	129-A	89	0	0	0	0
5	130-A	81	0	0	0	0
5	131-A	75	0	0	0	0
5	132-A	87	0	0	0	0
5	133-A	96	0	0	0	0
5	134-A	89	0	0	0	0
5	135-A	89	0	0	0	0
5	136-A	87	0	0	0	0
5	137-A	88	0	0	0	0
5	138-A	88	0	0	0	0
5	139-A	96	0	0	0	0
5	140-A	88	0	0	0	0
5	141-A	80	0	0	0	0
5	142-A	80	0	0	0	0
5	143-A	83	0	0	0	0
5	144-A	84	0	0	0	0
5	145-A	99	0	0	0	0
5	146-A	101	0	0	0	0
5	147-A	105	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	148-A	103	0	0	0	0
5	149-A	86	0	0	0	0
5	150-A	94	0	0	0	0
5	151-A	92	0	0	0	0
5	152-A	89	0	0	0	0
5	153-A	99	0	0	0	0
5	154-A	98	0	0	0	0
5	155-A	78	0	0	0	0
5	156-A	79	0	0	0	0
5	157-A	80	0	0	0	0
5	158-A	78	0	0	0	0
5	159-A	82	0	0	0	0
5	160-A	82	0	0	0	0
5	161-A	86	0	0	0	0
5	162-A	84	0	0	0	0
5	163-A	91	0	0	0	0
5	164-A	92	0	0	0	0
5	165-A	90	0	0	0	0
5	166-A	81	0	0	0	0
5	167-A	89	0	0	0	0
All	All	240066	211088	211070	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	6 0
1	2-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	9 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3-A	157/159 (99%)	150 (96%)	4 (2%)	3 (2%)	9	0
1	4-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	5	0
1	5-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	4	0
1	6-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	6	0
1	7-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	9	0
1	8-A	157/159 (99%)	142 (90%)	11 (7%)	4 (2%)	6	0
1	9-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	6	0
1	10-A	157/159 (99%)	146 (93%)	3 (2%)	8 (5%)	2	0
1	11-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	4	0
1	12-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	6	0
1	13-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	14	1
1	14-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	9	0
1	15-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	6	0
1	16-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	5	0
1	17-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	4	0
1	18-A	157/159 (99%)	142 (90%)	10 (6%)	5 (3%)	5	0
1	19-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	5	0
1	20-A	157/159 (99%)	148 (94%)	8 (5%)	1 (1%)	28	7
1	21-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	6	0
1	22-A	157/159 (99%)	145 (92%)	9 (6%)	3 (2%)	9	0
1	23-A	157/159 (99%)	148 (94%)	5 (3%)	4 (2%)	6	0
1	24-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	4	0
1	25-A	157/159 (99%)	145 (92%)	6 (4%)	6 (4%)	4	0
1	26-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	4	0
1	27-A	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	6	0
1	28-A	157/159 (99%)	143 (91%)	7 (4%)	7 (4%)	3	0
1	29-A	157/159 (99%)	139 (88%)	8 (5%)	10 (6%)	1	0
1	30-A	157/159 (99%)	138 (88%)	10 (6%)	9 (6%)	2	0
1	31-A	157/159 (99%)	136 (87%)	10 (6%)	11 (7%)	1	0
1	32-A	157/159 (99%)	137 (87%)	7 (4%)	13 (8%)	1	0
1	33-A	157/159 (99%)	137 (87%)	7 (4%)	13 (8%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	34-A	157/159 (99%)	139 (88%)	7 (4%)	11 (7%)	1	0
1	35-A	157/159 (99%)	141 (90%)	7 (4%)	9 (6%)	2	0
1	36-A	157/159 (99%)	140 (89%)	8 (5%)	9 (6%)	2	0
1	37-A	157/159 (99%)	137 (87%)	10 (6%)	10 (6%)	1	0
1	38-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	4	0
1	39-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	4	0
1	40-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	5	0
1	41-A	157/159 (99%)	142 (90%)	8 (5%)	7 (4%)	3	0
1	42-A	157/159 (99%)	146 (93%)	4 (2%)	7 (4%)	3	0
1	43-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	4	0
1	44-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	5	0
1	45-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	5	0
1	46-A	157/159 (99%)	148 (94%)	5 (3%)	4 (2%)	6	0
1	47-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	4	0
1	48-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	5	0
1	49-A	157/159 (99%)	145 (92%)	5 (3%)	7 (4%)	3	0
1	50-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	6	0
1	51-A	157/159 (99%)	146 (93%)	4 (2%)	7 (4%)	3	0
1	52-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	9	0
1	53-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	14	1
1	54-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	9	0
1	55-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	14	1
1	56-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	9	0
1	57-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	14	1
1	58-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	28	7
1	59-A	157/159 (99%)	148 (94%)	9 (6%)	0	100	100
1	60-A	157/159 (99%)	152 (97%)	2 (1%)	3 (2%)	9	0
1	61-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	14	1
1	62-A	157/159 (99%)	145 (92%)	9 (6%)	3 (2%)	9	0
1	63-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	14	1
1	64-A	157/159 (99%)	150 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	65-A	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
1	66-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	14	1
1	67-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	14	1
1	68-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	6	0
1	69-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	9	0
1	70-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	4	0
1	71-A	157/159 (99%)	144 (92%)	5 (3%)	8 (5%)	2	0
1	72-A	157/159 (99%)	144 (92%)	6 (4%)	7 (4%)	3	0
1	73-A	157/159 (99%)	147 (94%)	3 (2%)	7 (4%)	3	0
1	74-A	157/159 (99%)	143 (91%)	8 (5%)	6 (4%)	4	0
1	75-A	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	6	0
1	76-A	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	6	0
1	77-A	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	14	1
1	78-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	5	0
1	79-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	6	0
1	80-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	6	0
1	81-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	14	1
1	82-A	157/159 (99%)	143 (91%)	9 (6%)	5 (3%)	5	0
1	83-A	157/159 (99%)	146 (93%)	7 (4%)	4 (2%)	6	0
1	84-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	9	0
1	85-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	4	0
1	86-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	9	0
1	87-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	9	0
1	88-A	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
1	89-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	9	0
1	90-A	157/159 (99%)	148 (94%)	7 (4%)	2 (1%)	14	1
1	91-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	14	1
1	92-A	157/159 (99%)	146 (93%)	7 (4%)	4 (2%)	6	0
1	93-A	157/159 (99%)	147 (94%)	9 (6%)	1 (1%)	28	7
1	94-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	5	0
1	95-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	6	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	96-A	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	14	1
1	97-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	28	7
1	98-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	9	0
1	99-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	100-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	9	0
1	101-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	9	0
1	102-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	14	1
1	103-A	157/159 (99%)	150 (96%)	3 (2%)	4 (2%)	6	0
1	104-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	14	1
1	105-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	28	7
1	106-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	9	0
1	107-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	9	0
1	108-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	6	0
1	109-A	157/159 (99%)	143 (91%)	9 (6%)	5 (3%)	5	0
1	110-A	157/159 (99%)	139 (88%)	10 (6%)	8 (5%)	2	0
1	111-A	157/159 (99%)	142 (90%)	6 (4%)	9 (6%)	2	0
1	112-A	157/159 (99%)	141 (90%)	8 (5%)	8 (5%)	2	0
1	113-A	157/159 (99%)	141 (90%)	5 (3%)	11 (7%)	1	0
1	114-A	157/159 (99%)	138 (88%)	11 (7%)	8 (5%)	2	0
1	115-A	157/159 (99%)	145 (92%)	5 (3%)	7 (4%)	3	0
1	116-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	4	0
1	117-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	6	0
1	118-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	4	0
1	119-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	28	7
1	120-A	157/159 (99%)	144 (92%)	11 (7%)	2 (1%)	14	1
1	121-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	5	0
1	122-A	157/159 (99%)	142 (90%)	10 (6%)	5 (3%)	5	0
1	123-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	4	0
1	124-A	157/159 (99%)	144 (92%)	4 (2%)	9 (6%)	2	0
1	125-A	157/159 (99%)	142 (90%)	7 (4%)	8 (5%)	2	0
1	126-A	157/159 (99%)	148 (94%)	7 (4%)	2 (1%)	14	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	127-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	28	7
1	128-A	157/159 (99%)	146 (93%)	7 (4%)	4 (2%)	6	0
1	129-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	28	7
1	130-A	157/159 (99%)	144 (92%)	11 (7%)	2 (1%)	14	1
1	131-A	157/159 (99%)	141 (90%)	11 (7%)	5 (3%)	5	0
1	132-A	157/159 (99%)	140 (89%)	13 (8%)	4 (2%)	6	0
1	133-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	9	0
1	134-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	9	0
1	135-A	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	14	1
1	136-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	5	0
1	137-A	157/159 (99%)	144 (92%)	5 (3%)	8 (5%)	2	0
1	138-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	4	0
1	139-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	6	0
1	140-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	6	0
1	141-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	5	0
1	142-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	4	0
1	143-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	4	0
1	144-A	157/159 (99%)	143 (91%)	9 (6%)	5 (3%)	5	0
1	145-A	157/159 (99%)	141 (90%)	11 (7%)	5 (3%)	5	0
1	146-A	157/159 (99%)	143 (91%)	8 (5%)	6 (4%)	4	0
1	147-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	6	0
1	148-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	5	0
1	149-A	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	14	1
1	150-A	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	4	0
1	151-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	9	0
1	152-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	6	0
1	153-A	157/159 (99%)	150 (96%)	3 (2%)	4 (2%)	6	0
1	154-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	9	0
1	155-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	4	0
1	156-A	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	4	0
1	157-A	157/159 (99%)	142 (90%)	10 (6%)	5 (3%)	5	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	158-A	157/159 (99%)	140 (89%)	9 (6%)	8 (5%)	2	0
1	159-A	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	4	0
1	160-A	157/159 (99%)	141 (90%)	11 (7%)	5 (3%)	5	0
1	161-A	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	5	0
1	162-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	5	0
1	163-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	6	0
1	164-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	5	0
1	165-A	157/159 (99%)	144 (92%)	6 (4%)	7 (4%)	3	0
1	166-A	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	9	0
1	167-A	157/159 (99%)	145 (92%)	5 (3%)	7 (4%)	3	0
All	All	26219/26553 (99%)	24212 (92%)	1237 (5%)	770 (3%)	5	0

All (770) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	18	ASN
1	1-A	119	VAL
1	1-A	130	PRO
1	3-A	130	PRO
1	4-A	18	ASN
1	4-A	130	PRO
1	5-A	18	ASN
1	5-A	130	PRO
1	6-A	127	ASP
1	7-A	22	TRP
1	8-A	21	PRO
1	9-A	18	ASN
1	9-A	19	ALA
1	9-A	21	PRO
1	10-A	18	ASN
1	10-A	21	PRO
1	10-A	68	THR
1	11-A	18	ASN
1	11-A	21	PRO
1	11-A	22	TRP
1	12-A	16	MET
1	12-A	18	ASN
1	12-A	21	PRO

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Mol	Chain	Res	Type
1	12-A	22	TRP
1	14-A	21	PRO
1	14-A	22	TRP
1	15-A	17	GLU
1	15-A	130	PRO
1	15-A	131	ASP
1	16-A	19	ALA
1	16-A	130	PRO
1	17-A	20	MET
1	17-A	21	PRO
1	17-A	129	GLU
1	17-A	130	PRO
1	18-A	21	PRO
1	18-A	143	ALA
1	19-A	17	GLU
1	19-A	21	PRO
1	19-A	143	ALA
1	20-A	17	GLU
1	21-A	18	ASN
1	21-A	21	PRO
1	21-A	87	ASP
1	22-A	87	ASP
1	22-A	88	VAL
1	23-A	17	GLU
1	23-A	19	ALA
1	23-A	20	MET
1	23-A	88	VAL
1	24-A	20	MET
1	24-A	85	CYS
1	24-A	87	ASP
1	24-A	128	TYR
1	25-A	19	ALA
1	25-A	20	MET
1	26-A	17	GLU
1	26-A	18	ASN
1	26-A	19	ALA
1	26-A	20	MET
1	26-A	21	PRO
1	26-A	88	VAL
1	27-A	87	ASP
1	28-A	21	PRO
1	28-A	87	ASP

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Mol	Chain	Res	Type
1	28-A	88	VAL
1	29-A	20	MET
1	29-A	21	PRO
1	29-A	88	VAL
1	29-A	90	GLU
1	29-A	137	PHE
1	30-A	17	GLU
1	30-A	53	PRO
1	30-A	88	VAL
1	30-A	90	GLU
1	30-A	130	PRO
1	30-A	131	ASP
1	31-A	17	GLU
1	31-A	53	PRO
1	31-A	54	LEU
1	31-A	87	ASP
1	31-A	88	VAL
1	31-A	130	PRO
1	31-A	131	ASP
1	32-A	21	PRO
1	32-A	88	VAL
1	32-A	90	GLU
1	32-A	127	ASP
1	32-A	130	PRO
1	32-A	131	ASP
1	33-A	22	TRP
1	33-A	23	ASN
1	33-A	87	ASP
1	33-A	89	PRO
1	33-A	119	VAL
1	34-A	18	ASN
1	34-A	87	ASP
1	34-A	88	VAL
1	35-A	18	ASN
1	35-A	19	ALA
1	35-A	20	MET
1	35-A	23	ASN
1	35-A	90	GLU
1	35-A	119	VAL
1	36-A	17	GLU
1	36-A	19	ALA
1	36-A	87	ASP

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Mol	Chain	Res	Type
1	36-A	89	PRO
1	36-A	119	VAL
1	37-A	17	GLU
1	37-A	18	ASN
1	37-A	89	PRO
1	37-A	90	GLU
1	38-A	17	GLU
1	38-A	18	ASN
1	38-A	89	PRO
1	38-A	90	GLU
1	39-A	21	PRO
1	39-A	22	TRP
1	39-A	89	PRO
1	40-A	21	PRO
1	40-A	89	PRO
1	41-A	89	PRO
1	41-A	120	GLU
1	42-A	17	GLU
1	42-A	89	PRO
1	42-A	148	SER
1	43-A	17	GLU
1	43-A	87	ASP
1	43-A	89	PRO
1	44-A	88	VAL
1	44-A	89	PRO
1	45-A	18	ASN
1	45-A	88	VAL
1	45-A	89	PRO
1	46-A	18	ASN
1	46-A	88	VAL
1	47-A	18	ASN
1	47-A	85	CYS
1	47-A	88	VAL
1	48-A	85	CYS
1	48-A	88	VAL
1	48-A	119	VAL
1	49-A	85	CYS
1	49-A	88	VAL
1	49-A	119	VAL
1	49-A	120	GLU
1	50-A	119	VAL
1	50-A	120	GLU

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Mol	Chain	Res	Type
1	50-A	127	ASP
1	51-A	88	VAL
1	52-A	88	VAL
1	52-A	119	VAL
1	53-A	88	VAL
1	54-A	87	ASP
1	54-A	88	VAL
1	55-A	87	ASP
1	56-A	87	ASP
1	56-A	88	VAL
1	56-A	127	ASP
1	57-A	87	ASP
1	57-A	88	VAL
1	58-A	88	VAL
1	61-A	127	ASP
1	62-A	127	ASP
1	63-A	21	PRO
1	63-A	22	TRP
1	67-A	19	ALA
1	68-A	18	ASN
1	68-A	21	PRO
1	68-A	128	TYR
1	69-A	19	ALA
1	69-A	67	GLY
1	71-A	2	ILE
1	71-A	17	GLU
1	71-A	18	ASN
1	72-A	2	ILE
1	72-A	17	GLU
1	72-A	65	GLN
1	72-A	129	GLU
1	73-A	17	GLU
1	73-A	65	GLN
1	73-A	66	PRO
1	74-A	2	ILE
1	74-A	17	GLU
1	74-A	65	GLN
1	74-A	66	PRO
1	74-A	119	VAL
1	74-A	127	ASP
1	75-A	2	ILE
1	75-A	17	GLU

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Mol	Chain	Res	Type
1	75-A	87	ASP
1	76-A	20	MET
1	78-A	20	MET
1	79-A	130	PRO
1	80-A	126	PRO
1	80-A	128	TYR
1	81-A	130	PRO
1	81-A	131	ASP
1	82-A	127	ASP
1	83-A	129	GLU
1	84-A	131	ASP
1	85-A	127	ASP
1	85-A	131	ASP
1	86-A	127	ASP
1	86-A	131	ASP
1	87-A	127	ASP
1	91-A	129	GLU
1	91-A	130	PRO
1	92-A	130	PRO
1	92-A	131	ASP
1	93-A	17	GLU
1	94-A	18	ASN
1	94-A	122	ASP
1	95-A	122	ASP
1	96-A	52	ARG
1	98-A	143	ALA
1	102-A	18	ASN
1	104-A	17	GLU
1	106-A	21	PRO
1	107-A	21	PRO
1	108-A	21	PRO
1	108-A	87	ASP
1	110-A	19	ALA
1	110-A	20	MET
1	110-A	21	PRO
1	110-A	68	THR
1	111-A	19	ALA
1	111-A	21	PRO
1	111-A	22	TRP
1	111-A	121	GLY
1	111-A	131	ASP
1	112-A	2	ILE

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Mol	Chain	Res	Type
1	112-A	18	ASN
1	112-A	19	ALA
1	112-A	21	PRO
1	112-A	121	GLY
1	113-A	2	ILE
1	113-A	18	ASN
1	113-A	20	MET
1	113-A	21	PRO
1	113-A	120	GLU
1	113-A	143	ALA
1	114-A	20	MET
1	114-A	21	PRO
1	114-A	22	TRP
1	114-A	23	ASN
1	115-A	19	ALA
1	115-A	20	MET
1	115-A	21	PRO
1	115-A	22	TRP
1	115-A	23	ASN
1	115-A	119	VAL
1	116-A	18	ASN
1	116-A	19	ALA
1	116-A	20	MET
1	116-A	21	PRO
1	117-A	19	ALA
1	117-A	21	PRO
1	117-A	23	ASN
1	118-A	17	GLU
1	118-A	21	PRO
1	119-A	20	MET
1	120-A	23	ASN
1	120-A	120	GLU
1	121-A	23	ASN
1	121-A	121	GLY
1	121-A	130	PRO
1	121-A	131	ASP
1	123-A	88	VAL
1	123-A	120	GLU
1	124-A	21	PRO
1	124-A	22	TRP
1	124-A	23	ASN
1	124-A	87	ASP

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Mol	Chain	Res	Type
1	124-A	120	GLU
1	124-A	127	ASP
1	124-A	130	PRO
1	125-A	21	PRO
1	125-A	121	GLY
1	125-A	122	ASP
1	126-A	88	VAL
1	126-A	120	GLU
1	127-A	23	ASN
1	128-A	23	ASN
1	131-A	52	ARG
1	131-A	87	ASP
1	132-A	18	ASN
1	132-A	52	ARG
1	133-A	50	ILE
1	133-A	52	ARG
1	135-A	128	TYR
1	136-A	17	GLU
1	136-A	128	TYR
1	136-A	129	GLU
1	137-A	17	GLU
1	137-A	18	ASN
1	137-A	51	GLY
1	138-A	11	ASP
1	138-A	17	GLU
1	138-A	129	GLU
1	138-A	132	ASP
1	139-A	129	GLU
1	140-A	18	ASN
1	140-A	129	GLU
1	141-A	17	GLU
1	141-A	18	ASN
1	141-A	129	GLU
1	142-A	17	GLU
1	143-A	17	GLU
1	144-A	17	GLU
1	144-A	129	GLU
1	145-A	21	PRO
1	145-A	130	PRO
1	146-A	21	PRO
1	147-A	131	ASP
1	148-A	129	GLU

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Mol	Chain	Res	Type
1	148-A	130	PRO
1	148-A	137	PHE
1	149-A	130	PRO
1	149-A	131	ASP
1	150-A	128	TYR
1	150-A	129	GLU
1	150-A	131	ASP
1	150-A	137	PHE
1	152-A	67	GLY
1	154-A	67	GLY
1	156-A	65	GLN
1	156-A	131	ASP
1	157-A	87	ASP
1	157-A	129	GLU
1	157-A	131	ASP
1	158-A	87	ASP
1	158-A	130	PRO
1	159-A	65	GLN
1	159-A	66	PRO
1	159-A	87	ASP
1	159-A	129	GLU
1	159-A	130	PRO
1	160-A	65	GLN
1	160-A	129	GLU
1	160-A	130	PRO
1	160-A	131	ASP
1	161-A	18	ASN
1	161-A	130	PRO
1	161-A	131	ASP
1	162-A	128	TYR
1	162-A	130	PRO
1	162-A	131	ASP
1	163-A	130	PRO
1	163-A	131	ASP
1	164-A	128	TYR
1	164-A	129	GLU
1	164-A	130	PRO
1	164-A	132	ASP
1	165-A	68	THR
1	165-A	129	GLU
1	165-A	130	PRO
1	165-A	131	ASP

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Mol	Chain	Res	Type
1	165-A	132	ASP
1	166-A	68	THR
1	166-A	129	GLU
1	166-A	130	PRO
1	167-A	68	THR
1	167-A	129	GLU
1	167-A	130	PRO
1	167-A	131	ASP
1	167-A	132	ASP
1	2-A	18	ASN
1	2-A	129	GLU
1	3-A	17	GLU
1	6-A	130	PRO
1	7-A	137	PHE
1	8-A	16	MET
1	10-A	128	TYR
1	11-A	16	MET
1	11-A	68	THR
1	11-A	119	VAL
1	13-A	21	PRO
1	13-A	22	TRP
1	15-A	20	MET
1	16-A	21	PRO
1	17-A	120	GLU
1	18-A	120	GLU
1	19-A	144	ASP
1	25-A	88	VAL
1	27-A	18	ASN
1	27-A	19	ALA
1	28-A	19	ALA
1	28-A	90	GLU
1	30-A	50	ILE
1	32-A	17	GLU
1	32-A	87	ASP
1	32-A	89	PRO
1	32-A	119	VAL
1	32-A	128	TYR
1	32-A	129	GLU
1	33-A	17	GLU
1	33-A	18	ASN
1	33-A	86	GLY
1	33-A	88	VAL

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Mol	Chain	Res	Type
1	33-A	90	GLU
1	33-A	142	ASP
1	34-A	17	GLU
1	34-A	86	GLY
1	34-A	89	PRO
1	34-A	119	VAL
1	34-A	131	ASP
1	35-A	88	VAL
1	36-A	18	ASN
1	36-A	90	GLU
1	37-A	128	TYR
1	37-A	143	ALA
1	39-A	17	GLU
1	39-A	18	ASN
1	40-A	87	ASP
1	41-A	17	GLU
1	41-A	87	ASP
1	42-A	87	ASP
1	43-A	67	GLY
1	43-A	88	VAL
1	43-A	121	GLY
1	44-A	120	GLU
1	45-A	85	CYS
1	49-A	69	ASP
1	50-A	88	VAL
1	51-A	85	CYS
1	51-A	87	ASP
1	52-A	87	ASP
1	53-A	85	CYS
1	55-A	21	PRO
1	60-A	17	GLU
1	68-A	19	ALA
1	70-A	19	ALA
1	70-A	22	TRP
1	71-A	65	GLN
1	71-A	66	PRO
1	71-A	67	GLY
1	71-A	131	ASP
1	72-A	18	ASN
1	72-A	19	ALA
1	73-A	2	ILE
1	73-A	143	ALA

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Mol	Chain	Res	Type
1	75-A	127	ASP
1	76-A	17	GLU
1	77-A	18	ASN
1	77-A	21	PRO
1	78-A	50	ILE
1	82-A	128	TYR
1	83-A	127	ASP
1	83-A	128	TYR
1	84-A	127	ASP
1	84-A	137	PHE
1	85-A	87	ASP
1	85-A	120	GLU
1	85-A	137	PHE
1	87-A	126	PRO
1	89-A	131	ASP
1	90-A	130	PRO
1	92-A	129	GLU
1	94-A	19	ALA
1	94-A	121	GLY
1	96-A	17	GLU
1	100-A	18	ASN
1	100-A	21	PRO
1	101-A	17	GLU
1	101-A	18	ASN
1	103-A	17	GLU
1	103-A	18	ASN
1	104-A	18	ASN
1	105-A	18	ASN
1	106-A	18	ASN
1	106-A	51	GLY
1	108-A	17	GLU
1	108-A	86	GLY
1	109-A	49	SER
1	109-A	67	GLY
1	110-A	17	GLU
1	110-A	22	TRP
1	112-A	128	TYR
1	113-A	22	TRP
1	113-A	23	ASN
1	113-A	87	ASP
1	114-A	18	ASN
1	114-A	120	GLU

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Mol	Chain	Res	Type
1	115-A	18	ASN
1	122-A	121	GLY
1	122-A	136	VAL
1	123-A	21	PRO
1	125-A	23	ASN
1	125-A	120	GLU
1	125-A	130	PRO
1	128-A	121	GLY
1	129-A	121	GLY
1	130-A	67	GLY
1	131-A	121	GLY
1	134-A	121	GLY
1	134-A	122	ASP
1	136-A	18	ASN
1	136-A	130	PRO
1	137-A	132	ASP
1	140-A	132	ASP
1	142-A	132	ASP
1	144-A	18	ASN
1	148-A	131	ASP
1	150-A	86	GLY
1	151-A	67	GLY
1	153-A	67	GLY
1	155-A	18	ASN
1	155-A	65	GLN
1	155-A	67	GLY
1	156-A	119	VAL
1	157-A	130	PRO
1	158-A	21	PRO
1	158-A	66	PRO
1	159-A	67	GLY
1	160-A	90	GLU
1	161-A	128	TYR
1	164-A	131	ASP
1	165-A	21	PRO
1	165-A	22	TRP
1	1-A	17	GLU
1	2-A	130	PRO
1	5-A	127	ASP
1	8-A	128	TYR
1	10-A	17	GLU
1	14-A	17	GLU

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Mol	Chain	Res	Type
1	18-A	17	GLU
1	22-A	17	GLU
1	24-A	19	ALA
1	25-A	85	CYS
1	31-A	128	TYR
1	35-A	89	PRO
1	36-A	23	ASN
1	38-A	145	ALA
1	40-A	137	PHE
1	41-A	19	ALA
1	42-A	120	GLU
1	46-A	21	PRO
1	46-A	89	PRO
1	47-A	87	ASP
1	48-A	131	ASP
1	62-A	67	GLY
1	67-A	18	ASN
1	70-A	21	PRO
1	71-A	21	PRO
1	76-A	87	ASP
1	78-A	128	TYR
1	78-A	130	PRO
1	79-A	126	PRO
1	79-A	128	TYR
1	82-A	131	ASP
1	87-A	130	PRO
1	92-A	21	PRO
1	95-A	18	ASN
1	95-A	19	ALA
1	101-A	22	TRP
1	109-A	22	TRP
1	110-A	66	PRO
1	110-A	139	GLU
1	113-A	19	ALA
1	118-A	18	ASN
1	118-A	23	ASN
1	121-A	21	PRO
1	122-A	21	PRO
1	122-A	23	ASN
1	123-A	130	PRO
1	125-A	87	ASP
1	128-A	66	PRO

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Mol	Chain	Res	Type
1	132-A	128	TYR
1	137-A	11	ASP
1	137-A	130	PRO
1	138-A	137	PHE
1	141-A	130	PRO
1	144-A	130	PRO
1	145-A	18	ASN
1	146-A	66	PRO
1	146-A	120	GLU
1	147-A	137	PHE
1	153-A	18	ASN
1	154-A	18	ASN
1	157-A	66	PRO
1	158-A	69	ASP
1	158-A	129	GLU
1	163-A	129	GLU
1	167-A	66	PRO
1	5-A	87	ASP
1	10-A	16	MET
1	18-A	137	PHE
1	25-A	16	MET
1	28-A	17	GLU
1	29-A	50	ILE
1	29-A	53	PRO
1	30-A	18	ASN
1	31-A	86	GLY
1	31-A	90	GLU
1	32-A	20	MET
1	34-A	90	GLU
1	36-A	21	PRO
1	37-A	19	ALA
1	37-A	88	VAL
1	37-A	142	ASP
1	39-A	88	VAL
1	44-A	17	GLU
1	45-A	21	PRO
1	47-A	17	GLU
1	47-A	119	VAL
1	51-A	21	PRO
1	51-A	120	GLU
1	61-A	137	PHE
1	66-A	128	TYR

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Mol	Chain	Res	Type
1	70-A	18	ASN
1	73-A	18	ASN
1	73-A	21	PRO
1	80-A	21	PRO
1	82-A	129	GLU
1	83-A	131	ASP
1	85-A	21	PRO
1	97-A	21	PRO
1	102-A	17	GLU
1	107-A	17	GLU
1	109-A	89	PRO
1	112-A	20	MET
1	114-A	2	ILE
1	116-A	22	TRP
1	116-A	24	LEU
1	123-A	127	ASP
1	124-A	88	VAL
1	128-A	22	TRP
1	131-A	129	GLU
1	138-A	130	PRO
1	139-A	130	PRO
1	140-A	130	PRO
1	141-A	132	ASP
1	142-A	18	ASN
1	142-A	49	SER
1	142-A	129	GLU
1	143-A	132	ASP
1	144-A	19	ALA
1	145-A	19	ALA
1	146-A	130	PRO
1	147-A	129	GLU
1	152-A	21	PRO
1	152-A	22	TRP
1	152-A	131	ASP
1	153-A	22	TRP
1	153-A	129	GLU
1	156-A	18	ASN
1	158-A	22	TRP
1	163-A	18	ASN
1	167-A	50	ILE
1	4-A	21	PRO
1	7-A	20	MET

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Mol	Chain	Res	Type
1	9-A	16	MET
1	10-A	20	MET
1	16-A	129	GLU
1	21-A	127	ASP
1	25-A	21	PRO
1	27-A	88	VAL
1	28-A	20	MET
1	29-A	69	ASP
1	29-A	129	GLU
1	30-A	54	LEU
1	33-A	129	GLU
1	34-A	129	GLU
1	37-A	21	PRO
1	41-A	88	VAL
1	41-A	122	ASP
1	42-A	69	ASP
1	48-A	86	GLY
1	49-A	86	GLY
1	49-A	127	ASP
1	54-A	21	PRO
1	69-A	127	ASP
1	70-A	17	GLU
1	72-A	66	PRO
1	78-A	19	ALA
1	80-A	16	MET
1	82-A	130	PRO
1	90-A	18	ASN
1	94-A	128	TYR
1	98-A	144	ASP
1	107-A	137	PHE
1	114-A	19	ALA
1	134-A	54	LEU
1	143-A	16	MET
1	143-A	21	PRO
1	143-A	130	PRO
1	145-A	66	PRO
1	146-A	20	MET
1	146-A	129	GLU
1	156-A	66	PRO
1	156-A	130	PRO
1	158-A	65	GLN
1	4-A	137	PHE

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Mol	Chain	Res	Type
1	17-A	16	MET
1	24-A	18	ASN
1	31-A	129	GLU
1	33-A	20	MET
1	34-A	21	PRO
1	35-A	17	GLU
1	38-A	20	MET
1	60-A	129	GLU
1	62-A	22	TRP
1	70-A	67	GLY
1	89-A	130	PRO
1	98-A	21	PRO
1	100-A	87	ASP
1	111-A	17	GLU
1	111-A	18	ASN
1	111-A	130	PRO
1	113-A	126	PRO
1	122-A	22	TRP
1	123-A	11	ASP
1	124-A	129	GLU
1	125-A	88	VAL
1	131-A	51	GLY
1	137-A	50	ILE
1	139-A	17	GLU
1	147-A	136	VAL
1	148-A	50	ILE
1	4-A	129	GLU
1	5-A	52	ARG
1	40-A	88	VAL
1	76-A	21	PRO
1	103-A	21	PRO
1	103-A	86	GLY
1	109-A	21	PRO
1	132-A	121	GLY
1	142-A	21	PRO
1	143-A	129	GLU
1	151-A	21	PRO
1	151-A	136	VAL
1	154-A	130	PRO
1	155-A	21	PRO
1	155-A	66	PRO
1	161-A	129	GLU

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Mol	Chain	Res	Type
1	3-A	129	GLU
1	6-A	20	MET
1	16-A	20	MET
1	19-A	136	VAL
1	29-A	67	GLY
1	60-A	130	PRO
1	66-A	119	VAL
1	89-A	129	GLU
1	111-A	20	MET
1	118-A	20	MET
1	155-A	130	PRO
1	8-A	67	GLY
1	10-A	66	PRO
1	44-A	129	GLU
1	51-A	119	VAL
1	51-A	129	GLU
1	79-A	129	GLU
1	86-A	21	PRO
1	95-A	121	GLY
1	117-A	20	MET
1	130-A	21	PRO
1	133-A	51	GLY
1	137-A	129	GLU
1	150-A	21	PRO
1	162-A	66	PRO
1	5-A	129	GLU
1	6-A	129	GLU
1	42-A	88	VAL
1	118-A	136	VAL
1	139-A	21	PRO
1	112-A	126	PRO
1	135-A	52	ARG
1	162-A	129	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	2-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	3-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	4-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	5-A	136/136 (100%)	127 (93%)	9 (7%)	19	1
1	6-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	7-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	8-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	9-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	10-A	136/136 (100%)	126 (93%)	10 (7%)	16	1
1	11-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	12-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	13-A	136/136 (100%)	127 (93%)	9 (7%)	19	1
1	14-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	15-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	16-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	17-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	18-A	136/136 (100%)	128 (94%)	8 (6%)	23	2
1	19-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	20-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	21-A	136/136 (100%)	126 (93%)	10 (7%)	16	1
1	22-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	23-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	24-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	25-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	26-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	27-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	28-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	29-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	30-A	136/136 (100%)	115 (85%)	21 (15%)	3	0
1	31-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	32-A	136/136 (100%)	120 (88%)	16 (12%)	6	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	33-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	34-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	35-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	36-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	37-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	38-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	39-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	40-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	41-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	42-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	43-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	44-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	45-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	46-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	47-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	48-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	49-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	50-A	136/136 (100%)	115 (85%)	21 (15%)	3	0
1	51-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	52-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	53-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	54-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	55-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	56-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	57-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	58-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	59-A	136/136 (100%)	127 (93%)	9 (7%)	19	1
1	60-A	136/136 (100%)	114 (84%)	22 (16%)	3	0
1	61-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	62-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	63-A	136/136 (100%)	126 (93%)	10 (7%)	16	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	64-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	65-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	66-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	67-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	68-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	69-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	70-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	71-A	136/136 (100%)	127 (93%)	9 (7%)	19	1
1	72-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	73-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	74-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	75-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	76-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	77-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	78-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	79-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	80-A	136/136 (100%)	115 (85%)	21 (15%)	3	0
1	81-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	82-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	83-A	136/136 (100%)	127 (93%)	9 (7%)	19	1
1	84-A	136/136 (100%)	127 (93%)	9 (7%)	19	1
1	85-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	86-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	87-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	88-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	89-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	90-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	91-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	92-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	93-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	94-A	136/136 (100%)	119 (88%)	17 (12%)	5	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	95-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	96-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	97-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	98-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	99-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	100-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	101-A	136/136 (100%)	127 (93%)	9 (7%)	19	1
1	102-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	103-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	104-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	105-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	106-A	136/136 (100%)	114 (84%)	22 (16%)	3	0
1	107-A	136/136 (100%)	114 (84%)	22 (16%)	3	0
1	108-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	109-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	110-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	111-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	112-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	113-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	114-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	115-A	136/136 (100%)	115 (85%)	21 (15%)	3	0
1	116-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	117-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	118-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	119-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	120-A	136/136 (100%)	126 (93%)	10 (7%)	16	1
1	121-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	122-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	123-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	124-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	125-A	136/136 (100%)	124 (91%)	12 (9%)	12	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	126-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	127-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	128-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	129-A	136/136 (100%)	126 (93%)	10 (7%)	16	1
1	130-A	136/136 (100%)	128 (94%)	8 (6%)	23	2
1	131-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	132-A	136/136 (100%)	126 (93%)	10 (7%)	16	1
1	133-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	134-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	135-A	136/136 (100%)	125 (92%)	11 (8%)	14	1
1	136-A	136/136 (100%)	122 (90%)	14 (10%)	8	0
1	137-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	138-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	139-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	140-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	141-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	142-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	143-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	144-A	136/136 (100%)	113 (83%)	23 (17%)	2	0
1	145-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	146-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	147-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	148-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	149-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	150-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	151-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	152-A	136/136 (100%)	130 (96%)	6 (4%)	33	4
1	153-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	154-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	155-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	156-A	136/136 (100%)	117 (86%)	19 (14%)	4	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	157-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	158-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	159-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	160-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	161-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	162-A	136/136 (100%)	121 (89%)	15 (11%)	7	0
1	163-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	164-A	136/136 (100%)	119 (88%)	17 (12%)	5	0
1	165-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	166-A	136/136 (100%)	124 (91%)	12 (9%)	12	1
1	167-A	136/136 (100%)	115 (85%)	21 (15%)	3	0
All	All	22712/22712 (100%)	20232 (89%)	2480 (11%)	7	0

All (2480) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	4	LEU
1	1-A	20	MET
1	1-A	23	ASN
1	1-A	24	LEU
1	1-A	52	ARG
1	1-A	106	LYS
1	1-A	109	LYS
1	1-A	111	TYR
1	1-A	119	VAL
1	1-A	129	GLU
1	1-A	138	SER
1	1-A	148	SER
1	1-A	156	LEU
1	1-A	157	GLU
1	2-A	16	MET
1	2-A	17	GLU
1	2-A	33	ARG
1	2-A	38	LYS
1	2-A	52	ARG
1	2-A	106	LYS
1	2-A	109	LYS
1	2-A	119	VAL

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Mol	Chain	Res	Type
1	2-A	128	TYR
1	2-A	129	GLU
1	2-A	134	GLU
1	2-A	148	SER
1	2-A	156	LEU
1	2-A	159	ARG
1	3-A	1	MET
1	3-A	2	ILE
1	3-A	16	MET
1	3-A	17	GLU
1	3-A	20	MET
1	3-A	33	ARG
1	3-A	44	ARG
1	3-A	49	SER
1	3-A	52	ARG
1	3-A	59	ASN
1	3-A	106	LYS
1	3-A	118	GLU
1	3-A	119	VAL
1	3-A	128	TYR
1	3-A	129	GLU
1	3-A	135	SER
1	3-A	148	SER
1	4-A	4	LEU
1	4-A	11	ASP
1	4-A	17	GLU
1	4-A	20	MET
1	4-A	23	ASN
1	4-A	24	LEU
1	4-A	33	ARG
1	4-A	52	ARG
1	4-A	60	ILE
1	4-A	70	ASP
1	4-A	108	GLN
1	4-A	109	LYS
1	4-A	118	GLU
1	4-A	123	THR
1	4-A	132	ASP
1	5-A	17	GLU
1	5-A	20	MET
1	5-A	33	ARG
1	5-A	38	LYS

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Mol	Chain	Res	Type
1	5-A	60	ILE
1	5-A	70	ASP
1	5-A	108	GLN
1	5-A	128	TYR
1	5-A	129	GLU
1	6-A	1	MET
1	6-A	18	ASN
1	6-A	20	MET
1	6-A	24	LEU
1	6-A	33	ARG
1	6-A	36	LEU
1	6-A	37	ASN
1	6-A	52	ARG
1	6-A	70	ASP
1	6-A	79	ASP
1	6-A	108	GLN
1	6-A	118	GLU
1	6-A	123	THR
1	6-A	128	TYR
1	6-A	129	GLU
1	6-A	136	VAL
1	6-A	152	CYS
1	7-A	10	VAL
1	7-A	17	GLU
1	7-A	18	ASN
1	7-A	20	MET
1	7-A	33	ARG
1	7-A	36	LEU
1	7-A	38	LYS
1	7-A	52	ARG
1	7-A	70	ASP
1	7-A	79	ASP
1	7-A	87	ASP
1	7-A	108	GLN
1	7-A	123	THR
1	7-A	128	TYR
1	7-A	142	ASP
1	7-A	148	SER
1	7-A	156	LEU
1	8-A	1	MET
1	8-A	4	LEU
1	8-A	17	GLU

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Mol	Chain	Res	Type
1	8-A	18	ASN
1	8-A	20	MET
1	8-A	24	LEU
1	8-A	38	LYS
1	8-A	59	ASN
1	8-A	60	ILE
1	8-A	87	ASP
1	8-A	104	LEU
1	8-A	128	TYR
1	8-A	156	LEU
1	9-A	1	MET
1	9-A	16	MET
1	9-A	24	LEU
1	9-A	30	TRP
1	9-A	65	GLN
1	9-A	76	LYS
1	9-A	87	ASP
1	9-A	104	LEU
1	9-A	108	GLN
1	9-A	127	ASP
1	9-A	129	GLU
1	9-A	138	SER
1	9-A	156	LEU
1	10-A	1	MET
1	10-A	17	GLU
1	10-A	20	MET
1	10-A	59	ASN
1	10-A	104	LEU
1	10-A	106	LYS
1	10-A	118	GLU
1	10-A	126	PRO
1	10-A	127	ASP
1	10-A	156	LEU
1	11-A	1	MET
1	11-A	8	LEU
1	11-A	16	MET
1	11-A	17	GLU
1	11-A	18	ASN
1	11-A	20	MET
1	11-A	24	LEU
1	11-A	38	LYS
1	11-A	45	HIS

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Mol	Chain	Res	Type
1	11-A	87	ASP
1	11-A	104	LEU
1	11-A	106	LYS
1	11-A	120	GLU
1	11-A	129	GLU
1	11-A	139	GLU
1	11-A	156	LEU
1	12-A	1	MET
1	12-A	17	GLU
1	12-A	18	ASN
1	12-A	33	ARG
1	12-A	38	LYS
1	12-A	52	ARG
1	12-A	61	ILE
1	12-A	68	THR
1	12-A	88	VAL
1	12-A	104	LEU
1	12-A	106	LYS
1	12-A	118	GLU
1	12-A	128	TYR
1	12-A	129	GLU
1	12-A	134	GLU
1	12-A	138	SER
1	12-A	156	LEU
1	13-A	1	MET
1	13-A	10	VAL
1	13-A	18	ASN
1	13-A	58	LYS
1	13-A	104	LEU
1	13-A	106	LYS
1	13-A	118	GLU
1	13-A	128	TYR
1	13-A	129	GLU
1	14-A	1	MET
1	14-A	17	GLU
1	14-A	20	MET
1	14-A	24	LEU
1	14-A	33	ARG
1	14-A	37	ASN
1	14-A	44	ARG
1	14-A	61	ILE
1	14-A	65	GLN

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Mol	Chain	Res	Type
1	14-A	101	GLU
1	14-A	104	LEU
1	14-A	115	ILE
1	14-A	128	TYR
1	14-A	129	GLU
1	14-A	134	GLU
1	15-A	4	LEU
1	15-A	17	GLU
1	15-A	20	MET
1	15-A	33	ARG
1	15-A	38	LYS
1	15-A	52	ARG
1	15-A	61	ILE
1	15-A	65	GLN
1	15-A	87	ASP
1	15-A	101	GLU
1	15-A	104	LEU
1	15-A	109	LYS
1	15-A	118	GLU
1	15-A	129	GLU
1	15-A	148	SER
1	15-A	158	ARG
1	16-A	4	LEU
1	16-A	17	GLU
1	16-A	20	MET
1	16-A	22	TRP
1	16-A	28	LEU
1	16-A	32	LYS
1	16-A	33	ARG
1	16-A	52	ARG
1	16-A	59	ASN
1	16-A	61	ILE
1	16-A	118	GLU
1	16-A	129	GLU
1	16-A	134	GLU
1	16-A	158	ARG
1	17-A	16	MET
1	17-A	17	GLU
1	17-A	20	MET
1	17-A	33	ARG
1	17-A	52	ARG
1	17-A	61	ILE

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Mol	Chain	Res	Type
1	17-A	65	GLN
1	17-A	119	VAL
1	17-A	128	TYR
1	17-A	132	ASP
1	17-A	138	SER
1	18-A	10	VAL
1	18-A	18	ASN
1	18-A	23	ASN
1	18-A	61	ILE
1	18-A	104	LEU
1	18-A	119	VAL
1	18-A	138	SER
1	18-A	152	CYS
1	19-A	1	MET
1	19-A	8	LEU
1	19-A	18	ASN
1	19-A	22	TRP
1	19-A	32	LYS
1	19-A	36	LEU
1	19-A	52	ARG
1	19-A	76	LYS
1	19-A	134	GLU
1	19-A	135	SER
1	19-A	154	GLU
1	20-A	1	MET
1	20-A	8	LEU
1	20-A	20	MET
1	20-A	52	ARG
1	20-A	59	ASN
1	20-A	65	GLN
1	20-A	79	ASP
1	20-A	108	GLN
1	20-A	111	TYR
1	20-A	119	VAL
1	20-A	122	ASP
1	20-A	129	GLU
1	20-A	148	SER
1	20-A	152	CYS
1	20-A	157	GLU
1	21-A	24	LEU
1	21-A	28	LEU
1	21-A	32	LYS

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Mol	Chain	Res	Type
1	21-A	49	SER
1	21-A	65	GLN
1	21-A	70	ASP
1	21-A	106	LYS
1	21-A	119	VAL
1	21-A	128	TYR
1	21-A	157	GLU
1	22-A	16	MET
1	22-A	18	ASN
1	22-A	24	LEU
1	22-A	28	LEU
1	22-A	48	GLU
1	22-A	50	ILE
1	22-A	52	ARG
1	22-A	106	LYS
1	22-A	108	GLN
1	22-A	128	TYR
1	22-A	138	SER
1	22-A	157	GLU
1	23-A	1	MET
1	23-A	16	MET
1	23-A	18	ASN
1	23-A	23	ASN
1	23-A	28	LEU
1	23-A	50	ILE
1	23-A	52	ARG
1	23-A	59	ASN
1	23-A	62	LEU
1	23-A	119	VAL
1	23-A	128	TYR
1	23-A	148	SER
1	23-A	156	LEU
1	23-A	157	GLU
1	24-A	23	ASN
1	24-A	28	LEU
1	24-A	33	ARG
1	24-A	45	HIS
1	24-A	52	ARG
1	24-A	76	LYS
1	24-A	108	GLN
1	24-A	119	VAL
1	24-A	122	ASP

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Mol	Chain	Res	Type
1	24-A	127	ASP
1	24-A	148	SER
1	24-A	157	GLU
1	25-A	1	MET
1	25-A	11	ASP
1	25-A	23	ASN
1	25-A	28	LEU
1	25-A	52	ARG
1	25-A	76	LYS
1	25-A	88	VAL
1	25-A	106	LYS
1	25-A	119	VAL
1	25-A	120	GLU
1	25-A	129	GLU
1	25-A	139	GLU
1	25-A	142	ASP
1	25-A	148	SER
1	25-A	157	GLU
1	25-A	158	ARG
1	26-A	1	MET
1	26-A	18	ASN
1	26-A	23	ASN
1	26-A	24	LEU
1	26-A	28	LEU
1	26-A	33	ARG
1	26-A	52	ARG
1	26-A	60	ILE
1	26-A	76	LYS
1	26-A	87	ASP
1	26-A	106	LYS
1	26-A	108	GLN
1	27-A	1	MET
1	27-A	20	MET
1	27-A	21	PRO
1	27-A	24	LEU
1	27-A	28	LEU
1	27-A	33	ARG
1	27-A	52	ARG
1	27-A	58	LYS
1	27-A	60	ILE
1	27-A	76	LYS
1	27-A	87	ASP

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Mol	Chain	Res	Type
1	27-A	98	ARG
1	27-A	104	LEU
1	27-A	106	LYS
1	27-A	108	GLN
1	27-A	119	VAL
1	27-A	120	GLU
1	27-A	142	ASP
1	27-A	159	ARG
1	28-A	1	MET
1	28-A	18	ASN
1	28-A	49	SER
1	28-A	52	ARG
1	28-A	65	GLN
1	28-A	76	LYS
1	28-A	79	ASP
1	28-A	87	ASP
1	28-A	88	VAL
1	28-A	104	LEU
1	28-A	106	LYS
1	28-A	108	GLN
1	28-A	119	VAL
1	28-A	120	GLU
1	28-A	138	SER
1	28-A	148	SER
1	28-A	159	ARG
1	29-A	16	MET
1	29-A	18	ASN
1	29-A	20	MET
1	29-A	33	ARG
1	29-A	52	ARG
1	29-A	61	ILE
1	29-A	65	GLN
1	29-A	68	THR
1	29-A	76	LYS
1	29-A	88	VAL
1	29-A	104	LEU
1	29-A	106	LYS
1	29-A	108	GLN
1	29-A	118	GLU
1	29-A	119	VAL
1	29-A	120	GLU
1	29-A	127	ASP

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Mol	Chain	Res	Type
1	29-A	128	TYR
1	29-A	135	SER
1	29-A	142	ASP
1	30-A	2	ILE
1	30-A	10	VAL
1	30-A	17	GLU
1	30-A	18	ASN
1	30-A	33	ARG
1	30-A	49	SER
1	30-A	50	ILE
1	30-A	52	ARG
1	30-A	53	PRO
1	30-A	54	LEU
1	30-A	76	LYS
1	30-A	88	VAL
1	30-A	98	ARG
1	30-A	104	LEU
1	30-A	106	LYS
1	30-A	108	GLN
1	30-A	119	VAL
1	30-A	128	TYR
1	30-A	142	ASP
1	30-A	157	GLU
1	30-A	158	ARG
1	31-A	16	MET
1	31-A	23	ASN
1	31-A	33	ARG
1	31-A	54	LEU
1	31-A	65	GLN
1	31-A	76	LYS
1	31-A	87	ASP
1	31-A	98	ARG
1	31-A	104	LEU
1	31-A	106	LYS
1	31-A	109	LYS
1	31-A	129	GLU
1	31-A	142	ASP
1	31-A	156	LEU
1	32-A	1	MET
1	32-A	10	VAL
1	32-A	16	MET
1	32-A	17	GLU

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Mol	Chain	Res	Type
1	32-A	24	LEU
1	32-A	33	ARG
1	32-A	52	ARG
1	32-A	54	LEU
1	32-A	65	GLN
1	32-A	87	ASP
1	32-A	98	ARG
1	32-A	106	LYS
1	32-A	118	GLU
1	32-A	120	GLU
1	32-A	128	TYR
1	32-A	142	ASP
1	33-A	1	MET
1	33-A	2	ILE
1	33-A	16	MET
1	33-A	17	GLU
1	33-A	20	MET
1	33-A	33	ARG
1	33-A	88	VAL
1	33-A	89	PRO
1	33-A	106	LYS
1	33-A	131	ASP
1	33-A	139	GLU
1	33-A	142	ASP
1	33-A	158	ARG
1	34-A	2	ILE
1	34-A	16	MET
1	34-A	33	ARG
1	34-A	52	ARG
1	34-A	59	ASN
1	34-A	104	LEU
1	34-A	106	LYS
1	34-A	119	VAL
1	34-A	120	GLU
1	34-A	127	ASP
1	34-A	128	TYR
1	34-A	132	ASP
1	34-A	134	GLU
1	34-A	136	VAL
1	34-A	139	GLU
1	34-A	156	LEU
1	35-A	1	MET

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Mol	Chain	Res	Type
1	35-A	2	ILE
1	35-A	22	TRP
1	35-A	33	ARG
1	35-A	50	ILE
1	35-A	52	ARG
1	35-A	60	ILE
1	35-A	68	THR
1	35-A	79	ASP
1	35-A	104	LEU
1	35-A	106	LYS
1	35-A	108	GLN
1	35-A	127	ASP
1	35-A	148	SER
1	36-A	4	LEU
1	36-A	17	GLU
1	36-A	22	TRP
1	36-A	23	ASN
1	36-A	24	LEU
1	36-A	33	ARG
1	36-A	59	ASN
1	36-A	62	LEU
1	36-A	65	GLN
1	36-A	104	LEU
1	36-A	106	LYS
1	36-A	122	ASP
1	36-A	131	ASP
1	37-A	1	MET
1	37-A	17	GLU
1	37-A	21	PRO
1	37-A	23	ASN
1	37-A	33	ARG
1	37-A	36	LEU
1	37-A	65	GLN
1	37-A	79	ASP
1	37-A	98	ARG
1	37-A	108	GLN
1	37-A	118	GLU
1	37-A	122	ASP
1	37-A	131	ASP
1	37-A	142	ASP
1	37-A	156	LEU
1	38-A	1	MET

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Mol	Chain	Res	Type
1	38-A	10	VAL
1	38-A	17	GLU
1	38-A	20	MET
1	38-A	23	ASN
1	38-A	36	LEU
1	38-A	45	HIS
1	38-A	59	ASN
1	38-A	65	GLN
1	38-A	79	ASP
1	38-A	88	VAL
1	38-A	101	GLU
1	38-A	104	LEU
1	38-A	122	ASP
1	38-A	142	ASP
1	38-A	156	LEU
1	38-A	157	GLU
1	39-A	4	LEU
1	39-A	10	VAL
1	39-A	11	ASP
1	39-A	16	MET
1	39-A	23	ASN
1	39-A	32	LYS
1	39-A	65	GLN
1	39-A	70	ASP
1	39-A	79	ASP
1	39-A	88	VAL
1	39-A	119	VAL
1	39-A	120	GLU
1	39-A	123	THR
1	39-A	129	GLU
1	39-A	139	GLU
1	39-A	142	ASP
1	39-A	157	GLU
1	40-A	1	MET
1	40-A	16	MET
1	40-A	18	ASN
1	40-A	21	PRO
1	40-A	22	TRP
1	40-A	23	ASN
1	40-A	52	ARG
1	40-A	59	ASN
1	40-A	62	LEU

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Mol	Chain	Res	Type
1	40-A	88	VAL
1	40-A	104	LEU
1	40-A	120	GLU
1	40-A	122	ASP
1	40-A	129	GLU
1	40-A	157	GLU
1	40-A	158	ARG
1	41-A	8	LEU
1	41-A	16	MET
1	41-A	20	MET
1	41-A	23	ASN
1	41-A	32	LYS
1	41-A	44	ARG
1	41-A	48	GLU
1	41-A	62	LEU
1	41-A	66	PRO
1	41-A	79	ASP
1	41-A	87	ASP
1	41-A	106	LYS
1	41-A	108	GLN
1	41-A	119	VAL
1	41-A	120	GLU
1	41-A	158	ARG
1	42-A	1	MET
1	42-A	48	GLU
1	42-A	52	ARG
1	42-A	59	ASN
1	42-A	79	ASP
1	42-A	87	ASP
1	42-A	108	GLN
1	42-A	118	GLU
1	42-A	120	GLU
1	42-A	155	ILE
1	42-A	156	LEU
1	43-A	10	VAL
1	43-A	17	GLU
1	43-A	24	LEU
1	43-A	65	GLN
1	43-A	68	THR
1	43-A	87	ASP
1	43-A	118	GLU
1	43-A	119	VAL

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Mol	Chain	Res	Type
1	43-A	120	GLU
1	43-A	135	SER
1	43-A	156	LEU
1	44-A	16	MET
1	44-A	24	LEU
1	44-A	36	LEU
1	44-A	52	ARG
1	44-A	58	LYS
1	44-A	62	LEU
1	44-A	65	GLN
1	44-A	87	ASP
1	44-A	101	GLU
1	44-A	118	GLU
1	44-A	120	GLU
1	44-A	134	GLU
1	44-A	156	LEU
1	45-A	16	MET
1	45-A	17	GLU
1	45-A	24	LEU
1	45-A	33	ARG
1	45-A	36	LEU
1	45-A	44	ARG
1	45-A	52	ARG
1	45-A	58	LYS
1	45-A	65	GLN
1	45-A	87	ASP
1	45-A	98	ARG
1	45-A	106	LYS
1	45-A	118	GLU
1	45-A	120	GLU
1	45-A	132	ASP
1	45-A	135	SER
1	45-A	156	LEU
1	45-A	159	ARG
1	46-A	17	GLU
1	46-A	33	ARG
1	46-A	58	LYS
1	46-A	59	ASN
1	46-A	79	ASP
1	46-A	87	ASP
1	46-A	98	ARG
1	46-A	118	GLU

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Mol	Chain	Res	Type
1	46-A	120	GLU
1	46-A	129	GLU
1	46-A	132	ASP
1	46-A	138	SER
1	46-A	148	SER
1	46-A	156	LEU
1	46-A	159	ARG
1	47-A	4	LEU
1	47-A	23	ASN
1	47-A	33	ARG
1	47-A	36	LEU
1	47-A	45	HIS
1	47-A	52	ARG
1	47-A	58	LYS
1	47-A	59	ASN
1	47-A	85	CYS
1	47-A	98	ARG
1	47-A	118	GLU
1	47-A	148	SER
1	47-A	152	CYS
1	47-A	156	LEU
1	47-A	159	ARG
1	48-A	1	MET
1	48-A	20	MET
1	48-A	33	ARG
1	48-A	36	LEU
1	48-A	44	ARG
1	48-A	52	ARG
1	48-A	98	ARG
1	48-A	108	GLN
1	48-A	118	GLU
1	48-A	119	VAL
1	48-A	148	SER
1	48-A	156	LEU
1	49-A	20	MET
1	49-A	33	ARG
1	49-A	44	ARG
1	49-A	52	ARG
1	49-A	65	GLN
1	49-A	68	THR
1	49-A	88	VAL
1	49-A	118	GLU

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Mol	Chain	Res	Type
1	49-A	135	SER
1	49-A	144	ASP
1	49-A	158	ARG
1	50-A	1	MET
1	50-A	18	ASN
1	50-A	23	ASN
1	50-A	28	LEU
1	50-A	33	ARG
1	50-A	36	LEU
1	50-A	44	ARG
1	50-A	52	ARG
1	50-A	58	LYS
1	50-A	65	GLN
1	50-A	85	CYS
1	50-A	87	ASP
1	50-A	88	VAL
1	50-A	98	ARG
1	50-A	119	VAL
1	50-A	120	GLU
1	50-A	128	TYR
1	50-A	129	GLU
1	50-A	142	ASP
1	50-A	144	ASP
1	50-A	156	LEU
1	51-A	11	ASP
1	51-A	33	ARG
1	51-A	36	LEU
1	51-A	44	ARG
1	51-A	52	ARG
1	51-A	59	ASN
1	51-A	70	ASP
1	51-A	76	LYS
1	51-A	98	ARG
1	51-A	109	LYS
1	51-A	119	VAL
1	51-A	120	GLU
1	51-A	127	ASP
1	51-A	128	TYR
1	51-A	156	LEU
1	52-A	11	ASP
1	52-A	16	MET
1	52-A	18	ASN

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Mol	Chain	Res	Type
1	52-A	23	ASN
1	52-A	33	ARG
1	52-A	65	GLN
1	52-A	70	ASP
1	52-A	85	CYS
1	52-A	88	VAL
1	52-A	98	ARG
1	52-A	104	LEU
1	52-A	129	GLU
1	52-A	132	ASP
1	52-A	139	GLU
1	53-A	1	MET
1	53-A	11	ASP
1	53-A	24	LEU
1	53-A	33	ARG
1	53-A	52	ARG
1	53-A	59	ASN
1	53-A	87	ASP
1	53-A	88	VAL
1	53-A	101	GLU
1	53-A	104	LEU
1	53-A	118	GLU
1	53-A	127	ASP
1	53-A	128	TYR
1	53-A	138	SER
1	53-A	139	GLU
1	53-A	156	LEU
1	53-A	157	GLU
1	54-A	1	MET
1	54-A	17	GLU
1	54-A	23	ASN
1	54-A	24	LEU
1	54-A	33	ARG
1	54-A	48	GLU
1	54-A	58	LYS
1	54-A	59	ASN
1	54-A	76	LYS
1	54-A	104	LEU
1	54-A	106	LYS
1	54-A	122	ASP
1	54-A	127	ASP
1	54-A	128	TYR

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Mol	Chain	Res	Type
1	54-A	139	GLU
1	54-A	154	GLU
1	54-A	156	LEU
1	55-A	4	LEU
1	55-A	16	MET
1	55-A	18	ASN
1	55-A	23	ASN
1	55-A	24	LEU
1	55-A	33	ARG
1	55-A	52	ARG
1	55-A	70	ASP
1	55-A	98	ARG
1	55-A	104	LEU
1	55-A	106	LYS
1	55-A	108	GLN
1	55-A	118	GLU
1	55-A	122	ASP
1	55-A	132	ASP
1	55-A	138	SER
1	55-A	152	CYS
1	55-A	156	LEU
1	56-A	1	MET
1	56-A	17	GLU
1	56-A	18	ASN
1	56-A	23	ASN
1	56-A	24	LEU
1	56-A	33	ARG
1	56-A	59	ASN
1	56-A	79	ASP
1	56-A	98	ARG
1	56-A	106	LYS
1	56-A	108	GLN
1	56-A	118	GLU
1	56-A	127	ASP
1	57-A	1	MET
1	57-A	18	ASN
1	57-A	20	MET
1	57-A	24	LEU
1	57-A	30	TRP
1	57-A	33	ARG
1	57-A	54	LEU
1	57-A	61	ILE

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Mol	Chain	Res	Type
1	57-A	62	LEU
1	57-A	65	GLN
1	57-A	79	ASP
1	57-A	87	ASP
1	57-A	88	VAL
1	57-A	108	GLN
1	57-A	128	TYR
1	57-A	156	LEU
1	58-A	1	MET
1	58-A	8	LEU
1	58-A	16	MET
1	58-A	28	LEU
1	58-A	52	ARG
1	58-A	54	LEU
1	58-A	88	VAL
1	58-A	108	GLN
1	58-A	156	LEU
1	58-A	157	GLU
1	58-A	158	ARG
1	59-A	20	MET
1	59-A	23	ASN
1	59-A	37	ASN
1	59-A	52	ARG
1	59-A	101	GLU
1	59-A	104	LEU
1	59-A	108	GLN
1	59-A	138	SER
1	59-A	156	LEU
1	60-A	16	MET
1	60-A	18	ASN
1	60-A	20	MET
1	60-A	24	LEU
1	60-A	33	ARG
1	60-A	52	ARG
1	60-A	89	PRO
1	60-A	98	ARG
1	60-A	104	LEU
1	60-A	108	GLN
1	60-A	122	ASP
1	60-A	127	ASP
1	60-A	128	TYR
1	60-A	130	PRO

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Mol	Chain	Res	Type
1	60-A	138	SER
1	60-A	144	ASP
1	60-A	147	ASN
1	60-A	148	SER
1	60-A	156	LEU
1	60-A	157	GLU
1	60-A	158	ARG
1	60-A	159	ARG
1	61-A	16	MET
1	61-A	20	MET
1	61-A	28	LEU
1	61-A	33	ARG
1	61-A	49	SER
1	61-A	52	ARG
1	61-A	54	LEU
1	61-A	65	GLN
1	61-A	79	ASP
1	61-A	108	GLN
1	61-A	119	VAL
1	61-A	127	ASP
1	61-A	128	TYR
1	61-A	129	GLU
1	61-A	139	GLU
1	61-A	156	LEU
1	61-A	157	GLU
1	61-A	158	ARG
1	62-A	1	MET
1	62-A	20	MET
1	62-A	23	ASN
1	62-A	24	LEU
1	62-A	28	LEU
1	62-A	33	ARG
1	62-A	52	ARG
1	62-A	59	ASN
1	62-A	65	GLN
1	62-A	76	LYS
1	62-A	87	ASP
1	62-A	88	VAL
1	62-A	108	GLN
1	62-A	122	ASP
1	62-A	127	ASP
1	62-A	129	GLU

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Mol	Chain	Res	Type
1	62-A	139	GLU
1	62-A	156	LEU
1	63-A	18	ASN
1	63-A	24	LEU
1	63-A	33	ARG
1	63-A	76	LYS
1	63-A	87	ASP
1	63-A	88	VAL
1	63-A	108	GLN
1	63-A	138	SER
1	63-A	139	GLU
1	63-A	159	ARG
1	64-A	1	MET
1	64-A	2	ILE
1	64-A	20	MET
1	64-A	33	ARG
1	64-A	59	ASN
1	64-A	87	ASP
1	64-A	98	ARG
1	64-A	106	LYS
1	64-A	108	GLN
1	64-A	127	ASP
1	64-A	137	PHE
1	64-A	138	SER
1	64-A	148	SER
1	64-A	156	LEU
1	65-A	1	MET
1	65-A	2	ILE
1	65-A	16	MET
1	65-A	33	ARG
1	65-A	52	ARG
1	65-A	54	LEU
1	65-A	65	GLN
1	65-A	79	ASP
1	65-A	87	ASP
1	65-A	98	ARG
1	65-A	106	LYS
1	65-A	108	GLN
1	65-A	139	GLU
1	65-A	142	ASP
1	65-A	156	LEU
1	65-A	157	GLU

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Mol	Chain	Res	Type
1	66-A	1	MET
1	66-A	2	ILE
1	66-A	11	ASP
1	66-A	16	MET
1	66-A	20	MET
1	66-A	30	TRP
1	66-A	33	ARG
1	66-A	52	ARG
1	66-A	59	ASN
1	66-A	65	GLN
1	66-A	79	ASP
1	66-A	87	ASP
1	66-A	98	ARG
1	66-A	106	LYS
1	66-A	118	GLU
1	66-A	129	GLU
1	66-A	136	VAL
1	66-A	157	GLU
1	67-A	2	ILE
1	67-A	11	ASP
1	67-A	16	MET
1	67-A	18	ASN
1	67-A	20	MET
1	67-A	33	ARG
1	67-A	65	GLN
1	67-A	79	ASP
1	67-A	98	ARG
1	67-A	118	GLU
1	67-A	134	GLU
1	67-A	136	VAL
1	67-A	152	CYS
1	67-A	157	GLU
1	67-A	159	ARG
1	68-A	16	MET
1	68-A	20	MET
1	68-A	33	ARG
1	68-A	36	LEU
1	68-A	52	ARG
1	68-A	62	LEU
1	68-A	65	GLN
1	68-A	87	ASP
1	68-A	98	ARG

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Mol	Chain	Res	Type
1	68-A	118	GLU
1	68-A	127	ASP
1	68-A	159	ARG
1	69-A	1	MET
1	69-A	16	MET
1	69-A	20	MET
1	69-A	22	TRP
1	69-A	23	ASN
1	69-A	32	LYS
1	69-A	62	LEU
1	69-A	65	GLN
1	69-A	79	ASP
1	69-A	98	ARG
1	69-A	118	GLU
1	69-A	135	SER
1	69-A	142	ASP
1	69-A	159	ARG
1	70-A	1	MET
1	70-A	4	LEU
1	70-A	16	MET
1	70-A	18	ASN
1	70-A	20	MET
1	70-A	22	TRP
1	70-A	23	ASN
1	70-A	33	ARG
1	70-A	52	ARG
1	70-A	59	ASN
1	70-A	98	ARG
1	70-A	128	TYR
1	70-A	135	SER
1	70-A	138	SER
1	70-A	148	SER
1	71-A	18	ASN
1	71-A	22	TRP
1	71-A	70	ASP
1	71-A	88	VAL
1	71-A	98	ARG
1	71-A	120	GLU
1	71-A	123	THR
1	71-A	128	TYR
1	71-A	152	CYS
1	72-A	1	MET

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Mol	Chain	Res	Type
1	72-A	8	LEU
1	72-A	16	MET
1	72-A	18	ASN
1	72-A	20	MET
1	72-A	70	ASP
1	72-A	88	VAL
1	72-A	98	ARG
1	72-A	101	GLU
1	72-A	104	LEU
1	72-A	108	GLN
1	72-A	120	GLU
1	72-A	132	ASP
1	72-A	138	SER
1	72-A	152	CYS
1	72-A	154	GLU
1	73-A	8	LEU
1	73-A	10	VAL
1	73-A	16	MET
1	73-A	18	ASN
1	73-A	20	MET
1	73-A	21	PRO
1	73-A	52	ARG
1	73-A	65	GLN
1	73-A	98	ARG
1	73-A	104	LEU
1	73-A	108	GLN
1	73-A	118	GLU
1	73-A	120	GLU
1	73-A	148	SER
1	74-A	1	MET
1	74-A	8	LEU
1	74-A	18	ASN
1	74-A	20	MET
1	74-A	33	ARG
1	74-A	49	SER
1	74-A	65	GLN
1	74-A	79	ASP
1	74-A	89	PRO
1	74-A	104	LEU
1	74-A	118	GLU
1	74-A	119	VAL
1	74-A	132	ASP

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Mol	Chain	Res	Type
1	74-A	148	SER
1	74-A	152	CYS
1	75-A	1	MET
1	75-A	12	ARG
1	75-A	16	MET
1	75-A	18	ASN
1	75-A	33	ARG
1	75-A	52	ARG
1	75-A	65	GLN
1	75-A	79	ASP
1	75-A	88	VAL
1	75-A	108	GLN
1	75-A	128	TYR
1	75-A	137	PHE
1	75-A	156	LEU
1	76-A	12	ARG
1	76-A	16	MET
1	76-A	18	ASN
1	76-A	52	ARG
1	76-A	59	ASN
1	76-A	60	ILE
1	76-A	65	GLN
1	76-A	79	ASP
1	76-A	88	VAL
1	76-A	106	LYS
1	76-A	108	GLN
1	76-A	109	LYS
1	76-A	119	VAL
1	76-A	128	TYR
1	76-A	135	SER
1	76-A	156	LEU
1	76-A	158	ARG
1	76-A	159	ARG
1	77-A	12	ARG
1	77-A	18	ASN
1	77-A	36	LEU
1	77-A	52	ARG
1	77-A	59	ASN
1	77-A	65	GLN
1	77-A	76	LYS
1	77-A	106	LYS
1	77-A	108	GLN

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Mol	Chain	Res	Type
1	77-A	118	GLU
1	77-A	128	TYR
1	77-A	129	GLU
1	77-A	156	LEU
1	78-A	1	MET
1	78-A	4	LEU
1	78-A	12	ARG
1	78-A	18	ASN
1	78-A	33	ARG
1	78-A	36	LEU
1	78-A	52	ARG
1	78-A	65	GLN
1	78-A	76	LYS
1	78-A	79	ASP
1	78-A	88	VAL
1	78-A	104	LEU
1	78-A	106	LYS
1	78-A	118	GLU
1	78-A	128	TYR
1	78-A	135	SER
1	78-A	138	SER
1	78-A	158	ARG
1	79-A	1	MET
1	79-A	12	ARG
1	79-A	16	MET
1	79-A	36	LEU
1	79-A	48	GLU
1	79-A	52	ARG
1	79-A	59	ASN
1	79-A	76	LYS
1	79-A	88	VAL
1	79-A	109	LYS
1	79-A	123	THR
1	79-A	128	TYR
1	79-A	129	GLU
1	79-A	158	ARG
1	80-A	12	ARG
1	80-A	16	MET
1	80-A	17	GLU
1	80-A	18	ASN
1	80-A	33	ARG
1	80-A	44	ARG

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Mol	Chain	Res	Type
1	80-A	48	GLU
1	80-A	52	ARG
1	80-A	59	ASN
1	80-A	76	LYS
1	80-A	79	ASP
1	80-A	88	VAL
1	80-A	104	LEU
1	80-A	106	LYS
1	80-A	108	GLN
1	80-A	109	LYS
1	80-A	127	ASP
1	80-A	128	TYR
1	80-A	138	SER
1	80-A	142	ASP
1	80-A	148	SER
1	81-A	1	MET
1	81-A	16	MET
1	81-A	33	ARG
1	81-A	48	GLU
1	81-A	76	LYS
1	81-A	104	LEU
1	81-A	109	LYS
1	81-A	118	GLU
1	81-A	119	VAL
1	81-A	127	ASP
1	81-A	131	ASP
1	81-A	132	ASP
1	81-A	158	ARG
1	82-A	1	MET
1	82-A	2	ILE
1	82-A	10	VAL
1	82-A	16	MET
1	82-A	18	ASN
1	82-A	33	ARG
1	82-A	52	ARG
1	82-A	58	LYS
1	82-A	59	ASN
1	82-A	119	VAL
1	82-A	127	ASP
1	82-A	128	TYR
1	82-A	131	ASP
1	82-A	154	GLU

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Mol	Chain	Res	Type
1	83-A	1	MET
1	83-A	23	ASN
1	83-A	30	TRP
1	83-A	33	ARG
1	83-A	36	LEU
1	83-A	44	ARG
1	83-A	52	ARG
1	83-A	128	TYR
1	83-A	129	GLU
1	84-A	1	MET
1	84-A	18	ASN
1	84-A	23	ASN
1	84-A	36	LEU
1	84-A	58	LYS
1	84-A	65	GLN
1	84-A	118	GLU
1	84-A	127	ASP
1	84-A	129	GLU
1	85-A	1	MET
1	85-A	16	MET
1	85-A	36	LEU
1	85-A	54	LEU
1	85-A	58	LYS
1	85-A	87	ASP
1	85-A	88	VAL
1	85-A	104	LEU
1	85-A	106	LYS
1	85-A	127	ASP
1	85-A	134	GLU
1	85-A	148	SER
1	86-A	1	MET
1	86-A	16	MET
1	86-A	18	ASN
1	86-A	33	ARG
1	86-A	36	LEU
1	86-A	49	SER
1	86-A	54	LEU
1	86-A	65	GLN
1	86-A	104	LEU
1	86-A	120	GLU
1	86-A	127	ASP
1	86-A	129	GLU

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Mol	Chain	Res	Type
1	86-A	155	ILE
1	87-A	1	MET
1	87-A	18	ASN
1	87-A	23	ASN
1	87-A	36	LEU
1	87-A	54	LEU
1	87-A	58	LYS
1	87-A	98	ARG
1	87-A	104	LEU
1	87-A	119	VAL
1	87-A	122	ASP
1	87-A	127	ASP
1	88-A	1	MET
1	88-A	28	LEU
1	88-A	36	LEU
1	88-A	52	ARG
1	88-A	58	LYS
1	88-A	65	GLN
1	88-A	88	VAL
1	88-A	104	LEU
1	88-A	119	VAL
1	88-A	130	PRO
1	88-A	134	GLU
1	88-A	135	SER
1	88-A	138	SER
1	88-A	144	ASP
1	88-A	148	SER
1	88-A	158	ARG
1	89-A	1	MET
1	89-A	11	ASP
1	89-A	18	ASN
1	89-A	24	LEU
1	89-A	33	ARG
1	89-A	52	ARG
1	89-A	65	GLN
1	89-A	76	LYS
1	89-A	101	GLU
1	89-A	104	LEU
1	89-A	118	GLU
1	89-A	128	TYR
1	89-A	130	PRO
1	89-A	144	ASP

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Mol	Chain	Res	Type
1	90-A	1	MET
1	90-A	10	VAL
1	90-A	11	ASP
1	90-A	20	MET
1	90-A	23	ASN
1	90-A	36	LEU
1	90-A	52	ARG
1	90-A	54	LEU
1	90-A	98	ARG
1	90-A	104	LEU
1	90-A	120	GLU
1	90-A	134	GLU
1	90-A	136	VAL
1	90-A	142	ASP
1	90-A	144	ASP
1	90-A	154	GLU
1	91-A	16	MET
1	91-A	20	MET
1	91-A	24	LEU
1	91-A	36	LEU
1	91-A	54	LEU
1	91-A	87	ASP
1	91-A	88	VAL
1	91-A	101	GLU
1	91-A	104	LEU
1	91-A	120	GLU
1	91-A	132	ASP
1	91-A	134	GLU
1	91-A	142	ASP
1	91-A	144	ASP
1	92-A	1	MET
1	92-A	10	VAL
1	92-A	16	MET
1	92-A	33	ARG
1	92-A	36	LEU
1	92-A	52	ARG
1	92-A	59	ASN
1	92-A	87	ASP
1	92-A	88	VAL
1	92-A	101	GLU
1	92-A	109	LYS
1	92-A	142	ASP

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Mol	Chain	Res	Type
1	93-A	16	MET
1	93-A	17	GLU
1	93-A	18	ASN
1	93-A	24	LEU
1	93-A	32	LYS
1	93-A	33	ARG
1	93-A	36	LEU
1	93-A	48	GLU
1	93-A	52	ARG
1	93-A	87	ASP
1	93-A	88	VAL
1	93-A	109	LYS
1	93-A	122	ASP
1	93-A	128	TYR
1	93-A	157	GLU
1	94-A	16	MET
1	94-A	17	GLU
1	94-A	18	ASN
1	94-A	23	ASN
1	94-A	24	LEU
1	94-A	32	LYS
1	94-A	33	ARG
1	94-A	58	LYS
1	94-A	59	ASN
1	94-A	60	ILE
1	94-A	87	ASP
1	94-A	98	ARG
1	94-A	129	GLU
1	94-A	132	ASP
1	94-A	134	GLU
1	94-A	138	SER
1	94-A	156	LEU
1	95-A	2	ILE
1	95-A	16	MET
1	95-A	17	GLU
1	95-A	18	ASN
1	95-A	32	LYS
1	95-A	33	ARG
1	95-A	52	ARG
1	95-A	58	LYS
1	95-A	59	ASN
1	95-A	60	ILE

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Mol	Chain	Res	Type
1	95-A	85	CYS
1	95-A	87	ASP
1	95-A	89	PRO
1	95-A	104	LEU
1	95-A	118	GLU
1	95-A	120	GLU
1	95-A	129	GLU
1	96-A	1	MET
1	96-A	2	ILE
1	96-A	16	MET
1	96-A	17	GLU
1	96-A	24	LEU
1	96-A	33	ARG
1	96-A	59	ASN
1	96-A	65	GLN
1	96-A	66	PRO
1	96-A	87	ASP
1	96-A	88	VAL
1	96-A	101	GLU
1	96-A	104	LEU
1	96-A	106	LYS
1	96-A	109	LYS
1	96-A	119	VAL
1	96-A	122	ASP
1	96-A	157	GLU
1	96-A	159	ARG
1	97-A	4	LEU
1	97-A	18	ASN
1	97-A	20	MET
1	97-A	33	ARG
1	97-A	52	ARG
1	97-A	58	LYS
1	97-A	65	GLN
1	97-A	70	ASP
1	97-A	76	LYS
1	97-A	79	ASP
1	97-A	87	ASP
1	97-A	88	VAL
1	97-A	98	ARG
1	97-A	101	GLU
1	97-A	118	GLU
1	97-A	119	VAL

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Mol	Chain	Res	Type
1	97-A	123	THR
1	97-A	157	GLU
1	98-A	1	MET
1	98-A	16	MET
1	98-A	18	ASN
1	98-A	24	LEU
1	98-A	33	ARG
1	98-A	52	ARG
1	98-A	58	LYS
1	98-A	62	LEU
1	98-A	65	GLN
1	98-A	76	LYS
1	98-A	101	GLU
1	98-A	106	LYS
1	98-A	119	VAL
1	98-A	138	SER
1	99-A	18	ASN
1	99-A	24	LEU
1	99-A	33	ARG
1	99-A	52	ARG
1	99-A	58	LYS
1	99-A	65	GLN
1	99-A	68	THR
1	99-A	76	LYS
1	99-A	77	SER
1	99-A	87	ASP
1	99-A	104	LEU
1	99-A	106	LYS
1	99-A	109	LYS
1	99-A	128	TYR
1	99-A	135	SER
1	99-A	138	SER
1	99-A	158	ARG
1	100-A	20	MET
1	100-A	24	LEU
1	100-A	49	SER
1	100-A	52	ARG
1	100-A	58	LYS
1	100-A	59	ASN
1	100-A	60	ILE
1	100-A	65	GLN
1	100-A	79	ASP

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Mol	Chain	Res	Type
1	100-A	104	LEU
1	100-A	106	LYS
1	100-A	109	LYS
1	100-A	120	GLU
1	100-A	141	HIS
1	101-A	8	LEU
1	101-A	17	GLU
1	101-A	52	ARG
1	101-A	58	LYS
1	101-A	104	LEU
1	101-A	118	GLU
1	101-A	119	VAL
1	101-A	137	PHE
1	101-A	148	SER
1	102-A	1	MET
1	102-A	8	LEU
1	102-A	16	MET
1	102-A	17	GLU
1	102-A	18	ASN
1	102-A	52	ARG
1	102-A	58	LYS
1	102-A	68	THR
1	102-A	104	LEU
1	102-A	120	GLU
1	102-A	127	ASP
1	102-A	134	GLU
1	102-A	141	HIS
1	102-A	142	ASP
1	103-A	1	MET
1	103-A	17	GLU
1	103-A	18	ASN
1	103-A	23	ASN
1	103-A	36	LEU
1	103-A	45	HIS
1	103-A	52	ARG
1	103-A	58	LYS
1	103-A	65	GLN
1	103-A	104	LEU
1	103-A	120	GLU
1	103-A	129	GLU
1	103-A	139	GLU
1	103-A	141	HIS

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Mol	Chain	Res	Type
1	103-A	152	CYS
1	103-A	158	ARG
1	104-A	1	MET
1	104-A	23	ASN
1	104-A	36	LEU
1	104-A	45	HIS
1	104-A	76	LYS
1	104-A	87	ASP
1	104-A	108	GLN
1	104-A	138	SER
1	104-A	139	GLU
1	104-A	141	HIS
1	104-A	148	SER
1	105-A	1	MET
1	105-A	17	GLU
1	105-A	18	ASN
1	105-A	20	MET
1	105-A	23	ASN
1	105-A	24	LEU
1	105-A	36	LEU
1	105-A	45	HIS
1	105-A	59	ASN
1	105-A	65	GLN
1	105-A	79	ASP
1	105-A	108	GLN
1	105-A	109	LYS
1	105-A	120	GLU
1	105-A	128	TYR
1	105-A	132	ASP
1	105-A	141	HIS
1	105-A	148	SER
1	106-A	1	MET
1	106-A	4	LEU
1	106-A	17	GLU
1	106-A	23	ASN
1	106-A	24	LEU
1	106-A	36	LEU
1	106-A	49	SER
1	106-A	58	LYS
1	106-A	65	GLN
1	106-A	79	ASP
1	106-A	88	VAL

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Mol	Chain	Res	Type
1	106-A	106	LYS
1	106-A	108	GLN
1	106-A	122	ASP
1	106-A	129	GLU
1	106-A	132	ASP
1	106-A	137	PHE
1	106-A	141	HIS
1	106-A	148	SER
1	106-A	150	SER
1	106-A	152	CYS
1	106-A	159	ARG
1	107-A	16	MET
1	107-A	18	ASN
1	107-A	20	MET
1	107-A	21	PRO
1	107-A	23	ASN
1	107-A	24	LEU
1	107-A	52	ARG
1	107-A	58	LYS
1	107-A	59	ASN
1	107-A	60	ILE
1	107-A	79	ASP
1	107-A	87	ASP
1	107-A	88	VAL
1	107-A	104	LEU
1	107-A	106	LYS
1	107-A	108	GLN
1	107-A	119	VAL
1	107-A	129	GLU
1	107-A	135	SER
1	107-A	148	SER
1	107-A	156	LEU
1	107-A	159	ARG
1	108-A	1	MET
1	108-A	13	VAL
1	108-A	20	MET
1	108-A	23	ASN
1	108-A	24	LEU
1	108-A	49	SER
1	108-A	52	ARG
1	108-A	58	LYS
1	108-A	59	ASN

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Mol	Chain	Res	Type
1	108-A	98	ARG
1	108-A	104	LEU
1	108-A	106	LYS
1	108-A	108	GLN
1	108-A	127	ASP
1	108-A	138	SER
1	108-A	152	CYS
1	108-A	156	LEU
1	108-A	159	ARG
1	109-A	17	GLU
1	109-A	18	ASN
1	109-A	23	ASN
1	109-A	30	TRP
1	109-A	33	ARG
1	109-A	45	HIS
1	109-A	52	ARG
1	109-A	58	LYS
1	109-A	87	ASP
1	109-A	98	ARG
1	109-A	104	LEU
1	109-A	106	LYS
1	109-A	108	GLN
1	109-A	129	GLU
1	110-A	1	MET
1	110-A	18	ASN
1	110-A	20	MET
1	110-A	23	ASN
1	110-A	49	SER
1	110-A	59	ASN
1	110-A	76	LYS
1	110-A	98	ARG
1	110-A	106	LYS
1	110-A	108	GLN
1	110-A	118	GLU
1	110-A	129	GLU
1	110-A	135	SER
1	110-A	152	CYS
1	110-A	156	LEU
1	111-A	13	VAL
1	111-A	16	MET
1	111-A	18	ASN
1	111-A	65	GLN

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Mol	Chain	Res	Type
1	111-A	68	THR
1	111-A	76	LYS
1	111-A	98	ARG
1	111-A	106	LYS
1	111-A	108	GLN
1	111-A	118	GLU
1	111-A	156	LEU
1	111-A	157	GLU
1	112-A	16	MET
1	112-A	18	ASN
1	112-A	20	MET
1	112-A	54	LEU
1	112-A	59	ASN
1	112-A	61	ILE
1	112-A	68	THR
1	112-A	76	LYS
1	112-A	87	ASP
1	112-A	98	ARG
1	112-A	106	LYS
1	112-A	108	GLN
1	112-A	115	ILE
1	112-A	118	GLU
1	112-A	142	ASP
1	113-A	1	MET
1	113-A	2	ILE
1	113-A	4	LEU
1	113-A	23	ASN
1	113-A	33	ARG
1	113-A	52	ARG
1	113-A	54	LEU
1	113-A	58	LYS
1	113-A	60	ILE
1	113-A	65	GLN
1	113-A	68	THR
1	113-A	76	LYS
1	113-A	106	LYS
1	113-A	108	GLN
1	113-A	127	ASP
1	113-A	128	TYR
1	113-A	142	ASP
1	114-A	1	MET
1	114-A	2	ILE

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Mol	Chain	Res	Type
1	114-A	8	LEU
1	114-A	11	ASP
1	114-A	18	ASN
1	114-A	20	MET
1	114-A	33	ARG
1	114-A	52	ARG
1	114-A	58	LYS
1	114-A	59	ASN
1	114-A	76	LYS
1	114-A	87	ASP
1	114-A	104	LEU
1	114-A	106	LYS
1	114-A	120	GLU
1	114-A	122	ASP
1	114-A	127	ASP
1	114-A	128	TYR
1	114-A	142	ASP
1	114-A	158	ARG
1	115-A	1	MET
1	115-A	2	ILE
1	115-A	8	LEU
1	115-A	10	VAL
1	115-A	13	VAL
1	115-A	16	MET
1	115-A	20	MET
1	115-A	23	ASN
1	115-A	24	LEU
1	115-A	33	ARG
1	115-A	52	ARG
1	115-A	65	GLN
1	115-A	68	THR
1	115-A	87	ASP
1	115-A	109	LYS
1	115-A	119	VAL
1	115-A	122	ASP
1	115-A	132	ASP
1	115-A	136	VAL
1	115-A	157	GLU
1	115-A	158	ARG
1	116-A	1	MET
1	116-A	2	ILE
1	116-A	16	MET

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Mol	Chain	Res	Type
1	116-A	20	MET
1	116-A	23	ASN
1	116-A	24	LEU
1	116-A	27	ASP
1	116-A	44	ARG
1	116-A	52	ARG
1	116-A	64	SER
1	116-A	68	THR
1	116-A	87	ASP
1	116-A	109	LYS
1	116-A	132	ASP
1	116-A	138	SER
1	116-A	152	CYS
1	116-A	157	GLU
1	117-A	2	ILE
1	117-A	11	ASP
1	117-A	16	MET
1	117-A	18	ASN
1	117-A	23	ASN
1	117-A	24	LEU
1	117-A	28	LEU
1	117-A	52	ARG
1	117-A	58	LYS
1	117-A	68	THR
1	117-A	87	ASP
1	117-A	104	LEU
1	117-A	106	LYS
1	117-A	127	ASP
1	117-A	128	TYR
1	117-A	132	ASP
1	117-A	138	SER
1	117-A	148	SER
1	118-A	1	MET
1	118-A	2	ILE
1	118-A	4	LEU
1	118-A	16	MET
1	118-A	18	ASN
1	118-A	20	MET
1	118-A	23	ASN
1	118-A	24	LEU
1	118-A	33	ARG
1	118-A	52	ARG

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Mol	Chain	Res	Type
1	118-A	101	GLU
1	118-A	104	LEU
1	118-A	109	LYS
1	118-A	118	GLU
1	118-A	119	VAL
1	118-A	122	ASP
1	118-A	127	ASP
1	118-A	132	ASP
1	118-A	134	GLU
1	118-A	139	GLU
1	119-A	1	MET
1	119-A	2	ILE
1	119-A	18	ASN
1	119-A	22	TRP
1	119-A	23	ASN
1	119-A	36	LEU
1	119-A	52	ARG
1	119-A	65	GLN
1	119-A	70	ASP
1	119-A	79	ASP
1	119-A	87	ASP
1	119-A	101	GLU
1	119-A	118	GLU
1	119-A	119	VAL
1	119-A	122	ASP
1	119-A	157	GLU
1	119-A	159	ARG
1	120-A	23	ASN
1	120-A	33	ARG
1	120-A	36	LEU
1	120-A	58	LYS
1	120-A	79	ASP
1	120-A	87	ASP
1	120-A	108	GLN
1	120-A	119	VAL
1	120-A	122	ASP
1	120-A	159	ARG
1	121-A	1	MET
1	121-A	4	LEU
1	121-A	18	ASN
1	121-A	20	MET
1	121-A	33	ARG

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Mol	Chain	Res	Type
1	121-A	44	ARG
1	121-A	49	SER
1	121-A	52	ARG
1	121-A	79	ASP
1	121-A	87	ASP
1	121-A	101	GLU
1	121-A	108	GLN
1	121-A	118	GLU
1	121-A	122	ASP
1	121-A	128	TYR
1	121-A	129	GLU
1	121-A	131	ASP
1	121-A	158	ARG
1	122-A	16	MET
1	122-A	18	ASN
1	122-A	23	ASN
1	122-A	33	ARG
1	122-A	60	ILE
1	122-A	79	ASP
1	122-A	87	ASP
1	122-A	101	GLU
1	122-A	118	GLU
1	122-A	122	ASP
1	122-A	127	ASP
1	122-A	131	ASP
1	122-A	159	ARG
1	123-A	11	ASP
1	123-A	18	ASN
1	123-A	23	ASN
1	123-A	33	ARG
1	123-A	87	ASP
1	123-A	118	GLU
1	123-A	122	ASP
1	123-A	127	ASP
1	123-A	128	TYR
1	123-A	129	GLU
1	123-A	132	ASP
1	123-A	135	SER
1	123-A	148	SER
1	123-A	156	LEU
1	123-A	159	ARG
1	124-A	1	MET

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Mol	Chain	Res	Type
1	124-A	4	LEU
1	124-A	16	MET
1	124-A	33	ARG
1	124-A	52	ARG
1	124-A	119	VAL
1	124-A	128	TYR
1	124-A	132	ASP
1	124-A	148	SER
1	124-A	156	LEU
1	124-A	158	ARG
1	124-A	159	ARG
1	125-A	1	MET
1	125-A	8	LEU
1	125-A	17	GLU
1	125-A	24	LEU
1	125-A	28	LEU
1	125-A	33	ARG
1	125-A	59	ASN
1	125-A	61	ILE
1	125-A	87	ASP
1	125-A	118	GLU
1	125-A	129	GLU
1	125-A	148	SER
1	126-A	17	GLU
1	126-A	24	LEU
1	126-A	33	ARG
1	126-A	70	ASP
1	126-A	87	ASP
1	126-A	106	LYS
1	126-A	108	GLN
1	126-A	118	GLU
1	126-A	120	GLU
1	126-A	156	LEU
1	126-A	158	ARG
1	127-A	1	MET
1	127-A	24	LEU
1	127-A	28	LEU
1	127-A	33	ARG
1	127-A	65	GLN
1	127-A	104	LEU
1	127-A	118	GLU
1	127-A	123	THR

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Mol	Chain	Res	Type
1	127-A	129	GLU
1	127-A	132	ASP
1	127-A	135	SER
1	128-A	1	MET
1	128-A	16	MET
1	128-A	18	ASN
1	128-A	20	MET
1	128-A	22	TRP
1	128-A	24	LEU
1	128-A	33	ARG
1	128-A	52	ARG
1	128-A	104	LEU
1	128-A	119	VAL
1	128-A	120	GLU
1	128-A	127	ASP
1	128-A	132	ASP
1	128-A	154	GLU
1	129-A	1	MET
1	129-A	4	LEU
1	129-A	16	MET
1	129-A	20	MET
1	129-A	52	ARG
1	129-A	118	GLU
1	129-A	119	VAL
1	129-A	127	ASP
1	129-A	146	GLN
1	129-A	159	ARG
1	130-A	1	MET
1	130-A	16	MET
1	130-A	59	ASN
1	130-A	119	VAL
1	130-A	120	GLU
1	130-A	129	GLU
1	130-A	134	GLU
1	130-A	146	GLN
1	131-A	10	VAL
1	131-A	16	MET
1	131-A	20	MET
1	131-A	24	LEU
1	131-A	28	LEU
1	131-A	101	GLU
1	131-A	109	LYS

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Mol	Chain	Res	Type
1	131-A	115	ILE
1	131-A	119	VAL
1	131-A	129	GLU
1	131-A	134	GLU
1	131-A	146	GLN
1	132-A	10	VAL
1	132-A	16	MET
1	132-A	23	ASN
1	132-A	28	LEU
1	132-A	59	ASN
1	132-A	106	LYS
1	132-A	119	VAL
1	132-A	129	GLU
1	132-A	142	ASP
1	132-A	146	GLN
1	133-A	16	MET
1	133-A	18	ASN
1	133-A	28	LEU
1	133-A	52	ARG
1	133-A	106	LYS
1	133-A	109	LYS
1	133-A	118	GLU
1	133-A	119	VAL
1	133-A	129	GLU
1	133-A	142	ASP
1	133-A	146	GLN
1	134-A	1	MET
1	134-A	8	LEU
1	134-A	16	MET
1	134-A	20	MET
1	134-A	23	ASN
1	134-A	30	TRP
1	134-A	33	ARG
1	134-A	87	ASP
1	134-A	106	LYS
1	134-A	109	LYS
1	134-A	120	GLU
1	134-A	129	GLU
1	134-A	146	GLN
1	135-A	8	LEU
1	135-A	11	ASP
1	135-A	16	MET

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Mol	Chain	Res	Type
1	135-A	33	ARG
1	135-A	44	ARG
1	135-A	52	ARG
1	135-A	87	ASP
1	135-A	120	GLU
1	135-A	129	GLU
1	135-A	146	GLN
1	135-A	159	ARG
1	136-A	1	MET
1	136-A	10	VAL
1	136-A	16	MET
1	136-A	28	LEU
1	136-A	33	ARG
1	136-A	66	PRO
1	136-A	79	ASP
1	136-A	87	ASP
1	136-A	104	LEU
1	136-A	118	GLU
1	136-A	128	TYR
1	136-A	129	GLU
1	136-A	131	ASP
1	136-A	138	SER
1	137-A	13	VAL
1	137-A	16	MET
1	137-A	18	ASN
1	137-A	23	ASN
1	137-A	52	ARG
1	137-A	106	LYS
1	137-A	108	GLN
1	137-A	127	ASP
1	137-A	128	TYR
1	137-A	129	GLU
1	137-A	131	ASP
1	137-A	146	GLN
1	137-A	157	GLU
1	138-A	1	MET
1	138-A	2	ILE
1	138-A	10	VAL
1	138-A	11	ASP
1	138-A	16	MET
1	138-A	17	GLU
1	138-A	52	ARG

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Mol	Chain	Res	Type
1	138-A	59	ASN
1	138-A	70	ASP
1	138-A	76	LYS
1	138-A	108	GLN
1	138-A	118	GLU
1	138-A	128	TYR
1	138-A	129	GLU
1	138-A	138	SER
1	138-A	146	GLN
1	138-A	154	GLU
1	138-A	157	GLU
1	138-A	158	ARG
1	139-A	1	MET
1	139-A	18	ASN
1	139-A	23	ASN
1	139-A	24	LEU
1	139-A	52	ARG
1	139-A	68	THR
1	139-A	108	GLN
1	139-A	118	GLU
1	139-A	129	GLU
1	139-A	131	ASP
1	139-A	134	GLU
1	139-A	135	SER
1	139-A	152	CYS
1	139-A	154	GLU
1	139-A	156	LEU
1	139-A	157	GLU
1	140-A	1	MET
1	140-A	16	MET
1	140-A	18	ASN
1	140-A	23	ASN
1	140-A	24	LEU
1	140-A	59	ASN
1	140-A	87	ASP
1	140-A	108	GLN
1	140-A	118	GLU
1	140-A	129	GLU
1	140-A	131	ASP
1	140-A	138	SER
1	140-A	148	SER
1	140-A	152	CYS

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Mol	Chain	Res	Type
1	140-A	154	GLU
1	141-A	16	MET
1	141-A	24	LEU
1	141-A	36	LEU
1	141-A	52	ARG
1	141-A	65	GLN
1	141-A	68	THR
1	141-A	101	GLU
1	141-A	108	GLN
1	141-A	119	VAL
1	141-A	128	TYR
1	141-A	129	GLU
1	141-A	131	ASP
1	141-A	132	ASP
1	141-A	146	GLN
1	141-A	154	GLU
1	141-A	156	LEU
1	141-A	157	GLU
1	142-A	1	MET
1	142-A	8	LEU
1	142-A	10	VAL
1	142-A	16	MET
1	142-A	17	GLU
1	142-A	18	ASN
1	142-A	23	ASN
1	142-A	24	LEU
1	142-A	36	LEU
1	142-A	52	ARG
1	142-A	59	ASN
1	142-A	104	LEU
1	142-A	108	GLN
1	142-A	119	VAL
1	142-A	128	TYR
1	142-A	129	GLU
1	142-A	131	ASP
1	142-A	152	CYS
1	142-A	154	GLU
1	143-A	8	LEU
1	143-A	16	MET
1	143-A	17	GLU
1	143-A	18	ASN
1	143-A	20	MET

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Mol	Chain	Res	Type
1	143-A	44	ARG
1	143-A	52	ARG
1	143-A	87	ASP
1	143-A	106	LYS
1	143-A	118	GLU
1	143-A	122	ASP
1	143-A	128	TYR
1	143-A	129	GLU
1	143-A	131	ASP
1	143-A	142	ASP
1	143-A	154	GLU
1	144-A	1	MET
1	144-A	8	LEU
1	144-A	13	VAL
1	144-A	16	MET
1	144-A	17	GLU
1	144-A	36	LEU
1	144-A	44	ARG
1	144-A	48	GLU
1	144-A	52	ARG
1	144-A	79	ASP
1	144-A	87	ASP
1	144-A	88	VAL
1	144-A	106	LYS
1	144-A	108	GLN
1	144-A	112	LEU
1	144-A	118	GLU
1	144-A	123	THR
1	144-A	128	TYR
1	144-A	129	GLU
1	144-A	131	ASP
1	144-A	142	ASP
1	144-A	148	SER
1	144-A	157	GLU
1	145-A	4	LEU
1	145-A	10	VAL
1	145-A	11	ASP
1	145-A	16	MET
1	145-A	21	PRO
1	145-A	36	LEU
1	145-A	44	ARG
1	145-A	52	ARG

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Mol	Chain	Res	Type
1	145-A	60	ILE
1	145-A	106	LYS
1	145-A	108	GLN
1	145-A	109	LYS
1	145-A	112	LEU
1	145-A	120	GLU
1	145-A	122	ASP
1	145-A	129	GLU
1	145-A	154	GLU
1	146-A	8	LEU
1	146-A	10	VAL
1	146-A	16	MET
1	146-A	20	MET
1	146-A	21	PRO
1	146-A	36	LEU
1	146-A	44	ARG
1	146-A	52	ARG
1	146-A	60	ILE
1	146-A	101	GLU
1	146-A	106	LYS
1	146-A	109	LYS
1	146-A	118	GLU
1	146-A	120	GLU
1	146-A	127	ASP
1	146-A	129	GLU
1	146-A	137	PHE
1	146-A	139	GLU
1	146-A	148	SER
1	147-A	8	LEU
1	147-A	10	VAL
1	147-A	11	ASP
1	147-A	18	ASN
1	147-A	48	GLU
1	147-A	52	ARG
1	147-A	59	ASN
1	147-A	101	GLU
1	147-A	106	LYS
1	147-A	108	GLN
1	147-A	116	ASP
1	147-A	127	ASP
1	147-A	129	GLU
1	147-A	137	PHE

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Mol	Chain	Res	Type
1	147-A	142	ASP
1	147-A	148	SER
1	148-A	13	VAL
1	148-A	20	MET
1	148-A	28	LEU
1	148-A	52	ARG
1	148-A	85	CYS
1	148-A	101	GLU
1	148-A	109	LYS
1	148-A	118	GLU
1	148-A	119	VAL
1	148-A	120	GLU
1	148-A	129	GLU
1	148-A	131	ASP
1	148-A	134	GLU
1	148-A	137	PHE
1	148-A	142	ASP
1	148-A	157	GLU
1	149-A	16	MET
1	149-A	18	ASN
1	149-A	28	LEU
1	149-A	30	TRP
1	149-A	33	ARG
1	149-A	52	ARG
1	149-A	68	THR
1	149-A	106	LYS
1	149-A	120	GLU
1	149-A	129	GLU
1	149-A	137	PHE
1	149-A	156	LEU
1	150-A	13	VAL
1	150-A	16	MET
1	150-A	22	TRP
1	150-A	23	ASN
1	150-A	24	LEU
1	150-A	33	ARG
1	150-A	36	LEU
1	150-A	52	ARG
1	150-A	62	LEU
1	150-A	65	GLN
1	150-A	101	GLU
1	150-A	104	LEU

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Mol	Chain	Res	Type
1	150-A	109	LYS
1	150-A	110	LEU
1	150-A	118	GLU
1	150-A	156	LEU
1	151-A	2	ILE
1	151-A	18	ASN
1	151-A	23	ASN
1	151-A	24	LEU
1	151-A	33	ARG
1	151-A	36	LEU
1	151-A	48	GLU
1	151-A	52	ARG
1	151-A	59	ASN
1	151-A	60	ILE
1	151-A	65	GLN
1	151-A	70	ASP
1	151-A	85	CYS
1	151-A	104	LEU
1	151-A	137	PHE
1	151-A	138	SER
1	151-A	156	LEU
1	152-A	33	ARG
1	152-A	36	LEU
1	152-A	65	GLN
1	152-A	101	GLU
1	152-A	104	LEU
1	152-A	128	TYR
1	153-A	1	MET
1	153-A	16	MET
1	153-A	18	ASN
1	153-A	22	TRP
1	153-A	33	ARG
1	153-A	48	GLU
1	153-A	52	ARG
1	153-A	65	GLN
1	153-A	76	LYS
1	153-A	85	CYS
1	153-A	104	LEU
1	153-A	109	LYS
1	153-A	120	GLU
1	153-A	127	ASP
1	153-A	128	TYR

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Mol	Chain	Res	Type
1	153-A	129	GLU
1	153-A	142	ASP
1	153-A	156	LEU
1	153-A	158	ARG
1	153-A	159	ARG
1	154-A	1	MET
1	154-A	18	ASN
1	154-A	33	ARG
1	154-A	52	ARG
1	154-A	65	GLN
1	154-A	70	ASP
1	154-A	76	LYS
1	154-A	85	CYS
1	154-A	87	ASP
1	154-A	108	GLN
1	154-A	127	ASP
1	154-A	128	TYR
1	154-A	142	ASP
1	155-A	10	VAL
1	155-A	18	ASN
1	155-A	20	MET
1	155-A	27	ASP
1	155-A	52	ARG
1	155-A	65	GLN
1	155-A	68	THR
1	155-A	70	ASP
1	155-A	76	LYS
1	155-A	106	LYS
1	155-A	108	GLN
1	155-A	142	ASP
1	155-A	156	LEU
1	156-A	10	VAL
1	156-A	13	VAL
1	156-A	18	ASN
1	156-A	20	MET
1	156-A	23	ASN
1	156-A	27	ASP
1	156-A	33	ARG
1	156-A	36	LEU
1	156-A	45	HIS
1	156-A	49	SER
1	156-A	52	ARG

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Mol	Chain	Res	Type
1	156-A	64	SER
1	156-A	65	GLN
1	156-A	76	LYS
1	156-A	104	LEU
1	156-A	106	LYS
1	156-A	122	ASP
1	156-A	136	VAL
1	156-A	148	SER
1	157-A	1	MET
1	157-A	4	LEU
1	157-A	10	VAL
1	157-A	13	VAL
1	157-A	16	MET
1	157-A	17	GLU
1	157-A	18	ASN
1	157-A	24	LEU
1	157-A	27	ASP
1	157-A	33	ARG
1	157-A	59	ASN
1	157-A	64	SER
1	157-A	65	GLN
1	157-A	68	THR
1	157-A	76	LYS
1	157-A	120	GLU
1	157-A	122	ASP
1	157-A	132	ASP
1	157-A	148	SER
1	157-A	156	LEU
1	158-A	1	MET
1	158-A	13	VAL
1	158-A	16	MET
1	158-A	18	ASN
1	158-A	36	LEU
1	158-A	52	ARG
1	158-A	64	SER
1	158-A	65	GLN
1	158-A	68	THR
1	158-A	76	LYS
1	158-A	79	ASP
1	158-A	87	ASP
1	158-A	129	GLU
1	159-A	36	LEU

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Mol	Chain	Res	Type
1	159-A	52	ARG
1	159-A	64	SER
1	159-A	65	GLN
1	159-A	66	PRO
1	159-A	76	LYS
1	159-A	79	ASP
1	159-A	87	ASP
1	159-A	104	LEU
1	159-A	118	GLU
1	159-A	119	VAL
1	159-A	120	GLU
1	159-A	129	GLU
1	159-A	131	ASP
1	159-A	156	LEU
1	160-A	16	MET
1	160-A	20	MET
1	160-A	36	LEU
1	160-A	52	ARG
1	160-A	65	GLN
1	160-A	98	ARG
1	160-A	104	LEU
1	160-A	108	GLN
1	160-A	118	GLU
1	160-A	119	VAL
1	160-A	120	GLU
1	160-A	127	ASP
1	160-A	128	TYR
1	160-A	129	GLU
1	160-A	130	PRO
1	160-A	131	ASP
1	160-A	148	SER
1	160-A	156	LEU
1	161-A	16	MET
1	161-A	18	ASN
1	161-A	44	ARG
1	161-A	49	SER
1	161-A	52	ARG
1	161-A	65	GLN
1	161-A	66	PRO
1	161-A	98	ARG
1	161-A	104	LEU
1	161-A	108	GLN

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Mol	Chain	Res	Type
1	161-A	120	GLU
1	161-A	128	TYR
1	161-A	129	GLU
1	161-A	130	PRO
1	161-A	131	ASP
1	161-A	135	SER
1	161-A	137	PHE
1	161-A	138	SER
1	161-A	148	SER
1	161-A	156	LEU
1	162-A	1	MET
1	162-A	13	VAL
1	162-A	18	ASN
1	162-A	20	MET
1	162-A	33	ARG
1	162-A	65	GLN
1	162-A	87	ASP
1	162-A	98	ARG
1	162-A	104	LEU
1	162-A	108	GLN
1	162-A	128	TYR
1	162-A	129	GLU
1	162-A	130	PRO
1	162-A	132	ASP
1	162-A	158	ARG
1	163-A	10	VAL
1	163-A	13	VAL
1	163-A	16	MET
1	163-A	20	MET
1	163-A	23	ASN
1	163-A	59	ASN
1	163-A	68	THR
1	163-A	87	ASP
1	163-A	98	ARG
1	163-A	118	GLU
1	163-A	119	VAL
1	163-A	120	GLU
1	163-A	128	TYR
1	163-A	129	GLU
1	163-A	130	PRO
1	163-A	131	ASP
1	163-A	132	ASP

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Mol	Chain	Res	Type
1	163-A	156	LEU
1	164-A	16	MET
1	164-A	18	ASN
1	164-A	23	ASN
1	164-A	33	ARG
1	164-A	36	LEU
1	164-A	65	GLN
1	164-A	68	THR
1	164-A	79	ASP
1	164-A	106	LYS
1	164-A	118	GLU
1	164-A	127	ASP
1	164-A	128	TYR
1	164-A	129	GLU
1	164-A	130	PRO
1	164-A	135	SER
1	164-A	139	GLU
1	164-A	158	ARG
1	165-A	4	LEU
1	165-A	33	ARG
1	165-A	36	LEU
1	165-A	48	GLU
1	165-A	59	ASN
1	165-A	65	GLN
1	165-A	68	THR
1	165-A	79	ASP
1	165-A	87	ASP
1	165-A	131	ASP
1	165-A	132	ASP
1	165-A	135	SER
1	165-A	158	ARG
1	166-A	18	ASN
1	166-A	33	ARG
1	166-A	70	ASP
1	166-A	87	ASP
1	166-A	104	LEU
1	166-A	108	GLN
1	166-A	119	VAL
1	166-A	128	TYR
1	166-A	136	VAL
1	166-A	139	GLU
1	166-A	148	SER

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Mol	Chain	Res	Type
1	166-A	159	ARG
1	167-A	1	MET
1	167-A	10	VAL
1	167-A	13	VAL
1	167-A	33	ARG
1	167-A	49	SER
1	167-A	52	ARG
1	167-A	61	ILE
1	167-A	68	THR
1	167-A	79	ASP
1	167-A	87	ASP
1	167-A	98	ARG
1	167-A	104	LEU
1	167-A	120	GLU
1	167-A	127	ASP
1	167-A	128	TYR
1	167-A	130	PRO
1	167-A	131	ASP
1	167-A	132	ASP
1	167-A	134	GLU
1	167-A	154	GLU
1	167-A	158	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 668 ligands modelled in this entry, 334 are monoatomic - leaving 334 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FOL	1-A	201	-	27,34,34	1.37	3 (11%)	33,47,47	1.89	8 (24%)
4	NAP	1-A	204	-	44,52,52	1.69	9 (20%)	51,80,80	1.35	10 (19%)
2	FOL	10-A	201	-	27,34,34	1.36	3 (11%)	33,47,47	2.14	10 (30%)
4	NAP	10-A	204	-	44,52,52	1.73	8 (18%)	51,80,80	1.29	8 (15%)
2	FOL	100-A	201	-	27,34,34	1.72	4 (14%)	33,47,47	2.10	10 (30%)
4	NAP	100-A	204	-	44,52,52	1.76	9 (20%)	51,80,80	1.33	8 (15%)
2	FOL	101-A	201	-	27,34,34	1.38	3 (11%)	33,47,47	1.81	6 (18%)
4	NAP	101-A	204	-	44,52,52	1.74	10 (22%)	51,80,80	1.45	7 (13%)
2	FOL	102-A	201	-	27,34,34	1.21	3 (11%)	33,47,47	1.97	8 (24%)
4	NAP	102-A	204	-	44,52,52	1.78	9 (20%)	51,80,80	1.31	8 (15%)
2	FOL	103-A	201	-	27,34,34	1.36	3 (11%)	33,47,47	2.09	10 (30%)
4	NAP	103-A	204	-	44,52,52	1.81	9 (20%)	51,80,80	1.36	5 (9%)
2	FOL	104-A	201	-	27,34,34	1.37	5 (18%)	33,47,47	2.10	7 (21%)
4	NAP	104-A	204	-	44,52,52	1.79	10 (22%)	51,80,80	1.51	9 (17%)
2	FOL	105-A	201	-	27,34,34	1.57	4 (14%)	33,47,47	2.38	8 (24%)
4	NAP	105-A	204	-	44,52,52	1.77	9 (20%)	51,80,80	1.34	8 (15%)
2	FOL	106-A	201	-	27,34,34	1.41	4 (14%)	33,47,47	2.51	11 (33%)
4	NAP	106-A	204	-	44,52,52	1.81	10 (22%)	51,80,80	1.29	8 (15%)
2	FOL	107-A	201	-	27,34,34	1.46	4 (14%)	33,47,47	1.96	8 (24%)
4	NAP	107-A	204	-	44,52,52	1.77	10 (22%)	51,80,80	1.38	8 (15%)
2	FOL	108-A	201	-	27,34,34	1.30	3 (11%)	33,47,47	2.34	11 (33%)
4	NAP	108-A	204	-	44,52,52	1.69	10 (22%)	51,80,80	1.51	6 (11%)
2	FOL	109-A	201	-	27,34,34	1.35	3 (11%)	33,47,47	2.26	9 (27%)
4	NAP	109-A	204	-	44,52,52	1.66	10 (22%)	51,80,80	1.32	7 (13%)
2	FOL	11-A	201	-	27,34,34	1.30	3 (11%)	33,47,47	1.91	6 (18%)
4	NAP	11-A	204	-	44,52,52	1.72	9 (20%)	51,80,80	1.36	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	110-A	201	-	27,34,34	1.43	3 (11%)	33,47,47	2.48	9 (27%)
4	NAP	110-A	204	-	44,52,52	1.77	10 (22%)	51,80,80	1.30	8 (15%)
2	FOL	111-A	201	-	27,34,34	1.50	3 (11%)	33,47,47	1.91	6 (18%)
4	NAP	111-A	204	-	44,52,52	1.74	10 (22%)	51,80,80	1.32	8 (15%)
2	FOL	112-A	201	-	27,34,34	1.29	3 (11%)	33,47,47	2.28	8 (24%)
4	NAP	112-A	204	-	44,52,52	1.74	8 (18%)	51,80,80	1.31	8 (15%)
2	FOL	113-A	201	-	27,34,34	1.47	3 (11%)	33,47,47	2.21	8 (24%)
4	NAP	113-A	204	-	44,52,52	1.74	9 (20%)	51,80,80	1.29	9 (17%)
2	FOL	114-A	201	-	27,34,34	1.41	3 (11%)	33,47,47	2.25	9 (27%)
4	NAP	114-A	204	-	44,52,52	1.72	10 (22%)	51,80,80	1.30	9 (17%)
2	FOL	115-A	201	-	27,34,34	1.43	4 (14%)	33,47,47	2.39	10 (30%)
4	NAP	115-A	204	-	44,52,52	1.83	11 (25%)	51,80,80	1.54	11 (21%)
2	FOL	116-A	201	-	27,34,34	1.38	3 (11%)	33,47,47	1.84	8 (24%)
4	NAP	116-A	204	-	44,52,52	1.77	8 (18%)	51,80,80	1.33	8 (15%)
2	FOL	117-A	201	-	27,34,34	1.53	4 (14%)	33,47,47	1.46	4 (12%)
4	NAP	117-A	204	-	44,52,52	1.73	8 (18%)	51,80,80	1.52	10 (19%)
2	FOL	118-A	201	-	27,34,34	1.54	3 (11%)	33,47,47	2.20	14 (42%)
4	NAP	118-A	204	-	44,52,52	1.72	7 (15%)	51,80,80	2.17	10 (19%)
2	FOL	119-A	201	-	27,34,34	1.47	3 (11%)	33,47,47	1.85	7 (21%)
4	NAP	119-A	204	-	44,52,52	1.86	10 (22%)	51,80,80	1.84	10 (19%)
2	FOL	12-A	201	-	27,34,34	1.57	3 (11%)	33,47,47	1.79	7 (21%)
4	NAP	12-A	204	-	44,52,52	1.71	9 (20%)	51,80,80	1.33	10 (19%)
2	FOL	120-A	201	-	27,34,34	1.50	5 (18%)	33,47,47	1.82	8 (24%)
4	NAP	120-A	204	-	44,52,52	1.71	9 (20%)	51,80,80	1.27	6 (11%)
2	FOL	121-A	201	-	27,34,34	1.56	3 (11%)	33,47,47	1.72	7 (21%)
4	NAP	121-A	204	-	44,52,52	1.65	8 (18%)	51,80,80	1.25	7 (13%)
2	FOL	122-A	201	-	27,34,34	1.47	4 (14%)	33,47,47	1.84	8 (24%)
4	NAP	122-A	204	-	44,52,52	1.70	8 (18%)	51,80,80	1.27	8 (15%)
2	FOL	123-A	201	-	27,34,34	1.53	5 (18%)	33,47,47	1.60	4 (12%)
4	NAP	123-A	204	-	44,52,52	1.71	10 (22%)	51,80,80	1.40	7 (13%)
2	FOL	124-A	201	-	27,34,34	1.43	3 (11%)	33,47,47	1.97	10 (30%)
4	NAP	124-A	204	-	44,52,52	1.64	7 (15%)	51,80,80	1.32	8 (15%)
2	FOL	125-A	201	-	27,34,34	1.41	4 (14%)	33,47,47	2.09	7 (21%)
4	NAP	125-A	204	-	44,52,52	1.62	7 (15%)	51,80,80	1.33	8 (15%)
2	FOL	126-A	201	-	27,34,34	1.72	5 (18%)	33,47,47	2.96	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	126-A	204	-	44,52,52	1.64	7 (15%)	51,80,80	1.19	7 (13%)
2	FOL	127-A	201	-	27,34,34	1.38	3 (11%)	33,47,47	2.09	10 (30%)
4	NAP	127-A	204	-	44,52,52	1.68	8 (18%)	51,80,80	1.39	8 (15%)
2	FOL	128-A	201	-	27,34,34	1.36	3 (11%)	33,47,47	2.30	11 (33%)
4	NAP	128-A	204	-	44,52,52	1.71	9 (20%)	51,80,80	1.45	6 (11%)
2	FOL	129-A	201	-	27,34,34	1.57	3 (11%)	33,47,47	2.26	12 (36%)
4	NAP	129-A	204	-	44,52,52	1.72	8 (18%)	51,80,80	1.35	7 (13%)
2	FOL	13-A	201	-	27,34,34	1.54	4 (14%)	33,47,47	2.57	10 (30%)
4	NAP	13-A	204	-	44,52,52	1.70	9 (20%)	51,80,80	1.25	8 (15%)
2	FOL	130-A	201	-	27,34,34	1.44	3 (11%)	33,47,47	1.81	6 (18%)
4	NAP	130-A	204	-	44,52,52	1.68	8 (18%)	51,80,80	1.42	8 (15%)
2	FOL	131-A	201	-	27,34,34	1.38	4 (14%)	33,47,47	2.02	8 (24%)
4	NAP	131-A	204	-	44,52,52	1.63	7 (15%)	51,80,80	1.17	4 (7%)
2	FOL	132-A	201	-	27,34,34	1.56	5 (18%)	33,47,47	1.91	7 (21%)
4	NAP	132-A	204	-	44,52,52	1.57	8 (18%)	51,80,80	1.18	3 (5%)
2	FOL	133-A	201	-	27,34,34	1.43	3 (11%)	33,47,47	2.13	5 (15%)
4	NAP	133-A	204	-	44,52,52	1.65	9 (20%)	51,80,80	1.21	3 (5%)
2	FOL	134-A	201	-	27,34,34	1.54	4 (14%)	33,47,47	2.22	12 (36%)
4	NAP	134-A	204	-	44,52,52	1.58	8 (18%)	51,80,80	1.13	4 (7%)
2	FOL	135-A	201	-	27,34,34	1.47	4 (14%)	33,47,47	1.83	6 (18%)
4	NAP	135-A	204	-	44,52,52	1.70	7 (15%)	51,80,80	1.38	8 (15%)
2	FOL	136-A	201	-	27,34,34	1.35	3 (11%)	33,47,47	2.07	11 (33%)
4	NAP	136-A	204	-	44,52,52	1.71	7 (15%)	51,80,80	1.27	7 (13%)
2	FOL	137-A	201	-	27,34,34	1.49	3 (11%)	33,47,47	1.70	7 (21%)
4	NAP	137-A	204	-	44,52,52	1.69	6 (13%)	51,80,80	1.29	6 (11%)
2	FOL	138-A	201	-	27,34,34	1.29	3 (11%)	33,47,47	2.34	11 (33%)
4	NAP	138-A	204	-	44,52,52	1.66	9 (20%)	51,80,80	1.37	8 (15%)
2	FOL	139-A	201	-	27,34,34	1.48	4 (14%)	33,47,47	2.07	9 (27%)
4	NAP	139-A	204	-	44,52,52	1.64	8 (18%)	51,80,80	1.40	9 (17%)
2	FOL	14-A	201	-	27,34,34	1.43	4 (14%)	33,47,47	2.38	8 (24%)
4	NAP	14-A	204	-	44,52,52	1.72	9 (20%)	51,80,80	1.34	8 (15%)
2	FOL	140-A	201	-	27,34,34	1.28	4 (14%)	33,47,47	1.82	8 (24%)
4	NAP	140-A	204	-	44,52,52	1.71	9 (20%)	51,80,80	1.44	8 (15%)
2	FOL	141-A	201	-	27,34,34	1.37	3 (11%)	33,47,47	1.76	8 (24%)
4	NAP	141-A	204	-	44,52,52	1.67	8 (18%)	51,80,80	1.24	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	142-A	201	-	27,34,34	1.29	2 (7%)	33,47,47	1.99	9 (27%)
4	NAP	142-A	204	-	44,52,52	1.69	9 (20%)	51,80,80	1.39	9 (17%)
2	FOL	143-A	201	-	27,34,34	1.54	4 (14%)	33,47,47	1.81	6 (18%)
4	NAP	143-A	204	-	44,52,52	1.71	9 (20%)	51,80,80	1.24	7 (13%)
2	FOL	144-A	201	-	27,34,34	1.43	4 (14%)	33,47,47	2.59	14 (42%)
4	NAP	144-A	204	-	44,52,52	1.67	8 (18%)	51,80,80	1.30	8 (15%)
2	FOL	145-A	201	-	27,34,34	1.36	3 (11%)	33,47,47	1.90	6 (18%)
4	NAP	145-A	204	-	44,52,52	1.71	9 (20%)	51,80,80	1.32	8 (15%)
2	FOL	146-A	201	-	27,34,34	1.43	3 (11%)	33,47,47	1.86	6 (18%)
4	NAP	146-A	204	-	44,52,52	1.70	9 (20%)	51,80,80	1.28	8 (15%)
2	FOL	147-A	201	-	27,34,34	1.49	3 (11%)	33,47,47	1.84	10 (30%)
4	NAP	147-A	204	-	44,52,52	1.76	11 (25%)	51,80,80	1.32	7 (13%)
2	FOL	148-A	201	-	27,34,34	1.55	4 (14%)	33,47,47	1.90	5 (15%)
4	NAP	148-A	204	-	44,52,52	1.70	8 (18%)	51,80,80	1.38	6 (11%)
2	FOL	149-A	201	-	27,34,34	1.43	3 (11%)	33,47,47	2.08	7 (21%)
4	NAP	149-A	204	-	44,52,52	1.70	8 (18%)	51,80,80	1.30	7 (13%)
2	FOL	15-A	201	-	27,34,34	1.66	4 (14%)	33,47,47	2.18	8 (24%)
4	NAP	15-A	204	-	44,52,52	1.71	9 (20%)	51,80,80	1.40	7 (13%)
2	FOL	150-A	201	-	27,34,34	1.41	4 (14%)	33,47,47	1.67	4 (12%)
4	NAP	150-A	204	-	44,52,52	1.63	8 (18%)	51,80,80	1.37	8 (15%)
2	FOL	151-A	201	-	27,34,34	1.53	3 (11%)	33,47,47	1.88	7 (21%)
4	NAP	151-A	204	-	44,52,52	1.64	9 (20%)	51,80,80	1.37	9 (17%)
2	FOL	152-A	201	-	27,34,34	1.67	4 (14%)	33,47,47	2.02	8 (24%)
4	NAP	152-A	204	-	44,52,52	1.62	6 (13%)	51,80,80	1.17	5 (9%)
2	FOL	153-A	201	-	27,34,34	1.40	4 (14%)	33,47,47	1.97	10 (30%)
4	NAP	153-A	204	-	44,52,52	1.66	10 (22%)	51,80,80	1.18	5 (9%)
2	FOL	154-A	201	-	27,34,34	1.50	3 (11%)	33,47,47	1.78	6 (18%)
4	NAP	154-A	204	-	44,52,52	1.65	10 (22%)	51,80,80	1.42	6 (11%)
2	FOL	155-A	201	-	27,34,34	1.45	3 (11%)	33,47,47	2.01	9 (27%)
4	NAP	155-A	204	-	44,52,52	1.68	9 (20%)	51,80,80	1.28	7 (13%)
2	FOL	156-A	201	-	27,34,34	1.59	6 (22%)	33,47,47	2.40	8 (24%)
4	NAP	156-A	204	-	44,52,52	1.69	8 (18%)	51,80,80	1.30	8 (15%)
2	FOL	157-A	201	-	27,34,34	1.43	4 (14%)	33,47,47	1.84	9 (27%)
4	NAP	157-A	204	-	44,52,52	1.59	9 (20%)	51,80,80	1.18	3 (5%)
2	FOL	158-A	201	-	27,34,34	1.48	3 (11%)	33,47,47	1.96	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	158-A	204	-	44,52,52	1.55	8 (18%)	51,80,80	1.30	4 (7%)
2	FOL	159-A	201	-	27,34,34	1.37	5 (18%)	33,47,47	2.03	10 (30%)
4	NAP	159-A	204	-	44,52,52	1.55	6 (13%)	51,80,80	1.22	6 (11%)
2	FOL	16-A	201	-	27,34,34	1.47	5 (18%)	33,47,47	2.02	6 (18%)
4	NAP	16-A	204	-	44,52,52	1.73	9 (20%)	51,80,80	1.25	8 (15%)
2	FOL	160-A	201	-	27,34,34	1.52	4 (14%)	33,47,47	2.02	8 (24%)
4	NAP	160-A	204	-	44,52,52	1.70	9 (20%)	51,80,80	1.25	7 (13%)
2	FOL	161-A	201	-	27,34,34	1.28	4 (14%)	33,47,47	1.89	6 (18%)
4	NAP	161-A	204	-	44,52,52	1.70	9 (20%)	51,80,80	1.29	7 (13%)
2	FOL	162-A	201	-	27,34,34	1.51	4 (14%)	33,47,47	1.88	9 (27%)
4	NAP	162-A	204	-	44,52,52	1.68	8 (18%)	51,80,80	1.28	6 (11%)
2	FOL	163-A	201	-	27,34,34	1.31	5 (18%)	33,47,47	2.10	9 (27%)
4	NAP	163-A	204	-	44,52,52	1.68	8 (18%)	51,80,80	1.29	6 (11%)
2	FOL	164-A	201	-	27,34,34	1.46	4 (14%)	33,47,47	1.87	8 (24%)
4	NAP	164-A	204	-	44,52,52	1.63	9 (20%)	51,80,80	1.37	8 (15%)
2	FOL	165-A	201	-	27,34,34	1.47	4 (14%)	33,47,47	2.09	8 (24%)
4	NAP	165-A	204	-	44,52,52	1.75	10 (22%)	51,80,80	1.27	5 (9%)
2	FOL	166-A	201	-	27,34,34	1.53	4 (14%)	33,47,47	1.60	5 (15%)
4	NAP	166-A	204	-	44,52,52	1.65	8 (18%)	51,80,80	1.27	6 (11%)
2	FOL	167-A	201	-	27,34,34	1.51	3 (11%)	33,47,47	2.07	9 (27%)
4	NAP	167-A	204	-	44,52,52	1.68	8 (18%)	51,80,80	1.23	6 (11%)
2	FOL	17-A	201	-	27,34,34	1.49	3 (11%)	33,47,47	1.66	7 (21%)
4	NAP	17-A	204	-	44,52,52	1.73	8 (18%)	51,80,80	1.33	7 (13%)
2	FOL	18-A	201	-	27,34,34	1.45	3 (11%)	33,47,47	2.13	9 (27%)
4	NAP	18-A	204	-	44,52,52	1.73	9 (20%)	51,80,80	1.48	9 (17%)
2	FOL	19-A	201	-	27,34,34	1.55	3 (11%)	33,47,47	1.66	7 (21%)
4	NAP	19-A	204	-	44,52,52	1.75	9 (20%)	51,80,80	1.36	9 (17%)
2	FOL	2-A	201	-	27,34,34	1.49	3 (11%)	33,47,47	1.64	6 (18%)
4	NAP	2-A	204	-	44,52,52	1.68	9 (20%)	51,80,80	1.36	8 (15%)
2	FOL	20-A	201	-	27,34,34	1.44	3 (11%)	33,47,47	1.79	8 (24%)
4	NAP	20-A	204	-	44,52,52	1.73	8 (18%)	51,80,80	1.25	6 (11%)
2	FOL	21-A	201	-	27,34,34	1.69	3 (11%)	33,47,47	2.06	11 (33%)
4	NAP	21-A	204	-	44,52,52	1.70	9 (20%)	51,80,80	1.29	8 (15%)
2	FOL	22-A	201	-	27,34,34	1.45	3 (11%)	33,47,47	1.76	6 (18%)
4	NAP	22-A	204	-	44,52,52	1.77	10 (22%)	51,80,80	1.27	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	23-A	201	-	27,34,34	1.34	3 (11%)	33,47,47	2.16	11 (33%)
4	NAP	23-A	204	-	44,52,52	1.79	9 (20%)	51,80,80	1.38	11 (21%)
2	FOL	24-A	201	-	27,34,34	1.39	4 (14%)	33,47,47	2.02	12 (36%)
4	NAP	24-A	204	-	44,52,52	1.73	8 (18%)	51,80,80	1.28	8 (15%)
2	FOL	25-A	201	-	27,34,34	1.54	3 (11%)	33,47,47	2.26	8 (24%)
4	NAP	25-A	204	-	44,52,52	1.77	9 (20%)	51,80,80	1.38	7 (13%)
2	FOL	26-A	201	-	27,34,34	1.59	4 (14%)	33,47,47	2.16	11 (33%)
4	NAP	26-A	204	-	44,52,52	1.72	8 (18%)	51,80,80	1.28	7 (13%)
2	FOL	27-A	201	-	27,34,34	1.55	3 (11%)	33,47,47	1.77	4 (12%)
4	NAP	27-A	204	-	44,52,52	1.73	9 (20%)	51,80,80	1.30	7 (13%)
2	FOL	28-A	201	-	27,34,34	1.57	3 (11%)	33,47,47	1.75	6 (18%)
4	NAP	28-A	204	-	44,52,52	1.75	11 (25%)	51,80,80	1.29	6 (11%)
2	FOL	29-A	201	-	27,34,34	1.36	3 (11%)	33,47,47	1.95	7 (21%)
4	NAP	29-A	204	-	44,52,52	1.71	10 (22%)	51,80,80	1.31	6 (11%)
2	FOL	3-A	201	-	27,34,34	1.35	3 (11%)	33,47,47	1.76	7 (21%)
4	NAP	3-A	204	-	44,52,52	1.74	9 (20%)	51,80,80	1.30	7 (13%)
2	FOL	30-A	201	-	27,34,34	1.62	3 (11%)	33,47,47	1.83	8 (24%)
4	NAP	30-A	204	-	44,52,52	1.79	9 (20%)	51,80,80	1.29	7 (13%)
2	FOL	31-A	201	-	27,34,34	1.37	3 (11%)	33,47,47	2.37	13 (39%)
4	NAP	31-A	204	-	44,52,52	1.71	10 (22%)	51,80,80	1.21	3 (5%)
2	FOL	32-A	201	-	27,34,34	1.43	3 (11%)	33,47,47	1.81	7 (21%)
4	NAP	32-A	204	-	44,52,52	1.65	10 (22%)	51,80,80	1.22	3 (5%)
2	FOL	33-A	201	-	27,34,34	1.47	3 (11%)	33,47,47	1.85	7 (21%)
4	NAP	33-A	204	-	44,52,52	1.79	10 (22%)	51,80,80	1.36	8 (15%)
2	FOL	34-A	201	-	27,34,34	1.45	3 (11%)	33,47,47	2.30	14 (42%)
4	NAP	34-A	204	-	44,52,52	1.61	10 (22%)	51,80,80	1.15	5 (9%)
2	FOL	35-A	201	-	27,34,34	1.40	4 (14%)	33,47,47	1.72	5 (15%)
4	NAP	35-A	204	-	44,52,52	1.68	10 (22%)	51,80,80	1.42	7 (13%)
2	FOL	36-A	201	-	27,34,34	1.43	4 (14%)	33,47,47	1.88	7 (21%)
4	NAP	36-A	204	-	44,52,52	1.69	10 (22%)	51,80,80	1.26	8 (15%)
2	FOL	37-A	201	-	27,34,34	1.44	3 (11%)	33,47,47	1.96	9 (27%)
4	NAP	37-A	204	-	44,52,52	1.70	10 (22%)	51,80,80	1.21	7 (13%)
2	FOL	38-A	201	-	27,34,34	1.23	3 (11%)	33,47,47	2.08	7 (21%)
4	NAP	38-A	204	-	44,52,52	1.76	9 (20%)	51,80,80	1.34	9 (17%)
2	FOL	39-A	201	-	27,34,34	1.47	4 (14%)	33,47,47	2.48	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	39-A	204	-	44,52,52	1.82	9 (20%)	51,80,80	1.33	9 (17%)
2	FOL	4-A	201	-	27,34,34	1.55	3 (11%)	33,47,47	1.94	8 (24%)
4	NAP	4-A	204	-	44,52,52	1.71	8 (18%)	51,80,80	1.38	9 (17%)
2	FOL	40-A	201	-	27,34,34	1.49	3 (11%)	33,47,47	1.90	7 (21%)
4	NAP	40-A	204	-	44,52,52	1.75	9 (20%)	51,80,80	1.36	9 (17%)
2	FOL	41-A	201	-	27,34,34	1.52	3 (11%)	33,47,47	2.13	6 (18%)
4	NAP	41-A	204	-	44,52,52	1.75	10 (22%)	51,80,80	1.35	8 (15%)
2	FOL	42-A	201	-	27,34,34	1.65	3 (11%)	33,47,47	2.15	11 (33%)
4	NAP	42-A	204	-	44,52,52	1.77	10 (22%)	51,80,80	1.49	9 (17%)
2	FOL	43-A	201	-	27,34,34	1.39	4 (14%)	33,47,47	2.72	9 (27%)
4	NAP	43-A	204	-	44,52,52	1.72	8 (18%)	51,80,80	1.34	8 (15%)
2	FOL	44-A	201	-	27,34,34	1.51	3 (11%)	33,47,47	2.14	7 (21%)
4	NAP	44-A	204	-	44,52,52	1.73	9 (20%)	51,80,80	1.23	7 (13%)
2	FOL	45-A	201	-	27,34,34	1.45	3 (11%)	33,47,47	1.85	8 (24%)
4	NAP	45-A	204	-	44,52,52	1.71	9 (20%)	51,80,80	1.34	7 (13%)
2	FOL	46-A	201	-	27,34,34	1.51	4 (14%)	33,47,47	1.92	7 (21%)
4	NAP	46-A	204	-	44,52,52	1.70	8 (18%)	51,80,80	1.28	7 (13%)
2	FOL	47-A	201	-	27,34,34	1.55	3 (11%)	33,47,47	1.87	7 (21%)
4	NAP	47-A	204	-	44,52,52	1.74	9 (20%)	51,80,80	1.27	7 (13%)
2	FOL	48-A	201	-	27,34,34	1.46	3 (11%)	33,47,47	2.44	12 (36%)
4	NAP	48-A	204	-	44,52,52	1.74	8 (18%)	51,80,80	1.30	6 (11%)
2	FOL	49-A	201	-	27,34,34	1.32	3 (11%)	33,47,47	1.90	6 (18%)
4	NAP	49-A	204	-	44,52,52	1.73	8 (18%)	51,80,80	1.56	10 (19%)
2	FOL	5-A	201	-	27,34,34	1.47	4 (14%)	33,47,47	1.92	8 (24%)
4	NAP	5-A	204	-	44,52,52	1.69	8 (18%)	51,80,80	1.42	8 (15%)
2	FOL	50-A	201	-	27,34,34	1.52	3 (11%)	33,47,47	1.78	6 (18%)
4	NAP	50-A	204	-	44,52,52	1.78	10 (22%)	51,80,80	1.31	8 (15%)
2	FOL	51-A	201	-	27,34,34	1.51	3 (11%)	33,47,47	1.85	6 (18%)
4	NAP	51-A	204	-	44,52,52	1.78	10 (22%)	51,80,80	1.28	7 (13%)
2	FOL	52-A	201	-	27,34,34	1.69	4 (14%)	33,47,47	2.26	11 (33%)
4	NAP	52-A	204	-	44,52,52	1.76	9 (20%)	51,80,80	1.38	4 (7%)
2	FOL	53-A	201	-	27,34,34	1.55	3 (11%)	33,47,47	2.09	7 (21%)
4	NAP	53-A	204	-	44,52,52	1.74	8 (18%)	51,80,80	1.26	5 (9%)
2	FOL	54-A	201	-	27,34,34	1.36	3 (11%)	33,47,47	1.98	9 (27%)
4	NAP	54-A	204	-	44,52,52	1.69	8 (18%)	51,80,80	1.37	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	55-A	201	-	27,34,34	1.39	4 (14%)	33,47,47	1.82	8 (24%)
4	NAP	55-A	204	-	44,52,52	1.72	9 (20%)	51,80,80	1.32	7 (13%)
2	FOL	56-A	201	-	27,34,34	1.53	4 (14%)	33,47,47	2.10	7 (21%)
4	NAP	56-A	204	-	44,52,52	1.66	9 (20%)	51,80,80	1.93	7 (13%)
2	FOL	57-A	201	-	27,34,34	1.64	4 (14%)	33,47,47	2.20	14 (42%)
4	NAP	57-A	204	-	44,52,52	1.59	9 (20%)	51,80,80	2.12	3 (5%)
2	FOL	58-A	201	-	27,34,34	1.47	3 (11%)	33,47,47	2.35	12 (36%)
4	NAP	58-A	204	-	44,52,52	1.66	7 (15%)	51,80,80	1.12	3 (5%)
2	FOL	59-A	201	-	27,34,34	1.61	3 (11%)	33,47,47	2.05	11 (33%)
4	NAP	59-A	204	-	44,52,52	1.64	7 (15%)	51,80,80	1.30	5 (9%)
2	FOL	6-A	201	-	27,34,34	1.77	4 (14%)	33,47,47	2.31	9 (27%)
4	NAP	6-A	204	-	44,52,52	1.64	8 (18%)	51,80,80	1.26	7 (13%)
2	FOL	60-A	201	-	27,34,34	1.47	3 (11%)	33,47,47	1.89	6 (18%)
4	NAP	60-A	204	-	44,52,52	1.79	9 (20%)	51,80,80	1.33	7 (13%)
2	FOL	61-A	201	-	27,34,34	1.39	3 (11%)	33,47,47	1.93	8 (24%)
4	NAP	61-A	204	-	44,52,52	1.71	9 (20%)	51,80,80	1.28	7 (13%)
2	FOL	62-A	201	-	27,34,34	1.45	3 (11%)	33,47,47	2.11	10 (30%)
4	NAP	62-A	204	-	44,52,52	1.76	10 (22%)	51,80,80	1.42	10 (19%)
2	FOL	63-A	201	-	27,34,34	1.36	3 (11%)	33,47,47	2.36	12 (36%)
4	NAP	63-A	204	-	44,52,52	1.70	7 (15%)	51,80,80	1.32	7 (13%)
2	FOL	64-A	201	-	27,34,34	1.38	3 (11%)	33,47,47	2.02	12 (36%)
4	NAP	64-A	204	-	44,52,52	1.73	9 (20%)	51,80,80	1.28	6 (11%)
2	FOL	65-A	201	-	27,34,34	1.74	4 (14%)	33,47,47	1.88	10 (30%)
4	NAP	65-A	204	-	44,52,52	1.75	10 (22%)	51,80,80	1.25	7 (13%)
2	FOL	66-A	201	-	27,34,34	1.41	3 (11%)	33,47,47	1.95	9 (27%)
4	NAP	66-A	204	-	44,52,52	1.73	9 (20%)	51,80,80	1.26	8 (15%)
2	FOL	67-A	201	-	27,34,34	1.39	3 (11%)	33,47,47	2.05	9 (27%)
4	NAP	67-A	204	-	44,52,52	1.71	10 (22%)	51,80,80	1.32	6 (11%)
2	FOL	68-A	201	-	27,34,34	1.51	3 (11%)	33,47,47	1.81	6 (18%)
4	NAP	68-A	204	-	44,52,52	1.73	9 (20%)	51,80,80	1.13	6 (11%)
2	FOL	69-A	201	-	27,34,34	1.49	4 (14%)	33,47,47	1.95	7 (21%)
4	NAP	69-A	204	-	44,52,52	1.77	8 (18%)	51,80,80	1.21	7 (13%)
2	FOL	7-A	201	-	27,34,34	1.56	3 (11%)	33,47,47	2.01	7 (21%)
4	NAP	7-A	204	-	44,52,52	1.58	10 (22%)	51,80,80	1.19	3 (5%)
2	FOL	70-A	201	-	27,34,34	1.57	4 (14%)	33,47,47	2.38	10 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	70-A	204	-	44,52,52	1.77	8 (18%)	51,80,80	1.33	9 (17%)
2	FOL	71-A	201	-	27,34,34	1.42	3 (11%)	33,47,47	1.74	6 (18%)
4	NAP	71-A	204	-	44,52,52	1.73	10 (22%)	51,80,80	1.33	9 (17%)
2	FOL	72-A	201	-	27,34,34	1.39	3 (11%)	33,47,47	2.06	6 (18%)
4	NAP	72-A	204	-	44,52,52	1.73	11 (25%)	51,80,80	1.32	9 (17%)
2	FOL	73-A	201	-	27,34,34	1.59	3 (11%)	33,47,47	1.70	6 (18%)
4	NAP	73-A	204	-	44,52,52	1.72	11 (25%)	51,80,80	1.41	9 (17%)
2	FOL	74-A	201	-	27,34,34	1.63	3 (11%)	33,47,47	1.93	10 (30%)
4	NAP	74-A	204	-	44,52,52	1.72	10 (22%)	51,80,80	1.40	6 (11%)
2	FOL	75-A	201	-	27,34,34	1.39	3 (11%)	33,47,47	2.03	8 (24%)
4	NAP	75-A	204	-	44,52,52	1.74	8 (18%)	51,80,80	1.33	8 (15%)
2	FOL	76-A	201	-	27,34,34	1.65	3 (11%)	33,47,47	2.04	7 (21%)
4	NAP	76-A	204	-	44,52,52	1.75	10 (22%)	51,80,80	1.26	6 (11%)
2	FOL	77-A	201	-	27,34,34	1.56	5 (18%)	33,47,47	2.24	8 (24%)
4	NAP	77-A	204	-	44,52,52	1.70	9 (20%)	51,80,80	1.50	8 (15%)
2	FOL	78-A	201	-	27,34,34	1.35	3 (11%)	33,47,47	2.15	11 (33%)
4	NAP	78-A	204	-	44,52,52	1.68	9 (20%)	51,80,80	1.32	6 (11%)
2	FOL	79-A	201	-	27,34,34	1.33	3 (11%)	33,47,47	1.87	9 (27%)
4	NAP	79-A	204	-	44,52,52	1.74	11 (25%)	51,80,80	1.42	7 (13%)
2	FOL	8-A	201	-	27,34,34	1.50	3 (11%)	33,47,47	1.90	5 (15%)
4	NAP	8-A	204	-	44,52,52	1.59	9 (20%)	51,80,80	1.24	4 (7%)
2	FOL	80-A	201	-	27,34,34	1.57	3 (11%)	33,47,47	2.29	12 (36%)
4	NAP	80-A	204	-	44,52,52	1.75	9 (20%)	51,80,80	1.32	7 (13%)
2	FOL	81-A	201	-	27,34,34	1.49	4 (14%)	33,47,47	2.14	8 (24%)
4	NAP	81-A	204	-	44,52,52	1.69	8 (18%)	51,80,80	1.41	6 (11%)
2	FOL	82-A	201	-	27,34,34	1.54	4 (14%)	33,47,47	2.21	9 (27%)
4	NAP	82-A	204	-	44,52,52	1.68	9 (20%)	51,80,80	1.24	4 (7%)
2	FOL	83-A	201	-	27,34,34	1.68	4 (14%)	33,47,47	2.35	13 (39%)
4	NAP	83-A	204	-	44,52,52	1.64	9 (20%)	51,80,80	1.31	6 (11%)
2	FOL	84-A	201	-	27,34,34	1.37	3 (11%)	33,47,47	2.12	8 (24%)
4	NAP	84-A	204	-	44,52,52	1.67	8 (18%)	51,80,80	1.07	4 (7%)
2	FOL	85-A	201	-	27,34,34	1.46	4 (14%)	33,47,47	2.03	7 (21%)
4	NAP	85-A	204	-	44,52,52	1.72	9 (20%)	51,80,80	1.23	7 (13%)
2	FOL	86-A	201	-	27,34,34	1.35	3 (11%)	33,47,47	2.00	8 (24%)
4	NAP	86-A	204	-	44,52,52	1.69	9 (20%)	51,80,80	1.28	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	87-A	201	-	27,34,34	1.41	4 (14%)	33,47,47	2.06	10 (30%)
4	NAP	87-A	204	-	44,52,52	1.70	8 (18%)	51,80,80	1.26	6 (11%)
2	FOL	88-A	201	-	27,34,34	1.31	3 (11%)	33,47,47	1.80	7 (21%)
4	NAP	88-A	204	-	44,52,52	1.68	10 (22%)	51,80,80	1.40	8 (15%)
2	FOL	89-A	201	-	27,34,34	1.53	3 (11%)	33,47,47	2.09	9 (27%)
4	NAP	89-A	204	-	44,52,52	1.68	10 (22%)	51,80,80	1.39	7 (13%)
2	FOL	9-A	201	-	27,34,34	1.55	3 (11%)	33,47,47	1.76	9 (27%)
4	NAP	9-A	204	-	44,52,52	1.63	9 (20%)	51,80,80	1.18	5 (9%)
2	FOL	90-A	201	-	27,34,34	1.37	3 (11%)	33,47,47	1.64	6 (18%)
4	NAP	90-A	204	-	44,52,52	1.68	10 (22%)	51,80,80	1.46	10 (19%)
2	FOL	91-A	201	-	27,34,34	1.32	2 (7%)	33,47,47	1.91	9 (27%)
4	NAP	91-A	204	-	44,52,52	1.68	9 (20%)	51,80,80	1.23	7 (13%)
2	FOL	92-A	201	-	27,34,34	1.49	3 (11%)	33,47,47	2.35	8 (24%)
4	NAP	92-A	204	-	44,52,52	1.69	8 (18%)	51,80,80	1.29	8 (15%)
2	FOL	93-A	201	-	27,34,34	1.45	4 (14%)	33,47,47	2.05	8 (24%)
4	NAP	93-A	204	-	44,52,52	1.67	9 (20%)	51,80,80	1.35	7 (13%)
2	FOL	94-A	201	-	27,34,34	1.47	3 (11%)	33,47,47	1.86	10 (30%)
4	NAP	94-A	204	-	44,52,52	1.72	9 (20%)	51,80,80	1.27	6 (11%)
2	FOL	95-A	201	-	27,34,34	1.33	3 (11%)	33,47,47	1.76	8 (24%)
4	NAP	95-A	204	-	44,52,52	1.68	9 (20%)	51,80,80	1.33	6 (11%)
2	FOL	96-A	201	-	27,34,34	1.44	3 (11%)	33,47,47	1.67	7 (21%)
4	NAP	96-A	204	-	44,52,52	1.71	9 (20%)	51,80,80	1.23	5 (9%)
2	FOL	97-A	201	-	27,34,34	1.39	3 (11%)	33,47,47	2.01	9 (27%)
4	NAP	97-A	204	-	44,52,52	1.76	10 (22%)	51,80,80	1.22	7 (13%)
2	FOL	98-A	201	-	27,34,34	1.47	3 (11%)	33,47,47	1.85	4 (12%)
4	NAP	98-A	204	-	44,52,52	1.73	8 (18%)	51,80,80	1.28	7 (13%)
2	FOL	99-A	201	-	27,34,34	1.46	3 (11%)	33,47,47	1.96	8 (24%)
4	NAP	99-A	204	-	44,52,52	1.78	9 (20%)	51,80,80	1.44	7 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	1-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	1-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	10-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	10-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	100-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	100-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	101-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	101-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	102-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	102-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	103-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	103-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	104-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	104-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	105-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	105-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	106-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	106-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	107-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	107-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	108-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	108-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	109-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	109-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	11-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	11-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	110-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	110-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	111-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	111-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	112-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	112-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	113-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	113-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	114-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	114-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	115-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	115-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	116-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	116-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	117-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	117-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	118-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	118-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	119-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	119-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	12-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	12-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	120-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	120-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	121-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	121-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	122-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	122-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	123-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	123-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	124-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	124-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	125-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	125-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	126-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	126-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	127-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	127-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	128-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	128-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	129-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	129-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	13-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	13-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	130-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	130-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	131-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	131-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	132-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	132-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	133-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	133-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	134-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	134-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	135-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	135-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	136-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	136-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	137-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	137-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	138-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	138-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	139-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	139-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	14-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	14-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	140-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	140-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	141-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	141-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	142-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	142-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	143-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	143-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	144-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	144-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	145-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	145-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	146-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	146-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	147-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	147-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	148-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	148-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	149-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	149-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	15-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	15-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	150-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	150-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	151-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	151-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	152-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	152-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	153-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	153-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	154-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	154-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	155-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	155-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	156-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	156-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	157-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	157-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	158-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	158-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	159-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	159-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	16-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	16-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	160-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	160-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	161-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	161-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	162-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	162-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	163-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	163-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	164-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	164-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	165-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	165-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	166-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	166-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	167-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	167-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	17-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	17-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	18-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	18-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	19-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	19-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	2-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	2-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	20-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	20-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	21-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	21-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	22-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	22-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	23-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	23-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	24-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	24-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	25-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	25-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	26-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	26-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	27-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	27-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	28-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	28-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	29-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	29-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	3-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	3-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	30-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	30-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	31-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	31-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	32-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	32-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	33-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	33-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	34-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	34-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	35-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	35-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	36-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	36-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	37-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	37-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	38-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	38-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	39-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	39-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	4-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	4-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	40-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	40-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	41-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	41-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	42-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	42-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	43-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	43-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	44-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	44-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	45-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	45-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	46-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	46-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	47-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	47-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	48-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	48-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	49-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	49-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	5-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	5-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	50-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	50-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	51-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	51-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	52-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	52-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	53-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	53-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	54-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	54-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	55-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	55-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	56-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	56-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	57-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	57-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	58-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	58-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	59-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	59-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	6-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	6-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	60-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	60-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	61-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	61-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	62-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	62-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	63-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	63-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	64-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	64-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	65-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	65-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	66-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	66-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	67-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	67-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	68-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	68-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	69-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	69-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	7-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	7-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	70-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	70-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	71-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	71-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	72-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	72-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	73-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	73-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	74-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	74-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	75-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	75-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	76-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	76-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	77-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	77-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	78-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	78-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	79-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	79-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	8-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	8-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	80-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	80-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	81-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	81-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	82-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	82-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	83-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	83-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	84-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	84-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	85-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	85-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	86-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	86-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	87-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	87-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	88-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	88-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	89-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	89-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	9-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	9-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	90-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	90-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	91-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	91-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	92-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	92-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	93-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	93-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	94-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	94-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	95-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	95-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	96-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	96-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	97-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	97-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	98-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	98-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	99-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	99-A	204	-	-	0/27/67/67	0/5/5/5

All (2051) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-A	201	FOL	C8A-N1	-6.65	1.30	1.37
4	69-A	204	NAP	O3B-C3B	-6.57	1.27	1.43
4	25-A	204	NAP	O3B-C3B	-6.56	1.27	1.43
4	75-A	204	NAP	O3B-C3B	-6.51	1.28	1.43
4	22-A	204	NAP	O3B-C3B	-6.51	1.28	1.43
4	116-A	204	NAP	O3B-C3B	-6.45	1.28	1.43
4	26-A	204	NAP	O3B-C3B	-6.44	1.28	1.43
2	152-A	201	FOL	C8A-N1	-6.44	1.30	1.37
2	12-A	201	FOL	C8A-N1	-6.43	1.30	1.37
4	70-A	204	NAP	O3B-C3B	-6.42	1.28	1.43
4	23-A	204	NAP	O3B-C3B	-6.40	1.28	1.43
4	33-A	204	NAP	O3B-C3B	-6.38	1.28	1.43
4	52-A	204	NAP	O3B-C3B	-6.38	1.28	1.43
4	30-A	204	NAP	O3B-C3B	-6.36	1.28	1.43
4	74-A	204	NAP	O3B-C3B	-6.36	1.28	1.43
4	71-A	204	NAP	O3B-C3B	-6.36	1.28	1.43
4	19-A	204	NAP	O3B-C3B	-6.33	1.28	1.43
4	68-A	204	NAP	O3B-C3B	-6.33	1.28	1.43
2	15-A	201	FOL	C8A-N1	-6.32	1.30	1.37
4	11-A	204	NAP	O3B-C3B	-6.32	1.28	1.43
2	7-A	201	FOL	C8A-N1	-6.31	1.30	1.37
4	64-A	204	NAP	O3B-C3B	-6.31	1.28	1.43
4	99-A	204	NAP	O3B-C3B	-6.30	1.28	1.43
4	147-A	204	NAP	O3B-C3B	-6.27	1.28	1.43
4	17-A	204	NAP	O3B-C3B	-6.27	1.28	1.43
4	76-A	204	NAP	O3B-C3B	-6.27	1.28	1.43
4	67-A	204	NAP	O3B-C3B	-6.26	1.28	1.43
4	51-A	204	NAP	O3B-C3B	-6.25	1.28	1.43
4	24-A	204	NAP	O3B-C3B	-6.25	1.28	1.43
4	27-A	204	NAP	O3B-C3B	-6.24	1.28	1.43
4	20-A	204	NAP	O3B-C3B	-6.23	1.28	1.43
2	9-A	201	FOL	C8A-N1	-6.23	1.30	1.37
4	60-A	204	NAP	O3B-C3B	-6.22	1.28	1.43
2	76-A	201	FOL	C8A-N1	-6.22	1.30	1.37
4	10-A	204	NAP	O3B-C3B	-6.22	1.28	1.43
4	122-A	204	NAP	O3B-C3B	-6.21	1.28	1.43
4	18-A	204	NAP	O3B-C3B	-6.21	1.28	1.43
4	106-A	204	NAP	O3B-C3B	-6.21	1.28	1.43
4	4-A	204	NAP	O3B-C3B	-6.20	1.28	1.43
4	65-A	204	NAP	O3B-C3B	-6.19	1.28	1.43
4	145-A	204	NAP	O3B-C3B	-6.19	1.28	1.43
4	140-A	204	NAP	O3B-C3B	-6.19	1.28	1.43
2	21-A	201	FOL	C8A-N1	-6.19	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	39-A	204	NAP	O3B-C3B	-6.18	1.28	1.43
4	103-A	204	NAP	O3B-C3B	-6.17	1.28	1.43
4	62-A	204	NAP	O3B-C3B	-6.16	1.28	1.43
4	40-A	204	NAP	O3B-C3B	-6.16	1.28	1.43
4	117-A	204	NAP	O3B-C3B	-6.15	1.28	1.43
2	59-A	201	FOL	C8A-N1	-6.15	1.30	1.37
2	42-A	201	FOL	C8A-N1	-6.14	1.30	1.37
4	165-A	204	NAP	O3B-C3B	-6.14	1.28	1.43
4	115-A	204	NAP	O3B-C3B	-6.13	1.28	1.43
2	19-A	201	FOL	C8A-N1	-6.12	1.30	1.37
4	149-A	204	NAP	O3B-C3B	-6.12	1.28	1.43
4	53-A	204	NAP	O3B-C3B	-6.12	1.28	1.43
4	129-A	204	NAP	O3B-C3B	-6.12	1.28	1.43
4	16-A	204	NAP	O3B-C3B	-6.12	1.28	1.43
4	80-A	204	NAP	O3B-C3B	-6.12	1.28	1.43
4	77-A	204	NAP	O3B-C3B	-6.12	1.28	1.43
4	38-A	204	NAP	O3B-C3B	-6.11	1.28	1.43
4	3-A	204	NAP	O3B-C3B	-6.11	1.28	1.43
4	28-A	204	NAP	O3B-C3B	-6.11	1.28	1.43
4	50-A	204	NAP	O3B-C3B	-6.09	1.28	1.43
4	49-A	204	NAP	O3B-C3B	-6.09	1.28	1.43
4	128-A	204	NAP	O3B-C3B	-6.09	1.28	1.43
4	127-A	204	NAP	O3B-C3B	-6.09	1.28	1.43
4	151-A	204	NAP	O3B-C3B	-6.09	1.28	1.43
4	42-A	204	NAP	O3B-C3B	-6.08	1.29	1.43
2	73-A	201	FOL	C8A-N1	-6.07	1.30	1.37
2	50-A	201	FOL	C8A-N1	-6.07	1.30	1.37
4	78-A	204	NAP	O3B-C3B	-6.07	1.29	1.43
4	98-A	204	NAP	O3B-C3B	-6.06	1.29	1.43
4	163-A	204	NAP	O3B-C3B	-6.06	1.29	1.43
4	161-A	204	NAP	O3B-C3B	-6.06	1.29	1.43
4	63-A	204	NAP	O3B-C3B	-6.06	1.29	1.43
4	124-A	204	NAP	O3B-C3B	-6.06	1.29	1.43
4	104-A	204	NAP	O3B-C3B	-6.05	1.29	1.43
4	55-A	204	NAP	O3B-C3B	-6.05	1.29	1.43
4	126-A	204	NAP	O3B-C3B	-6.05	1.29	1.43
4	100-A	204	NAP	O3B-C3B	-6.05	1.29	1.43
4	85-A	204	NAP	O3B-C3B	-6.05	1.29	1.43
4	119-A	204	NAP	O3B-C3B	-6.04	1.29	1.43
2	4-A	201	FOL	C8A-N1	-6.04	1.30	1.37
4	79-A	204	NAP	O3B-C3B	-6.03	1.29	1.43
4	72-A	204	NAP	O3B-C3B	-6.02	1.29	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	162-A	204	NAP	O3B-C3B	-6.02	1.29	1.43
4	47-A	204	NAP	O3B-C3B	-6.02	1.29	1.43
4	114-A	204	NAP	O3B-C3B	-6.01	1.29	1.43
4	141-A	204	NAP	O3B-C3B	-6.01	1.29	1.43
4	66-A	204	NAP	O3B-C3B	-6.00	1.29	1.43
4	123-A	204	NAP	O3B-C3B	-6.00	1.29	1.43
4	146-A	204	NAP	O3B-C3B	-6.00	1.29	1.43
4	143-A	204	NAP	O3B-C3B	-5.99	1.29	1.43
4	5-A	204	NAP	O3B-C3B	-5.99	1.29	1.43
4	97-A	204	NAP	O3B-C3B	-5.99	1.29	1.43
4	153-A	204	NAP	O3B-C3B	-5.99	1.29	1.43
4	148-A	204	NAP	O3B-C3B	-5.99	1.29	1.43
4	35-A	204	NAP	O3B-C3B	-5.98	1.29	1.43
4	73-A	204	NAP	O3B-C3B	-5.97	1.29	1.43
4	15-A	204	NAP	O3B-C3B	-5.97	1.29	1.43
4	105-A	204	NAP	O3B-C3B	-5.96	1.29	1.43
4	86-A	204	NAP	O3B-C3B	-5.96	1.29	1.43
2	117-A	201	FOL	C8A-N1	-5.96	1.30	1.37
4	21-A	204	NAP	O3B-C3B	-5.95	1.29	1.43
4	110-A	204	NAP	O3B-C3B	-5.95	1.29	1.43
4	156-A	204	NAP	O3B-C3B	-5.94	1.29	1.43
4	139-A	204	NAP	O3B-C3B	-5.94	1.29	1.43
4	102-A	204	NAP	O3B-C3B	-5.94	1.29	1.43
4	1-A	204	NAP	O3B-C3B	-5.93	1.29	1.43
4	107-A	204	NAP	O3B-C3B	-5.93	1.29	1.43
4	13-A	204	NAP	O3B-C3B	-5.92	1.29	1.43
2	47-A	201	FOL	C8A-N1	-5.92	1.30	1.37
4	48-A	204	NAP	O3B-C3B	-5.92	1.29	1.43
4	144-A	204	NAP	O3B-C3B	-5.92	1.29	1.43
2	74-A	201	FOL	C8A-N1	-5.92	1.30	1.37
4	37-A	204	NAP	O3B-C3B	-5.91	1.29	1.43
4	130-A	204	NAP	O3B-C3B	-5.89	1.29	1.43
4	167-A	204	NAP	O3B-C3B	-5.89	1.29	1.43
4	120-A	204	NAP	O3B-C3B	-5.89	1.29	1.43
4	135-A	204	NAP	O3B-C3B	-5.88	1.29	1.43
4	164-A	204	NAP	O3B-C3B	-5.88	1.29	1.43
4	61-A	204	NAP	O3B-C3B	-5.88	1.29	1.43
2	83-A	201	FOL	C8A-N1	-5.88	1.31	1.37
4	101-A	204	NAP	O3B-C3B	-5.87	1.29	1.43
4	91-A	204	NAP	O3B-C3B	-5.87	1.29	1.43
2	8-A	201	FOL	C8A-N1	-5.87	1.31	1.37
4	166-A	204	NAP	O3B-C3B	-5.85	1.29	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	14-A	204	NAP	O3B-C3B	-5.84	1.29	1.43
4	142-A	204	NAP	O3B-C3B	-5.84	1.29	1.43
4	45-A	204	NAP	O3B-C3B	-5.84	1.29	1.43
4	87-A	204	NAP	O3B-C3B	-5.82	1.29	1.43
4	2-A	204	NAP	O3B-C3B	-5.82	1.29	1.43
4	160-A	204	NAP	O3B-C3B	-5.81	1.29	1.43
4	36-A	204	NAP	O3B-C3B	-5.81	1.29	1.43
4	113-A	204	NAP	O3B-C3B	-5.81	1.29	1.43
4	12-A	204	NAP	O3B-C3B	-5.80	1.29	1.43
4	41-A	204	NAP	O3B-C3B	-5.80	1.29	1.43
4	118-A	204	NAP	O3B-C3B	-5.79	1.29	1.43
4	150-A	204	NAP	O3B-C3B	-5.79	1.29	1.43
4	136-A	204	NAP	O3B-C3B	-5.78	1.29	1.43
4	96-A	204	NAP	O3B-C3B	-5.78	1.29	1.43
4	88-A	204	NAP	O3B-C3B	-5.78	1.29	1.43
4	29-A	204	NAP	O3B-C3B	-5.78	1.29	1.43
4	92-A	204	NAP	O3B-C3B	-5.78	1.29	1.43
4	59-A	204	NAP	O3B-C3B	-5.78	1.29	1.43
4	44-A	204	NAP	O3B-C3B	-5.77	1.29	1.43
4	125-A	204	NAP	O3B-C3B	-5.75	1.29	1.43
4	43-A	204	NAP	O3B-C3B	-5.75	1.29	1.43
4	90-A	204	NAP	O3B-C3B	-5.74	1.29	1.43
4	121-A	204	NAP	O3B-C3B	-5.73	1.29	1.43
4	152-A	204	NAP	O3B-C3B	-5.73	1.29	1.43
4	154-A	204	NAP	O3B-C3B	-5.73	1.29	1.43
4	138-A	204	NAP	O3B-C3B	-5.72	1.29	1.43
4	54-A	204	NAP	O3B-C3B	-5.71	1.29	1.43
4	112-A	204	NAP	O3B-C3B	-5.71	1.29	1.43
4	111-A	204	NAP	O3B-C3B	-5.69	1.29	1.43
2	89-A	201	FOL	C8A-N1	-5.67	1.31	1.37
2	45-A	201	FOL	C8A-N1	-5.66	1.31	1.37
4	89-A	204	NAP	O3B-C3B	-5.66	1.29	1.43
4	137-A	204	NAP	O3B-C3B	-5.66	1.29	1.43
2	2-A	201	FOL	C8A-N1	-5.66	1.31	1.37
4	93-A	204	NAP	O3B-C3B	-5.64	1.30	1.43
2	57-A	201	FOL	C8A-N1	-5.62	1.31	1.37
2	70-A	201	FOL	C8A-N1	-5.61	1.31	1.37
4	155-A	204	NAP	O3B-C3B	-5.61	1.30	1.43
2	56-A	201	FOL	C8A-N1	-5.60	1.31	1.37
2	110-A	201	FOL	C8A-N1	-5.60	1.31	1.37
2	118-A	201	FOL	C8A-N1	-5.58	1.31	1.37
4	46-A	204	NAP	O3B-C3B	-5.58	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	71-A	201	FOL	C8A-N1	-5.58	1.31	1.37
4	81-A	204	NAP	O3B-C3B	-5.57	1.30	1.43
2	51-A	201	FOL	C8A-N1	-5.57	1.31	1.37
2	20-A	201	FOL	C8A-N1	-5.57	1.31	1.37
2	134-A	201	FOL	C8A-N1	-5.56	1.31	1.37
2	167-A	201	FOL	C8A-N1	-5.56	1.31	1.37
2	151-A	201	FOL	C8A-N1	-5.53	1.31	1.37
2	32-A	201	FOL	C8A-N1	-5.51	1.31	1.37
4	94-A	204	NAP	O3B-C3B	-5.49	1.30	1.43
2	92-A	201	FOL	C8A-N1	-5.49	1.31	1.37
4	131-A	204	NAP	O3B-C3B	-5.46	1.30	1.43
4	58-A	204	NAP	O3B-C3B	-5.46	1.30	1.43
2	160-A	201	FOL	C8A-N1	-5.43	1.31	1.37
2	129-A	201	FOL	C8A-N1	-5.43	1.31	1.37
2	158-A	201	FOL	C8A-N1	-5.43	1.31	1.37
2	68-A	201	FOL	C8A-N1	-5.42	1.31	1.37
2	143-A	201	FOL	C8A-N1	-5.41	1.31	1.37
2	137-A	201	FOL	C8A-N1	-5.40	1.31	1.37
2	162-A	201	FOL	C8A-N1	-5.39	1.31	1.37
2	146-A	201	FOL	C8A-N1	-5.38	1.31	1.37
2	119-A	201	FOL	C8A-N1	-5.37	1.31	1.37
2	30-A	201	FOL	C8A-N1	-5.37	1.31	1.37
2	28-A	201	FOL	C8A-N1	-5.36	1.31	1.37
2	1-A	201	FOL	C8A-N1	-5.35	1.31	1.37
2	22-A	201	FOL	C8A-N1	-5.35	1.31	1.37
2	132-A	201	FOL	C8A-N1	-5.34	1.31	1.37
2	34-A	201	FOL	C8A-N1	-5.34	1.31	1.37
4	95-A	204	NAP	O3B-C3B	-5.34	1.30	1.43
2	126-A	201	FOL	C8A-N1	-5.34	1.31	1.37
2	23-A	201	FOL	C8A-N1	-5.34	1.31	1.37
4	34-A	204	NAP	O3B-C3B	-5.33	1.30	1.43
2	27-A	201	FOL	C8A-N1	-5.32	1.31	1.37
2	154-A	201	FOL	C8A-N1	-5.30	1.31	1.37
2	157-A	201	FOL	C8A-N1	-5.30	1.31	1.37
2	111-A	201	FOL	C8A-N1	-5.29	1.31	1.37
2	94-A	201	FOL	C8A-N1	-5.28	1.31	1.37
4	32-A	204	NAP	O3B-C3B	-5.28	1.30	1.43
2	98-A	201	FOL	C8A-N1	-5.28	1.31	1.37
4	31-A	204	NAP	O3B-C3B	-5.28	1.30	1.43
2	65-A	201	FOL	C8A-N1	-5.28	1.31	1.37
2	40-A	201	FOL	C8A-N1	-5.27	1.31	1.37
4	82-A	204	NAP	O3B-C3B	-5.26	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	44-A	201	FOL	C8A-N1	-5.26	1.31	1.37
2	17-A	201	FOL	C8A-N1	-5.24	1.31	1.37
4	84-A	204	NAP	O3B-C3B	-5.23	1.30	1.43
2	66-A	201	FOL	C8A-N1	-5.22	1.31	1.37
2	39-A	201	FOL	C8A-N1	-5.21	1.31	1.37
4	108-A	204	NAP	O3B-C3B	-5.20	1.31	1.43
2	69-A	201	FOL	C8A-N1	-5.19	1.31	1.37
2	36-A	201	FOL	C8A-N1	-5.18	1.31	1.37
2	62-A	201	FOL	C8A-N1	-5.18	1.31	1.37
2	133-A	201	FOL	C8A-N1	-5.17	1.31	1.37
2	53-A	201	FOL	C8A-N1	-5.15	1.31	1.37
2	77-A	201	FOL	C8A-N1	-5.15	1.31	1.37
2	121-A	201	FOL	C8A-N1	-5.15	1.31	1.37
2	18-A	201	FOL	C8A-N1	-5.14	1.31	1.37
2	147-A	201	FOL	C8A-N1	-5.13	1.31	1.37
2	85-A	201	FOL	C8A-N1	-5.11	1.31	1.37
2	105-A	201	FOL	C8A-N1	-5.11	1.31	1.37
4	157-A	204	NAP	O3B-C3B	-5.10	1.31	1.43
2	100-A	201	FOL	C8A-N1	-5.08	1.31	1.37
4	83-A	204	NAP	O3B-C3B	-5.08	1.31	1.43
2	16-A	201	FOL	C8A-N1	-5.08	1.31	1.37
2	25-A	201	FOL	C8A-N1	-5.07	1.31	1.37
4	158-A	204	NAP	O3B-C3B	-5.07	1.31	1.43
2	41-A	201	FOL	C8A-N1	-5.06	1.31	1.37
2	26-A	201	FOL	C8A-N1	-5.06	1.31	1.37
4	57-A	204	NAP	O3B-C3B	-5.06	1.31	1.43
4	56-A	204	NAP	O3B-C3B	-5.05	1.31	1.43
2	33-A	201	FOL	C8A-N1	-5.05	1.31	1.37
2	72-A	201	FOL	C8A-N1	-5.04	1.31	1.37
2	58-A	201	FOL	C8A-N1	-5.04	1.31	1.37
2	113-A	201	FOL	C8A-N1	-5.02	1.31	1.37
2	52-A	201	FOL	C8A-N1	-5.01	1.31	1.37
4	133-A	204	NAP	O3B-C3B	-5.00	1.31	1.43
2	148-A	201	FOL	C8A-N1	-5.00	1.31	1.37
4	9-A	204	NAP	O3B-C3B	-4.99	1.31	1.43
2	136-A	201	FOL	C8A-N1	-4.99	1.31	1.37
2	123-A	201	FOL	C8A-N1	-4.98	1.31	1.37
2	37-A	201	FOL	C8A-N1	-4.97	1.32	1.37
4	6-A	204	NAP	O3B-C3B	-4.96	1.31	1.43
2	96-A	201	FOL	C8A-N1	-4.95	1.32	1.37
2	139-A	201	FOL	C8A-N1	-4.95	1.32	1.37
2	144-A	201	FOL	C8A-N1	-4.95	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	8-A	204	NAP	O3B-C3B	-4.95	1.31	1.43
2	124-A	201	FOL	C8A-N1	-4.94	1.32	1.37
4	132-A	204	NAP	O3B-C3B	-4.93	1.31	1.43
2	13-A	201	FOL	C8A-N1	-4.91	1.32	1.37
2	145-A	201	FOL	C8A-N1	-4.90	1.32	1.37
4	159-A	204	NAP	O3B-C3B	-4.90	1.31	1.43
2	55-A	201	FOL	C8A-N1	-4.89	1.32	1.37
4	109-A	204	NAP	O3B-C3B	-4.89	1.31	1.43
2	149-A	201	FOL	C8A-N1	-4.88	1.32	1.37
2	82-A	201	FOL	C8A-N1	-4.87	1.32	1.37
4	134-A	204	NAP	O3B-C3B	-4.86	1.31	1.43
2	99-A	201	FOL	C8A-N1	-4.86	1.32	1.37
2	153-A	201	FOL	C8A-N1	-4.85	1.32	1.37
2	109-A	201	FOL	C8A-N1	-4.85	1.32	1.37
2	164-A	201	FOL	C8A-N1	-4.85	1.32	1.37
2	155-A	201	FOL	C8A-N1	-4.83	1.32	1.37
2	46-A	201	FOL	C8A-N1	-4.83	1.32	1.37
2	43-A	201	FOL	C8A-N1	-4.82	1.32	1.37
2	48-A	201	FOL	C8A-N1	-4.80	1.32	1.37
2	67-A	201	FOL	C8A-N1	-4.78	1.32	1.37
2	166-A	201	FOL	C8A-N1	-4.77	1.32	1.37
2	60-A	201	FOL	C8A-N1	-4.77	1.32	1.37
2	35-A	201	FOL	C8A-N1	-4.76	1.32	1.37
2	115-A	201	FOL	C8A-N1	-4.76	1.32	1.37
2	108-A	201	FOL	C8A-N1	-4.75	1.32	1.37
2	141-A	201	FOL	C8A-N1	-4.74	1.32	1.37
2	91-A	201	FOL	C8A-N1	-4.74	1.32	1.37
2	78-A	201	FOL	C8A-N1	-4.71	1.32	1.37
2	103-A	201	FOL	C8A-N1	-4.70	1.32	1.37
4	7-A	204	NAP	O3B-C3B	-4.69	1.32	1.43
2	14-A	201	FOL	C8A-N1	-4.69	1.32	1.37
2	114-A	201	FOL	C8A-N1	-4.68	1.32	1.37
2	107-A	201	FOL	C8A-N1	-4.67	1.32	1.37
2	11-A	201	FOL	C8A-N1	-4.66	1.32	1.37
2	5-A	201	FOL	C8A-N1	-4.65	1.32	1.37
2	80-A	201	FOL	C8A-N1	-4.65	1.32	1.37
2	130-A	201	FOL	C8A-N1	-4.65	1.32	1.37
2	54-A	201	FOL	C8A-N1	-4.63	1.32	1.37
2	116-A	201	FOL	C8A-N1	-4.61	1.32	1.37
2	3-A	201	FOL	C8A-N1	-4.60	1.32	1.37
2	75-A	201	FOL	C8A-N1	-4.59	1.32	1.37
2	150-A	201	FOL	C8A-N1	-4.55	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	135-A	201	FOL	C8A-N1	-4.55	1.32	1.37
2	101-A	201	FOL	C8A-N1	-4.54	1.32	1.37
2	84-A	201	FOL	C8A-N1	-4.52	1.32	1.37
2	112-A	201	FOL	C8A-N1	-4.52	1.32	1.37
2	24-A	201	FOL	C8A-N1	-4.51	1.32	1.37
2	122-A	201	FOL	C8A-N1	-4.49	1.32	1.37
2	140-A	201	FOL	C8A-N1	-4.48	1.32	1.37
2	81-A	201	FOL	C8A-N1	-4.45	1.32	1.37
2	93-A	201	FOL	C8A-N1	-4.41	1.32	1.37
2	61-A	201	FOL	C8A-N1	-4.41	1.32	1.37
2	87-A	201	FOL	C8A-N1	-4.41	1.32	1.37
2	86-A	201	FOL	C8A-N1	-4.40	1.32	1.37
2	90-A	201	FOL	C8A-N1	-4.40	1.32	1.37
2	31-A	201	FOL	C8A-N1	-4.39	1.32	1.37
2	95-A	201	FOL	C8A-N1	-4.39	1.32	1.37
2	165-A	201	FOL	C8A-N1	-4.38	1.32	1.37
2	79-A	201	FOL	C8A-N1	-4.38	1.32	1.37
2	120-A	201	FOL	C8A-N1	-4.37	1.32	1.37
4	119-A	204	NAP	O4B-C4B	-4.34	1.35	1.45
2	64-A	201	FOL	C8A-N1	-4.33	1.32	1.37
2	63-A	201	FOL	C8A-N1	-4.31	1.32	1.37
2	125-A	201	FOL	C8A-N1	-4.31	1.32	1.37
2	142-A	201	FOL	C8A-N1	-4.28	1.32	1.37
2	10-A	201	FOL	C8A-N1	-4.21	1.32	1.37
2	156-A	201	FOL	C8A-N1	-4.10	1.32	1.37
2	131-A	201	FOL	C8A-N1	-4.10	1.32	1.37
2	100-A	201	FOL	CA-N	-4.08	1.40	1.46
2	49-A	201	FOL	C8A-N1	-4.07	1.32	1.37
2	65-A	201	FOL	CA-N	-4.06	1.40	1.46
2	159-A	201	FOL	C8A-N1	-4.01	1.33	1.37
2	88-A	201	FOL	C8A-N1	-3.96	1.33	1.37
2	102-A	201	FOL	C8A-N1	-3.95	1.33	1.37
2	97-A	201	FOL	C8A-N1	-3.92	1.33	1.37
2	52-A	201	FOL	CA-N	-3.90	1.41	1.46
4	39-A	204	NAP	C2D-C1D	-3.90	1.47	1.53
2	156-A	201	FOL	CA-N	-3.88	1.41	1.46
4	33-A	204	NAP	O4B-C4B	-3.79	1.36	1.45
4	112-A	204	NAP	C2D-C1D	-3.76	1.47	1.53
2	138-A	201	FOL	C8A-N1	-3.75	1.33	1.37
2	29-A	201	FOL	C8A-N1	-3.75	1.33	1.37
4	113-A	204	NAP	C2D-C1D	-3.74	1.47	1.53
4	107-A	204	NAP	C2D-C1D	-3.73	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	38-A	201	FOL	C8A-N1	-3.71	1.33	1.37
2	127-A	201	FOL	C8A-N1	-3.61	1.33	1.37
4	165-A	204	NAP	C2D-C1D	-3.59	1.47	1.53
4	118-A	204	NAP	C2D-C1D	-3.56	1.48	1.53
4	111-A	204	NAP	C2D-C1D	-3.56	1.48	1.53
4	104-A	204	NAP	C2D-C1D	-3.56	1.48	1.53
2	106-A	201	FOL	C8A-N1	-3.55	1.33	1.37
4	100-A	204	NAP	C2D-C1D	-3.55	1.48	1.53
4	106-A	204	NAP	C2D-C1D	-3.52	1.48	1.53
4	115-A	204	NAP	C2D-C1D	-3.50	1.48	1.53
2	161-A	201	FOL	C8A-N1	-3.49	1.33	1.37
4	157-A	204	NAP	C2D-C1D	-3.45	1.48	1.53
4	22-A	204	NAP	C2D-C1D	-3.44	1.48	1.53
4	85-A	204	NAP	C2D-C1D	-3.41	1.48	1.53
4	18-A	204	NAP	C2D-C1D	-3.41	1.48	1.53
4	14-A	204	NAP	C2D-C1D	-3.38	1.48	1.53
4	101-A	204	NAP	C2D-C1D	-3.37	1.48	1.53
2	163-A	201	FOL	C8A-N1	-3.37	1.33	1.37
4	95-A	204	NAP	C2D-C1D	-3.37	1.48	1.53
4	2-A	204	NAP	C2D-C1D	-3.36	1.48	1.53
4	17-A	204	NAP	C2D-C1D	-3.34	1.48	1.53
4	12-A	204	NAP	C2D-C1D	-3.33	1.48	1.53
4	105-A	204	NAP	C2D-C1D	-3.32	1.48	1.53
4	23-A	204	NAP	C2D-C1D	-3.31	1.48	1.53
4	99-A	204	NAP	C2D-C1D	-3.31	1.48	1.53
4	83-A	204	NAP	C2D-C1D	-3.31	1.48	1.53
4	63-A	204	NAP	C2D-C1D	-3.30	1.48	1.53
4	110-A	204	NAP	C2D-C1D	-3.30	1.48	1.53
4	108-A	204	NAP	C2D-C1D	-3.30	1.48	1.53
4	147-A	204	NAP	C2D-C1D	-3.29	1.48	1.53
4	65-A	204	NAP	C2D-C1D	-3.28	1.48	1.53
4	94-A	204	NAP	C2D-C1D	-3.26	1.48	1.53
4	116-A	204	NAP	C2D-C1D	-3.25	1.48	1.53
4	117-A	204	NAP	C2D-C1D	-3.25	1.48	1.53
4	15-A	204	NAP	C2D-C1D	-3.25	1.48	1.53
4	97-A	204	NAP	C2D-C1D	-3.24	1.48	1.53
4	155-A	204	NAP	C2D-C1D	-3.22	1.48	1.53
4	89-A	204	NAP	C2D-C1D	-3.21	1.48	1.53
4	86-A	204	NAP	C2D-C1D	-3.21	1.48	1.53
4	148-A	204	NAP	C2D-C1D	-3.21	1.48	1.53
4	166-A	204	NAP	C2D-C1D	-3.20	1.48	1.53
4	16-A	204	NAP	C2D-C1D	-3.20	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	98-A	204	NAP	C2D-C1D	-3.20	1.48	1.53
4	119-A	204	NAP	C2D-C1D	-3.20	1.48	1.53
4	96-A	204	NAP	C2D-C1D	-3.20	1.48	1.53
4	109-A	204	NAP	C2D-C1D	-3.19	1.48	1.53
2	104-A	201	FOL	C8A-N1	-3.19	1.33	1.37
4	102-A	204	NAP	O4B-C4B	-3.18	1.37	1.45
4	81-A	204	NAP	C2D-C1D	-3.18	1.48	1.53
4	42-A	204	NAP	O4B-C4B	-3.18	1.37	1.45
4	50-A	204	NAP	O4B-C4B	-3.17	1.37	1.45
4	9-A	204	NAP	C2D-C1D	-3.17	1.48	1.53
4	82-A	204	NAP	C2D-C1D	-3.17	1.48	1.53
4	61-A	204	NAP	C2D-C1D	-3.16	1.48	1.53
4	13-A	204	NAP	C2D-C1D	-3.16	1.48	1.53
4	10-A	204	NAP	C2D-C1D	-3.15	1.48	1.53
4	88-A	204	NAP	C2D-C1D	-3.14	1.48	1.53
4	132-A	204	NAP	C2D-C1D	-3.13	1.48	1.53
4	87-A	204	NAP	C2D-C1D	-3.12	1.48	1.53
4	7-A	204	NAP	C2D-C1D	-3.12	1.48	1.53
4	64-A	204	NAP	C2D-C1D	-3.12	1.48	1.53
4	5-A	204	NAP	C2D-C1D	-3.12	1.48	1.53
4	72-A	204	NAP	C2D-C1D	-3.11	1.48	1.53
4	103-A	204	NAP	C2D-C1D	-3.11	1.48	1.53
4	146-A	204	NAP	C2D-C1D	-3.10	1.48	1.53
4	66-A	204	NAP	C2D-C1D	-3.10	1.48	1.53
4	114-A	204	NAP	C2D-C1D	-3.09	1.48	1.53
4	92-A	204	NAP	C2D-C1D	-3.09	1.48	1.53
4	11-A	204	NAP	C2D-C1D	-3.09	1.48	1.53
4	62-A	204	NAP	C2D-C1D	-3.09	1.48	1.53
4	29-A	204	NAP	C2D-C1D	-3.08	1.48	1.53
4	70-A	204	NAP	C2D-C1D	-3.08	1.48	1.53
4	20-A	204	NAP	C2D-C1D	-3.07	1.48	1.53
4	24-A	204	NAP	O4B-C4B	-3.07	1.38	1.45
4	161-A	204	NAP	C2D-C1D	-3.07	1.48	1.53
4	150-A	204	NAP	C2D-C1D	-3.07	1.48	1.53
4	143-A	204	NAP	C2D-C1D	-3.07	1.48	1.53
4	6-A	204	NAP	C2D-C1D	-3.06	1.48	1.53
4	19-A	204	NAP	C2D-C1D	-3.06	1.48	1.53
4	60-A	204	NAP	C2D-C1D	-3.06	1.48	1.53
4	133-A	204	NAP	C2D-C1D	-3.06	1.48	1.53
4	80-A	204	NAP	C2D-C1D	-3.05	1.48	1.53
4	118-A	204	NAP	O4B-C4B	-3.05	1.38	1.45
4	131-A	204	NAP	C2D-C1D	-3.04	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	152-A	204	NAP	C2D-C1D	-3.03	1.48	1.53
4	115-A	204	NAP	O7N-C7N	-3.03	1.18	1.24
4	135-A	204	NAP	C2D-C1D	-3.03	1.48	1.53
4	137-A	204	NAP	C2D-C1D	-3.03	1.48	1.53
4	71-A	204	NAP	C2D-C1D	-3.02	1.48	1.53
4	154-A	204	NAP	C2D-C1D	-3.02	1.48	1.53
4	151-A	204	NAP	C2D-C1D	-3.02	1.48	1.53
4	56-A	204	NAP	C2D-C1D	-3.02	1.48	1.53
4	74-A	204	NAP	C2D-C1D	-3.02	1.48	1.53
2	128-A	201	FOL	C8A-N1	-3.02	1.34	1.37
4	144-A	204	NAP	C2D-C1D	-3.01	1.48	1.53
4	156-A	204	NAP	C2D-C1D	-3.01	1.48	1.53
4	1-A	204	NAP	C2D-C1D	-3.01	1.48	1.53
4	136-A	204	NAP	C2D-C1D	-2.99	1.48	1.53
4	167-A	204	NAP	C2D-C1D	-2.99	1.48	1.53
4	142-A	204	NAP	C2D-C1D	-2.99	1.48	1.53
4	84-A	204	NAP	C2D-C1D	-2.99	1.48	1.53
4	53-A	204	NAP	C2D-C1D	-2.99	1.48	1.53
4	145-A	204	NAP	C2D-C1D	-2.98	1.48	1.53
4	24-A	204	NAP	C2D-C1D	-2.98	1.48	1.53
4	30-A	204	NAP	C2D-C1D	-2.98	1.48	1.53
4	21-A	204	NAP	C2D-C1D	-2.98	1.48	1.53
4	102-A	204	NAP	C2D-C1D	-2.98	1.48	1.53
4	79-A	204	NAP	C2D-C1D	-2.97	1.48	1.53
4	43-A	204	NAP	C2D-C1D	-2.97	1.48	1.53
4	75-A	204	NAP	C2D-C1D	-2.97	1.48	1.53
4	55-A	204	NAP	C2D-C1D	-2.97	1.48	1.53
4	160-A	204	NAP	C2D-C1D	-2.96	1.48	1.53
4	51-A	204	NAP	O4B-C4B	-2.96	1.38	1.45
4	159-A	204	NAP	C2D-C1D	-2.95	1.48	1.53
4	94-A	204	NAP	O4B-C4B	-2.95	1.38	1.45
4	128-A	204	NAP	C2D-C1D	-2.95	1.49	1.53
4	28-A	204	NAP	C2D-C1D	-2.94	1.49	1.53
4	80-A	204	NAP	O4B-C4B	-2.94	1.38	1.45
4	123-A	204	NAP	C2D-C1D	-2.94	1.49	1.53
4	20-A	204	NAP	O4B-C4B	-2.93	1.38	1.45
4	120-A	204	NAP	C2D-C1D	-2.93	1.49	1.53
4	34-A	204	NAP	O4B-C4B	-2.93	1.38	1.45
4	38-A	204	NAP	O4B-C4B	-2.93	1.38	1.45
4	47-A	204	NAP	C2D-C1D	-2.92	1.49	1.53
4	73-A	204	NAP	C2D-C1D	-2.92	1.49	1.53
4	44-A	204	NAP	C2D-C1D	-2.92	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	82-A	204	NAP	O4B-C4B	-2.92	1.38	1.45
4	67-A	204	NAP	C2D-C1D	-2.92	1.49	1.53
4	21-A	204	NAP	O4B-C4B	-2.92	1.38	1.45
4	91-A	204	NAP	C2D-C1D	-2.92	1.49	1.53
4	140-A	204	NAP	C2D-C1D	-2.91	1.49	1.53
4	134-A	204	NAP	C2D-C1D	-2.91	1.49	1.53
4	25-A	204	NAP	C2D-C1D	-2.91	1.49	1.53
4	53-A	204	NAP	O4B-C4B	-2.90	1.38	1.45
4	76-A	204	NAP	C2D-C1D	-2.89	1.49	1.53
4	38-A	204	NAP	C2D-C1D	-2.89	1.49	1.53
4	97-A	204	NAP	O4B-C4B	-2.88	1.38	1.45
4	25-A	204	NAP	O4B-C4B	-2.87	1.38	1.45
4	23-A	204	NAP	O4B-C4B	-2.87	1.38	1.45
4	93-A	204	NAP	C2D-C1D	-2.87	1.49	1.53
4	162-A	204	NAP	C2D-C1D	-2.86	1.49	1.53
4	49-A	204	NAP	O4B-C4B	-2.86	1.38	1.45
4	129-A	204	NAP	C2D-C1D	-2.85	1.49	1.53
4	18-A	204	NAP	O4B-C4B	-2.85	1.38	1.45
4	69-A	204	NAP	C2D-C1D	-2.85	1.49	1.53
4	95-A	204	NAP	O4B-C4B	-2.85	1.38	1.45
4	33-A	204	NAP	O7N-C7N	-2.85	1.18	1.24
4	41-A	204	NAP	O4B-C4B	-2.85	1.38	1.45
4	31-A	204	NAP	C2D-C1D	-2.84	1.49	1.53
4	54-A	204	NAP	C2D-C1D	-2.84	1.49	1.53
4	77-A	204	NAP	C2D-C1D	-2.84	1.49	1.53
4	55-A	204	NAP	O4B-C4B	-2.84	1.38	1.45
4	39-A	204	NAP	O4B-C4B	-2.84	1.38	1.45
4	38-A	204	NAP	C2D-C3D	-2.84	1.45	1.53
4	121-A	204	NAP	C2D-C1D	-2.83	1.49	1.53
4	98-A	204	NAP	O4B-C4B	-2.83	1.38	1.45
4	149-A	204	NAP	C2D-C1D	-2.83	1.49	1.53
4	19-A	204	NAP	O4B-C4B	-2.83	1.38	1.45
4	163-A	204	NAP	C2D-C1D	-2.82	1.49	1.53
4	39-A	204	NAP	C2D-C3D	-2.82	1.46	1.53
4	107-A	204	NAP	O4B-C4B	-2.82	1.38	1.45
4	99-A	204	NAP	O4B-C4B	-2.82	1.38	1.45
4	52-A	204	NAP	O4B-C4B	-2.82	1.38	1.45
4	153-A	204	NAP	C2D-C1D	-2.81	1.49	1.53
4	40-A	204	NAP	C2D-C1D	-2.81	1.49	1.53
4	96-A	204	NAP	O4B-C4B	-2.81	1.38	1.45
4	138-A	204	NAP	C2D-C1D	-2.80	1.49	1.53
4	93-A	204	NAP	O4B-C4B	-2.79	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	60-A	204	NAP	O4B-C4B	-2.79	1.38	1.45
4	48-A	204	NAP	C2D-C1D	-2.79	1.49	1.53
4	108-A	204	NAP	O7N-C7N	-2.79	1.18	1.24
4	164-A	204	NAP	C2D-C1D	-2.78	1.49	1.53
4	69-A	204	NAP	O4B-C4B	-2.78	1.38	1.45
4	36-A	204	NAP	O4B-C4B	-2.78	1.38	1.45
4	52-A	204	NAP	C2D-C1D	-2.78	1.49	1.53
4	122-A	204	NAP	C2D-C1D	-2.78	1.49	1.53
4	130-A	204	NAP	C2D-C1D	-2.78	1.49	1.53
4	54-A	204	NAP	O4B-C4B	-2.77	1.38	1.45
4	8-A	204	NAP	C2D-C1D	-2.77	1.49	1.53
2	143-A	201	FOL	CA-N	-2.77	1.42	1.46
4	165-A	204	NAP	C3D-C4D	-2.77	1.45	1.53
4	90-A	204	NAP	C2D-C1D	-2.77	1.49	1.53
4	67-A	204	NAP	O4B-C4B	-2.76	1.38	1.45
4	58-A	204	NAP	C2D-C1D	-2.76	1.49	1.53
4	117-A	204	NAP	O4B-C4B	-2.76	1.38	1.45
4	26-A	204	NAP	O4B-C4B	-2.76	1.38	1.45
4	35-A	204	NAP	O4B-C4B	-2.76	1.38	1.45
4	3-A	204	NAP	C2D-C1D	-2.76	1.49	1.53
4	11-A	204	NAP	O4B-C4B	-2.76	1.38	1.45
4	22-A	204	NAP	O4B-C4B	-2.76	1.38	1.45
4	81-A	204	NAP	O4B-C4B	-2.75	1.38	1.45
4	158-A	204	NAP	C2D-C1D	-2.75	1.49	1.53
2	77-A	201	FOL	CA-N	-2.75	1.42	1.46
4	139-A	204	NAP	C2D-C1D	-2.75	1.49	1.53
4	78-A	204	NAP	C2D-C1D	-2.75	1.49	1.53
4	127-A	204	NAP	C2D-C1D	-2.75	1.49	1.53
4	62-A	204	NAP	O4B-C4B	-2.74	1.38	1.45
4	137-A	204	NAP	O4B-C4B	-2.74	1.38	1.45
4	100-A	204	NAP	O4B-C4B	-2.73	1.38	1.45
4	68-A	204	NAP	O4B-C4B	-2.73	1.38	1.45
4	77-A	204	NAP	O4B-C4B	-2.73	1.38	1.45
4	138-A	204	NAP	O4B-C4B	-2.73	1.38	1.45
4	17-A	204	NAP	O4B-C4B	-2.73	1.38	1.45
4	27-A	204	NAP	C2D-C1D	-2.72	1.49	1.53
4	6-A	204	NAP	O7N-C7N	-2.72	1.18	1.24
4	126-A	204	NAP	C2D-C1D	-2.72	1.49	1.53
4	103-A	204	NAP	O4B-C4B	-2.72	1.38	1.45
4	12-A	204	NAP	O4B-C4B	-2.72	1.38	1.45
4	37-A	204	NAP	C2D-C1D	-2.72	1.49	1.53
4	68-A	204	NAP	C2D-C1D	-2.72	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	41-A	204	NAP	C2D-C1D	-2.72	1.49	1.53
4	16-A	204	NAP	O4B-C4B	-2.72	1.38	1.45
4	124-A	204	NAP	C2D-C1D	-2.71	1.49	1.53
4	136-A	204	NAP	O4B-C4B	-2.71	1.38	1.45
4	115-A	204	NAP	O4B-C4B	-2.71	1.38	1.45
4	4-A	204	NAP	C2D-C1D	-2.71	1.49	1.53
4	116-A	204	NAP	O4B-C4B	-2.71	1.38	1.45
4	149-A	204	NAP	O4B-C4B	-2.71	1.38	1.45
2	106-A	201	FOL	CA-N	-2.70	1.42	1.46
4	32-A	204	NAP	C2D-C1D	-2.70	1.49	1.53
4	120-A	204	NAP	O4B-C4B	-2.70	1.38	1.45
4	70-A	204	NAP	O4B-C4B	-2.69	1.38	1.45
4	101-A	204	NAP	O4B-C4B	-2.69	1.38	1.45
4	37-A	204	NAP	O4B-C4B	-2.69	1.38	1.45
4	124-A	204	NAP	O4B-C4B	-2.69	1.38	1.45
4	13-A	204	NAP	O4B-C4B	-2.69	1.38	1.45
4	92-A	204	NAP	O4B-C4B	-2.68	1.38	1.45
4	141-A	204	NAP	C2D-C1D	-2.68	1.49	1.53
4	31-A	204	NAP	O7N-C7N	-2.68	1.18	1.24
4	45-A	204	NAP	C2D-C1D	-2.67	1.49	1.53
4	46-A	204	NAP	C2D-C1D	-2.67	1.49	1.53
4	14-A	204	NAP	O4B-C4B	-2.67	1.39	1.45
4	78-A	204	NAP	O4B-C4B	-2.67	1.39	1.45
4	110-A	204	NAP	O4B-C4B	-2.65	1.39	1.45
4	42-A	204	NAP	C2D-C1D	-2.65	1.49	1.53
4	90-A	204	NAP	O4B-C4B	-2.64	1.39	1.45
4	59-A	204	NAP	C2D-C1D	-2.64	1.49	1.53
4	65-A	204	NAP	O4B-C4B	-2.64	1.39	1.45
4	91-A	204	NAP	O4B-C4B	-2.64	1.39	1.45
4	41-A	204	NAP	O7N-C7N	-2.64	1.18	1.24
4	44-A	204	NAP	O4B-C4B	-2.64	1.39	1.45
4	32-A	204	NAP	O4B-C4B	-2.64	1.39	1.45
4	34-A	204	NAP	C2D-C1D	-2.63	1.49	1.53
4	130-A	204	NAP	O4B-C4B	-2.63	1.39	1.45
4	51-A	204	NAP	C2D-C1D	-2.63	1.49	1.53
4	131-A	204	NAP	O4B-C4B	-2.63	1.39	1.45
4	135-A	204	NAP	O4B-C4B	-2.63	1.39	1.45
4	104-A	204	NAP	O4B-C4B	-2.62	1.39	1.45
4	40-A	204	NAP	O4B-C4B	-2.62	1.39	1.45
4	79-A	204	NAP	O4B-C4B	-2.62	1.39	1.45
4	89-A	204	NAP	O4B-C4B	-2.62	1.39	1.45
4	105-A	204	NAP	O4B-C4B	-2.62	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	27-A	204	NAP	O4B-C4B	-2.62	1.39	1.45
4	66-A	204	NAP	O4B-C4B	-2.61	1.39	1.45
4	46-A	204	NAP	O4B-C4B	-2.61	1.39	1.45
4	106-A	204	NAP	O4B-C4B	-2.61	1.39	1.45
4	49-A	204	NAP	O7N-C7N	-2.61	1.18	1.24
4	48-A	204	NAP	O4B-C4B	-2.61	1.39	1.45
4	4-A	204	NAP	O4B-C4B	-2.60	1.39	1.45
4	26-A	204	NAP	C2D-C1D	-2.60	1.49	1.53
4	35-A	204	NAP	C2D-C1D	-2.60	1.49	1.53
4	36-A	204	NAP	C2D-C1D	-2.59	1.49	1.53
4	134-A	204	NAP	O4B-C4B	-2.59	1.39	1.45
4	145-A	204	NAP	O4B-C4B	-2.58	1.39	1.45
4	35-A	204	NAP	O7N-C7N	-2.58	1.18	1.24
4	57-A	204	NAP	C2D-C1D	-2.58	1.49	1.53
4	114-A	204	NAP	O4B-C4B	-2.58	1.39	1.45
4	111-A	204	NAP	O4B-C4B	-2.58	1.39	1.45
4	150-A	204	NAP	O4B-C4B	-2.57	1.39	1.45
4	43-A	204	NAP	O4B-C4B	-2.56	1.39	1.45
4	125-A	204	NAP	O4B-C4B	-2.56	1.39	1.45
4	83-A	204	NAP	O7N-C7N	-2.56	1.18	1.24
4	132-A	204	NAP	O4B-C4B	-2.56	1.39	1.45
4	64-A	204	NAP	O4B-C4B	-2.55	1.39	1.45
4	5-A	204	NAP	O4B-C4B	-2.55	1.39	1.45
4	9-A	204	NAP	O7N-C7N	-2.55	1.18	1.24
4	75-A	204	NAP	O4B-C4B	-2.55	1.39	1.45
4	139-A	204	NAP	O4B-C4B	-2.55	1.39	1.45
4	59-A	204	NAP	O4B-C4B	-2.54	1.39	1.45
4	45-A	204	NAP	O4B-C4B	-2.53	1.39	1.45
4	73-A	204	NAP	O4B-C4B	-2.53	1.39	1.45
4	112-A	204	NAP	O4B-C4B	-2.53	1.39	1.45
4	74-A	204	NAP	O4B-C4B	-2.52	1.39	1.45
4	32-A	204	NAP	O7N-C7N	-2.52	1.19	1.24
4	148-A	204	NAP	O4B-C4B	-2.52	1.39	1.45
4	47-A	204	NAP	O4B-C4B	-2.52	1.39	1.45
4	15-A	204	NAP	O4B-C4B	-2.52	1.39	1.45
4	151-A	204	NAP	O4B-C4B	-2.51	1.39	1.45
4	131-A	204	NAP	O7N-C7N	-2.51	1.19	1.24
4	122-A	204	NAP	O4B-C4B	-2.51	1.39	1.45
4	10-A	204	NAP	O4B-C4B	-2.51	1.39	1.45
4	3-A	204	NAP	O4B-C4B	-2.51	1.39	1.45
4	63-A	204	NAP	O4B-C4B	-2.50	1.39	1.45
4	8-A	204	NAP	O7N-C7N	-2.50	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	109-A	204	NAP	O4B-C4B	-2.50	1.39	1.45
4	49-A	204	NAP	C2D-C1D	-2.50	1.49	1.53
4	82-A	204	NAP	O7N-C7N	-2.50	1.19	1.24
2	126-A	201	FOL	CB-CA	-2.49	1.50	1.53
4	150-A	204	NAP	O7N-C7N	-2.49	1.19	1.24
4	30-A	204	NAP	O4B-C4B	-2.49	1.39	1.45
4	76-A	204	NAP	O4B-C4B	-2.49	1.39	1.45
4	56-A	204	NAP	O4B-C4B	-2.49	1.39	1.45
4	121-A	204	NAP	O4B-C4B	-2.49	1.39	1.45
4	147-A	204	NAP	O4B-C4B	-2.48	1.39	1.45
4	89-A	204	NAP	O7N-C7N	-2.48	1.19	1.24
4	140-A	204	NAP	O4B-C4B	-2.48	1.39	1.45
4	166-A	204	NAP	O4B-C4B	-2.48	1.39	1.45
4	156-A	204	NAP	O4B-C4B	-2.47	1.39	1.45
4	123-A	204	NAP	O4B-C4B	-2.47	1.39	1.45
4	144-A	204	NAP	O4B-C4B	-2.47	1.39	1.45
4	71-A	204	NAP	O4B-C4B	-2.46	1.39	1.45
4	157-A	204	NAP	O7N-C7N	-2.46	1.19	1.24
4	28-A	204	NAP	O4B-C4B	-2.46	1.39	1.45
4	113-A	204	NAP	O4B-C4B	-2.45	1.39	1.45
4	133-A	204	NAP	O4B-C4B	-2.45	1.39	1.45
4	153-A	204	NAP	O4B-C4B	-2.45	1.39	1.45
4	61-A	204	NAP	O4B-C4B	-2.45	1.39	1.45
4	57-A	204	NAP	O4B-C4B	-2.44	1.39	1.45
4	96-A	204	NAP	O7N-C7N	-2.44	1.19	1.24
4	25-A	204	NAP	O7N-C7N	-2.44	1.19	1.24
4	9-A	204	NAP	O4B-C4B	-2.44	1.39	1.45
4	159-A	204	NAP	O4B-C4B	-2.43	1.39	1.45
4	146-A	204	NAP	O4B-C4B	-2.43	1.39	1.45
4	160-A	204	NAP	O4B-C4B	-2.43	1.39	1.45
4	125-A	204	NAP	C2D-C1D	-2.43	1.49	1.53
4	152-A	204	NAP	O4B-C4B	-2.42	1.39	1.45
4	31-A	204	NAP	O4B-C4B	-2.42	1.39	1.45
4	36-A	204	NAP	O7N-C7N	-2.42	1.19	1.24
4	129-A	204	NAP	O4B-C4B	-2.41	1.39	1.45
4	72-A	204	NAP	O7N-C7N	-2.41	1.19	1.24
4	110-A	204	NAP	O7N-C7N	-2.41	1.19	1.24
4	88-A	204	NAP	O4B-C4B	-2.41	1.39	1.45
4	141-A	204	NAP	O4B-C4B	-2.41	1.39	1.45
4	50-A	204	NAP	C2D-C1D	-2.40	1.49	1.53
4	158-A	204	NAP	O7N-C7N	-2.39	1.19	1.24
4	167-A	204	NAP	O4B-C4B	-2.39	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	58-A	204	NAP	O4B-C4B	-2.39	1.39	1.45
4	86-A	204	NAP	O4B-C4B	-2.39	1.39	1.45
4	143-A	204	NAP	O4B-C4B	-2.39	1.39	1.45
4	109-A	204	NAP	O7N-C7N	-2.39	1.19	1.24
4	155-A	204	NAP	O4B-C4B	-2.38	1.39	1.45
4	2-A	204	NAP	O4B-C4B	-2.38	1.39	1.45
4	42-A	204	NAP	O7N-C7N	-2.38	1.19	1.24
4	72-A	204	NAP	O4B-C4B	-2.37	1.39	1.45
2	123-A	201	FOL	CA-N	-2.36	1.43	1.46
4	161-A	204	NAP	O4B-C4B	-2.36	1.39	1.45
4	160-A	204	NAP	O7N-C7N	-2.36	1.19	1.24
4	147-A	204	NAP	O7N-C7N	-2.36	1.19	1.24
4	154-A	204	NAP	O4B-C4B	-2.36	1.39	1.45
4	148-A	204	NAP	O7N-C7N	-2.35	1.19	1.24
4	90-A	204	NAP	O7N-C7N	-2.35	1.19	1.24
4	79-A	204	NAP	O7N-C7N	-2.35	1.19	1.24
4	162-A	204	NAP	O4B-C4B	-2.34	1.39	1.45
4	108-A	204	NAP	O4B-C4B	-2.34	1.39	1.45
4	163-A	204	NAP	O4B-C4B	-2.34	1.39	1.45
4	33-A	204	NAP	C2D-C1D	-2.34	1.49	1.53
4	127-A	204	NAP	O4B-C4B	-2.33	1.39	1.45
4	157-A	204	NAP	O4B-C4B	-2.33	1.39	1.45
4	146-A	204	NAP	O7N-C7N	-2.33	1.19	1.24
4	29-A	204	NAP	O4B-C4B	-2.33	1.39	1.45
4	51-A	204	NAP	O7N-C7N	-2.32	1.19	1.24
4	87-A	204	NAP	O4B-C4B	-2.32	1.39	1.45
4	38-A	204	NAP	O7N-C7N	-2.30	1.19	1.24
4	97-A	204	NAP	O7N-C7N	-2.29	1.19	1.24
4	165-A	204	NAP	O4B-C4B	-2.29	1.39	1.45
4	153-A	204	NAP	O7N-C7N	-2.29	1.19	1.24
4	85-A	204	NAP	O4B-C4B	-2.28	1.39	1.45
4	74-A	204	NAP	O7N-C7N	-2.28	1.19	1.24
4	7-A	204	NAP	O7N-C7N	-2.28	1.19	1.24
4	126-A	204	NAP	O4B-C4B	-2.28	1.39	1.45
4	32-A	204	NAP	C2D-C3D	-2.27	1.47	1.53
4	128-A	204	NAP	O4B-C4B	-2.27	1.39	1.45
2	156-A	201	FOL	CB-CA	-2.27	1.50	1.53
2	77-A	201	FOL	CB-CA	-2.27	1.50	1.53
4	99-A	204	NAP	O7N-C7N	-2.26	1.19	1.24
4	156-A	204	NAP	O7N-C7N	-2.26	1.19	1.24
2	132-A	201	FOL	CA-N	-2.26	1.43	1.46
4	1-A	204	NAP	O4B-C4B	-2.26	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	93-A	204	NAP	O7N-C7N	-2.26	1.19	1.24
4	103-A	204	NAP	O7N-C7N	-2.26	1.19	1.24
4	84-A	204	NAP	O4B-C4B	-2.25	1.39	1.45
4	108-A	204	NAP	C2D-C3D	-2.25	1.47	1.53
4	50-A	204	NAP	O7N-C7N	-2.25	1.19	1.24
4	22-A	204	NAP	C2D-C3D	-2.23	1.47	1.53
4	142-A	204	NAP	O4B-C4B	-2.23	1.40	1.45
4	47-A	204	NAP	O7N-C7N	-2.23	1.19	1.24
4	8-A	204	NAP	O4B-C4B	-2.22	1.40	1.45
4	44-A	204	NAP	O7N-C7N	-2.22	1.19	1.24
4	6-A	204	NAP	O4B-C4B	-2.22	1.40	1.45
2	16-A	201	FOL	CA-N	-2.21	1.43	1.46
4	91-A	204	NAP	O7N-C7N	-2.21	1.19	1.24
4	22-A	204	NAP	O7N-C7N	-2.21	1.19	1.24
4	164-A	204	NAP	O4B-C4B	-2.21	1.40	1.45
4	45-A	204	NAP	O7N-C7N	-2.21	1.19	1.24
4	14-A	204	NAP	C2D-C3D	-2.20	1.47	1.53
4	162-A	204	NAP	O7N-C7N	-2.20	1.19	1.24
4	37-A	204	NAP	O7N-C7N	-2.20	1.19	1.24
4	29-A	204	NAP	C2D-C3D	-2.19	1.47	1.53
4	167-A	204	NAP	O7N-C7N	-2.18	1.19	1.24
2	35-A	201	FOL	CA-N	-2.17	1.43	1.46
4	83-A	204	NAP	O4B-C4B	-2.17	1.40	1.45
4	86-A	204	NAP	C2D-C3D	-2.17	1.47	1.53
4	63-A	204	NAP	C2N-C3N	-2.17	1.35	1.39
4	18-A	204	NAP	O7N-C7N	-2.16	1.19	1.24
4	68-A	204	NAP	C2D-C3D	-2.16	1.47	1.53
4	111-A	204	NAP	C2D-C3D	-2.15	1.47	1.53
4	73-A	204	NAP	C2D-C3D	-2.15	1.47	1.53
4	158-A	204	NAP	O4B-C4B	-2.15	1.40	1.45
4	147-A	204	NAP	C2D-C3D	-2.14	1.47	1.53
4	123-A	204	NAP	O7N-C7N	-2.14	1.19	1.24
4	163-A	204	NAP	O7N-C7N	-2.14	1.19	1.24
4	57-A	204	NAP	C2D-C3D	-2.13	1.47	1.53
4	104-A	204	NAP	O7N-C7N	-2.13	1.19	1.24
4	66-A	204	NAP	O7N-C7N	-2.12	1.19	1.24
4	153-A	204	NAP	C2D-C3D	-2.12	1.47	1.53
2	6-A	201	FOL	CA-N	-2.12	1.43	1.46
4	54-A	204	NAP	O7N-C7N	-2.11	1.19	1.24
4	65-A	204	NAP	C2D-C3D	-2.10	1.47	1.53
4	108-A	204	NAP	C2N-C3N	-2.10	1.35	1.39
4	28-A	204	NAP	C2D-C3D	-2.10	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	140-A	204	NAP	O7N-C7N	-2.10	1.19	1.24
4	71-A	204	NAP	O7N-C7N	-2.09	1.19	1.24
4	107-A	204	NAP	C2D-C3D	-2.09	1.47	1.53
4	7-A	204	NAP	O4B-C4B	-2.09	1.40	1.45
4	72-A	204	NAP	C2D-C3D	-2.08	1.47	1.53
4	133-A	204	NAP	O7N-C7N	-2.08	1.19	1.24
4	85-A	204	NAP	O7N-C7N	-2.07	1.19	1.24
4	151-A	204	NAP	O7N-C7N	-2.07	1.19	1.24
4	11-A	204	NAP	O7N-C7N	-2.06	1.19	1.24
4	110-A	204	NAP	C2D-C3D	-2.06	1.48	1.53
4	88-A	204	NAP	C2D-C3D	-2.06	1.48	1.53
4	60-A	204	NAP	C2D-C3D	-2.05	1.48	1.53
4	104-A	204	NAP	C2D-C3D	-2.05	1.48	1.53
4	2-A	204	NAP	O7N-C7N	-2.04	1.20	1.24
4	65-A	204	NAP	O7N-C7N	-2.04	1.20	1.24
4	61-A	204	NAP	O7N-C7N	-2.04	1.20	1.24
4	2-A	204	NAP	C2D-C3D	-2.04	1.48	1.53
2	135-A	201	FOL	CA-N	-2.04	1.43	1.46
4	64-A	204	NAP	C2D-C3D	-2.04	1.48	1.53
4	62-A	204	NAP	O7N-C7N	-2.04	1.20	1.24
4	40-A	204	NAP	O7N-C7N	-2.03	1.20	1.24
4	157-A	204	NAP	C2D-C3D	-2.03	1.48	1.53
4	33-A	204	NAP	C2D-C3D	-2.03	1.48	1.53
4	13-A	204	NAP	C2D-C3D	-2.03	1.48	1.53
4	4-A	204	NAP	O7N-C7N	-2.02	1.20	1.24
2	159-A	201	FOL	CA-N	-2.02	1.43	1.46
2	36-A	201	FOL	CA-N	-2.02	1.43	1.46
4	149-A	204	NAP	O7N-C7N	-2.02	1.20	1.24
4	88-A	204	NAP	O7N-C7N	-2.01	1.20	1.24
4	164-A	204	NAP	O7N-C7N	-2.01	1.20	1.24
4	56-A	204	NAP	C2N-C3N	-2.01	1.35	1.39
4	67-A	204	NAP	C2D-C3D	-2.01	1.48	1.53
4	30-A	204	NAP	C2D-C3D	-2.01	1.48	1.53
4	73-A	204	NAP	O7N-C7N	-2.01	1.20	1.24
4	34-A	204	NAP	C2D-C3D	-2.00	1.48	1.53
4	165-A	204	NAP	O7N-C7N	-2.00	1.20	1.24
4	78-A	204	NAP	O7N-C7N	-2.00	1.20	1.24
2	163-A	201	FOL	C8A-N8	2.00	1.36	1.34
4	106-A	204	NAP	P2B-O2B	2.00	1.63	1.59
4	134-A	204	NAP	C5A-N7A	2.00	1.46	1.39
4	147-A	204	NAP	C6A-N6A	2.00	1.42	1.34
4	78-A	204	NAP	C8A-N7A	2.00	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	153-A	204	NAP	O4D-C1D	2.00	1.44	1.41
2	107-A	201	FOL	C2-N3	2.01	1.36	1.33
4	105-A	204	NAP	C5A-N7A	2.01	1.46	1.39
4	34-A	204	NAP	O4D-C1D	2.01	1.44	1.41
2	123-A	201	FOL	C2-N3	2.01	1.36	1.33
4	161-A	204	NAP	C5A-N7A	2.01	1.46	1.39
2	153-A	201	FOL	C2-N3	2.01	1.36	1.33
4	113-A	204	NAP	C5A-N7A	2.01	1.46	1.39
4	127-A	204	NAP	C5A-N7A	2.01	1.46	1.39
2	140-A	201	FOL	C4A-C8A	2.02	1.44	1.41
4	50-A	204	NAP	C6N-N1N	2.02	1.40	1.35
4	97-A	204	NAP	P2B-O2B	2.02	1.63	1.59
4	62-A	204	NAP	O4D-C1D	2.02	1.44	1.41
4	155-A	204	NAP	C6N-N1N	2.02	1.40	1.35
4	154-A	204	NAP	C6N-N1N	2.02	1.40	1.35
4	114-A	204	NAP	P2B-O2B	2.02	1.63	1.59
4	89-A	204	NAP	C5A-N7A	2.02	1.46	1.39
4	4-A	204	NAP	C8A-N7A	2.02	1.38	1.34
4	79-A	204	NAP	C6N-N1N	2.02	1.40	1.35
4	64-A	204	NAP	O4D-C1D	2.03	1.44	1.41
4	90-A	204	NAP	O4D-C1D	2.03	1.44	1.41
4	147-A	204	NAP	P2B-O2B	2.03	1.63	1.59
4	21-A	204	NAP	P2B-O2B	2.03	1.63	1.59
2	115-A	201	FOL	CB-CA	2.03	1.56	1.53
4	128-A	204	NAP	C5A-N7A	2.03	1.46	1.39
4	79-A	204	NAP	C5A-N7A	2.03	1.46	1.39
2	104-A	201	FOL	C2-N3	2.03	1.36	1.33
4	90-A	204	NAP	P2B-O2B	2.03	1.63	1.59
4	76-A	204	NAP	C5A-N7A	2.04	1.46	1.39
4	52-A	204	NAP	C5A-N7A	2.04	1.46	1.39
4	165-A	204	NAP	C5A-N7A	2.04	1.46	1.39
4	143-A	204	NAP	P2B-O2B	2.04	1.63	1.59
4	158-A	204	NAP	C8A-N7A	2.04	1.38	1.34
4	80-A	204	NAP	C6N-N1N	2.04	1.40	1.35
4	47-A	204	NAP	C6N-N1N	2.04	1.40	1.35
4	53-A	204	NAP	C6N-N1N	2.04	1.40	1.35
2	140-A	201	FOL	CB-CA	2.04	1.56	1.53
4	27-A	204	NAP	C5A-N7A	2.04	1.46	1.39
4	87-A	204	NAP	C6N-N1N	2.04	1.40	1.35
4	2-A	204	NAP	P2B-O2B	2.04	1.63	1.59
4	151-A	204	NAP	P2B-O2B	2.04	1.63	1.59
4	1-A	204	NAP	C5A-N7A	2.04	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	152-A	204	NAP	C8A-N7A	2.04	1.38	1.34
4	9-A	204	NAP	O4D-C1D	2.05	1.44	1.41
4	48-A	204	NAP	C6N-N1N	2.05	1.40	1.35
2	16-A	201	FOL	C7-N8	2.05	1.35	1.31
4	64-A	204	NAP	C6N-N1N	2.05	1.40	1.35
4	164-A	204	NAP	C5A-N7A	2.05	1.46	1.39
4	71-A	204	NAP	P2B-O2B	2.05	1.63	1.59
4	78-A	204	NAP	O4D-C1D	2.05	1.44	1.41
2	150-A	201	FOL	C2-N3	2.05	1.36	1.33
4	132-A	204	NAP	O4D-C1D	2.05	1.44	1.41
4	42-A	204	NAP	P2B-O2B	2.06	1.63	1.59
4	153-A	204	NAP	C6N-N1N	2.06	1.40	1.35
2	157-A	201	FOL	C4-C4A	2.06	1.45	1.41
4	80-A	204	NAP	C5A-N7A	2.06	1.46	1.39
4	55-A	204	NAP	C5A-N7A	2.06	1.46	1.39
4	154-A	204	NAP	C5A-N7A	2.06	1.46	1.39
2	43-A	201	FOL	C7-N8	2.06	1.35	1.31
4	51-A	204	NAP	C6N-N1N	2.06	1.40	1.35
4	15-A	204	NAP	C5A-N7A	2.06	1.46	1.39
4	156-A	204	NAP	C6N-N1N	2.07	1.40	1.35
2	132-A	201	FOL	C2-N3	2.07	1.36	1.33
4	120-A	204	NAP	P2B-O2B	2.07	1.63	1.59
4	151-A	204	NAP	C5A-N7A	2.07	1.46	1.39
4	35-A	204	NAP	C8A-N7A	2.07	1.38	1.34
2	46-A	201	FOL	C4A-C8A	2.07	1.44	1.41
4	2-A	204	NAP	C6N-N1N	2.07	1.40	1.35
4	68-A	204	NAP	O4D-C1D	2.07	1.44	1.41
4	158-A	204	NAP	O4D-C1D	2.07	1.44	1.41
2	134-A	201	FOL	C2-N3	2.07	1.36	1.33
4	79-A	204	NAP	P2B-O2B	2.07	1.63	1.59
4	65-A	204	NAP	C6N-N1N	2.08	1.40	1.35
4	114-A	204	NAP	C5A-N7A	2.08	1.46	1.39
4	110-A	204	NAP	C8A-N7A	2.08	1.38	1.34
4	143-A	204	NAP	C6N-N1N	2.08	1.40	1.35
4	141-A	204	NAP	C6N-N1N	2.08	1.40	1.35
4	130-A	204	NAP	C6N-N1N	2.08	1.40	1.35
4	134-A	204	NAP	O4D-C1D	2.08	1.44	1.41
4	100-A	204	NAP	C5A-N7A	2.08	1.46	1.39
4	142-A	204	NAP	C6N-N1N	2.09	1.40	1.35
4	52-A	204	NAP	C6N-N1N	2.09	1.40	1.35
2	159-A	201	FOL	C8A-N8	2.09	1.37	1.34
4	41-A	204	NAP	C8A-N7A	2.09	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	56-A	204	NAP	C6N-N1N	2.09	1.40	1.35
4	76-A	204	NAP	P2B-O2B	2.09	1.63	1.59
4	115-A	204	NAP	P2B-O2B	2.09	1.63	1.59
4	94-A	204	NAP	C6N-N1N	2.09	1.40	1.35
4	35-A	204	NAP	C5A-N7A	2.10	1.46	1.39
2	34-A	201	FOL	C4A-C8A	2.10	1.44	1.41
2	139-A	201	FOL	C4A-C8A	2.10	1.44	1.41
4	125-A	204	NAP	C6N-N1N	2.10	1.40	1.35
2	151-A	201	FOL	C4A-C8A	2.10	1.44	1.41
4	67-A	204	NAP	C5A-N7A	2.10	1.46	1.39
4	7-A	204	NAP	P2B-O2B	2.10	1.63	1.59
4	59-A	204	NAP	P2B-O2B	2.10	1.63	1.59
4	7-A	204	NAP	O4D-C1D	2.10	1.44	1.41
4	123-A	204	NAP	C6N-N1N	2.10	1.40	1.35
2	5-A	201	FOL	C8A-N8	2.10	1.37	1.34
4	138-A	204	NAP	P2B-O2B	2.10	1.63	1.59
4	90-A	204	NAP	C6N-N1N	2.10	1.40	1.35
4	129-A	204	NAP	P2B-O2B	2.10	1.63	1.59
4	7-A	204	NAP	C6N-N1N	2.11	1.40	1.35
4	89-A	204	NAP	C8A-N7A	2.11	1.38	1.34
2	148-A	201	FOL	C2-N3	2.11	1.36	1.33
4	157-A	204	NAP	P2B-O2B	2.11	1.63	1.59
4	57-A	204	NAP	C6N-N1N	2.11	1.40	1.35
4	5-A	204	NAP	C6N-N1N	2.11	1.40	1.35
4	76-A	204	NAP	O4D-C1D	2.11	1.44	1.41
4	10-A	204	NAP	C6N-N1N	2.12	1.40	1.35
4	146-A	204	NAP	C6N-N1N	2.12	1.40	1.35
4	58-A	204	NAP	C6N-N1N	2.12	1.40	1.35
4	62-A	204	NAP	C6N-N1N	2.12	1.40	1.35
4	12-A	204	NAP	C6N-N1N	2.12	1.40	1.35
4	84-A	204	NAP	O4D-C1D	2.12	1.44	1.41
4	143-A	204	NAP	O4D-C1D	2.12	1.44	1.41
4	124-A	204	NAP	C6N-N1N	2.13	1.40	1.35
4	145-A	204	NAP	C6N-N1N	2.13	1.41	1.35
2	120-A	201	FOL	C8A-N8	2.13	1.37	1.34
2	7-A	201	FOL	C4A-C8A	2.13	1.44	1.41
4	161-A	204	NAP	C6N-N1N	2.13	1.41	1.35
4	74-A	204	NAP	C5A-N7A	2.13	1.46	1.39
2	117-A	201	FOL	C2-N3	2.13	1.36	1.33
4	106-A	204	NAP	C5A-N7A	2.13	1.46	1.39
4	44-A	204	NAP	C6N-N1N	2.13	1.41	1.35
4	31-A	204	NAP	O4D-C1D	2.13	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	43-A	204	NAP	C6N-N1N	2.13	1.41	1.35
4	37-A	204	NAP	P2B-O2B	2.13	1.63	1.59
4	77-A	204	NAP	O4D-C1D	2.14	1.44	1.41
4	134-A	204	NAP	P2B-O2B	2.14	1.63	1.59
4	36-A	204	NAP	P2B-O2B	2.14	1.63	1.59
2	126-A	201	FOL	C2-N3	2.14	1.36	1.33
4	124-A	204	NAP	C8A-N7A	2.14	1.38	1.34
4	140-A	204	NAP	C6N-N1N	2.14	1.41	1.35
4	28-A	204	NAP	C5A-N7A	2.14	1.46	1.39
4	96-A	204	NAP	C6N-N1N	2.14	1.41	1.35
2	56-A	201	FOL	CB-CA	2.15	1.56	1.53
4	138-A	204	NAP	C6N-N1N	2.15	1.41	1.35
4	73-A	204	NAP	O4D-C1D	2.15	1.44	1.41
4	34-A	204	NAP	C6N-N1N	2.15	1.41	1.35
4	145-A	204	NAP	C5A-N7A	2.15	1.46	1.39
2	145-A	201	FOL	C4A-C8A	2.15	1.44	1.41
2	83-A	201	FOL	CB-CA	2.15	1.56	1.53
4	145-A	204	NAP	C8A-N7A	2.15	1.38	1.34
2	46-A	201	FOL	CB-CA	2.15	1.56	1.53
4	93-A	204	NAP	O4D-C1D	2.16	1.44	1.41
2	131-A	201	FOL	C8A-N8	2.16	1.37	1.34
4	154-A	204	NAP	P2B-O2B	2.16	1.63	1.59
4	115-A	204	NAP	C5A-N7A	2.16	1.46	1.39
4	6-A	204	NAP	P2B-O2B	2.16	1.63	1.59
4	15-A	204	NAP	C6N-N1N	2.16	1.41	1.35
2	87-A	201	FOL	C2-N3	2.16	1.36	1.33
4	109-A	204	NAP	P2B-O2B	2.16	1.63	1.59
4	7-A	204	NAP	C8A-N7A	2.17	1.38	1.34
4	60-A	204	NAP	C6N-N1N	2.17	1.41	1.35
4	144-A	204	NAP	C6N-N1N	2.17	1.41	1.35
4	55-A	204	NAP	C6N-N1N	2.17	1.41	1.35
4	88-A	204	NAP	C6N-N1N	2.17	1.41	1.35
4	39-A	204	NAP	C8A-N7A	2.17	1.38	1.34
4	155-A	204	NAP	C8A-N7A	2.17	1.38	1.34
4	3-A	204	NAP	C6N-N1N	2.17	1.41	1.35
2	128-A	201	FOL	C4A-C8A	2.17	1.44	1.41
2	8-A	201	FOL	C4A-C8A	2.17	1.44	1.41
4	13-A	204	NAP	C8A-N7A	2.18	1.38	1.34
4	82-A	204	NAP	C8A-N7A	2.18	1.38	1.34
4	153-A	204	NAP	C8A-N7A	2.18	1.38	1.34
4	77-A	204	NAP	P2B-O2B	2.18	1.63	1.59
4	104-A	204	NAP	C6N-N1N	2.19	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-A	201	FOL	C4A-C8A	2.19	1.44	1.41
4	105-A	204	NAP	C6N-N1N	2.19	1.41	1.35
4	45-A	204	NAP	P2B-O2B	2.19	1.63	1.59
4	139-A	204	NAP	C6N-N1N	2.19	1.41	1.35
2	23-A	201	FOL	C4-C4A	2.19	1.45	1.41
4	107-A	204	NAP	P2B-O2B	2.19	1.63	1.59
4	83-A	204	NAP	P2B-O2B	2.19	1.63	1.59
2	122-A	201	FOL	C8A-N8	2.19	1.37	1.34
4	80-A	204	NAP	C8A-N7A	2.19	1.38	1.34
4	74-A	204	NAP	C8A-N7A	2.19	1.38	1.34
4	122-A	204	NAP	C6N-N1N	2.20	1.41	1.35
4	3-A	204	NAP	P2B-O2B	2.20	1.63	1.59
4	161-A	204	NAP	C8A-N7A	2.20	1.38	1.34
4	88-A	204	NAP	O4D-C1D	2.20	1.44	1.41
4	95-A	204	NAP	C6N-N1N	2.20	1.41	1.35
4	119-A	204	NAP	C3B-C4B	2.21	1.58	1.53
4	71-A	204	NAP	C8A-N7A	2.21	1.38	1.34
4	67-A	204	NAP	O4D-C1D	2.21	1.44	1.41
4	89-A	204	NAP	C6N-N1N	2.21	1.41	1.35
2	55-A	201	FOL	CB-CA	2.21	1.56	1.53
4	61-A	204	NAP	C6N-N1N	2.21	1.41	1.35
4	101-A	204	NAP	C5A-N7A	2.21	1.46	1.39
2	85-A	201	FOL	C2-N3	2.22	1.36	1.33
2	131-A	201	FOL	C4A-C8A	2.22	1.44	1.41
4	21-A	204	NAP	C6N-N1N	2.22	1.41	1.35
4	120-A	204	NAP	C8A-N7A	2.22	1.38	1.34
4	132-A	204	NAP	P2B-O2B	2.23	1.63	1.59
2	57-A	201	FOL	CB-CA	2.23	1.56	1.53
4	86-A	204	NAP	O4D-C1D	2.23	1.44	1.41
4	1-A	204	NAP	C6N-N1N	2.23	1.41	1.35
4	112-A	204	NAP	C8A-N7A	2.23	1.38	1.34
4	13-A	204	NAP	C6N-N1N	2.23	1.41	1.35
4	11-A	204	NAP	C6N-N1N	2.23	1.41	1.35
4	116-A	204	NAP	C8A-N7A	2.23	1.38	1.34
4	139-A	204	NAP	C8A-N7A	2.23	1.38	1.34
4	154-A	204	NAP	O4D-C1D	2.23	1.44	1.41
2	35-A	201	FOL	C4A-C8A	2.23	1.44	1.41
4	81-A	204	NAP	P2B-O2B	2.23	1.63	1.59
2	120-A	201	FOL	C7-N8	2.23	1.35	1.31
4	121-A	204	NAP	C6N-N1N	2.24	1.41	1.35
4	97-A	204	NAP	C6N-N1N	2.24	1.41	1.35
4	150-A	204	NAP	O4D-C1D	2.24	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	78-A	204	NAP	C6N-N1N	2.24	1.41	1.35
4	66-A	204	NAP	C6N-N1N	2.24	1.41	1.35
4	117-A	204	NAP	O4D-C1D	2.24	1.44	1.41
4	87-A	204	NAP	O4D-C1D	2.24	1.44	1.41
2	133-A	201	FOL	C4A-C8A	2.24	1.44	1.41
2	82-A	201	FOL	C4A-C8A	2.24	1.44	1.41
4	50-A	204	NAP	P2B-O2B	2.24	1.63	1.59
4	103-A	204	NAP	C6N-N1N	2.24	1.41	1.35
4	16-A	204	NAP	P2B-O2B	2.25	1.63	1.59
4	85-A	204	NAP	P2B-O2B	2.25	1.63	1.59
4	99-A	204	NAP	C6N-N1N	2.25	1.41	1.35
4	162-A	204	NAP	C8A-N7A	2.25	1.38	1.34
4	91-A	204	NAP	C6N-N1N	2.25	1.41	1.35
4	107-A	204	NAP	C8A-N7A	2.25	1.38	1.34
4	22-A	204	NAP	C6N-N1N	2.25	1.41	1.35
4	14-A	204	NAP	C6N-N1N	2.26	1.41	1.35
4	118-A	204	NAP	C8A-N7A	2.26	1.38	1.34
4	108-A	204	NAP	C7N-N7N	2.26	1.37	1.33
4	28-A	204	NAP	P2B-O2B	2.26	1.63	1.59
4	165-A	204	NAP	C8A-N7A	2.26	1.38	1.34
4	79-A	204	NAP	C8A-N7A	2.26	1.38	1.34
4	142-A	204	NAP	O4D-C1D	2.26	1.44	1.41
4	151-A	204	NAP	C8A-N7A	2.26	1.38	1.34
2	32-A	201	FOL	C4A-C8A	2.26	1.45	1.41
4	72-A	204	NAP	C6N-N1N	2.26	1.41	1.35
4	45-A	204	NAP	C8A-N7A	2.26	1.38	1.34
2	41-A	201	FOL	C4A-C8A	2.27	1.45	1.41
4	37-A	204	NAP	C8A-N7A	2.27	1.38	1.34
4	32-A	204	NAP	C8A-N7A	2.27	1.38	1.34
2	152-A	201	FOL	C2-N3	2.27	1.36	1.33
4	74-A	204	NAP	O4D-C1D	2.27	1.44	1.41
4	42-A	204	NAP	C8A-N7A	2.27	1.38	1.34
4	166-A	204	NAP	P2B-O2B	2.28	1.63	1.59
4	22-A	204	NAP	O4D-C1D	2.28	1.44	1.41
4	122-A	204	NAP	C8A-N7A	2.28	1.38	1.34
4	87-A	204	NAP	C8A-N7A	2.28	1.39	1.34
4	106-A	204	NAP	C6N-N1N	2.28	1.41	1.35
4	13-A	204	NAP	O4D-C1D	2.28	1.44	1.41
4	91-A	204	NAP	O4D-C1D	2.28	1.44	1.41
2	82-A	201	FOL	C4-C4A	2.28	1.45	1.41
4	108-A	204	NAP	C6N-N1N	2.29	1.41	1.35
4	138-A	204	NAP	C8A-N7A	2.29	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	72-A	201	FOL	C4-C4A	2.29	1.45	1.41
4	147-A	204	NAP	O4D-C1D	2.29	1.44	1.41
4	94-A	204	NAP	O4D-C1D	2.29	1.44	1.41
4	92-A	204	NAP	C6N-N1N	2.29	1.41	1.35
4	136-A	204	NAP	O4D-C1D	2.29	1.44	1.41
4	135-A	204	NAP	O4D-C1D	2.29	1.44	1.41
4	142-A	204	NAP	P2B-O2B	2.29	1.63	1.59
4	100-A	204	NAP	C6N-N1N	2.29	1.41	1.35
4	29-A	204	NAP	P2B-O2B	2.29	1.63	1.59
4	66-A	204	NAP	O4D-C1D	2.29	1.44	1.41
4	113-A	204	NAP	C8A-N7A	2.30	1.39	1.34
4	71-A	204	NAP	C6N-N1N	2.30	1.41	1.35
4	33-A	204	NAP	C8A-N7A	2.30	1.39	1.34
4	148-A	204	NAP	O4D-C1D	2.30	1.44	1.41
4	156-A	204	NAP	C8A-N7A	2.30	1.39	1.34
4	29-A	204	NAP	C8A-N7A	2.30	1.39	1.34
4	92-A	204	NAP	O4D-C1D	2.31	1.44	1.41
4	111-A	204	NAP	C8A-N7A	2.31	1.39	1.34
4	29-A	204	NAP	C6N-N1N	2.31	1.41	1.35
4	47-A	204	NAP	C8A-N7A	2.31	1.39	1.34
4	164-A	204	NAP	C8A-N7A	2.31	1.39	1.34
4	138-A	204	NAP	O4D-C1D	2.31	1.44	1.41
2	157-A	201	FOL	C2-N3	2.31	1.36	1.33
2	165-A	201	FOL	C2-N3	2.31	1.36	1.33
4	109-A	204	NAP	C6N-N1N	2.31	1.41	1.35
4	137-A	204	NAP	O4D-C1D	2.31	1.44	1.41
4	68-A	204	NAP	C6N-N1N	2.31	1.41	1.35
4	166-A	204	NAP	O4D-C1D	2.31	1.44	1.41
4	41-A	204	NAP	P2B-O2B	2.32	1.63	1.59
4	95-A	204	NAP	O4D-C1D	2.32	1.44	1.41
4	72-A	204	NAP	C8A-N7A	2.32	1.39	1.34
4	57-A	204	NAP	P2B-O2B	2.32	1.63	1.59
2	24-A	201	FOL	CB-CA	2.32	1.56	1.53
4	93-A	204	NAP	C6N-N1N	2.32	1.41	1.35
4	52-A	204	NAP	C8A-N7A	2.32	1.39	1.34
4	117-A	204	NAP	C8A-N7A	2.32	1.39	1.34
4	106-A	204	NAP	C8A-N7A	2.32	1.39	1.34
4	44-A	204	NAP	C8A-N7A	2.32	1.39	1.34
2	26-A	201	FOL	CB-CA	2.32	1.56	1.53
2	163-A	201	FOL	C2-N3	2.32	1.36	1.33
2	109-A	201	FOL	C4A-C8A	2.32	1.45	1.41
4	28-A	204	NAP	C6N-N1N	2.33	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	62-A	204	NAP	P2B-O2B	2.33	1.63	1.59
4	144-A	204	NAP	C8A-N7A	2.33	1.39	1.34
4	128-A	204	NAP	P2B-O2B	2.33	1.63	1.59
4	22-A	204	NAP	C8A-N7A	2.33	1.39	1.34
4	77-A	204	NAP	C8A-N7A	2.33	1.39	1.34
4	83-A	204	NAP	O4D-C1D	2.33	1.44	1.41
4	54-A	204	NAP	C8A-N7A	2.33	1.39	1.34
4	102-A	204	NAP	C6N-N1N	2.33	1.41	1.35
4	102-A	204	NAP	P2B-O2B	2.33	1.63	1.59
4	36-A	204	NAP	C6N-N1N	2.33	1.41	1.35
4	46-A	204	NAP	C8A-N7A	2.33	1.39	1.34
4	67-A	204	NAP	C6N-N1N	2.33	1.41	1.35
2	132-A	201	FOL	C4A-C8A	2.34	1.45	1.41
2	14-A	201	FOL	CB-CA	2.34	1.56	1.53
4	75-A	204	NAP	O4D-C1D	2.34	1.44	1.41
4	5-A	204	NAP	O4D-C1D	2.34	1.44	1.41
4	116-A	204	NAP	C6N-N1N	2.34	1.41	1.35
4	157-A	204	NAP	C8A-N7A	2.34	1.39	1.34
4	79-A	204	NAP	O4D-C1D	2.34	1.44	1.41
4	1-A	204	NAP	O4D-C1D	2.34	1.44	1.41
4	16-A	204	NAP	O4D-C1D	2.34	1.44	1.41
4	141-A	204	NAP	C8A-N7A	2.34	1.39	1.34
4	101-A	204	NAP	C6N-N1N	2.34	1.41	1.35
4	73-A	204	NAP	C6N-N1N	2.34	1.41	1.35
4	155-A	204	NAP	P2B-O2B	2.34	1.63	1.59
4	160-A	204	NAP	P2B-O2B	2.34	1.63	1.59
4	115-A	204	NAP	C6N-N1N	2.35	1.41	1.35
4	56-A	204	NAP	P2B-O2B	2.35	1.63	1.59
2	95-A	201	FOL	C4A-C8A	2.35	1.45	1.41
4	144-A	204	NAP	O4D-C1D	2.35	1.44	1.41
4	18-A	204	NAP	C6N-N1N	2.35	1.41	1.35
4	40-A	204	NAP	C6N-N1N	2.35	1.41	1.35
4	3-A	204	NAP	C8A-N7A	2.35	1.39	1.34
4	12-A	204	NAP	C8A-N7A	2.35	1.39	1.34
4	3-A	204	NAP	O4D-C1D	2.36	1.44	1.41
2	13-A	201	FOL	C4A-C8A	2.36	1.45	1.41
4	126-A	204	NAP	C8A-N7A	2.36	1.39	1.34
4	107-A	204	NAP	C6N-N1N	2.36	1.41	1.35
4	32-A	204	NAP	C6N-N1N	2.36	1.41	1.35
4	63-A	204	NAP	C8A-N7A	2.36	1.39	1.34
4	114-A	204	NAP	C6N-N1N	2.36	1.41	1.35
4	80-A	204	NAP	O4D-C1D	2.36	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	104-A	204	NAP	C8A-N7A	2.36	1.39	1.34
2	108-A	201	FOL	C4A-C8A	2.36	1.45	1.41
2	136-A	201	FOL	C4A-C8A	2.37	1.45	1.41
4	8-A	204	NAP	O4D-C1D	2.37	1.44	1.41
2	113-A	201	FOL	C4A-C8A	2.37	1.45	1.41
2	161-A	201	FOL	C4A-C8A	2.37	1.45	1.41
4	42-A	204	NAP	C6N-N1N	2.37	1.41	1.35
4	111-A	204	NAP	P2B-O2B	2.37	1.63	1.59
4	18-A	204	NAP	C8A-N7A	2.37	1.39	1.34
4	34-A	204	NAP	C8A-N7A	2.37	1.39	1.34
4	112-A	204	NAP	C6N-N1N	2.37	1.41	1.35
4	77-A	204	NAP	C6N-N1N	2.37	1.41	1.35
4	14-A	204	NAP	C8A-N7A	2.38	1.39	1.34
4	154-A	204	NAP	C8A-N7A	2.38	1.39	1.34
4	111-A	204	NAP	C6N-N1N	2.38	1.41	1.35
4	98-A	204	NAP	C6N-N1N	2.38	1.41	1.35
4	65-A	204	NAP	O4D-C1D	2.38	1.44	1.41
2	1-A	201	FOL	C4-C4A	2.38	1.45	1.41
4	123-A	204	NAP	O4D-C1D	2.38	1.44	1.41
2	101-A	201	FOL	C4A-C8A	2.38	1.45	1.41
4	126-A	204	NAP	O4D-C1D	2.39	1.44	1.41
2	116-A	201	FOL	C4A-C8A	2.39	1.45	1.41
4	49-A	204	NAP	C8A-N7A	2.39	1.39	1.34
4	19-A	204	NAP	C6N-N1N	2.39	1.41	1.35
4	51-A	204	NAP	P2B-O2B	2.39	1.63	1.59
2	162-A	201	FOL	C2-N3	2.39	1.36	1.33
4	98-A	204	NAP	O4D-C1D	2.39	1.44	1.41
4	72-A	204	NAP	P2B-O2B	2.39	1.63	1.59
4	65-A	204	NAP	C8A-N7A	2.39	1.39	1.34
4	76-A	204	NAP	C8A-N7A	2.39	1.39	1.34
4	163-A	204	NAP	C8A-N7A	2.40	1.39	1.34
2	37-A	201	FOL	C4A-C8A	2.40	1.45	1.41
4	133-A	204	NAP	O4D-C1D	2.40	1.44	1.41
4	85-A	204	NAP	O4D-C1D	2.40	1.44	1.41
4	30-A	204	NAP	C8A-N7A	2.40	1.39	1.34
2	81-A	201	FOL	C4-C4A	2.40	1.45	1.41
4	27-A	204	NAP	C6N-N1N	2.41	1.41	1.35
4	76-A	204	NAP	C6N-N1N	2.41	1.41	1.35
4	113-A	204	NAP	C6N-N1N	2.41	1.41	1.35
2	1-A	201	FOL	C4A-C8A	2.41	1.45	1.41
4	31-A	204	NAP	C6N-N1N	2.41	1.41	1.35
2	56-A	201	FOL	C4A-C8A	2.41	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	37-A	204	NAP	O4D-C1D	2.41	1.44	1.41
2	110-A	201	FOL	C4A-C8A	2.41	1.45	1.41
4	9-A	204	NAP	P2B-O2B	2.41	1.63	1.59
4	32-A	204	NAP	P2B-O2B	2.42	1.63	1.59
4	24-A	204	NAP	O4D-C1D	2.42	1.44	1.41
4	51-A	204	NAP	C8A-N7A	2.42	1.39	1.34
2	159-A	201	FOL	C2-N3	2.42	1.36	1.33
4	36-A	204	NAP	C8A-N7A	2.42	1.39	1.34
2	11-A	201	FOL	C4A-C8A	2.42	1.45	1.41
4	117-A	204	NAP	C6N-N1N	2.42	1.41	1.35
2	156-A	201	FOL	C2-N3	2.42	1.36	1.33
4	97-A	204	NAP	C8A-N7A	2.42	1.39	1.34
2	125-A	201	FOL	C2-N3	2.42	1.36	1.33
4	70-A	204	NAP	O4D-C1D	2.42	1.44	1.41
4	121-A	204	NAP	C8A-N7A	2.42	1.39	1.34
4	61-A	204	NAP	O4D-C1D	2.42	1.44	1.41
4	11-A	204	NAP	C8A-N7A	2.43	1.39	1.34
4	130-A	204	NAP	O4D-C1D	2.43	1.44	1.41
4	72-A	204	NAP	O4D-C1D	2.43	1.44	1.41
4	41-A	204	NAP	C6N-N1N	2.43	1.41	1.35
2	75-A	201	FOL	C4-C4A	2.43	1.46	1.41
4	167-A	204	NAP	C8A-N7A	2.43	1.39	1.34
4	35-A	204	NAP	C6N-N1N	2.44	1.41	1.35
4	86-A	204	NAP	C8A-N7A	2.44	1.39	1.34
4	119-A	204	NAP	C8A-N7A	2.44	1.39	1.34
4	70-A	204	NAP	C6N-N1N	2.44	1.41	1.35
4	37-A	204	NAP	C6N-N1N	2.44	1.41	1.35
2	159-A	201	FOL	C4-C4A	2.44	1.46	1.41
4	75-A	204	NAP	C6N-N1N	2.44	1.41	1.35
4	101-A	204	NAP	C8A-N7A	2.44	1.39	1.34
2	15-A	201	FOL	CB-CA	2.44	1.56	1.53
4	82-A	204	NAP	P2B-O2B	2.44	1.63	1.59
2	161-A	201	FOL	C2-N3	2.44	1.36	1.33
4	166-A	204	NAP	C8A-N7A	2.45	1.39	1.34
4	155-A	204	NAP	O4D-C1D	2.45	1.44	1.41
4	29-A	204	NAP	O4D-C1D	2.45	1.44	1.41
4	110-A	204	NAP	C6N-N1N	2.45	1.41	1.35
4	160-A	204	NAP	O4D-C1D	2.45	1.44	1.41
4	38-A	204	NAP	C8A-N7A	2.45	1.39	1.34
4	24-A	204	NAP	C8A-N7A	2.45	1.39	1.34
2	125-A	201	FOL	C4A-C8A	2.45	1.45	1.41
4	48-A	204	NAP	C8A-N7A	2.45	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	20-A	204	NAP	C8A-N7A	2.45	1.39	1.34
4	75-A	204	NAP	C8A-N7A	2.46	1.39	1.34
4	149-A	204	NAP	C8A-N7A	2.46	1.39	1.34
4	19-A	204	NAP	C8A-N7A	2.46	1.39	1.34
4	109-A	204	NAP	C8A-N7A	2.46	1.39	1.34
4	146-A	204	NAP	C8A-N7A	2.46	1.39	1.34
4	16-A	204	NAP	C6N-N1N	2.46	1.41	1.35
4	14-A	204	NAP	O4D-C1D	2.46	1.44	1.41
4	8-A	204	NAP	C7N-N7N	2.46	1.37	1.33
4	69-A	204	NAP	C8A-N7A	2.46	1.39	1.34
4	159-A	204	NAP	C8A-N7A	2.46	1.39	1.34
4	33-A	204	NAP	O4D-C1D	2.46	1.44	1.41
4	39-A	204	NAP	C6N-N1N	2.46	1.41	1.35
4	131-A	204	NAP	C8A-N7A	2.47	1.39	1.34
4	100-A	204	NAP	C8A-N7A	2.47	1.39	1.34
4	19-A	204	NAP	P2B-O2B	2.47	1.63	1.59
4	19-A	204	NAP	O4D-C1D	2.47	1.44	1.41
2	158-A	201	FOL	C4-C4A	2.47	1.46	1.41
4	5-A	204	NAP	C8A-N7A	2.47	1.39	1.34
4	1-A	204	NAP	C8A-N7A	2.47	1.39	1.34
4	94-A	204	NAP	P2B-O2B	2.47	1.63	1.59
4	10-A	204	NAP	C8A-N7A	2.48	1.39	1.34
4	86-A	204	NAP	P2B-O2B	2.48	1.63	1.59
4	69-A	204	NAP	C6N-N1N	2.48	1.41	1.35
4	8-A	204	NAP	P2B-O2B	2.48	1.63	1.59
4	68-A	204	NAP	C8A-N7A	2.48	1.39	1.34
2	88-A	201	FOL	C4A-C8A	2.48	1.45	1.41
2	33-A	201	FOL	CB-CA	2.48	1.56	1.53
4	84-A	204	NAP	C8A-N7A	2.48	1.39	1.34
2	141-A	201	FOL	C4A-C8A	2.48	1.45	1.41
4	35-A	204	NAP	O4D-C1D	2.48	1.44	1.41
4	21-A	204	NAP	O4D-C1D	2.49	1.44	1.41
4	46-A	204	NAP	P2B-O2B	2.49	1.63	1.59
4	52-A	204	NAP	O4D-C1D	2.49	1.44	1.41
4	149-A	204	NAP	O4D-C1D	2.49	1.44	1.41
2	153-A	201	FOL	C4A-C8A	2.49	1.45	1.41
4	158-A	204	NAP	C2A-N3A	2.49	1.36	1.32
4	59-A	204	NAP	C8A-N7A	2.49	1.39	1.34
2	91-A	201	FOL	C4-C4A	2.49	1.46	1.41
4	83-A	204	NAP	C2A-N3A	2.49	1.36	1.32
2	112-A	201	FOL	C4A-C8A	2.49	1.45	1.41
2	66-A	201	FOL	C4A-C8A	2.50	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	38-A	204	NAP	C6N-N1N	2.50	1.41	1.35
2	166-A	201	FOL	C2-N3	2.50	1.36	1.33
4	119-A	204	NAP	P2B-O2B	2.50	1.63	1.59
4	114-A	204	NAP	C8A-N7A	2.50	1.39	1.34
2	143-A	201	FOL	C4A-C8A	2.50	1.45	1.41
4	91-A	204	NAP	C8A-N7A	2.50	1.39	1.34
2	9-A	201	FOL	C4A-C8A	2.50	1.45	1.41
4	17-A	204	NAP	C6N-N1N	2.50	1.41	1.35
2	69-A	201	FOL	CB-CA	2.50	1.56	1.53
4	50-A	204	NAP	C8A-N7A	2.51	1.39	1.34
2	123-A	201	FOL	C4A-C8A	2.51	1.45	1.41
4	71-A	204	NAP	O4D-C1D	2.51	1.44	1.41
4	74-A	204	NAP	C6N-N1N	2.51	1.41	1.35
2	164-A	201	FOL	C2-N3	2.51	1.36	1.33
4	12-A	204	NAP	P2B-O2B	2.51	1.64	1.59
4	161-A	204	NAP	O4D-C1D	2.52	1.44	1.41
2	149-A	201	FOL	C4A-C8A	2.52	1.45	1.41
2	22-A	201	FOL	C4A-C8A	2.52	1.45	1.41
4	23-A	204	NAP	C6N-N1N	2.52	1.42	1.35
2	77-A	201	FOL	C4-C4A	2.53	1.46	1.41
4	154-A	204	NAP	C2A-N3A	2.53	1.36	1.32
4	55-A	204	NAP	C8A-N7A	2.53	1.39	1.34
2	16-A	201	FOL	C4-C4A	2.53	1.46	1.41
4	98-A	204	NAP	C8A-N7A	2.53	1.39	1.34
2	36-A	201	FOL	C4A-C8A	2.53	1.45	1.41
4	26-A	204	NAP	C6N-N1N	2.53	1.42	1.35
4	119-A	204	NAP	O4D-C1D	2.53	1.44	1.41
4	17-A	204	NAP	C8A-N7A	2.53	1.39	1.34
4	25-A	204	NAP	C6N-N1N	2.53	1.42	1.35
2	71-A	201	FOL	C4-C4A	2.53	1.46	1.41
2	118-A	201	FOL	C4A-C8A	2.54	1.45	1.41
4	99-A	204	NAP	O4D-C1D	2.54	1.44	1.41
4	55-A	204	NAP	O4D-C1D	2.54	1.44	1.41
4	40-A	204	NAP	C8A-N7A	2.54	1.39	1.34
4	20-A	204	NAP	O4D-C1D	2.54	1.44	1.41
4	88-A	204	NAP	C8A-N7A	2.54	1.39	1.34
2	10-A	201	FOL	C4A-C8A	2.54	1.45	1.41
4	61-A	204	NAP	C8A-N7A	2.54	1.39	1.34
4	17-A	204	NAP	O4D-C1D	2.54	1.44	1.41
4	26-A	204	NAP	C8A-N7A	2.54	1.39	1.34
2	79-A	201	FOL	C4-C4A	2.55	1.46	1.41
2	84-A	201	FOL	C8A-N8	2.55	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	144-A	201	FOL	CB-CA	2.55	1.56	1.53
4	67-A	204	NAP	C8A-N7A	2.55	1.39	1.34
4	69-A	204	NAP	O4D-C1D	2.55	1.44	1.41
2	114-A	201	FOL	C4A-C8A	2.55	1.45	1.41
2	39-A	201	FOL	C4A-C8A	2.55	1.45	1.41
4	33-A	204	NAP	C7N-N7N	2.55	1.38	1.33
4	120-A	204	NAP	C6N-N1N	2.55	1.42	1.35
2	14-A	201	FOL	C4A-C8A	2.56	1.45	1.41
4	136-A	204	NAP	C8A-N7A	2.56	1.39	1.34
4	116-A	204	NAP	O4D-C1D	2.56	1.44	1.41
4	23-A	204	NAP	P2B-O2B	2.56	1.64	1.59
2	55-A	201	FOL	C4A-C8A	2.56	1.45	1.41
4	20-A	204	NAP	C6N-N1N	2.56	1.42	1.35
2	154-A	201	FOL	C4A-C8A	2.56	1.45	1.41
4	23-A	204	NAP	O4D-C1D	2.56	1.44	1.41
4	118-A	204	NAP	C6N-N1N	2.56	1.42	1.35
2	75-A	201	FOL	C4A-C8A	2.57	1.45	1.41
4	135-A	204	NAP	C2A-N3A	2.57	1.36	1.32
2	160-A	201	FOL	C2-N3	2.57	1.36	1.33
2	78-A	201	FOL	C4-C4A	2.57	1.46	1.41
2	43-A	201	FOL	C4A-C8A	2.58	1.45	1.41
2	4-A	201	FOL	C4A-C8A	2.58	1.45	1.41
2	167-A	201	FOL	C4A-C8A	2.58	1.45	1.41
4	30-A	204	NAP	C6N-N1N	2.58	1.42	1.35
2	20-A	201	FOL	C4-C4A	2.58	1.46	1.41
4	33-A	204	NAP	P2B-O2B	2.58	1.64	1.59
4	28-A	204	NAP	O4D-C1D	2.58	1.44	1.41
4	125-A	204	NAP	C8A-N7A	2.58	1.39	1.34
4	123-A	204	NAP	C2A-N3A	2.58	1.36	1.32
4	77-A	204	NAP	C2A-N3A	2.59	1.36	1.32
4	25-A	204	NAP	C8A-N7A	2.59	1.39	1.34
4	73-A	204	NAP	P2B-O2B	2.59	1.64	1.59
4	140-A	204	NAP	O4D-C1D	2.59	1.44	1.41
4	127-A	204	NAP	C8A-N7A	2.59	1.39	1.34
4	27-A	204	NAP	C8A-N7A	2.59	1.39	1.34
2	138-A	201	FOL	C4A-C8A	2.59	1.45	1.41
4	132-A	204	NAP	C8A-N7A	2.59	1.39	1.34
2	140-A	201	FOL	C4-C4A	2.60	1.46	1.41
2	23-A	201	FOL	C4A-C8A	2.60	1.45	1.41
4	85-A	204	NAP	C8A-N7A	2.60	1.39	1.34
4	148-A	204	NAP	C8A-N7A	2.60	1.39	1.34
2	34-A	201	FOL	C4-C4A	2.60	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	129-A	204	NAP	C8A-N7A	2.60	1.39	1.34
2	145-A	201	FOL	C4-C4A	2.60	1.46	1.41
2	156-A	201	FOL	C4A-C8A	2.61	1.45	1.41
4	23-A	204	NAP	C8A-N7A	2.61	1.39	1.34
4	95-A	204	NAP	C8A-N7A	2.61	1.39	1.34
4	82-A	204	NAP	O4D-C1D	2.61	1.44	1.41
4	36-A	204	NAP	O4D-C1D	2.61	1.44	1.41
4	122-A	204	NAP	O4D-C1D	2.61	1.44	1.41
4	58-A	204	NAP	C8A-N7A	2.61	1.39	1.34
2	161-A	201	FOL	C4-C4A	2.61	1.46	1.41
2	54-A	201	FOL	C4A-C8A	2.61	1.45	1.41
2	59-A	201	FOL	C4A-C8A	2.62	1.45	1.41
2	126-A	201	FOL	C4A-C8A	2.62	1.45	1.41
4	53-A	204	NAP	C8A-N7A	2.62	1.39	1.34
4	128-A	204	NAP	O4D-C1D	2.62	1.44	1.41
4	119-A	204	NAP	C6N-N1N	2.62	1.42	1.35
2	157-A	201	FOL	C4A-C8A	2.62	1.45	1.41
4	67-A	204	NAP	C2A-N3A	2.62	1.36	1.32
2	83-A	201	FOL	C4-C4A	2.63	1.46	1.41
4	105-A	204	NAP	C8A-N7A	2.63	1.39	1.34
4	138-A	204	NAP	C2A-N3A	2.63	1.36	1.32
2	93-A	201	FOL	C4A-C8A	2.63	1.45	1.41
4	39-A	204	NAP	O4D-C1D	2.63	1.44	1.41
4	26-A	204	NAP	O4D-C1D	2.63	1.44	1.41
2	104-A	201	FOL	C4A-C8A	2.63	1.45	1.41
4	28-A	204	NAP	C8A-N7A	2.63	1.39	1.34
2	69-A	201	FOL	C4A-C8A	2.63	1.45	1.41
4	160-A	204	NAP	C8A-N7A	2.63	1.39	1.34
2	119-A	201	FOL	C4A-C8A	2.64	1.45	1.41
4	143-A	204	NAP	C8A-N7A	2.64	1.39	1.34
4	89-A	204	NAP	O4D-C1D	2.64	1.44	1.41
2	127-A	201	FOL	C4A-C8A	2.64	1.45	1.41
2	103-A	201	FOL	C4A-C8A	2.64	1.45	1.41
4	150-A	204	NAP	C8A-N7A	2.64	1.39	1.34
4	102-A	204	NAP	O4D-C1D	2.65	1.44	1.41
2	150-A	201	FOL	C4A-C8A	2.65	1.45	1.41
4	92-A	204	NAP	C8A-N7A	2.65	1.39	1.34
2	67-A	201	FOL	C4-C4A	2.65	1.46	1.41
4	34-A	204	NAP	C7N-N7N	2.66	1.38	1.33
4	150-A	204	NAP	C2A-N3A	2.66	1.36	1.32
2	115-A	201	FOL	C4A-C8A	2.66	1.45	1.41
4	11-A	204	NAP	O4D-C1D	2.66	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	144-A	201	FOL	C4A-C8A	2.66	1.45	1.41
2	47-A	201	FOL	C4A-C8A	2.66	1.45	1.41
2	48-A	201	FOL	C4A-C8A	2.66	1.45	1.41
4	81-A	204	NAP	C2A-N3A	2.66	1.36	1.32
4	31-A	204	NAP	C8A-N7A	2.67	1.39	1.34
4	123-A	204	NAP	P2B-O2B	2.67	1.64	1.59
4	49-A	204	NAP	O4D-C1D	2.67	1.45	1.41
2	69-A	201	FOL	C4-C4A	2.68	1.46	1.41
4	108-A	204	NAP	O4D-C1D	2.68	1.45	1.41
2	74-A	201	FOL	C4-C4A	2.68	1.46	1.41
4	93-A	204	NAP	C8A-N7A	2.68	1.39	1.34
2	38-A	201	FOL	C4A-C8A	2.68	1.45	1.41
4	81-A	204	NAP	O4D-C1D	2.68	1.45	1.41
4	151-A	204	NAP	C2A-N3A	2.68	1.36	1.32
4	167-A	204	NAP	O4D-C1D	2.68	1.45	1.41
2	117-A	201	FOL	C4A-C8A	2.68	1.45	1.41
4	60-A	204	NAP	C8A-N7A	2.68	1.39	1.34
4	12-A	204	NAP	O4D-C1D	2.68	1.45	1.41
4	146-A	204	NAP	O4D-C1D	2.69	1.45	1.41
4	70-A	204	NAP	C8A-N7A	2.69	1.39	1.34
2	102-A	201	FOL	C4-C4A	2.69	1.46	1.41
4	9-A	204	NAP	C7N-N7N	2.69	1.38	1.33
2	102-A	201	FOL	C4A-C8A	2.69	1.45	1.41
4	157-A	204	NAP	C2A-N3A	2.69	1.36	1.32
4	120-A	204	NAP	O4D-C1D	2.69	1.45	1.41
4	15-A	204	NAP	O4D-C1D	2.69	1.45	1.41
2	163-A	201	FOL	C4A-C8A	2.70	1.45	1.41
2	2-A	201	FOL	C4A-C8A	2.70	1.45	1.41
2	104-A	201	FOL	C8A-N8	2.70	1.37	1.34
4	128-A	204	NAP	C8A-N7A	2.70	1.39	1.34
4	102-A	204	NAP	C8A-N7A	2.70	1.39	1.34
4	51-A	204	NAP	O4D-C1D	2.70	1.45	1.41
4	96-A	204	NAP	O4D-C1D	2.70	1.45	1.41
2	49-A	201	FOL	C4A-C8A	2.70	1.45	1.41
4	24-A	204	NAP	C6N-N1N	2.70	1.42	1.35
2	31-A	201	FOL	C4A-C8A	2.70	1.45	1.41
4	95-A	204	NAP	P2B-O2B	2.70	1.64	1.59
4	88-A	204	NAP	C2A-N3A	2.70	1.36	1.32
4	4-A	204	NAP	O4D-C1D	2.70	1.45	1.41
2	88-A	201	FOL	C4-C4A	2.71	1.46	1.41
4	53-A	204	NAP	O4D-C1D	2.71	1.45	1.41
4	103-A	204	NAP	C8A-N7A	2.71	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	32-A	201	FOL	C4-C4A	2.71	1.46	1.41
2	96-A	201	FOL	C4A-C8A	2.71	1.45	1.41
2	49-A	201	FOL	C4-C4A	2.72	1.46	1.41
4	139-A	204	NAP	O4D-C1D	2.72	1.45	1.41
2	16-A	201	FOL	C4A-C8A	2.72	1.45	1.41
4	83-A	204	NAP	C8A-N7A	2.72	1.39	1.34
4	10-A	204	NAP	O4D-C1D	2.72	1.45	1.41
4	139-A	204	NAP	C2A-N3A	2.72	1.36	1.32
2	134-A	201	FOL	C4A-C8A	2.72	1.45	1.41
2	14-A	201	FOL	C4-C4A	2.72	1.46	1.41
4	86-A	204	NAP	C2A-N3A	2.72	1.36	1.32
4	148-A	204	NAP	C2A-N3A	2.72	1.36	1.32
2	7-A	201	FOL	C4-C4A	2.73	1.46	1.41
2	99-A	201	FOL	C4A-C8A	2.73	1.45	1.41
4	64-A	204	NAP	C2A-N3A	2.73	1.36	1.32
2	70-A	201	FOL	C4-C4A	2.73	1.46	1.41
2	90-A	201	FOL	C4A-C8A	2.73	1.45	1.41
2	5-A	201	FOL	C4A-C8A	2.73	1.45	1.41
2	68-A	201	FOL	C4-C4A	2.73	1.46	1.41
2	58-A	201	FOL	C4-C4A	2.73	1.46	1.41
4	96-A	204	NAP	C8A-N7A	2.73	1.39	1.34
4	99-A	204	NAP	C8A-N7A	2.74	1.39	1.34
4	64-A	204	NAP	C8A-N7A	2.74	1.39	1.34
2	146-A	201	FOL	C4A-C8A	2.74	1.45	1.41
4	135-A	204	NAP	C8A-N7A	2.74	1.39	1.34
4	93-A	204	NAP	C2A-N3A	2.74	1.36	1.32
4	133-A	204	NAP	C8A-N7A	2.74	1.39	1.34
2	160-A	201	FOL	C4A-C8A	2.75	1.45	1.41
4	66-A	204	NAP	C8A-N7A	2.75	1.39	1.34
4	101-A	204	NAP	P2B-O2B	2.75	1.64	1.59
4	54-A	204	NAP	O4D-C1D	2.75	1.45	1.41
4	130-A	204	NAP	C8A-N7A	2.75	1.39	1.34
2	132-A	201	FOL	C4-C4A	2.75	1.46	1.41
4	42-A	204	NAP	O4D-C1D	2.75	1.45	1.41
4	130-A	204	NAP	C2A-N3A	2.75	1.36	1.32
4	132-A	204	NAP	C2A-N3A	2.75	1.36	1.32
4	114-A	204	NAP	O4D-C1D	2.76	1.45	1.41
2	12-A	201	FOL	C4A-C8A	2.76	1.45	1.41
4	34-A	204	NAP	C2A-N3A	2.76	1.36	1.32
4	43-A	204	NAP	C8A-N7A	2.76	1.39	1.34
2	63-A	201	FOL	C4A-C8A	2.76	1.45	1.41
2	112-A	201	FOL	C4-C4A	2.76	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	142-A	201	FOL	C4-C4A	2.76	1.46	1.41
2	25-A	201	FOL	C4A-C8A	2.77	1.45	1.41
2	104-A	201	FOL	C4-C4A	2.77	1.46	1.41
4	27-A	204	NAP	O4D-C1D	2.77	1.45	1.41
4	129-A	204	NAP	O4D-C1D	2.77	1.45	1.41
2	18-A	201	FOL	C4A-C8A	2.78	1.45	1.41
4	16-A	204	NAP	C8A-N7A	2.78	1.39	1.34
4	73-A	204	NAP	C2A-N3A	2.78	1.36	1.32
2	40-A	201	FOL	C4A-C8A	2.78	1.45	1.41
4	15-A	204	NAP	C8A-N7A	2.78	1.39	1.34
4	147-A	204	NAP	C8A-N7A	2.78	1.39	1.34
2	72-A	201	FOL	C4A-C8A	2.78	1.45	1.41
2	130-A	201	FOL	C4A-C8A	2.78	1.45	1.41
4	61-A	204	NAP	C2A-N3A	2.79	1.36	1.32
2	2-A	201	FOL	C4-C4A	2.79	1.46	1.41
2	107-A	201	FOL	C4A-C8A	2.79	1.45	1.41
4	109-A	204	NAP	C7N-N7N	2.79	1.38	1.33
4	62-A	204	NAP	C2A-N3A	2.79	1.36	1.32
4	115-A	204	NAP	C8A-N7A	2.79	1.39	1.34
2	105-A	201	FOL	CB-CA	2.79	1.57	1.53
4	123-A	204	NAP	C8A-N7A	2.79	1.39	1.34
2	146-A	201	FOL	C4-C4A	2.79	1.46	1.41
2	147-A	201	FOL	C4A-C8A	2.79	1.45	1.41
4	57-A	204	NAP	C2A-N3A	2.80	1.36	1.32
4	15-A	204	NAP	C2A-N3A	2.80	1.36	1.32
4	145-A	204	NAP	O4D-C1D	2.80	1.45	1.41
4	133-A	204	NAP	C2A-N3A	2.80	1.36	1.32
4	127-A	204	NAP	O4D-C1D	2.80	1.45	1.41
2	22-A	201	FOL	C4-C4A	2.80	1.46	1.41
4	163-A	204	NAP	O4D-C1D	2.80	1.45	1.41
2	33-A	201	FOL	C4-C4A	2.80	1.46	1.41
4	73-A	204	NAP	C8A-N7A	2.80	1.39	1.34
4	81-A	204	NAP	C8A-N7A	2.81	1.39	1.34
4	121-A	204	NAP	O4D-C1D	2.81	1.45	1.41
4	8-A	204	NAP	C8A-N7A	2.81	1.39	1.34
4	9-A	204	NAP	C8A-N7A	2.81	1.39	1.34
2	62-A	201	FOL	C4-C4A	2.81	1.46	1.41
4	18-A	204	NAP	O4D-C1D	2.82	1.45	1.41
2	84-A	201	FOL	C4-C4A	2.82	1.46	1.41
2	97-A	201	FOL	C4A-C8A	2.82	1.46	1.41
2	95-A	201	FOL	C4-C4A	2.82	1.46	1.41
4	82-A	204	NAP	C2A-N3A	2.82	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	148-A	201	FOL	C4-C4A	2.82	1.46	1.41
2	93-A	201	FOL	CB-CA	2.82	1.57	1.53
2	87-A	201	FOL	C4A-C8A	2.82	1.46	1.41
2	19-A	201	FOL	C4A-C8A	2.82	1.46	1.41
2	44-A	201	FOL	C4A-C8A	2.83	1.46	1.41
2	85-A	201	FOL	C4A-C8A	2.83	1.46	1.41
4	25-A	204	NAP	O4D-C1D	2.83	1.45	1.41
4	60-A	204	NAP	O4D-C1D	2.83	1.45	1.41
4	101-A	204	NAP	O4D-C1D	2.83	1.45	1.41
2	94-A	201	FOL	C4A-C8A	2.83	1.46	1.41
2	158-A	201	FOL	C4A-C8A	2.83	1.46	1.41
4	162-A	204	NAP	O4D-C1D	2.83	1.45	1.41
4	90-A	204	NAP	C8A-N7A	2.84	1.40	1.34
4	35-A	204	NAP	C2A-N3A	2.84	1.36	1.32
2	139-A	201	FOL	C4-C4A	2.84	1.46	1.41
4	159-A	204	NAP	C7N-N7N	2.84	1.38	1.33
2	116-A	201	FOL	C4-C4A	2.84	1.46	1.41
4	50-A	204	NAP	O4D-C1D	2.85	1.45	1.41
2	50-A	201	FOL	C4-C4A	2.85	1.46	1.41
2	156-A	201	FOL	C4-C4A	2.85	1.46	1.41
2	108-A	201	FOL	C4-C4A	2.85	1.46	1.41
4	155-A	204	NAP	C2A-N3A	2.85	1.36	1.32
4	94-A	204	NAP	C8A-N7A	2.85	1.40	1.34
4	140-A	204	NAP	C8A-N7A	2.85	1.40	1.34
2	121-A	201	FOL	C4A-C8A	2.85	1.46	1.41
2	57-A	201	FOL	C4-C4A	2.85	1.46	1.41
2	131-A	201	FOL	C4-C4A	2.86	1.46	1.41
2	20-A	201	FOL	C4A-C8A	2.86	1.46	1.41
2	63-A	201	FOL	C4-C4A	2.86	1.46	1.41
4	163-A	204	NAP	C2A-N3A	2.86	1.36	1.32
2	124-A	201	FOL	C4A-C8A	2.86	1.46	1.41
2	45-A	201	FOL	C4A-C8A	2.86	1.46	1.41
2	122-A	201	FOL	C4A-C8A	2.86	1.46	1.41
4	107-A	204	NAP	O4D-C1D	2.86	1.45	1.41
4	119-A	204	NAP	C2A-N3A	2.86	1.37	1.32
2	42-A	201	FOL	C4A-C8A	2.86	1.46	1.41
4	164-A	204	NAP	O4D-C1D	2.86	1.45	1.41
2	120-A	201	FOL	C4A-C8A	2.86	1.46	1.41
4	115-A	204	NAP	O4D-C1D	2.86	1.45	1.41
4	74-A	204	NAP	C2A-N3A	2.87	1.37	1.32
4	56-A	204	NAP	C8A-N7A	2.87	1.40	1.34
2	70-A	201	FOL	C4A-C8A	2.87	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	73-A	201	FOL	C4A-C8A	2.87	1.46	1.41
4	140-A	204	NAP	C2A-N3A	2.87	1.37	1.32
2	155-A	201	FOL	C4-C4A	2.87	1.46	1.41
4	141-A	204	NAP	O4D-C1D	2.88	1.45	1.41
2	19-A	201	FOL	C4-C4A	2.88	1.46	1.41
2	29-A	201	FOL	C4A-C8A	2.88	1.46	1.41
4	30-A	204	NAP	O4D-C1D	2.88	1.45	1.41
2	29-A	201	FOL	C4-C4A	2.88	1.46	1.41
2	152-A	201	FOL	C4A-C8A	2.88	1.46	1.41
2	61-A	201	FOL	C4A-C8A	2.88	1.46	1.41
4	165-A	204	NAP	O4D-C1D	2.88	1.45	1.41
4	165-A	204	NAP	C2A-N3A	2.89	1.37	1.32
4	104-A	204	NAP	O4D-C1D	2.89	1.45	1.41
4	153-A	204	NAP	C2A-N3A	2.89	1.37	1.32
4	18-A	204	NAP	C7N-N7N	2.89	1.38	1.33
2	81-A	201	FOL	C4A-C8A	2.89	1.46	1.41
4	17-A	204	NAP	C2A-N3A	2.89	1.37	1.32
4	84-A	204	NAP	P2B-O2B	2.89	1.64	1.59
4	29-A	204	NAP	C2A-N3A	2.90	1.37	1.32
4	131-A	204	NAP	C2A-N3A	2.90	1.37	1.32
2	10-A	201	FOL	C4-C4A	2.90	1.46	1.41
2	111-A	201	FOL	C4A-C8A	2.90	1.46	1.41
4	113-A	204	NAP	O4D-C1D	2.90	1.45	1.41
4	137-A	204	NAP	C2A-N3A	2.90	1.37	1.32
2	64-A	201	FOL	C4A-C8A	2.90	1.46	1.41
4	38-A	204	NAP	C2A-N3A	2.90	1.37	1.32
2	35-A	201	FOL	C4-C4A	2.90	1.46	1.41
2	38-A	201	FOL	C4-C4A	2.90	1.46	1.41
2	55-A	201	FOL	C4-C4A	2.91	1.46	1.41
4	47-A	204	NAP	O4D-C1D	2.91	1.45	1.41
4	162-A	204	NAP	C2A-N3A	2.91	1.37	1.32
2	39-A	201	FOL	CB-CA	2.91	1.57	1.53
2	92-A	201	FOL	C4A-C8A	2.91	1.46	1.41
2	78-A	201	FOL	C4A-C8A	2.91	1.46	1.41
2	61-A	201	FOL	C4-C4A	2.91	1.46	1.41
2	36-A	201	FOL	C4-C4A	2.91	1.46	1.41
2	129-A	201	FOL	C4A-C8A	2.92	1.46	1.41
2	71-A	201	FOL	C4A-C8A	2.92	1.46	1.41
2	17-A	201	FOL	C4-C4A	2.92	1.46	1.41
2	98-A	201	FOL	C4A-C8A	2.93	1.46	1.41
4	125-A	204	NAP	C2A-N3A	2.93	1.37	1.32
2	165-A	201	FOL	C4A-C8A	2.93	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	106-A	201	FOL	C4-C4A	2.93	1.46	1.41
2	4-A	201	FOL	C4-C4A	2.93	1.46	1.41
4	5-A	204	NAP	C2A-N3A	2.93	1.37	1.32
4	40-A	204	NAP	O4D-C1D	2.94	1.45	1.41
2	133-A	201	FOL	C4-C4A	2.94	1.46	1.41
4	31-A	204	NAP	C7N-N7N	2.94	1.38	1.33
4	41-A	204	NAP	O4D-C1D	2.94	1.45	1.41
2	3-A	201	FOL	C4-C4A	2.94	1.47	1.41
4	59-A	204	NAP	C2A-N3A	2.94	1.37	1.32
2	153-A	201	FOL	C4-C4A	2.94	1.47	1.41
2	110-A	201	FOL	C4-C4A	2.94	1.47	1.41
4	164-A	204	NAP	C2A-N3A	2.94	1.37	1.32
4	46-A	204	NAP	O4D-C1D	2.94	1.45	1.41
4	164-A	204	NAP	C7N-N7N	2.95	1.38	1.33
4	133-A	204	NAP	P2B-O2B	2.95	1.64	1.59
2	86-A	201	FOL	C4A-C8A	2.95	1.46	1.41
4	57-A	204	NAP	C8A-N7A	2.95	1.40	1.34
4	21-A	204	NAP	C2A-N3A	2.95	1.37	1.32
4	127-A	204	NAP	C2A-N3A	2.95	1.37	1.32
4	90-A	204	NAP	C2A-N3A	2.95	1.37	1.32
2	50-A	201	FOL	C4A-C8A	2.95	1.46	1.41
4	48-A	204	NAP	O4D-C1D	2.95	1.45	1.41
4	128-A	204	NAP	C2A-N3A	2.96	1.37	1.32
4	103-A	204	NAP	O4D-C1D	2.96	1.45	1.41
2	52-A	201	FOL	C4A-C8A	2.96	1.46	1.41
4	166-A	204	NAP	C2A-N3A	2.96	1.37	1.32
4	92-A	204	NAP	C2A-N3A	2.96	1.37	1.32
2	52-A	201	FOL	C4-C4A	2.96	1.47	1.41
4	21-A	204	NAP	C8A-N7A	2.96	1.40	1.34
2	113-A	201	FOL	C4-C4A	2.96	1.47	1.41
4	101-A	204	NAP	C2A-N3A	2.96	1.37	1.32
2	8-A	201	FOL	C4-C4A	2.97	1.47	1.41
2	41-A	201	FOL	C4-C4A	2.97	1.47	1.41
4	95-A	204	NAP	C2A-N3A	2.97	1.37	1.32
4	59-A	204	NAP	C7N-N7N	2.97	1.38	1.33
4	42-A	204	NAP	C2A-N3A	2.98	1.37	1.32
4	36-A	204	NAP	C2A-N3A	2.98	1.37	1.32
2	79-A	201	FOL	C4A-C8A	2.98	1.46	1.41
4	121-A	204	NAP	C2A-N3A	2.98	1.37	1.32
4	40-A	204	NAP	C2A-N3A	2.98	1.37	1.32
4	6-A	204	NAP	C8A-N7A	2.98	1.40	1.34
2	45-A	201	FOL	C4-C4A	2.98	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-A	201	FOL	C4A-C8A	2.99	1.46	1.41
2	163-A	201	FOL	C4-C4A	2.99	1.47	1.41
2	117-A	201	FOL	C4-C4A	2.99	1.47	1.41
4	142-A	204	NAP	C8A-N7A	3.00	1.40	1.34
4	97-A	204	NAP	O4D-C1D	3.00	1.45	1.41
4	25-A	204	NAP	C7N-N7N	3.00	1.38	1.33
2	96-A	201	FOL	C4-C4A	3.00	1.47	1.41
2	103-A	201	FOL	C4-C4A	3.01	1.47	1.41
2	74-A	201	FOL	C4A-C8A	3.01	1.46	1.41
4	157-A	204	NAP	C7N-N7N	3.01	1.38	1.33
4	96-A	204	NAP	C2A-N3A	3.01	1.37	1.32
4	26-A	204	NAP	C2A-N3A	3.01	1.37	1.32
4	110-A	204	NAP	O4D-C1D	3.02	1.45	1.41
4	150-A	204	NAP	C7N-N7N	3.02	1.38	1.33
4	124-A	204	NAP	C2A-N3A	3.02	1.37	1.32
4	158-A	204	NAP	C7N-N7N	3.02	1.38	1.33
2	106-A	201	FOL	C4A-C8A	3.02	1.46	1.41
2	15-A	201	FOL	C4A-C8A	3.02	1.46	1.41
4	44-A	204	NAP	O4D-C1D	3.03	1.45	1.41
4	100-A	204	NAP	O4D-C1D	3.03	1.45	1.41
2	73-A	201	FOL	C4-C4A	3.03	1.47	1.41
2	11-A	201	FOL	C4-C4A	3.03	1.47	1.41
2	86-A	201	FOL	C4-C4A	3.04	1.47	1.41
2	66-A	201	FOL	C4-C4A	3.04	1.47	1.41
4	147-A	204	NAP	C2A-N3A	3.04	1.37	1.32
4	14-A	204	NAP	C2A-N3A	3.04	1.37	1.32
2	137-A	201	FOL	C4A-C8A	3.04	1.46	1.41
4	149-A	204	NAP	C2A-N3A	3.04	1.37	1.32
4	72-A	204	NAP	C2A-N3A	3.04	1.37	1.32
4	75-A	204	NAP	C2A-N3A	3.04	1.37	1.32
2	135-A	201	FOL	C4A-C8A	3.04	1.46	1.41
4	18-A	204	NAP	C2A-N3A	3.04	1.37	1.32
4	70-A	204	NAP	C2A-N3A	3.05	1.37	1.32
4	11-A	204	NAP	C2A-N3A	3.05	1.37	1.32
4	55-A	204	NAP	C2A-N3A	3.05	1.37	1.32
2	97-A	201	FOL	C4-C4A	3.05	1.47	1.41
2	18-A	201	FOL	C4-C4A	3.05	1.47	1.41
4	43-A	204	NAP	C2A-N3A	3.06	1.37	1.32
2	51-A	201	FOL	C4A-C8A	3.06	1.46	1.41
2	139-A	201	FOL	CB-CA	3.06	1.57	1.53
4	32-A	204	NAP	C7N-N7N	3.06	1.39	1.33
4	163-A	204	NAP	C7N-N7N	3.06	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	138-A	201	FOL	C4-C4A	3.06	1.47	1.41
4	109-A	204	NAP	O4D-C1D	3.06	1.45	1.41
2	123-A	201	FOL	C4-C4A	3.06	1.47	1.41
4	10-A	204	NAP	C2A-N3A	3.07	1.37	1.32
2	60-A	201	FOL	C4A-C8A	3.07	1.46	1.41
4	85-A	204	NAP	C2A-N3A	3.07	1.37	1.32
2	143-A	201	FOL	C4-C4A	3.07	1.47	1.41
4	113-A	204	NAP	C2A-N3A	3.07	1.37	1.32
2	24-A	201	FOL	C4-C4A	3.07	1.47	1.41
4	101-A	204	NAP	C7N-N7N	3.07	1.39	1.33
2	58-A	201	FOL	CB-CA	3.07	1.57	1.53
4	11-A	204	NAP	C7N-N7N	3.07	1.39	1.33
4	89-A	204	NAP	C7N-N7N	3.08	1.39	1.33
4	145-A	204	NAP	C2A-N3A	3.08	1.37	1.32
2	54-A	201	FOL	C4-C4A	3.08	1.47	1.41
2	51-A	201	FOL	C4-C4A	3.08	1.47	1.41
4	2-A	204	NAP	C2A-N3A	3.08	1.37	1.32
2	128-A	201	FOL	C4-C4A	3.08	1.47	1.41
4	32-A	204	NAP	C2A-N3A	3.08	1.37	1.32
2	87-A	201	FOL	C4-C4A	3.08	1.47	1.41
2	107-A	201	FOL	C4-C4A	3.09	1.47	1.41
2	85-A	201	FOL	C4-C4A	3.09	1.47	1.41
4	34-A	204	NAP	P2B-O2B	3.09	1.65	1.59
2	31-A	201	FOL	C4-C4A	3.09	1.47	1.41
2	164-A	201	FOL	C4A-C8A	3.09	1.46	1.41
2	27-A	201	FOL	C4A-C8A	3.09	1.46	1.41
2	70-A	201	FOL	CB-CA	3.10	1.57	1.53
4	131-A	204	NAP	C7N-N7N	3.10	1.39	1.33
2	134-A	201	FOL	C4-C4A	3.10	1.47	1.41
2	162-A	201	FOL	C4-C4A	3.10	1.47	1.41
2	93-A	201	FOL	C4-C4A	3.10	1.47	1.41
2	77-A	201	FOL	C4A-C8A	3.10	1.46	1.41
4	132-A	204	NAP	C7N-N7N	3.11	1.39	1.33
4	152-A	204	NAP	C2A-N3A	3.12	1.37	1.32
4	6-A	204	NAP	C7N-N7N	3.12	1.39	1.33
2	100-A	201	FOL	C4A-C8A	3.12	1.46	1.41
2	105-A	201	FOL	C4-C4A	3.12	1.47	1.41
4	8-A	204	NAP	C2A-N3A	3.12	1.37	1.32
4	45-A	204	NAP	C2A-N3A	3.13	1.37	1.32
4	78-A	204	NAP	C7N-N7N	3.13	1.39	1.33
4	110-A	204	NAP	C7N-N7N	3.13	1.39	1.33
4	54-A	204	NAP	C2A-N3A	3.13	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	120-A	204	NAP	C2A-N3A	3.13	1.37	1.32
4	91-A	204	NAP	C2A-N3A	3.13	1.37	1.32
4	142-A	204	NAP	C2A-N3A	3.13	1.37	1.32
4	105-A	204	NAP	C7N-N7N	3.13	1.39	1.33
2	162-A	201	FOL	C4A-C8A	3.13	1.46	1.41
4	45-A	204	NAP	O4D-C1D	3.13	1.45	1.41
2	160-A	201	FOL	C4-C4A	3.13	1.47	1.41
4	53-A	204	NAP	C2A-N3A	3.14	1.37	1.32
4	111-A	204	NAP	O4D-C1D	3.14	1.45	1.41
4	146-A	204	NAP	C7N-N7N	3.15	1.39	1.33
2	24-A	201	FOL	C4A-C8A	3.15	1.46	1.41
2	37-A	201	FOL	C4-C4A	3.15	1.47	1.41
2	89-A	201	FOL	C4A-C8A	3.15	1.46	1.41
2	44-A	201	FOL	C4-C4A	3.15	1.47	1.41
2	67-A	201	FOL	C4A-C8A	3.15	1.46	1.41
2	25-A	201	FOL	C4-C4A	3.15	1.47	1.41
4	15-A	204	NAP	C7N-N7N	3.15	1.39	1.33
4	112-A	204	NAP	O4D-C1D	3.16	1.45	1.41
2	26-A	201	FOL	C4A-C8A	3.16	1.46	1.41
2	125-A	201	FOL	C4-C4A	3.16	1.47	1.41
4	122-A	204	NAP	C2A-N3A	3.16	1.37	1.32
4	22-A	204	NAP	C7N-N7N	3.16	1.39	1.33
2	144-A	201	FOL	C4-C4A	3.16	1.47	1.41
2	47-A	201	FOL	C4-C4A	3.16	1.47	1.41
4	58-A	204	NAP	C7N-N7N	3.16	1.39	1.33
4	62-A	204	NAP	C8A-N7A	3.17	1.40	1.34
2	39-A	201	FOL	C4-C4A	3.17	1.47	1.41
4	10-A	204	NAP	C7N-N7N	3.17	1.39	1.33
4	151-A	204	NAP	C7N-N7N	3.17	1.39	1.33
4	161-A	204	NAP	C2A-N3A	3.18	1.37	1.32
2	130-A	201	FOL	C4-C4A	3.18	1.47	1.41
4	27-A	204	NAP	C7N-N7N	3.18	1.39	1.33
4	78-A	204	NAP	C2A-N3A	3.18	1.37	1.32
2	141-A	201	FOL	C4-C4A	3.18	1.47	1.41
2	109-A	201	FOL	C4-C4A	3.18	1.47	1.41
4	19-A	204	NAP	C7N-N7N	3.18	1.39	1.33
4	133-A	204	NAP	C7N-N7N	3.18	1.39	1.33
2	13-A	201	FOL	C4-C4A	3.18	1.47	1.41
4	33-A	204	NAP	C2A-N3A	3.19	1.37	1.32
2	166-A	201	FOL	C4A-C8A	3.19	1.46	1.41
4	144-A	204	NAP	C2A-N3A	3.19	1.37	1.32
4	167-A	204	NAP	C2A-N3A	3.19	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	63-A	204	NAP	C2A-N3A	3.19	1.37	1.32
4	56-A	204	NAP	C2A-N3A	3.19	1.37	1.32
4	26-A	204	NAP	C7N-N7N	3.19	1.39	1.33
4	12-A	204	NAP	C7N-N7N	3.19	1.39	1.33
4	66-A	204	NAP	C7N-N7N	3.19	1.39	1.33
4	71-A	204	NAP	C2A-N3A	3.20	1.37	1.32
4	160-A	204	NAP	C2A-N3A	3.20	1.37	1.32
4	98-A	204	NAP	C2A-N3A	3.20	1.37	1.32
2	17-A	201	FOL	C4A-C8A	3.21	1.46	1.41
2	99-A	201	FOL	C4-C4A	3.21	1.47	1.41
2	149-A	201	FOL	C4-C4A	3.21	1.47	1.41
2	115-A	201	FOL	C4-C4A	3.21	1.47	1.41
2	83-A	201	FOL	C4A-C8A	3.21	1.46	1.41
4	27-A	204	NAP	C2A-N3A	3.21	1.37	1.32
4	126-A	204	NAP	C2A-N3A	3.21	1.37	1.32
4	79-A	204	NAP	C2A-N3A	3.21	1.37	1.32
4	25-A	204	NAP	C2A-N3A	3.21	1.37	1.32
2	28-A	201	FOL	C4A-C8A	3.21	1.46	1.41
4	49-A	204	NAP	C2A-N3A	3.22	1.37	1.32
4	36-A	204	NAP	C7N-N7N	3.22	1.39	1.33
2	62-A	201	FOL	C4A-C8A	3.22	1.46	1.41
4	146-A	204	NAP	C2A-N3A	3.22	1.37	1.32
4	71-A	204	NAP	C7N-N7N	3.22	1.39	1.33
2	118-A	201	FOL	C4-C4A	3.22	1.47	1.41
4	4-A	204	NAP	C2A-N3A	3.22	1.37	1.32
4	139-A	204	NAP	C7N-N7N	3.22	1.39	1.33
4	154-A	204	NAP	C7N-N7N	3.22	1.39	1.33
4	107-A	204	NAP	C2A-N3A	3.22	1.37	1.32
4	109-A	204	NAP	C2A-N3A	3.22	1.37	1.32
4	112-A	204	NAP	C2A-N3A	3.23	1.37	1.32
2	21-A	201	FOL	C4A-C8A	3.23	1.46	1.41
2	21-A	201	FOL	C4-C4A	3.23	1.47	1.41
2	68-A	201	FOL	C4A-C8A	3.23	1.46	1.41
4	111-A	204	NAP	C7N-N7N	3.24	1.39	1.33
4	156-A	204	NAP	C2A-N3A	3.24	1.37	1.32
2	5-A	201	FOL	C4-C4A	3.24	1.47	1.41
2	167-A	201	FOL	C4-C4A	3.24	1.47	1.41
2	46-A	201	FOL	C4-C4A	3.24	1.47	1.41
4	7-A	204	NAP	C7N-N7N	3.24	1.39	1.33
2	80-A	201	FOL	C4-C4A	3.25	1.47	1.41
4	39-A	204	NAP	C2A-N3A	3.25	1.37	1.32
4	114-A	204	NAP	C2A-N3A	3.25	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	92-A	201	FOL	C4-C4A	3.25	1.47	1.41
2	101-A	201	FOL	C4-C4A	3.25	1.47	1.41
4	162-A	204	NAP	C7N-N7N	3.25	1.39	1.33
4	89-A	204	NAP	C2A-N3A	3.25	1.37	1.32
2	151-A	201	FOL	C4-C4A	3.25	1.47	1.41
4	97-A	204	NAP	C7N-N7N	3.26	1.39	1.33
4	129-A	204	NAP	C2A-N3A	3.26	1.37	1.32
4	52-A	204	NAP	C2A-N3A	3.26	1.37	1.32
2	9-A	201	FOL	C4-C4A	3.26	1.47	1.41
4	153-A	204	NAP	C7N-N7N	3.26	1.39	1.33
4	35-A	204	NAP	C7N-N7N	3.26	1.39	1.33
4	134-A	204	NAP	C2A-N3A	3.26	1.37	1.32
2	60-A	201	FOL	C4-C4A	3.26	1.47	1.41
4	31-A	204	NAP	C2A-N3A	3.26	1.37	1.32
4	99-A	204	NAP	C2A-N3A	3.26	1.37	1.32
2	136-A	201	FOL	C4-C4A	3.26	1.47	1.41
4	159-A	204	NAP	C2A-N3A	3.27	1.37	1.32
4	23-A	204	NAP	C2A-N3A	3.27	1.37	1.32
2	164-A	201	FOL	C4-C4A	3.27	1.47	1.41
4	69-A	204	NAP	C2A-N3A	3.27	1.37	1.32
2	57-A	201	FOL	C4A-C8A	3.27	1.46	1.41
4	22-A	204	NAP	C2A-N3A	3.27	1.37	1.32
2	137-A	201	FOL	C4-C4A	3.27	1.47	1.41
4	17-A	204	NAP	C7N-N7N	3.27	1.39	1.33
4	68-A	204	NAP	C7N-N7N	3.27	1.39	1.33
4	136-A	204	NAP	C2A-N3A	3.28	1.37	1.32
2	150-A	201	FOL	C4-C4A	3.28	1.47	1.41
2	43-A	201	FOL	C4-C4A	3.28	1.47	1.41
2	124-A	201	FOL	C4-C4A	3.28	1.47	1.41
2	155-A	201	FOL	C4A-C8A	3.28	1.46	1.41
4	107-A	204	NAP	C7N-N7N	3.28	1.39	1.33
4	91-A	204	NAP	C7N-N7N	3.28	1.39	1.33
4	16-A	204	NAP	C2A-N3A	3.28	1.37	1.32
2	90-A	201	FOL	C4-C4A	3.28	1.47	1.41
4	106-A	204	NAP	O4D-C1D	3.29	1.45	1.41
4	24-A	204	NAP	C2A-N3A	3.29	1.37	1.32
2	12-A	201	FOL	C4-C4A	3.29	1.47	1.41
4	129-A	204	NAP	C7N-N7N	3.29	1.39	1.33
4	9-A	204	NAP	C2A-N3A	3.29	1.37	1.32
4	87-A	204	NAP	C2A-N3A	3.29	1.37	1.32
4	74-A	204	NAP	C7N-N7N	3.29	1.39	1.33
2	80-A	201	FOL	C4A-C8A	3.30	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	94-A	204	NAP	C7N-N7N	3.30	1.39	1.33
4	93-A	204	NAP	C7N-N7N	3.30	1.39	1.33
2	15-A	201	FOL	C4-C4A	3.30	1.47	1.41
4	43-A	204	NAP	O4D-C1D	3.30	1.45	1.41
4	100-A	204	NAP	C7N-N7N	3.30	1.39	1.33
4	54-A	204	NAP	C7N-N7N	3.31	1.39	1.33
4	56-A	204	NAP	C7N-N7N	3.31	1.39	1.33
2	76-A	201	FOL	C4A-C8A	3.31	1.46	1.41
4	3-A	204	NAP	C2A-N3A	3.31	1.37	1.32
4	49-A	204	NAP	C7N-N7N	3.31	1.39	1.33
4	30-A	204	NAP	C2A-N3A	3.31	1.37	1.32
2	165-A	201	FOL	C4-C4A	3.32	1.47	1.41
4	160-A	204	NAP	C7N-N7N	3.32	1.39	1.33
4	24-A	204	NAP	C7N-N7N	3.32	1.39	1.33
2	27-A	201	FOL	C4-C4A	3.32	1.47	1.41
4	37-A	204	NAP	C2A-N3A	3.32	1.37	1.32
4	77-A	204	NAP	C7N-N7N	3.32	1.39	1.33
2	148-A	201	FOL	CB-CA	3.32	1.57	1.53
4	20-A	204	NAP	C7N-N7N	3.33	1.39	1.33
4	166-A	204	NAP	C7N-N7N	3.33	1.39	1.33
2	100-A	201	FOL	C4-C4A	3.33	1.47	1.41
4	165-A	204	NAP	C7N-N7N	3.33	1.39	1.33
4	16-A	204	NAP	C7N-N7N	3.33	1.39	1.33
4	21-A	204	NAP	C7N-N7N	3.33	1.39	1.33
4	60-A	204	NAP	C2A-N3A	3.33	1.37	1.32
4	106-A	204	NAP	C7N-N7N	3.33	1.39	1.33
4	81-A	204	NAP	C7N-N7N	3.33	1.39	1.33
2	152-A	201	FOL	C4-C4A	3.34	1.47	1.41
4	28-A	204	NAP	C2A-N3A	3.34	1.37	1.32
4	28-A	204	NAP	C7N-N7N	3.34	1.39	1.33
2	111-A	201	FOL	C4-C4A	3.34	1.47	1.41
4	96-A	204	NAP	C7N-N7N	3.34	1.39	1.33
4	23-A	204	NAP	C7N-N7N	3.35	1.39	1.33
4	116-A	204	NAP	C2A-N3A	3.35	1.37	1.32
4	82-A	204	NAP	C7N-N7N	3.36	1.39	1.33
2	64-A	201	FOL	C4-C4A	3.36	1.47	1.41
4	117-A	204	NAP	C2A-N3A	3.36	1.37	1.32
4	37-A	204	NAP	C7N-N7N	3.36	1.39	1.33
4	141-A	204	NAP	C7N-N7N	3.37	1.39	1.33
2	147-A	201	FOL	C4-C4A	3.37	1.47	1.41
2	30-A	201	FOL	C4A-C8A	3.37	1.46	1.41
4	63-A	204	NAP	C7N-N7N	3.37	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	121-A	201	FOL	C4-C4A	3.37	1.47	1.41
2	126-A	201	FOL	C4-C4A	3.37	1.47	1.41
4	41-A	204	NAP	C7N-N7N	3.38	1.39	1.33
4	83-A	204	NAP	C7N-N7N	3.38	1.39	1.33
4	13-A	204	NAP	C7N-N7N	3.38	1.39	1.33
4	126-A	204	NAP	C7N-N7N	3.38	1.39	1.33
4	105-A	204	NAP	O4D-C1D	3.38	1.45	1.41
4	115-A	204	NAP	C2A-N3A	3.38	1.37	1.32
4	12-A	204	NAP	C2A-N3A	3.38	1.37	1.32
4	102-A	204	NAP	C2A-N3A	3.39	1.37	1.32
4	147-A	204	NAP	C7N-N7N	3.39	1.39	1.33
4	65-A	204	NAP	C2A-N3A	3.39	1.37	1.32
4	57-A	204	NAP	C7N-N7N	3.39	1.39	1.33
4	111-A	204	NAP	C2A-N3A	3.39	1.37	1.32
4	99-A	204	NAP	C7N-N7N	3.40	1.39	1.33
4	104-A	204	NAP	C2A-N3A	3.40	1.37	1.32
4	95-A	204	NAP	C7N-N7N	3.40	1.39	1.33
2	154-A	201	FOL	C4-C4A	3.40	1.47	1.41
4	155-A	204	NAP	C7N-N7N	3.41	1.39	1.33
2	65-A	201	FOL	C4-C4A	3.41	1.47	1.41
2	135-A	201	FOL	C4-C4A	3.41	1.47	1.41
4	134-A	204	NAP	C7N-N7N	3.41	1.39	1.33
2	53-A	201	FOL	C4A-C8A	3.41	1.47	1.41
4	141-A	204	NAP	C2A-N3A	3.41	1.37	1.32
4	41-A	204	NAP	C2A-N3A	3.41	1.37	1.32
4	20-A	204	NAP	C2A-N3A	3.41	1.37	1.32
4	88-A	204	NAP	C7N-N7N	3.42	1.39	1.33
4	92-A	204	NAP	C7N-N7N	3.42	1.39	1.33
4	103-A	204	NAP	C2A-N3A	3.42	1.37	1.32
4	51-A	204	NAP	C7N-N7N	3.42	1.39	1.33
2	129-A	201	FOL	C4-C4A	3.43	1.47	1.41
4	13-A	204	NAP	C2A-N3A	3.43	1.37	1.32
2	98-A	201	FOL	C4-C4A	3.43	1.47	1.41
4	14-A	204	NAP	C7N-N7N	3.43	1.39	1.33
4	123-A	204	NAP	C7N-N7N	3.43	1.39	1.33
4	6-A	204	NAP	C2A-N3A	3.43	1.37	1.32
4	128-A	204	NAP	C7N-N7N	3.43	1.39	1.33
4	94-A	204	NAP	C2A-N3A	3.44	1.37	1.32
2	56-A	201	FOL	C4-C4A	3.44	1.47	1.41
2	122-A	201	FOL	C4-C4A	3.44	1.47	1.41
2	59-A	201	FOL	C4-C4A	3.45	1.47	1.41
4	79-A	204	NAP	C7N-N7N	3.45	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	115-A	204	NAP	C7N-N7N	3.45	1.39	1.33
2	94-A	201	FOL	C4-C4A	3.45	1.47	1.41
4	127-A	204	NAP	C7N-N7N	3.45	1.39	1.33
2	42-A	201	FOL	C4-C4A	3.46	1.47	1.41
4	143-A	204	NAP	C2A-N3A	3.46	1.37	1.32
4	65-A	204	NAP	C7N-N7N	3.46	1.39	1.33
2	76-A	201	FOL	C4-C4A	3.46	1.47	1.41
4	105-A	204	NAP	C2A-N3A	3.46	1.37	1.32
4	46-A	204	NAP	C2A-N3A	3.47	1.38	1.32
2	6-A	201	FOL	C4-C4A	3.47	1.48	1.41
4	112-A	204	NAP	C7N-N7N	3.47	1.39	1.33
4	124-A	204	NAP	C7N-N7N	3.48	1.39	1.33
4	58-A	204	NAP	C2A-N3A	3.48	1.38	1.32
4	84-A	204	NAP	C7N-N7N	3.48	1.39	1.33
4	100-A	204	NAP	C2A-N3A	3.48	1.38	1.32
4	76-A	204	NAP	C2A-N3A	3.48	1.38	1.32
4	117-A	204	NAP	C7N-N7N	3.49	1.39	1.33
4	118-A	204	NAP	C7N-N7N	3.49	1.39	1.33
2	114-A	201	FOL	C4-C4A	3.49	1.48	1.41
4	75-A	204	NAP	C7N-N7N	3.50	1.39	1.33
2	119-A	201	FOL	C4-C4A	3.50	1.48	1.41
4	86-A	204	NAP	C7N-N7N	3.50	1.39	1.33
4	51-A	204	NAP	C2A-N3A	3.50	1.38	1.32
4	145-A	204	NAP	C7N-N7N	3.50	1.39	1.33
4	148-A	204	NAP	C7N-N7N	3.51	1.39	1.33
4	73-A	204	NAP	C7N-N7N	3.51	1.39	1.33
4	84-A	204	NAP	C2A-N3A	3.52	1.38	1.32
4	161-A	204	NAP	C7N-N7N	3.52	1.39	1.33
2	89-A	201	FOL	C4-C4A	3.52	1.48	1.41
4	53-A	204	NAP	C7N-N7N	3.52	1.39	1.33
4	103-A	204	NAP	C7N-N7N	3.52	1.39	1.33
4	108-A	204	NAP	C2A-N3A	3.52	1.38	1.32
4	1-A	204	NAP	C7N-N7N	3.52	1.39	1.33
2	28-A	201	FOL	C4-C4A	3.52	1.48	1.41
4	114-A	204	NAP	C7N-N7N	3.52	1.39	1.33
4	68-A	204	NAP	C2A-N3A	3.53	1.38	1.32
2	53-A	201	FOL	C4-C4A	3.53	1.48	1.41
4	80-A	204	NAP	C7N-N7N	3.53	1.39	1.33
4	1-A	204	NAP	C2A-N3A	3.54	1.38	1.32
4	122-A	204	NAP	C7N-N7N	3.54	1.39	1.33
4	167-A	204	NAP	C7N-N7N	3.54	1.39	1.33
4	121-A	204	NAP	C7N-N7N	3.54	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	67-A	204	NAP	C7N-N7N	3.54	1.39	1.33
2	65-A	201	FOL	C4A-C8A	3.55	1.47	1.41
4	72-A	204	NAP	C7N-N7N	3.55	1.39	1.33
4	2-A	204	NAP	C7N-N7N	3.55	1.39	1.33
2	166-A	201	FOL	C4-C4A	3.55	1.48	1.41
4	50-A	204	NAP	C2A-N3A	3.55	1.38	1.32
4	144-A	204	NAP	C7N-N7N	3.56	1.39	1.33
4	76-A	204	NAP	C7N-N7N	3.56	1.39	1.33
4	64-A	204	NAP	C7N-N7N	3.57	1.40	1.33
2	127-A	201	FOL	C4-C4A	3.57	1.48	1.41
4	50-A	204	NAP	C7N-N7N	3.58	1.40	1.33
4	120-A	204	NAP	C7N-N7N	3.58	1.40	1.33
4	45-A	204	NAP	C7N-N7N	3.58	1.40	1.33
4	118-A	204	NAP	C2A-N3A	3.58	1.38	1.32
4	4-A	204	NAP	C7N-N7N	3.59	1.40	1.33
4	156-A	204	NAP	C7N-N7N	3.59	1.40	1.33
4	104-A	204	NAP	C7N-N7N	3.60	1.40	1.33
4	38-A	204	NAP	C7N-N7N	3.60	1.40	1.33
4	140-A	204	NAP	C7N-N7N	3.60	1.40	1.33
4	48-A	204	NAP	C7N-N7N	3.60	1.40	1.33
2	105-A	201	FOL	C4A-C8A	3.60	1.47	1.41
4	97-A	204	NAP	C2A-N3A	3.60	1.38	1.32
4	69-A	204	NAP	C7N-N7N	3.61	1.40	1.33
4	19-A	204	NAP	C2A-N3A	3.61	1.38	1.32
4	44-A	204	NAP	C2A-N3A	3.61	1.38	1.32
4	98-A	204	NAP	C7N-N7N	3.61	1.40	1.33
4	143-A	204	NAP	C7N-N7N	3.61	1.40	1.33
4	80-A	204	NAP	C2A-N3A	3.61	1.38	1.32
4	66-A	204	NAP	C2A-N3A	3.63	1.38	1.32
4	47-A	204	NAP	C7N-N7N	3.63	1.40	1.33
2	40-A	201	FOL	C4-C4A	3.63	1.48	1.41
4	142-A	204	NAP	C7N-N7N	3.64	1.40	1.33
4	119-A	204	NAP	C7N-N7N	3.65	1.40	1.33
4	110-A	204	NAP	C2A-N3A	3.65	1.38	1.32
4	7-A	204	NAP	C2A-N3A	3.65	1.38	1.32
4	44-A	204	NAP	C7N-N7N	3.65	1.40	1.33
2	120-A	201	FOL	C4-C4A	3.65	1.48	1.41
4	149-A	204	NAP	C7N-N7N	3.66	1.40	1.33
4	152-A	204	NAP	C7N-N7N	3.66	1.40	1.33
4	30-A	204	NAP	C7N-N7N	3.68	1.40	1.33
4	47-A	204	NAP	C2A-N3A	3.68	1.38	1.32
4	85-A	204	NAP	C7N-N7N	3.68	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	81-A	201	FOL	CB-CA	3.68	1.58	1.53
4	29-A	204	NAP	C7N-N7N	3.68	1.40	1.33
4	48-A	204	NAP	C2A-N3A	3.69	1.38	1.32
4	116-A	204	NAP	C7N-N7N	3.69	1.40	1.33
4	62-A	204	NAP	C7N-N7N	3.71	1.40	1.33
4	39-A	204	NAP	C7N-N7N	3.71	1.40	1.33
4	55-A	204	NAP	C7N-N7N	3.72	1.40	1.33
4	106-A	204	NAP	C2A-N3A	3.72	1.38	1.32
2	82-A	201	FOL	CB-CA	3.73	1.58	1.53
4	87-A	204	NAP	C7N-N7N	3.73	1.40	1.33
4	31-A	204	NAP	P2B-O2B	3.73	1.66	1.59
4	125-A	204	NAP	C7N-N7N	3.74	1.40	1.33
4	46-A	204	NAP	C7N-N7N	3.74	1.40	1.33
4	130-A	204	NAP	C7N-N7N	3.74	1.40	1.33
4	113-A	204	NAP	C7N-N7N	3.74	1.40	1.33
4	42-A	204	NAP	C7N-N7N	3.75	1.40	1.33
4	70-A	204	NAP	C7N-N7N	3.76	1.40	1.33
4	90-A	204	NAP	C7N-N7N	3.79	1.40	1.33
4	52-A	204	NAP	C7N-N7N	3.79	1.40	1.33
4	61-A	204	NAP	C7N-N7N	3.79	1.40	1.33
4	5-A	204	NAP	C7N-N7N	3.81	1.40	1.33
4	60-A	204	NAP	C7N-N7N	3.83	1.40	1.33
2	13-A	201	FOL	CB-CA	3.84	1.58	1.53
2	48-A	201	FOL	C4-C4A	3.85	1.48	1.41
2	26-A	201	FOL	C4-C4A	3.88	1.48	1.41
2	30-A	201	FOL	C4-C4A	3.91	1.48	1.41
4	40-A	204	NAP	C7N-N7N	3.93	1.40	1.33
4	43-A	204	NAP	C7N-N7N	3.93	1.40	1.33
4	138-A	204	NAP	C7N-N7N	3.95	1.40	1.33
4	3-A	204	NAP	C7N-N7N	3.96	1.40	1.33
4	102-A	204	NAP	C7N-N7N	4.01	1.40	1.33
4	135-A	204	NAP	C7N-N7N	4.02	1.40	1.33
4	137-A	204	NAP	C7N-N7N	4.11	1.41	1.33
4	136-A	204	NAP	C7N-N7N	4.14	1.41	1.33

All (2571) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	126-A	201	FOL	CA-N-C	-9.89	108.59	122.15
2	6-A	201	FOL	CB-CA-CT	-8.16	100.42	112.28
2	156-A	201	FOL	CB-CA-N	-8.05	97.99	110.22
2	92-A	201	FOL	CB-CA-CT	-7.88	100.83	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	43-A	201	FOL	CB-CA-CT	-7.52	101.36	112.28
2	77-A	201	FOL	CB-CA-N	-7.17	99.32	110.22
2	106-A	201	FOL	CG-CB-CA	-7.13	98.96	113.19
2	109-A	201	FOL	CB-CA-CT	-6.96	102.17	112.28
2	133-A	201	FOL	C4A-C4-N3	-6.94	113.61	123.48
4	118-A	204	NAP	O2N-PN-O5D	-6.67	76.64	108.14
2	113-A	201	FOL	CB-CA-CT	-6.66	102.60	112.28
2	76-A	201	FOL	C4A-C4-N3	-6.61	114.07	123.48
2	8-A	201	FOL	C4A-C4-N3	-6.46	114.29	123.48
2	56-A	201	FOL	C4A-C4-N3	-6.38	114.40	123.48
2	31-A	201	FOL	CB-CA-CT	-6.35	103.06	112.28
2	53-A	201	FOL	C4A-C4-N3	-6.33	114.47	123.48
2	13-A	201	FOL	C4A-C4-N3	-6.25	114.59	123.48
2	98-A	201	FOL	C4A-C4-N3	-6.18	114.68	123.48
2	48-A	201	FOL	CG-CB-CA	-6.14	100.92	113.19
4	56-A	204	NAP	O2N-PN-O5D	-6.06	79.54	108.14
2	154-A	201	FOL	C4A-C4-N3	-6.04	114.88	123.48
2	38-A	201	FOL	C4A-C8A-N8	-6.02	115.58	123.07
2	160-A	201	FOL	C4A-C4-N3	-6.01	114.93	123.48
2	111-A	201	FOL	C4A-C4-N3	-5.98	114.97	123.48
2	136-A	201	FOL	C4A-C4-N3	-5.93	115.04	123.48
2	152-A	201	FOL	CB-CA-CT	-5.88	103.75	112.28
2	167-A	201	FOL	C4A-C4-N3	-5.87	115.12	123.48
4	77-A	204	NAP	C4A-C5A-N7A	-5.87	103.74	109.41
4	57-A	204	NAP	O2N-PN-O5D	-5.86	80.48	108.14
2	51-A	201	FOL	C4A-C4-N3	-5.85	115.16	123.48
2	149-A	201	FOL	CG-CB-CA	-5.84	101.52	113.19
2	134-A	201	FOL	C4A-C4-N3	-5.83	115.18	123.48
2	164-A	201	FOL	C4A-C4-N3	-5.81	115.21	123.48
2	151-A	201	FOL	C4A-C4-N3	-5.81	115.22	123.48
2	18-A	201	FOL	CB-CA-CT	-5.80	103.86	112.28
2	107-A	201	FOL	C4A-C4-N3	-5.79	115.24	123.48
2	126-A	201	FOL	C4A-C4-N3	-5.77	115.27	123.48
2	100-A	201	FOL	CB-CA-N	-5.74	101.51	110.22
4	101-A	204	NAP	C4A-C5A-N7A	-5.70	103.91	109.41
2	6-A	201	FOL	C4A-C4-N3	-5.66	115.42	123.48
2	27-A	201	FOL	C4A-C4-N3	-5.66	115.43	123.48
2	110-A	201	FOL	C4A-C4-N3	-5.63	115.46	123.48
2	125-A	201	FOL	C4A-C4-N3	-5.62	115.48	123.48
2	58-A	201	FOL	C4A-C8A-N8	-5.60	116.10	123.07
2	28-A	201	FOL	C4A-C4-N3	-5.57	115.55	123.48
2	105-A	201	FOL	C4A-C4-N3	-5.56	115.56	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	113-A	201	FOL	C4A-C4-N3	-5.55	115.58	123.48
4	35-A	204	NAP	C4A-C5A-N7A	-5.55	104.05	109.41
2	77-A	201	FOL	C4A-C4-N3	-5.54	115.60	123.48
2	15-A	201	FOL	C4A-C4-N3	-5.53	115.61	123.48
2	44-A	201	FOL	C4A-C4-N3	-5.52	115.63	123.48
2	108-A	201	FOL	CB-CA-CT	-5.50	104.29	112.28
2	19-A	201	FOL	C4A-C4-N3	-5.49	115.67	123.48
2	118-A	201	FOL	C4A-C4-N3	-5.48	115.68	123.48
2	36-A	201	FOL	C4A-C4-N3	-5.48	115.69	123.48
2	104-A	201	FOL	C4A-C8A-N8	-5.47	116.26	123.07
2	89-A	201	FOL	CB-CA-CT	-5.47	104.34	112.28
2	7-A	201	FOL	C4A-C4-N3	-5.46	115.71	123.48
2	83-A	201	FOL	C4A-C4-N3	-5.45	115.72	123.48
4	45-A	204	NAP	C4A-C5A-N7A	-5.42	104.17	109.41
2	143-A	201	FOL	C4A-C4-N3	-5.42	115.76	123.48
2	121-A	201	FOL	C4A-C4-N3	-5.42	115.77	123.48
2	119-A	201	FOL	C4A-C4-N3	-5.41	115.78	123.48
2	66-A	201	FOL	C4A-C4-N3	-5.40	115.80	123.48
4	74-A	204	NAP	C4A-C5A-N7A	-5.38	104.21	109.41
4	158-A	204	NAP	C4A-C5A-N7A	-5.38	104.21	109.41
2	4-A	201	FOL	C4A-C4-N3	-5.37	115.83	123.48
2	115-A	201	FOL	C4A-C4-N3	-5.37	115.83	123.48
2	41-A	201	FOL	C4A-C8A-N8	-5.37	116.39	123.07
4	89-A	204	NAP	C4A-C5A-N7A	-5.34	104.25	109.41
2	123-A	201	FOL	C4A-C4-N3	-5.33	115.89	123.48
2	57-A	201	FOL	C4A-C4-N3	-5.32	115.90	123.48
4	88-A	204	NAP	C4A-C5A-N7A	-5.31	104.28	109.41
2	68-A	201	FOL	C4A-C4-N3	-5.31	115.92	123.48
2	74-A	201	FOL	C4A-C4-N3	-5.31	115.93	123.48
2	54-A	201	FOL	C4A-C4-N3	-5.29	115.95	123.48
2	155-A	201	FOL	C4A-C4-N3	-5.29	115.95	123.48
2	75-A	201	FOL	C4A-C8A-N8	-5.28	116.50	123.07
2	42-A	201	FOL	C4A-C4-N3	-5.26	115.99	123.48
2	80-A	201	FOL	NA2-C2-N3	-5.26	113.83	120.26
2	14-A	201	FOL	C4A-C4-N3	-5.26	116.00	123.48
2	67-A	201	FOL	C4A-C4-N3	-5.25	116.01	123.48
2	69-A	201	FOL	C4A-C4-N3	-5.25	116.01	123.48
2	112-A	201	FOL	C4A-C4-N3	-5.24	116.03	123.48
2	146-A	201	FOL	C4A-C4-N3	-5.24	116.03	123.48
2	152-A	201	FOL	C4A-C4-N3	-5.21	116.06	123.48
2	128-A	201	FOL	C4A-C8A-N8	-5.21	116.59	123.07
2	102-A	201	FOL	C4A-C8A-N8	-5.20	116.60	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	106-A	201	FOL	CA-N-C	-5.19	115.03	122.15
2	100-A	201	FOL	C4A-C4-N3	-5.18	116.11	123.48
2	16-A	201	FOL	CB-CA-N	-5.18	102.35	110.22
4	145-A	204	NAP	C4A-C5A-N7A	-5.18	104.41	109.41
2	49-A	201	FOL	C4A-C8A-N8	-5.18	116.62	123.07
2	163-A	201	FOL	C4A-C4-N3	-5.17	116.12	123.48
2	42-A	201	FOL	CB-CA-CT	-5.15	104.81	112.28
2	55-A	201	FOL	C4A-C4-N3	-5.15	116.16	123.48
2	148-A	201	FOL	C4A-C4-N3	-5.13	116.17	123.48
2	25-A	201	FOL	C4A-C4-N3	-5.13	116.18	123.48
4	52-A	204	NAP	C4A-C5A-N7A	-5.12	104.46	109.41
2	145-A	201	FOL	C4A-C4-N3	-5.12	116.19	123.48
2	72-A	201	FOL	C4A-C4-N3	-5.12	116.20	123.48
2	50-A	201	FOL	C4A-C4-N3	-5.12	116.20	123.48
4	148-A	204	NAP	C4A-C5A-N7A	-5.10	104.48	109.41
2	125-A	201	FOL	CA-N-C	-5.10	115.16	122.15
4	140-A	204	NAP	C4A-C5A-N7A	-5.09	104.49	109.41
4	154-A	204	NAP	C4A-C5A-N7A	-5.09	104.49	109.41
2	108-A	201	FOL	C4A-C4-N3	-5.09	116.23	123.48
2	38-A	201	FOL	C4A-C4-N3	-5.09	116.24	123.48
2	78-A	201	FOL	C4A-C8A-N8	-5.08	116.74	123.07
2	18-A	201	FOL	C4A-C4-N3	-5.08	116.25	123.48
2	49-A	201	FOL	C4A-C4-N3	-5.07	116.26	123.48
2	61-A	201	FOL	C4A-C4-N3	-5.07	116.27	123.48
4	49-A	204	NAP	C4A-C5A-N7A	-5.06	104.52	109.41
2	99-A	201	FOL	C4A-C4-N3	-5.04	116.31	123.48
2	22-A	201	FOL	C4A-C4-N3	-5.04	116.31	123.48
4	99-A	204	NAP	C4A-C5A-N7A	-5.04	104.55	109.41
2	130-A	201	FOL	C4A-C4-N3	-5.04	116.31	123.48
4	55-A	204	NAP	C4A-C5A-N7A	-5.03	104.55	109.41
2	128-A	201	FOL	C4A-C4-N3	-5.03	116.32	123.48
2	62-A	201	FOL	C4A-C4-N3	-5.02	116.33	123.48
2	29-A	201	FOL	C4A-C8A-N8	-5.02	116.82	123.07
2	161-A	201	FOL	C4A-C8A-N8	-5.02	116.82	123.07
2	103-A	201	FOL	C4A-C8A-N8	-5.01	116.83	123.07
2	132-A	201	FOL	C4A-C4-N3	-5.00	116.36	123.48
2	46-A	201	FOL	C4A-C8A-N8	-5.00	116.85	123.07
2	41-A	201	FOL	C4A-C4-N3	-5.00	116.37	123.48
2	104-A	201	FOL	C4A-C4-N3	-5.00	116.37	123.48
4	73-A	204	NAP	C4A-C5A-N7A	-5.00	104.58	109.41
2	43-A	201	FOL	NA2-C2-N3	-4.99	114.15	120.26
2	47-A	201	FOL	C4A-C4-N3	-4.99	116.38	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	63-A	201	FOL	C4A-C4-N3	-4.99	116.38	123.48
2	109-A	201	FOL	C4A-C4-N3	-4.98	116.39	123.48
2	101-A	201	FOL	CA-N-C	-4.98	115.33	122.15
2	142-A	201	FOL	C4A-C8A-N8	-4.98	116.88	123.07
2	63-A	201	FOL	C4A-C8A-N8	-4.98	116.88	123.07
2	29-A	201	FOL	C4A-C4-N3	-4.97	116.41	123.48
4	7-A	204	NAP	C4A-C5A-N7A	-4.97	104.61	109.41
2	60-A	201	FOL	C4A-C4-N3	-4.96	116.42	123.48
4	138-A	204	NAP	C4A-C5A-N7A	-4.96	104.62	109.41
2	79-A	201	FOL	C4A-C4-N3	-4.96	116.42	123.48
2	166-A	201	FOL	C4A-C4-N3	-4.96	116.42	123.48
2	23-A	201	FOL	C4A-C8A-N8	-4.96	116.90	123.07
2	150-A	201	FOL	C4A-C4-N3	-4.96	116.42	123.48
2	81-A	201	FOL	C4A-C8A-N8	-4.95	116.90	123.07
2	117-A	201	FOL	C4A-C4-N3	-4.95	116.43	123.48
4	142-A	204	NAP	C4A-C5A-N7A	-4.95	104.63	109.41
4	135-A	204	NAP	C4A-C5A-N7A	-4.94	104.63	109.41
2	75-A	201	FOL	C4A-C4-N3	-4.94	116.44	123.48
2	43-A	201	FOL	C4A-C8A-N8	-4.94	116.92	123.07
4	151-A	204	NAP	C4A-C5A-N7A	-4.94	104.64	109.41
2	135-A	201	FOL	C4A-C4-N3	-4.94	116.45	123.48
2	78-A	201	FOL	C4A-C4-N3	-4.93	116.46	123.48
2	124-A	201	FOL	C4A-C4-N3	-4.93	116.46	123.48
2	21-A	201	FOL	CB-CA-N	-4.93	102.73	110.22
2	103-A	201	FOL	C4A-C4-N3	-4.93	116.46	123.48
2	97-A	201	FOL	C4A-C4-N3	-4.92	116.47	123.48
2	48-A	201	FOL	NA2-C2-N3	-4.91	114.25	120.26
2	122-A	201	FOL	C4A-C4-N3	-4.91	116.49	123.48
2	1-A	201	FOL	C4A-C4-N3	-4.91	116.49	123.48
4	163-A	204	NAP	C4A-C5A-N7A	-4.91	104.67	109.41
2	70-A	201	FOL	C4A-C4-N3	-4.90	116.51	123.48
4	92-A	204	NAP	C4A-C5A-N7A	-4.89	104.68	109.41
2	84-A	201	FOL	C4A-C4-N3	-4.89	116.52	123.48
4	81-A	204	NAP	C4A-C5A-N7A	-4.89	104.69	109.41
2	156-A	201	FOL	C4A-C4-N3	-4.89	116.53	123.48
2	129-A	201	FOL	C4A-C4-N3	-4.88	116.53	123.48
2	10-A	201	FOL	C4A-C8A-N8	-4.88	117.00	123.07
2	156-A	201	FOL	CB-CA-CT	-4.88	105.20	112.28
4	14-A	204	NAP	C4A-C5A-N7A	-4.87	104.71	109.41
2	108-A	201	FOL	C4A-C8A-N8	-4.86	117.02	123.07
2	72-A	201	FOL	C4A-C8A-N8	-4.86	117.02	123.07
4	67-A	204	NAP	C4A-C5A-N7A	-4.86	104.71	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	71-A	201	FOL	C4A-C4-N3	-4.86	116.56	123.48
4	25-A	204	NAP	C4A-C5A-N7A	-4.86	104.72	109.41
2	120-A	201	FOL	NA2-C2-N3	-4.86	114.32	120.26
4	128-A	204	NAP	C4A-C5A-N7A	-4.85	104.73	109.41
2	39-A	201	FOL	C4A-C4-N3	-4.84	116.59	123.48
2	26-A	201	FOL	C4A-C4-N3	-4.84	116.59	123.48
2	163-A	201	FOL	C4A-C8A-N8	-4.84	117.05	123.07
2	106-A	201	FOL	C4A-C8A-N8	-4.83	117.06	123.07
2	11-A	201	FOL	C4A-C4-N3	-4.82	116.62	123.48
2	45-A	201	FOL	C4A-C4-N3	-4.81	116.63	123.48
4	123-A	204	NAP	C4A-C5A-N7A	-4.81	104.76	109.41
2	82-A	201	FOL	C4A-C4-N3	-4.80	116.64	123.48
4	108-A	204	NAP	C4A-C5A-N7A	-4.79	104.78	109.41
4	104-A	204	NAP	C4A-C5A-N7A	-4.78	104.79	109.41
2	131-A	201	FOL	C4A-C8A-N8	-4.78	117.12	123.07
4	107-A	204	NAP	C4A-C5A-N7A	-4.77	104.80	109.41
4	10-A	204	NAP	C4A-C5A-N7A	-4.77	104.80	109.41
2	41-A	201	FOL	C7-C6-N5	-4.77	117.67	120.80
2	161-A	201	FOL	C4A-C4-N3	-4.76	116.71	123.48
2	133-A	201	FOL	CG-CB-CA	-4.75	103.70	113.19
2	31-A	201	FOL	C4A-C4-N3	-4.75	116.72	123.48
2	88-A	201	FOL	C4A-C4-N3	-4.73	116.74	123.48
2	85-A	201	FOL	C4A-C4-N3	-4.72	116.76	123.48
2	25-A	201	FOL	CB-CA-CT	-4.72	105.43	112.28
4	105-A	204	NAP	C4A-C5A-N7A	-4.72	104.85	109.41
2	141-A	201	FOL	C4A-C4-N3	-4.71	116.77	123.48
2	106-A	201	FOL	C4A-C4-N3	-4.70	116.79	123.48
2	144-A	201	FOL	C4A-C4-N3	-4.70	116.79	123.48
2	32-A	201	FOL	C4A-C4-N3	-4.69	116.80	123.48
2	80-A	201	FOL	C4A-C8A-N8	-4.69	117.23	123.07
2	65-A	201	FOL	C4A-C4-N3	-4.69	116.81	123.48
2	116-A	201	FOL	C4A-C4-N3	-4.68	116.81	123.48
4	15-A	204	NAP	C4A-C5A-N7A	-4.68	104.88	109.41
4	17-A	204	NAP	C4A-C5A-N7A	-4.68	104.89	109.41
4	139-A	204	NAP	C4A-C5A-N7A	-4.68	104.89	109.41
4	127-A	204	NAP	C4A-C5A-N7A	-4.67	104.89	109.41
2	93-A	201	FOL	C4A-C8A-N8	-4.67	117.25	123.07
4	18-A	204	NAP	C4A-C5A-N7A	-4.67	104.90	109.41
2	37-A	201	FOL	C4A-C4-N3	-4.67	116.83	123.48
4	91-A	204	NAP	C4A-C5A-N7A	-4.66	104.90	109.41
2	131-A	201	FOL	NA2-C2-N3	-4.65	114.57	120.26
2	97-A	201	FOL	C4A-C8A-N8	-4.65	117.28	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	88-A	201	FOL	C4A-C8A-N8	-4.65	117.28	123.07
2	77-A	201	FOL	C4A-C8A-N8	-4.65	117.29	123.07
2	93-A	201	FOL	C4A-C4-N3	-4.64	116.88	123.48
4	2-A	204	NAP	C4A-C5A-N7A	-4.64	104.93	109.41
2	82-A	201	FOL	C4A-C8A-N8	-4.63	117.30	123.07
4	164-A	204	NAP	C4A-C5A-N7A	-4.63	104.94	109.41
2	91-A	201	FOL	C4A-C4-N3	-4.63	116.90	123.48
2	31-A	201	FOL	C4A-C8A-N8	-4.63	117.31	123.07
4	64-A	204	NAP	C4A-C5A-N7A	-4.62	104.95	109.41
2	67-A	201	FOL	C4A-C8A-N8	-4.61	117.33	123.07
2	46-A	201	FOL	C4A-C4-N3	-4.61	116.92	123.48
2	40-A	201	FOL	C4A-C4-N3	-4.61	116.92	123.48
4	95-A	204	NAP	C4A-C5A-N7A	-4.61	104.96	109.41
2	94-A	201	FOL	C4A-C4-N3	-4.61	116.93	123.48
2	59-A	201	FOL	C4A-C8A-N8	-4.59	117.36	123.07
2	58-A	201	FOL	C4A-C4-N3	-4.58	116.96	123.48
2	59-A	201	FOL	C4A-C4-N3	-4.58	116.97	123.48
2	84-A	201	FOL	C4A-C8A-N8	-4.57	117.38	123.07
4	106-A	204	NAP	C4A-C5A-N7A	-4.56	105.00	109.41
2	35-A	201	FOL	C4A-C8A-N8	-4.56	117.39	123.07
2	21-A	201	FOL	C4A-C4-N3	-4.56	116.99	123.48
2	64-A	201	FOL	C4A-C4-N3	-4.55	117.01	123.48
2	12-A	201	FOL	C4A-C4-N3	-4.55	117.01	123.48
2	52-A	201	FOL	CB-CA-N	-4.55	103.31	110.22
4	5-A	204	NAP	C4A-C5A-N7A	-4.54	105.02	109.41
2	138-A	201	FOL	C4A-C8A-N8	-4.54	117.42	123.07
2	159-A	201	FOL	C4A-C8A-N8	-4.54	117.42	123.07
2	89-A	201	FOL	C4A-C4-N3	-4.54	117.03	123.48
2	114-A	201	FOL	C4A-C4-N3	-4.53	117.03	123.48
4	119-A	204	NAP	C4A-C5A-N7A	-4.53	105.03	109.41
2	142-A	201	FOL	C4A-C4-N3	-4.53	117.03	123.48
2	165-A	201	FOL	C4A-C4-N3	-4.53	117.04	123.48
2	35-A	201	FOL	C4A-C4-N3	-4.53	117.04	123.48
2	137-A	201	FOL	C4A-C4-N3	-4.52	117.05	123.48
4	4-A	204	NAP	C4A-C5A-N7A	-4.51	105.05	109.41
2	81-A	201	FOL	C4A-C4-N3	-4.51	117.06	123.48
2	22-A	201	FOL	C4A-C8A-N8	-4.51	117.46	123.07
2	43-A	201	FOL	C4A-C4-N3	-4.51	117.07	123.48
2	3-A	201	FOL	C4A-C4-N3	-4.50	117.07	123.48
2	1-A	201	FOL	C4A-C8A-N8	-4.50	117.47	123.07
2	138-A	201	FOL	C4A-C4-N3	-4.50	117.08	123.48
4	144-A	204	NAP	C4A-C5A-N7A	-4.50	105.06	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	145-A	201	FOL	C4A-C8A-N8	-4.49	117.48	123.07
2	91-A	201	FOL	C4A-C8A-N8	-4.49	117.48	123.07
2	14-A	201	FOL	C4A-C8A-N8	-4.49	117.48	123.07
4	162-A	204	NAP	C4A-C5A-N7A	-4.49	105.08	109.41
2	87-A	201	FOL	C4A-C4-N3	-4.48	117.11	123.48
2	102-A	201	FOL	C4A-C4-N3	-4.47	117.11	123.48
4	79-A	204	NAP	C4A-C5A-N7A	-4.47	105.09	109.41
2	61-A	201	FOL	C4A-C8A-N8	-4.46	117.52	123.07
4	62-A	204	NAP	C4A-C5A-N7A	-4.46	105.10	109.41
2	79-A	201	FOL	C4A-C8A-N8	-4.46	117.52	123.07
2	34-A	201	FOL	C4A-C8A-N8	-4.46	117.52	123.07
2	149-A	201	FOL	C4A-C4-N3	-4.45	117.14	123.48
4	42-A	204	NAP	C4A-C5A-N7A	-4.45	105.11	109.41
4	47-A	204	NAP	C4A-C5A-N7A	-4.45	105.11	109.41
2	23-A	201	FOL	CB-CA-CT	-4.45	105.82	112.28
2	20-A	201	FOL	C4A-C4-N3	-4.44	117.16	123.48
2	11-A	201	FOL	C4A-C8A-N8	-4.44	117.55	123.07
4	147-A	204	NAP	C4A-C5A-N7A	-4.44	105.12	109.41
2	148-A	201	FOL	C4A-C8A-N8	-4.43	117.55	123.07
4	8-A	204	NAP	C4A-C5A-N7A	-4.43	105.13	109.41
4	109-A	204	NAP	C4A-C5A-N7A	-4.43	105.13	109.41
2	17-A	201	FOL	C4A-C4-N3	-4.43	117.18	123.48
2	112-A	201	FOL	C4A-C8A-N8	-4.43	117.56	123.07
2	86-A	201	FOL	C4A-C4-N3	-4.42	117.18	123.48
2	37-A	201	FOL	C4A-C8A-N8	-4.41	117.58	123.07
2	140-A	201	FOL	C4A-C8A-N8	-4.41	117.58	123.07
2	25-A	201	FOL	C4A-C8A-N8	-4.41	117.58	123.07
4	93-A	204	NAP	C4A-C5A-N7A	-4.41	105.15	109.41
4	98-A	204	NAP	C4A-C5A-N7A	-4.40	105.16	109.41
4	32-A	204	NAP	C4A-C5A-N7A	-4.40	105.16	109.41
2	39-A	201	FOL	C4A-C8A-N8	-4.40	117.60	123.07
4	116-A	204	NAP	C4A-C5A-N7A	-4.40	105.16	109.41
2	159-A	201	FOL	C4A-C4-N3	-4.39	117.23	123.48
4	53-A	204	NAP	C4A-C5A-N7A	-4.39	105.17	109.41
2	44-A	201	FOL	C4A-C8A-N8	-4.39	117.61	123.07
2	52-A	201	FOL	C4A-C8A-N8	-4.39	117.61	123.07
2	95-A	201	FOL	C4A-C8A-N8	-4.39	117.61	123.07
4	59-A	204	NAP	C4A-C5A-N7A	-4.39	105.17	109.41
2	13-A	201	FOL	C4A-C8A-N8	-4.38	117.61	123.07
2	144-A	201	FOL	CB-CA-CT	-4.38	105.92	112.28
4	155-A	204	NAP	C4A-C5A-N7A	-4.38	105.18	109.41
4	103-A	204	NAP	C4A-C5A-N7A	-4.38	105.18	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	143-A	204	NAP	C4A-C5A-N7A	-4.38	105.18	109.41
2	80-A	201	FOL	C4A-C4-N3	-4.37	117.26	123.48
2	146-A	201	FOL	CB-CA-CT	-4.37	105.93	112.28
4	108-A	204	NAP	O3D-C3D-C2D	-4.37	97.82	111.83
2	87-A	201	FOL	CB-CA-CT	-4.37	105.93	112.28
4	51-A	204	NAP	C4A-C5A-N7A	-4.37	105.19	109.41
4	46-A	204	NAP	C4A-C5A-N7A	-4.37	105.19	109.41
2	101-A	201	FOL	C4A-C4-N3	-4.36	117.27	123.48
2	60-A	201	FOL	C4A-C8A-N8	-4.36	117.65	123.07
4	43-A	204	NAP	C4A-C5A-N7A	-4.35	105.21	109.41
2	16-A	201	FOL	C4A-C8A-N8	-4.35	117.66	123.07
2	144-A	201	FOL	C4A-C8A-N8	-4.34	117.66	123.07
2	34-A	201	FOL	C4A-C4-N3	-4.34	117.31	123.48
4	22-A	204	NAP	C4A-C5A-N7A	-4.33	105.22	109.41
2	5-A	201	FOL	C4A-C4-N3	-4.33	117.31	123.48
2	48-A	201	FOL	C4A-C4-N3	-4.33	117.31	123.48
2	127-A	201	FOL	C4A-C8A-N8	-4.33	117.68	123.07
2	2-A	201	FOL	C4A-C4-N3	-4.33	117.32	123.48
2	116-A	201	FOL	C4A-C8A-N8	-4.33	117.68	123.07
2	40-A	201	FOL	NA2-C2-N3	-4.32	114.97	120.26
4	130-A	204	NAP	C4A-C5A-N7A	-4.32	105.23	109.41
2	147-A	201	FOL	C4A-C4-N3	-4.31	117.34	123.48
2	45-A	201	FOL	C4A-C8A-N8	-4.31	117.71	123.07
2	132-A	201	FOL	C4A-C8A-N8	-4.30	117.72	123.07
4	137-A	204	NAP	C4A-C5A-N7A	-4.30	105.26	109.41
4	75-A	204	NAP	C4A-C5A-N7A	-4.30	105.26	109.41
4	86-A	204	NAP	C4A-C5A-N7A	-4.29	105.26	109.41
4	40-A	204	NAP	C4A-C5A-N7A	-4.29	105.26	109.41
4	120-A	204	NAP	C4A-C5A-N7A	-4.29	105.26	109.41
4	115-A	204	NAP	C4A-C5A-N7A	-4.29	105.27	109.41
4	29-A	204	NAP	C4A-C5A-N7A	-4.29	105.27	109.41
4	11-A	204	NAP	C4A-C5A-N7A	-4.28	105.27	109.41
4	61-A	204	NAP	C4A-C5A-N7A	-4.28	105.27	109.41
4	157-A	204	NAP	C4A-C5A-N7A	-4.28	105.28	109.41
4	90-A	204	NAP	C4A-C5A-N7A	-4.28	105.28	109.41
4	96-A	204	NAP	C4A-C5A-N7A	-4.28	105.28	109.41
2	90-A	201	FOL	C4A-C4-N3	-4.27	117.40	123.48
4	83-A	204	NAP	C4A-C5A-N7A	-4.27	105.28	109.41
2	158-A	201	FOL	C4A-C4-N3	-4.26	117.41	123.48
4	30-A	204	NAP	C4A-C5A-N7A	-4.25	105.31	109.41
2	9-A	201	FOL	C4A-C4-N3	-4.24	117.44	123.48
2	10-A	201	FOL	C4A-C4-N3	-4.24	117.44	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	153-A	201	FOL	C4A-C8A-N8	-4.24	117.79	123.07
4	54-A	204	NAP	C4A-C5A-N7A	-4.24	105.31	109.41
2	149-A	201	FOL	C4A-C8A-N8	-4.24	117.80	123.07
2	36-A	201	FOL	C4A-C8A-N8	-4.23	117.81	123.07
4	125-A	204	NAP	C4A-C5A-N7A	-4.23	105.33	109.41
2	4-A	201	FOL	C4A-C8A-N8	-4.23	117.81	123.07
2	5-A	201	FOL	C4A-C8A-N8	-4.22	117.81	123.07
2	109-A	201	FOL	C4A-C8A-N8	-4.22	117.82	123.07
2	92-A	201	FOL	C4A-C4-N3	-4.21	117.48	123.48
4	19-A	204	NAP	C4A-C5A-N7A	-4.21	105.34	109.41
2	133-A	201	FOL	C4A-C8A-N8	-4.20	117.84	123.07
4	3-A	204	NAP	C4A-C5A-N7A	-4.20	105.35	109.41
2	165-A	201	FOL	NA2-C2-N3	-4.20	115.12	120.26
2	16-A	201	FOL	NA2-C2-N3	-4.20	115.12	120.26
4	38-A	204	NAP	C4A-C5A-N7A	-4.20	105.35	109.41
2	162-A	201	FOL	C4A-C4-N3	-4.20	117.51	123.48
2	99-A	201	FOL	C4A-C8A-N8	-4.19	117.85	123.07
2	33-A	201	FOL	C4A-C8A-N8	-4.19	117.85	123.07
4	121-A	204	NAP	C4A-C5A-N7A	-4.19	105.36	109.41
4	102-A	204	NAP	C4A-C5A-N7A	-4.19	105.36	109.41
4	146-A	204	NAP	C4A-C5A-N7A	-4.19	105.36	109.41
4	133-A	204	NAP	C4A-C5A-N7A	-4.19	105.37	109.41
2	70-A	201	FOL	CB-CA-CT	-4.18	106.21	112.28
4	82-A	204	NAP	C4A-C5A-N7A	-4.18	105.37	109.41
2	69-A	201	FOL	C4A-C8A-N8	-4.18	117.87	123.07
4	72-A	204	NAP	C4A-C5A-N7A	-4.18	105.37	109.41
2	53-A	201	FOL	CB-CA-N	-4.18	103.88	110.22
2	149-A	201	FOL	NA2-C2-N3	-4.17	115.16	120.26
4	78-A	204	NAP	C4A-C5A-N7A	-4.17	105.38	109.41
2	120-A	201	FOL	C4A-C4-N3	-4.16	117.55	123.48
4	100-A	204	NAP	C4A-C5A-N7A	-4.16	105.39	109.41
2	54-A	201	FOL	C4A-C8A-N8	-4.15	117.90	123.07
2	59-A	201	FOL	CA-N-C	-4.15	116.47	122.15
4	165-A	204	NAP	C4A-C5A-N7A	-4.14	105.41	109.41
2	147-A	201	FOL	NA2-C2-N3	-4.14	115.19	120.26
2	45-A	201	FOL	CG-CB-CA	-4.13	104.95	113.19
2	83-A	201	FOL	C4A-C8A-N8	-4.12	117.94	123.07
2	156-A	201	FOL	C4A-C8A-N8	-4.12	117.94	123.07
2	125-A	201	FOL	C4A-C8A-N8	-4.11	117.95	123.07
4	112-A	204	NAP	C4A-C5A-N7A	-4.11	105.44	109.41
2	87-A	201	FOL	C4A-C8A-N8	-4.10	117.96	123.07
2	70-A	201	FOL	C4A-C8A-N8	-4.10	117.97	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	139-A	201	FOL	C4A-C8A-N8	-4.10	117.97	123.07
2	126-A	201	FOL	O-C-C11	-4.10	113.67	120.94
2	105-A	201	FOL	C4A-C8A-N8	-4.10	117.97	123.07
2	92-A	201	FOL	C4A-C8A-N8	-4.10	117.97	123.07
2	146-A	201	FOL	C4A-C8A-N8	-4.10	117.97	123.07
4	132-A	204	NAP	C4A-C5A-N7A	-4.09	105.45	109.41
2	82-A	201	FOL	CA-N-C	-4.09	116.54	122.15
2	157-A	201	FOL	C4A-C8A-N8	-4.09	117.98	123.07
2	157-A	201	FOL	C4A-C4-N3	-4.09	117.66	123.48
2	55-A	201	FOL	C4A-C8A-N8	-4.08	117.99	123.07
4	150-A	204	NAP	C4A-C5A-N7A	-4.08	105.47	109.41
2	3-A	201	FOL	C4A-C8A-N8	-4.08	117.99	123.07
2	56-A	201	FOL	C4A-C8A-N8	-4.07	118.00	123.07
2	139-A	201	FOL	C4A-C4-N3	-4.07	117.69	123.48
2	44-A	201	FOL	CB-CA-CT	-4.07	106.37	112.28
4	152-A	204	NAP	C4A-C5A-N7A	-4.06	105.49	109.41
2	71-A	201	FOL	C4A-C8A-N8	-4.06	118.02	123.07
2	73-A	201	FOL	C4A-C8A-N8	-4.06	118.02	123.07
2	162-A	201	FOL	C4A-C8A-N8	-4.05	118.02	123.07
4	111-A	204	NAP	C4A-C5A-N7A	-4.05	105.49	109.41
2	5-A	201	FOL	NA2-C2-N3	-4.05	115.31	120.26
4	21-A	204	NAP	C4A-C5A-N7A	-4.04	105.50	109.41
2	62-A	201	FOL	C4A-C8A-N8	-4.04	118.04	123.07
2	30-A	201	FOL	C4A-C4-N3	-4.04	117.73	123.48
2	159-A	201	FOL	CG-CB-CA	-4.03	105.15	113.19
2	150-A	201	FOL	C4A-C8A-N8	-4.01	118.08	123.07
4	60-A	204	NAP	C4A-C5A-N7A	-4.00	105.54	109.41
2	7-A	201	FOL	C4A-C8A-N8	-4.00	118.09	123.07
4	87-A	204	NAP	C4A-C5A-N7A	-4.00	105.55	109.41
4	44-A	204	NAP	C4A-C5A-N7A	-3.99	105.56	109.41
2	67-A	201	FOL	CG-CB-CA	-3.99	105.23	113.19
2	165-A	201	FOL	C4A-C8A-N8	-3.98	118.11	123.07
4	12-A	204	NAP	C4A-C5A-N7A	-3.98	105.56	109.41
2	85-A	201	FOL	C4A-C8A-N8	-3.98	118.12	123.07
2	96-A	201	FOL	C4A-C4-N3	-3.97	117.83	123.48
2	164-A	201	FOL	C4A-C8A-N8	-3.97	118.13	123.07
2	24-A	201	FOL	C4A-C8A-N8	-3.97	118.13	123.07
2	42-A	201	FOL	C4A-C8A-N8	-3.96	118.14	123.07
2	107-A	201	FOL	C4A-C8A-N8	-3.96	118.14	123.07
2	64-A	201	FOL	NA2-C2-N3	-3.96	115.42	120.26
2	73-A	201	FOL	C4A-C4-N3	-3.95	117.86	123.48
4	41-A	204	NAP	C4A-C5A-N7A	-3.95	105.59	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	20-A	201	FOL	C4A-C8A-N8	-3.95	118.16	123.07
4	36-A	204	NAP	C4A-C5A-N7A	-3.95	105.60	109.41
4	160-A	204	NAP	C4A-C5A-N7A	-3.95	105.60	109.41
4	23-A	204	NAP	C4A-C5A-N7A	-3.94	105.60	109.41
2	147-A	201	FOL	C4A-C8A-N8	-3.94	118.17	123.07
2	68-A	201	FOL	C4A-C8A-N8	-3.94	118.17	123.07
2	57-A	201	FOL	C4A-C8A-N8	-3.93	118.18	123.07
2	64-A	201	FOL	C4A-C8A-N8	-3.93	118.18	123.07
2	131-A	201	FOL	C4A-C4-N3	-3.92	117.90	123.48
2	86-A	201	FOL	C4A-C8A-N8	-3.92	118.19	123.07
4	119-A	204	NAP	O2N-PN-O5D	-3.91	89.66	108.14
2	141-A	201	FOL	C4A-C8A-N8	-3.91	118.20	123.07
2	101-A	201	FOL	C4A-C8A-N8	-3.91	118.21	123.07
2	24-A	201	FOL	C4A-C4-N3	-3.90	117.92	123.48
4	124-A	204	NAP	C4A-C5A-N7A	-3.90	105.64	109.41
2	95-A	201	FOL	C4A-C4-N3	-3.90	117.94	123.48
4	27-A	204	NAP	C4A-C5A-N7A	-3.89	105.65	109.41
4	6-A	204	NAP	C4A-C5A-N7A	-3.89	105.65	109.41
2	32-A	201	FOL	C4A-C8A-N8	-3.89	118.23	123.07
2	51-A	201	FOL	C4A-C8A-N8	-3.89	118.23	123.07
4	71-A	204	NAP	C4A-C5A-N7A	-3.88	105.66	109.41
2	2-A	201	FOL	C4A-C8A-N8	-3.88	118.24	123.07
2	127-A	201	FOL	NA2-C2-N3	-3.87	115.52	120.26
4	50-A	204	NAP	C4A-C5A-N7A	-3.87	105.67	109.41
4	131-A	204	NAP	C4A-C5A-N7A	-3.87	105.67	109.41
2	48-A	201	FOL	C4A-C8A-N8	-3.87	118.25	123.07
4	16-A	204	NAP	C4A-C5A-N7A	-3.87	105.67	109.41
2	135-A	201	FOL	NA2-C2-N3	-3.87	115.53	120.26
4	26-A	204	NAP	C4A-C5A-N7A	-3.87	105.67	109.41
4	28-A	204	NAP	C4A-C5A-N7A	-3.86	105.68	109.41
4	24-A	204	NAP	C4A-C5A-N7A	-3.86	105.68	109.41
4	80-A	204	NAP	C4A-C5A-N7A	-3.86	105.69	109.41
2	18-A	201	FOL	C4A-C8A-N8	-3.86	118.27	123.07
2	90-A	201	FOL	C4A-C8A-N8	-3.85	118.27	123.07
2	17-A	201	FOL	C4A-C8A-N8	-3.85	118.27	123.07
2	8-A	201	FOL	C4A-C8A-N8	-3.85	118.28	123.07
2	127-A	201	FOL	C4A-C4-N3	-3.85	118.01	123.48
2	106-A	201	FOL	CB-CA-CT	-3.84	106.70	112.28
2	160-A	201	FOL	CB-CA-CT	-3.84	106.70	112.28
2	81-A	201	FOL	CG-CB-CA	-3.83	105.54	113.19
2	137-A	201	FOL	C4A-C8A-N8	-3.83	118.31	123.07
4	161-A	204	NAP	C4A-C5A-N7A	-3.83	105.71	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	115-A	201	FOL	C4A-C8A-N8	-3.82	118.31	123.07
4	9-A	204	NAP	C4A-C5A-N7A	-3.82	105.72	109.41
2	52-A	201	FOL	C4A-C4-N3	-3.82	118.05	123.48
2	113-A	201	FOL	C4A-C8A-N8	-3.82	118.32	123.07
4	110-A	204	NAP	C4A-C5A-N7A	-3.81	105.72	109.41
4	153-A	204	NAP	C4A-C5A-N7A	-3.81	105.73	109.41
2	53-A	201	FOL	C4A-C8A-N8	-3.81	118.33	123.07
4	97-A	204	NAP	C4A-C5A-N7A	-3.80	105.74	109.41
2	134-A	201	FOL	C4A-C8A-N8	-3.80	118.34	123.07
4	13-A	204	NAP	C4A-C5A-N7A	-3.80	105.74	109.41
4	90-A	204	NAP	O7N-C7N-N7N	-3.80	117.18	122.58
4	134-A	204	NAP	C4A-C5A-N7A	-3.80	105.74	109.41
2	40-A	201	FOL	C4A-C8A-N8	-3.79	118.35	123.07
2	89-A	201	FOL	NA2-C2-N3	-3.79	115.63	120.26
4	141-A	204	NAP	C4A-C5A-N7A	-3.79	105.75	109.41
4	58-A	204	NAP	C4A-C5A-N7A	-3.78	105.75	109.41
4	48-A	204	NAP	C4A-C5A-N7A	-3.78	105.76	109.41
2	80-A	201	FOL	O-C-N	-3.77	115.56	122.46
4	136-A	204	NAP	C4A-C5A-N7A	-3.77	105.77	109.41
4	117-A	204	NAP	C4A-C5A-N7A	-3.76	105.77	109.41
2	96-A	201	FOL	C4A-C8A-N8	-3.76	118.39	123.07
4	39-A	204	NAP	C4A-C5A-N7A	-3.75	105.78	109.41
4	66-A	204	NAP	C4A-C5A-N7A	-3.75	105.78	109.41
2	37-A	201	FOL	CB-CA-N	-3.75	104.53	110.22
2	166-A	201	FOL	C4A-C8A-N8	-3.74	118.41	123.07
2	155-A	201	FOL	NA2-C2-N3	-3.74	115.68	120.26
2	157-A	201	FOL	NA2-C2-N3	-3.73	115.69	120.26
4	56-A	204	NAP	C4A-C5A-N7A	-3.73	105.81	109.41
2	155-A	201	FOL	C4A-C8A-N8	-3.72	118.43	123.07
2	100-A	201	FOL	C4A-C8A-N8	-3.71	118.45	123.07
4	85-A	204	NAP	C4A-C5A-N7A	-3.71	105.83	109.41
2	130-A	201	FOL	C4A-C8A-N8	-3.71	118.45	123.07
4	20-A	204	NAP	C4A-C5A-N7A	-3.70	105.83	109.41
4	65-A	204	NAP	C4A-C5A-N7A	-3.70	105.84	109.41
2	120-A	201	FOL	C4A-C8A-N8	-3.69	118.47	123.07
2	158-A	201	FOL	C4A-C8A-N8	-3.68	118.48	123.07
2	94-A	201	FOL	C4A-C8A-N8	-3.68	118.49	123.07
2	16-A	201	FOL	C4A-C4-N3	-3.68	118.25	123.48
2	153-A	201	FOL	C4A-C4-N3	-3.68	118.25	123.48
2	129-A	201	FOL	C16-C11-C12	-3.67	113.49	118.58
2	136-A	201	FOL	C4A-C8A-N8	-3.66	118.51	123.07
2	66-A	201	FOL	C4A-C8A-N8	-3.66	118.52	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	118-A	201	FOL	CB-CA-CT	-3.65	106.98	112.28
4	1-A	204	NAP	C4A-C5A-N7A	-3.65	105.88	109.41
2	144-A	201	FOL	NA2-C2-N3	-3.65	115.80	120.26
2	119-A	201	FOL	CB-CA-CT	-3.65	106.99	112.28
4	70-A	204	NAP	C4A-C5A-N7A	-3.63	105.90	109.41
2	135-A	201	FOL	C4A-C8A-N8	-3.63	118.55	123.07
4	94-A	204	NAP	C4A-C5A-N7A	-3.63	105.90	109.41
2	143-A	201	FOL	C4A-C8A-N8	-3.62	118.56	123.07
4	113-A	204	NAP	C4A-C5A-N7A	-3.62	105.91	109.41
4	159-A	204	NAP	C4A-C5A-N7A	-3.61	105.92	109.41
4	63-A	204	NAP	C4A-C5A-N7A	-3.61	105.92	109.41
4	115-A	204	NAP	O7N-C7N-N7N	-3.61	117.44	122.58
2	20-A	201	FOL	NA2-C2-N3	-3.61	115.84	120.26
2	128-A	201	FOL	CA-N-C	-3.60	117.21	122.15
2	31-A	201	FOL	NA2-C2-N3	-3.59	115.87	120.26
2	65-A	201	FOL	C4A-C8A-N8	-3.58	118.61	123.07
4	156-A	204	NAP	C4A-C5A-N7A	-3.57	105.96	109.41
2	140-A	201	FOL	C4A-C4-N3	-3.57	118.40	123.48
4	37-A	204	NAP	C4A-C5A-N7A	-3.56	105.97	109.41
2	74-A	201	FOL	C4A-C8A-N8	-3.56	118.64	123.07
4	31-A	204	NAP	C4A-C5A-N7A	-3.56	105.97	109.41
4	118-A	204	NAP	N3A-C2A-N1A	-3.55	125.77	128.86
2	122-A	201	FOL	NA2-C2-N3	-3.54	115.93	120.26
2	97-A	201	FOL	CB-CA-CT	-3.53	107.16	112.28
2	72-A	201	FOL	O-C-C11	-3.53	114.68	120.94
4	57-A	204	NAP	C4A-C5A-N7A	-3.53	106.00	109.41
4	129-A	204	NAP	C4A-C5A-N7A	-3.52	106.01	109.41
2	114-A	201	FOL	CA-N-C	-3.52	117.33	122.15
2	26-A	201	FOL	C4A-C8A-N8	-3.51	118.70	123.07
2	118-A	201	FOL	C4A-C8A-N8	-3.50	118.72	123.07
4	119-A	204	NAP	C1B-N9A-C4A	-3.47	120.64	126.64
2	114-A	201	FOL	C4A-C8A-N8	-3.47	118.75	123.07
4	114-A	204	NAP	C4A-C5A-N7A	-3.44	106.08	109.41
2	123-A	201	FOL	C4A-C8A-N8	-3.44	118.78	123.07
2	121-A	201	FOL	C4A-C8A-N8	-3.43	118.80	123.07
2	98-A	201	FOL	C4A-C8A-N8	-3.43	118.80	123.07
2	33-A	201	FOL	C4A-C4-N3	-3.43	118.60	123.48
2	135-A	201	FOL	CB-CA-N	-3.42	105.03	110.22
2	44-A	201	FOL	CA-N-C	-3.41	117.48	122.15
2	47-A	201	FOL	C4A-C8A-N8	-3.41	118.83	123.07
4	119-A	204	NAP	O4B-C4B-C5B	-3.41	97.90	109.40
2	10-A	201	FOL	NA2-C2-N3	-3.41	116.09	120.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	59-A	201	FOL	NA2-C2-N3	-3.40	116.10	120.26
4	149-A	204	NAP	C4A-C5A-N7A	-3.39	106.13	109.41
4	18-A	204	NAP	O7N-C7N-N7N	-3.39	117.76	122.58
4	34-A	204	NAP	C4A-C5A-N7A	-3.38	106.14	109.41
4	76-A	204	NAP	C4A-C5A-N7A	-3.38	106.14	109.41
4	126-A	204	NAP	C4A-C5A-N7A	-3.38	106.14	109.41
2	34-A	201	FOL	C15-C14-C13	-3.36	114.34	119.04
4	82-A	204	NAP	O4B-C4B-C5B	-3.35	98.08	109.40
2	66-A	201	FOL	C13-C14-N10	-3.34	114.30	121.03
2	127-A	201	FOL	O-C-C11	-3.34	115.01	120.94
2	162-A	201	FOL	CB-CA-CT	-3.33	107.45	112.28
2	110-A	201	FOL	C4A-C8A-N8	-3.33	118.93	123.07
2	43-A	201	FOL	C7-C6-N5	-3.33	118.61	120.80
2	27-A	201	FOL	C4A-C8A-N8	-3.32	118.93	123.07
2	162-A	201	FOL	NA2-C2-N3	-3.32	116.20	120.26
2	134-A	201	FOL	CB-CA-CT	-3.31	107.47	112.28
2	50-A	201	FOL	C4A-C8A-N8	-3.31	118.95	123.07
2	63-A	201	FOL	O-C-C11	-3.30	115.08	120.94
4	156-A	204	NAP	N3A-C2A-N1A	-3.30	125.98	128.86
2	41-A	201	FOL	O-C-N	-3.30	116.43	122.46
4	166-A	204	NAP	C4A-C5A-N7A	-3.29	106.23	109.41
4	104-A	204	NAP	O3D-C3D-C2D	-3.29	101.28	111.83
2	167-A	201	FOL	CB-CA-N	-3.29	105.23	110.22
2	9-A	201	FOL	C4A-C8A-N8	-3.28	118.98	123.07
2	119-A	201	FOL	C4A-C8A-N8	-3.28	118.99	123.07
2	19-A	201	FOL	C4A-C8A-N8	-3.27	119.00	123.07
2	129-A	201	FOL	C4A-C8A-N8	-3.26	119.01	123.07
2	117-A	201	FOL	C4A-C8A-N8	-3.25	119.03	123.07
2	126-A	201	FOL	C4A-C8A-N8	-3.24	119.03	123.07
2	122-A	201	FOL	C4A-C8A-N8	-3.22	119.06	123.07
2	152-A	201	FOL	C4A-C8A-N8	-3.21	119.07	123.07
2	93-A	201	FOL	NA2-C2-N3	-3.21	116.34	120.26
2	81-A	201	FOL	NA2-C2-N3	-3.20	116.34	120.26
2	143-A	201	FOL	CB-CA-N	-3.20	105.36	110.22
4	129-A	204	NAP	O2A-PA-O5B	-3.20	93.04	108.14
2	85-A	201	FOL	CG-CB-CA	-3.18	106.84	113.19
2	114-A	201	FOL	NA2-C2-N3	-3.16	116.39	120.26
2	151-A	201	FOL	C4A-C8A-N8	-3.16	119.14	123.07
4	68-A	204	NAP	C4A-C5A-N7A	-3.16	106.36	109.41
4	33-A	204	NAP	C4A-C5A-N7A	-3.15	106.37	109.41
2	74-A	201	FOL	C16-C11-C12	-3.14	114.23	118.58
2	167-A	201	FOL	C4A-C8A-N8	-3.14	119.16	123.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	127-A	201	FOL	CA-N-C	-3.13	117.86	122.15
4	33-A	204	NAP	O4B-C4B-C5B	-3.13	98.85	109.40
2	30-A	201	FOL	NA2-C2-N3	-3.12	116.45	120.26
4	79-A	204	NAP	N3A-C2A-N1A	-3.11	126.15	128.86
2	23-A	201	FOL	C4A-C4-N3	-3.11	119.05	123.48
2	51-A	201	FOL	O-C-C11	-3.11	115.42	120.94
2	84-A	201	FOL	CA-N-C	-3.11	117.89	122.15
2	57-A	201	FOL	C6-N5-C4A	-3.11	114.72	118.44
4	118-A	204	NAP	C4A-C5A-N7A	-3.11	106.41	109.41
2	163-A	201	FOL	NA2-C2-N3	-3.09	116.48	120.26
2	153-A	201	FOL	NA2-C2-N3	-3.09	116.49	120.26
2	104-A	201	FOL	NA2-C2-N3	-3.08	116.49	120.26
4	115-A	204	NAP	N3A-C2A-N1A	-3.08	126.17	128.86
2	94-A	201	FOL	O-C-C11	-3.08	115.47	120.94
2	89-A	201	FOL	C4A-C8A-N8	-3.08	119.23	123.07
2	124-A	201	FOL	C4A-C8A-N8	-3.07	119.24	123.07
4	128-A	204	NAP	O2A-PA-O5B	-3.07	93.65	108.14
2	64-A	201	FOL	C13-C14-N10	-3.06	114.86	121.03
2	154-A	201	FOL	C4A-C8A-N8	-3.06	119.26	123.07
2	38-A	201	FOL	C7-C6-N5	-3.06	118.79	120.80
2	159-A	201	FOL	NA2-C2-N3	-3.06	116.52	120.26
2	107-A	201	FOL	CB-CA-CT	-3.06	107.85	112.28
2	108-A	201	FOL	NA2-C2-N3	-3.05	116.53	120.26
2	100-A	201	FOL	CG-CB-CA	-3.05	107.11	113.19
2	96-A	201	FOL	CB-CA-CT	-3.04	107.86	112.28
2	159-A	201	FOL	C7-C6-N5	-3.04	118.80	120.80
4	114-A	204	NAP	N3A-C2A-N1A	-3.04	126.21	128.86
2	21-A	201	FOL	C4A-C8A-N8	-3.04	119.29	123.07
2	142-A	201	FOL	C7-C6-N5	-3.04	118.80	120.80
2	9-A	201	FOL	NA2-C2-N3	-3.04	116.55	120.26
2	70-A	201	FOL	O-C-C11	-3.03	115.56	120.94
2	115-A	201	FOL	CA-N-C	-3.03	118.00	122.15
2	94-A	201	FOL	NA2-C2-N3	-3.03	116.55	120.26
2	151-A	201	FOL	CB-CA-CT	-3.03	107.89	112.28
2	102-A	201	FOL	NA2-C2-N3	-3.02	116.56	120.26
2	163-A	201	FOL	CG-CB-CA	-3.02	107.16	113.19
2	145-A	201	FOL	CB-CA-CT	-3.02	107.91	112.28
2	12-A	201	FOL	C4A-C8A-N8	-3.01	119.32	123.07
4	42-A	204	NAP	O4B-C4B-C5B	-2.99	99.30	109.40
2	111-A	201	FOL	C4A-C8A-N8	-2.98	119.36	123.07
2	141-A	201	FOL	O-C-C11	-2.98	115.65	120.94
4	69-A	204	NAP	C4A-C5A-N7A	-2.98	106.53	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	126-A	201	FOL	CB-CA-CT	-2.98	107.95	112.28
4	117-A	204	NAP	O2N-PN-O5D	-2.97	94.10	108.14
2	115-A	201	FOL	NA2-C2-N3	-2.96	116.64	120.26
2	166-A	201	FOL	NA2-C2-N3	-2.94	116.66	120.26
2	112-A	201	FOL	NA2-C2-N3	-2.94	116.67	120.26
2	80-A	201	FOL	C7-C6-N5	-2.93	118.87	120.80
2	39-A	201	FOL	NA2-C2-N3	-2.93	116.68	120.26
2	99-A	201	FOL	O-C-N	-2.93	117.10	122.46
2	128-A	201	FOL	NA2-C2-N3	-2.93	116.68	120.26
2	113-A	201	FOL	CG-CB-CA	-2.91	107.37	113.19
4	79-A	204	NAP	O2A-PA-O5B	-2.91	94.42	108.14
2	29-A	201	FOL	NA2-C2-N3	-2.91	116.71	120.26
4	28-A	204	NAP	O2A-PA-O5B	-2.91	94.42	108.14
2	97-A	201	FOL	NA2-C2-N3	-2.89	116.72	120.26
4	38-A	204	NAP	O2D-C2D-C3D	-2.89	102.57	111.83
4	119-A	204	NAP	N3A-C2A-N1A	-2.89	126.34	128.86
4	123-A	204	NAP	N3A-C2A-N1A	-2.89	126.34	128.86
2	30-A	201	FOL	CB-CA-CT	-2.89	108.09	112.28
4	122-A	204	NAP	C4A-C5A-N7A	-2.88	106.63	109.41
2	90-A	201	FOL	NA2-C2-N3	-2.88	116.74	120.26
2	86-A	201	FOL	NA2-C2-N3	-2.88	116.74	120.26
4	42-A	204	NAP	O2A-PA-O5B	-2.88	94.55	108.14
2	63-A	201	FOL	CB-CA-CT	-2.87	108.11	112.28
2	4-A	201	FOL	C16-C11-C12	-2.87	114.60	118.58
2	30-A	201	FOL	C4A-C8A-N8	-2.87	119.50	123.07
2	36-A	201	FOL	CB-CA-N	-2.86	105.88	110.22
4	121-A	204	NAP	N3A-C2A-N1A	-2.86	126.36	128.86
2	78-A	201	FOL	CB-CA-N	-2.86	105.88	110.22
2	6-A	201	FOL	C4A-C8A-N8	-2.85	119.52	123.07
2	32-A	201	FOL	NA2-C2-N3	-2.85	116.78	120.26
2	153-A	201	FOL	O-C-C11	-2.85	115.89	120.94
2	134-A	201	FOL	CA-N-C	-2.84	118.25	122.15
2	28-A	201	FOL	C4A-C8A-N8	-2.84	119.53	123.07
4	117-A	204	NAP	N3A-C2A-N1A	-2.83	126.39	128.86
2	26-A	201	FOL	CA-N-C	-2.83	118.27	122.15
2	100-A	201	FOL	C9-C6-C7	-2.83	116.60	121.38
4	3-A	204	NAP	O2A-PA-O5B	-2.82	94.81	108.14
2	85-A	201	FOL	CB-CA-CT	-2.81	108.20	112.28
4	29-A	204	NAP	O2A-PA-O5B	-2.81	94.89	108.14
4	80-A	204	NAP	O2A-PA-O5B	-2.80	94.91	108.14
2	15-A	201	FOL	C4A-C8A-N8	-2.80	119.58	123.07
2	103-A	201	FOL	NA2-C2-N3	-2.79	116.84	120.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-A	204	NAP	N3A-C2A-N1A	-2.79	126.43	128.86
2	102-A	201	FOL	O-C-C11	-2.79	116.00	120.94
2	57-A	201	FOL	C16-C11-C12	-2.78	114.73	118.58
4	49-A	204	NAP	O2A-PA-O5B	-2.78	95.02	108.14
4	71-A	204	NAP	N3A-C2A-N1A	-2.76	126.45	128.86
2	115-A	201	FOL	C13-C14-N10	-2.76	115.47	121.03
4	12-A	204	NAP	N3A-C2A-N1A	-2.76	126.46	128.86
2	24-A	201	FOL	NA2-C2-N3	-2.75	116.89	120.26
2	65-A	201	FOL	C9-C6-C7	-2.75	116.73	121.38
4	99-A	204	NAP	O2A-PA-O5B	-2.75	95.17	108.14
4	40-A	204	NAP	N3A-C2A-N1A	-2.74	126.47	128.86
2	86-A	201	FOL	CB-CA-CT	-2.74	108.31	112.28
4	27-A	204	NAP	O2A-PA-O5B	-2.73	95.24	108.14
4	93-A	204	NAP	O2A-PA-O5B	-2.73	95.26	108.14
4	127-A	204	NAP	O2A-PA-O5B	-2.72	95.29	108.14
4	19-A	204	NAP	N3A-C2A-N1A	-2.72	126.49	128.86
2	17-A	201	FOL	CB-CA-CT	-2.71	108.34	112.28
2	144-A	201	FOL	C13-C14-N10	-2.71	115.56	121.03
4	130-A	204	NAP	O2A-PA-O5B	-2.71	95.34	108.14
4	49-A	204	NAP	O7N-C7N-N7N	-2.71	118.73	122.58
2	62-A	201	FOL	NA2-C2-N3	-2.71	116.95	120.26
2	76-A	201	FOL	C9-C6-C7	-2.70	116.81	121.38
2	68-A	201	FOL	NA2-C2-N3	-2.70	116.96	120.26
2	95-A	201	FOL	NA2-C2-N3	-2.70	116.96	120.26
4	154-A	204	NAP	O2A-PA-O5B	-2.70	95.41	108.14
2	126-A	201	FOL	C9-C6-C7	-2.69	116.82	121.38
2	9-A	201	FOL	O-C-C11	-2.68	116.18	120.94
4	122-A	204	NAP	O2A-PA-O5B	-2.68	95.48	108.14
2	132-A	201	FOL	CB-CA-CT	-2.68	108.40	112.28
2	130-A	201	FOL	NA2-C2-N3	-2.68	116.99	120.26
4	4-A	204	NAP	O2A-PA-O5B	-2.67	95.52	108.14
4	11-A	204	NAP	N3A-C2A-N1A	-2.67	126.53	128.86
2	9-A	201	FOL	CA-N-C	-2.67	118.49	122.15
4	125-A	204	NAP	N3A-C2A-N1A	-2.67	126.53	128.86
4	94-A	204	NAP	O2A-PA-O5B	-2.66	95.57	108.14
4	138-A	204	NAP	O2A-PA-O5B	-2.66	95.59	108.14
2	65-A	201	FOL	C6-N5-C4A	-2.66	115.25	118.44
2	92-A	201	FOL	NA2-C2-N3	-2.65	117.01	120.26
4	54-A	204	NAP	O2A-PA-O5B	-2.65	95.62	108.14
4	106-A	204	NAP	N3A-C2A-N1A	-2.65	126.55	128.86
2	109-A	201	FOL	NA2-C2-N3	-2.65	117.02	120.26
2	84-A	201	FOL	NA2-C2-N3	-2.65	117.02	120.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	123-A	204	NAP	O2A-PA-O5B	-2.64	95.67	108.14
2	83-A	201	FOL	C16-C11-C12	-2.64	114.92	118.58
4	137-A	204	NAP	O2A-PA-O5B	-2.64	95.67	108.14
2	105-A	201	FOL	NA2-C2-N3	-2.64	117.04	120.26
2	134-A	201	FOL	O-C-N	-2.63	117.64	122.46
2	76-A	201	FOL	C4A-C8A-N8	-2.63	119.79	123.07
2	14-A	201	FOL	CB-CA-CT	-2.63	108.46	112.28
2	134-A	201	FOL	CG-CB-CA	-2.63	107.94	113.19
2	34-A	201	FOL	NA2-C2-N3	-2.63	117.05	120.26
4	90-A	204	NAP	N3A-C2A-N1A	-2.62	126.58	128.86
2	75-A	201	FOL	C7-C6-N5	-2.62	119.08	120.80
2	26-A	201	FOL	O-C-N	-2.61	117.68	122.46
2	136-A	201	FOL	CB-CA-N	-2.61	106.25	110.22
4	61-A	204	NAP	O2A-PA-O5B	-2.61	95.81	108.14
4	100-A	204	NAP	N3A-C2A-N1A	-2.61	126.58	128.86
2	161-A	201	FOL	C7-C6-N5	-2.61	119.08	120.80
2	83-A	201	FOL	C6-N5-C4A	-2.61	115.31	118.44
4	122-A	204	NAP	N3A-C2A-N1A	-2.61	126.59	128.86
4	120-A	204	NAP	N3A-C2A-N1A	-2.60	126.59	128.86
2	23-A	201	FOL	NA2-C2-N3	-2.59	117.09	120.26
4	44-A	204	NAP	O2A-PA-O5B	-2.59	95.90	108.14
4	73-A	204	NAP	N3A-C2A-N1A	-2.59	126.60	128.86
4	15-A	204	NAP	O2A-PA-O5B	-2.58	95.94	108.14
2	75-A	201	FOL	NA2-C2-N3	-2.58	117.10	120.26
2	158-A	201	FOL	C6-N5-C4A	-2.58	115.34	118.44
4	124-A	204	NAP	O2A-PA-O5B	-2.58	95.95	108.14
4	103-A	204	NAP	O2A-PA-O5B	-2.58	95.96	108.14
2	47-A	201	FOL	CG-CB-CA	-2.57	108.05	113.19
4	62-A	204	NAP	N3A-C2A-N1A	-2.57	126.62	128.86
4	165-A	204	NAP	O2A-PA-O5B	-2.57	96.01	108.14
4	60-A	204	NAP	O2A-PA-O5B	-2.57	96.01	108.14
4	75-A	204	NAP	O2A-PA-O5B	-2.57	96.02	108.14
2	72-A	201	FOL	CA-N-C	-2.57	118.63	122.15
2	160-A	201	FOL	C4A-C8A-N8	-2.56	119.88	123.07
4	87-A	204	NAP	O2A-PA-O5B	-2.56	96.04	108.14
4	63-A	204	NAP	O2A-PA-O5B	-2.56	96.05	108.14
4	113-A	204	NAP	N3A-C2A-N1A	-2.56	126.63	128.86
4	136-A	204	NAP	O2A-PA-O5B	-2.56	96.05	108.14
2	57-A	201	FOL	NA2-C2-N3	-2.56	117.13	120.26
2	20-A	201	FOL	CB-CA-CT	-2.56	108.57	112.28
2	21-A	201	FOL	C16-C11-C12	-2.55	115.05	118.58
2	87-A	201	FOL	C16-C11-C12	-2.55	115.05	118.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	62-A	204	NAP	O2A-PA-O5B	-2.55	96.12	108.14
4	156-A	204	NAP	O2A-PA-O5B	-2.55	96.12	108.14
4	104-A	204	NAP	O2A-PA-O5B	-2.54	96.13	108.14
2	138-A	201	FOL	NA2-C2-N3	-2.54	117.15	120.26
4	2-A	204	NAP	O3D-C3D-C2D	-2.54	103.70	111.83
4	167-A	204	NAP	C4A-C5A-N7A	-2.53	106.96	109.41
4	75-A	204	NAP	N3A-C2A-N1A	-2.53	126.65	128.86
2	37-A	201	FOL	C9-C6-C7	-2.53	117.09	121.38
2	124-A	201	FOL	NA2-C2-N3	-2.53	117.16	120.26
4	84-A	204	NAP	C4A-C5A-N7A	-2.53	106.97	109.41
4	150-A	204	NAP	O7N-C7N-N7N	-2.52	118.99	122.58
4	167-A	204	NAP	O2A-PA-O5B	-2.52	96.22	108.14
4	16-A	204	NAP	O2A-PA-O5B	-2.52	96.24	108.14
2	52-A	201	FOL	NA2-C2-N3	-2.52	117.18	120.26
4	150-A	204	NAP	O2A-PA-O5B	-2.51	96.28	108.14
2	158-A	201	FOL	C16-C11-C12	-2.51	115.10	118.58
4	41-A	204	NAP	O2A-PA-O5B	-2.51	96.31	108.14
4	13-A	204	NAP	O2A-PA-O5B	-2.51	96.31	108.14
4	117-A	204	NAP	O2A-PA-O5B	-2.51	96.31	108.14
4	113-A	204	NAP	O2A-PA-O5B	-2.50	96.32	108.14
2	7-A	201	FOL	CG-CB-CA	-2.50	108.19	113.19
4	5-A	204	NAP	O2A-PA-O5B	-2.50	96.33	108.14
4	78-A	204	NAP	O2A-PA-O5B	-2.50	96.33	108.14
4	139-A	204	NAP	O7N-C7N-N7N	-2.50	119.03	122.58
2	106-A	201	FOL	NA2-C2-N3	-2.50	117.21	120.26
2	21-A	201	FOL	C9-C6-C7	-2.49	117.17	121.38
4	69-A	204	NAP	N3A-C2A-N1A	-2.49	126.69	128.86
4	43-A	204	NAP	N3A-C2A-N1A	-2.48	126.70	128.86
4	95-A	204	NAP	O2A-PA-O5B	-2.48	96.43	108.14
2	10-A	201	FOL	C7-C6-N5	-2.48	119.17	120.80
2	39-A	201	FOL	CB-CA-CT	-2.48	108.69	112.28
4	23-A	204	NAP	O2N-PN-O5D	-2.48	96.45	108.14
4	18-A	204	NAP	N3A-C2A-N1A	-2.47	126.70	128.86
4	70-A	204	NAP	N3A-C2A-N1A	-2.47	126.71	128.86
4	12-A	204	NAP	O2A-PA-O5B	-2.47	96.49	108.14
4	159-A	204	NAP	N3A-C2A-N1A	-2.47	126.71	128.86
4	98-A	204	NAP	O2A-PA-O5B	-2.47	96.50	108.14
4	45-A	204	NAP	O2A-PA-O5B	-2.46	96.52	108.14
4	125-A	204	NAP	O2A-PA-O5B	-2.46	96.52	108.14
4	74-A	204	NAP	O2A-PA-O5B	-2.46	96.52	108.14
2	77-A	201	FOL	CB-CA-CT	-2.46	108.71	112.28
2	54-A	201	FOL	C13-C14-N10	-2.46	116.08	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	108-A	204	NAP	O7N-C7N-N7N	-2.45	119.09	122.58
2	124-A	201	FOL	CB-CA-CT	-2.45	108.72	112.28
4	14-A	204	NAP	O2A-PA-O5B	-2.45	96.56	108.14
2	47-A	201	FOL	C6-C9-N10	-2.45	107.67	113.15
2	74-A	201	FOL	CB-CA-N	-2.45	106.50	110.22
4	77-A	204	NAP	O2A-PA-O5B	-2.45	96.59	108.14
4	139-A	204	NAP	O2A-PA-O5B	-2.45	96.59	108.14
4	25-A	204	NAP	O2A-PA-O5B	-2.44	96.60	108.14
4	6-A	204	NAP	O3D-C3D-C2D	-2.44	104.00	111.83
4	6-A	204	NAP	N3A-C2A-N1A	-2.44	126.73	128.86
4	43-A	204	NAP	O2A-PA-O5B	-2.44	96.62	108.14
2	51-A	201	FOL	CB-CA-CT	-2.44	108.74	112.28
4	116-A	204	NAP	O2A-PA-O5B	-2.44	96.62	108.14
2	110-A	201	FOL	CB-CA-CT	-2.44	108.75	112.28
4	73-A	204	NAP	O2A-PA-O5B	-2.44	96.64	108.14
4	91-A	204	NAP	O2A-PA-O5B	-2.43	96.65	108.14
2	144-A	201	FOL	O-C-C11	-2.43	116.62	120.94
4	166-A	204	NAP	O2A-PA-O5B	-2.43	96.68	108.14
2	73-A	201	FOL	NA2-C2-N3	-2.43	117.30	120.26
4	1-A	204	NAP	O2A-PA-O5B	-2.42	96.70	108.14
4	111-A	204	NAP	O2A-PA-O5B	-2.42	96.72	108.14
4	148-A	204	NAP	O2A-PA-O5B	-2.42	96.72	108.14
4	55-A	204	NAP	O2A-PA-O5B	-2.42	96.72	108.14
2	167-A	201	FOL	C13-C14-N10	-2.42	116.16	121.03
4	86-A	204	NAP	O2A-PA-O5B	-2.41	96.75	108.14
4	118-A	204	NAP	O2A-PA-O5B	-2.41	96.75	108.14
2	65-A	201	FOL	CB-CA-N	-2.41	106.56	110.22
4	112-A	204	NAP	N3A-C2A-N1A	-2.41	126.76	128.86
2	64-A	201	FOL	O-C-C11	-2.41	116.67	120.94
4	149-A	204	NAP	O2A-PA-O5B	-2.40	96.79	108.14
4	111-A	204	NAP	N3A-C2A-N1A	-2.40	126.77	128.86
4	50-A	204	NAP	O2A-PA-O5B	-2.40	96.81	108.14
2	52-A	201	FOL	C13-C14-N10	-2.40	116.20	121.03
4	90-A	204	NAP	O2A-PA-O5B	-2.40	96.83	108.14
4	30-A	204	NAP	O2A-PA-O5B	-2.39	96.85	108.14
4	17-A	204	NAP	O2A-PA-O5B	-2.39	96.86	108.14
2	83-A	201	FOL	NA2-C2-N3	-2.39	117.34	120.26
4	110-A	204	NAP	N3A-C2A-N1A	-2.39	126.78	128.86
4	76-A	204	NAP	O2A-PA-O5B	-2.38	96.88	108.14
2	118-A	201	FOL	NA2-C2-N3	-2.38	117.35	120.26
4	164-A	204	NAP	O7N-C7N-N7N	-2.38	119.20	122.58
4	66-A	204	NAP	O2A-PA-O5B	-2.38	96.92	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	36-A	204	NAP	O2A-PA-O5B	-2.38	96.92	108.14
2	59-A	201	FOL	C7-C6-N5	-2.37	119.24	120.80
4	67-A	204	NAP	O2A-PA-O5B	-2.37	96.93	108.14
2	42-A	201	FOL	C16-C11-C12	-2.37	115.29	118.58
4	53-A	204	NAP	O2A-PA-O5B	-2.37	96.94	108.14
4	23-A	204	NAP	O2A-PA-O5B	-2.37	96.94	108.14
4	119-A	204	NAP	O2A-PA-O5B	-2.37	96.96	108.14
4	126-A	204	NAP	O2A-PA-O5B	-2.37	96.96	108.14
4	112-A	204	NAP	O2A-PA-O5B	-2.37	96.96	108.14
4	85-A	204	NAP	O2A-PA-O5B	-2.36	96.98	108.14
4	23-A	204	NAP	N3A-C2A-N1A	-2.36	126.80	128.86
4	46-A	204	NAP	O2A-PA-O5B	-2.36	96.99	108.14
4	56-A	204	NAP	O4D-C4D-C5D	-2.36	101.44	109.40
4	164-A	204	NAP	O2A-PA-O5B	-2.36	97.00	108.14
4	11-A	204	NAP	O2A-PA-O5B	-2.36	97.00	108.14
4	31-A	204	NAP	O2X-P2B-O1X	-2.36	101.27	110.50
4	48-A	204	NAP	O2A-PA-O5B	-2.36	97.01	108.14
2	138-A	201	FOL	C15-C14-C13	-2.36	115.75	119.04
4	81-A	204	NAP	N3A-C2A-N1A	-2.36	126.81	128.86
4	38-A	204	NAP	N3A-C2A-N1A	-2.35	126.81	128.86
4	142-A	204	NAP	O2A-PA-O5B	-2.35	97.03	108.14
4	97-A	204	NAP	O2A-PA-O5B	-2.35	97.03	108.14
4	115-A	204	NAP	O2A-PA-O5B	-2.35	97.04	108.14
4	22-A	204	NAP	O2A-PA-O5B	-2.35	97.05	108.14
2	3-A	201	FOL	CG-CB-CA	-2.35	108.50	113.19
4	129-A	204	NAP	N3A-C2A-N1A	-2.35	126.81	128.86
4	39-A	204	NAP	O2A-PA-O5B	-2.35	97.06	108.14
2	118-A	201	FOL	O-C-N	-2.35	118.17	122.46
2	67-A	201	FOL	NA2-C2-N3	-2.34	117.39	120.26
4	100-A	204	NAP	O2A-PA-O5B	-2.34	97.09	108.14
4	56-A	204	NAP	O7N-C7N-C3N	-2.34	116.89	119.62
4	101-A	204	NAP	O2A-PA-O5B	-2.34	97.10	108.14
4	92-A	204	NAP	O2A-PA-O5B	-2.34	97.11	108.14
4	5-A	204	NAP	N3A-C2A-N1A	-2.33	126.82	128.86
2	23-A	201	FOL	C13-C14-N10	-2.33	116.34	121.03
4	135-A	204	NAP	C1B-N9A-C4A	-2.33	122.61	126.64
4	26-A	204	NAP	O2A-PA-O5B	-2.33	97.16	108.14
4	69-A	204	NAP	O2A-PA-O5B	-2.33	97.16	108.14
4	114-A	204	NAP	O2A-PA-O5B	-2.32	97.17	108.14
4	88-A	204	NAP	O2A-PA-O5B	-2.32	97.17	108.14
2	101-A	201	FOL	NA2-C2-N3	-2.32	117.42	120.26
4	24-A	204	NAP	O2A-PA-O5B	-2.32	97.19	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	42-A	204	NAP	C1B-N9A-C4A	-2.32	122.63	126.64
4	110-A	204	NAP	O2A-PA-O5B	-2.32	97.20	108.14
2	137-A	201	FOL	NA2-C2-N3	-2.31	117.43	120.26
4	140-A	204	NAP	O2A-PA-O5B	-2.31	97.22	108.14
4	161-A	204	NAP	O2A-PA-O5B	-2.31	97.24	108.14
4	65-A	204	NAP	O2A-PA-O5B	-2.31	97.24	108.14
4	143-A	204	NAP	O2A-PA-O5B	-2.31	97.24	108.14
4	13-A	204	NAP	O3D-C3D-C2D	-2.31	104.44	111.83
4	96-A	204	NAP	O2A-PA-O5B	-2.31	97.25	108.14
4	35-A	204	NAP	O2A-PA-O5B	-2.31	97.25	108.14
4	40-A	204	NAP	O2A-PA-O5B	-2.31	97.25	108.14
2	79-A	201	FOL	CB-CA-CT	-2.31	108.94	112.28
2	87-A	201	FOL	NA2-C2-N3	-2.30	117.44	120.26
2	17-A	201	FOL	NA2-C2-N3	-2.30	117.45	120.26
4	126-A	204	NAP	N3A-C2A-N1A	-2.30	126.85	128.86
4	144-A	204	NAP	N3A-C2A-N1A	-2.30	126.86	128.86
4	144-A	204	NAP	O2A-PA-O5B	-2.30	97.30	108.14
4	107-A	204	NAP	N3A-C2A-N1A	-2.29	126.86	128.86
4	72-A	204	NAP	N3A-C2A-N1A	-2.29	126.86	128.86
4	68-A	204	NAP	N3A-C2A-N1A	-2.29	126.86	128.86
4	163-A	204	NAP	O2A-PA-O5B	-2.29	97.34	108.14
4	135-A	204	NAP	O2A-PA-O5B	-2.29	97.34	108.14
4	146-A	204	NAP	N3A-C2A-N1A	-2.28	126.87	128.86
4	139-A	204	NAP	C1B-N9A-C4A	-2.28	122.70	126.64
2	1-A	201	FOL	C13-C14-N10	-2.28	116.44	121.03
4	10-A	204	NAP	N3A-C2A-N1A	-2.28	126.88	128.86
2	118-A	201	FOL	C15-C14-C13	-2.28	115.86	119.04
2	54-A	201	FOL	CB-CA-CT	-2.27	108.98	112.28
4	64-A	204	NAP	O2A-PA-O5B	-2.27	97.41	108.14
4	141-A	204	NAP	O2A-PA-O5B	-2.27	97.41	108.14
2	24-A	201	FOL	C13-C14-N10	-2.27	116.46	121.03
2	2-A	201	FOL	CG-CB-CA	-2.27	108.66	113.19
2	58-A	201	FOL	NA2-C2-N3	-2.27	117.49	120.26
2	129-A	201	FOL	C15-C14-C13	-2.27	115.87	119.04
4	145-A	204	NAP	N3A-C2A-N1A	-2.27	126.88	128.86
4	130-A	204	NAP	N3A-C2A-N1A	-2.27	126.88	128.86
4	49-A	204	NAP	O2N-PN-O5D	-2.26	97.45	108.14
4	160-A	204	NAP	O2A-PA-O5B	-2.26	97.45	108.14
2	161-A	201	FOL	NA2-C2-N3	-2.26	117.49	120.26
2	49-A	201	FOL	NA2-C2-N3	-2.26	117.49	120.26
4	81-A	204	NAP	N6A-C6A-N1A	-2.26	114.28	118.77
2	23-A	201	FOL	C7-C6-N5	-2.26	119.31	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	127-A	204	NAP	N3A-C2A-N1A	-2.26	126.89	128.86
2	122-A	201	FOL	CB-CA-CT	-2.26	109.00	112.28
4	153-A	204	NAP	O2A-PA-O5B	-2.26	97.48	108.14
2	64-A	201	FOL	CB-CA-CT	-2.26	109.01	112.28
4	10-A	204	NAP	O2A-PA-O5B	-2.25	97.50	108.14
4	2-A	204	NAP	O2A-PA-O5B	-2.25	97.51	108.14
2	46-A	201	FOL	C7-C6-N5	-2.25	119.32	120.80
2	108-A	201	FOL	C13-C14-N10	-2.24	116.51	121.03
2	142-A	201	FOL	NA2-C2-N3	-2.24	117.52	120.26
2	139-A	201	FOL	C16-C11-C12	-2.24	115.47	118.58
2	58-A	201	FOL	C13-C14-N10	-2.24	116.52	121.03
4	47-A	204	NAP	O2A-PA-O5B	-2.24	97.56	108.14
4	152-A	204	NAP	O2A-PA-O5B	-2.24	97.58	108.14
4	70-A	204	NAP	O2A-PA-O5B	-2.24	97.58	108.14
4	89-A	204	NAP	O2A-PA-O5B	-2.24	97.58	108.14
4	128-A	204	NAP	N3A-C2A-N1A	-2.23	126.91	128.86
4	151-A	204	NAP	C1B-N9A-C4A	-2.23	122.78	126.64
4	145-A	204	NAP	O2A-PA-O5B	-2.23	97.62	108.14
4	39-A	204	NAP	O3D-C3D-C2D	-2.22	104.71	111.83
4	151-A	204	NAP	O2A-PA-O5B	-2.22	97.65	108.14
4	141-A	204	NAP	N3A-C2A-N1A	-2.22	126.92	128.86
2	95-A	201	FOL	O-C-N	-2.22	118.41	122.46
4	72-A	204	NAP	O2A-PA-O5B	-2.22	97.68	108.14
2	134-A	201	FOL	O-C-C11	-2.22	117.01	120.94
4	147-A	204	NAP	N3A-C2A-N1A	-2.21	126.93	128.86
4	151-A	204	NAP	N3A-C2A-N1A	-2.21	126.93	128.86
4	83-A	204	NAP	O3D-C3D-C2D	-2.21	104.76	111.83
4	51-A	204	NAP	O2A-PA-O5B	-2.21	97.72	108.14
4	147-A	204	NAP	O2A-PA-O5B	-2.21	97.72	108.14
4	140-A	204	NAP	N3A-C2A-N1A	-2.20	126.94	128.86
4	102-A	204	NAP	C1B-N9A-C4A	-2.20	122.83	126.64
2	21-A	201	FOL	C6-N5-C4A	-2.20	115.80	118.44
2	10-A	201	FOL	O-C-N	-2.20	118.44	122.46
4	120-A	204	NAP	O2A-PA-O5B	-2.20	97.76	108.14
2	94-A	201	FOL	C9-C6-C7	-2.20	117.66	121.38
4	162-A	204	NAP	O2A-PA-O5B	-2.20	97.77	108.14
2	164-A	201	FOL	CB-CA-CT	-2.20	109.10	112.28
2	125-A	201	FOL	CG-CB-CA	-2.19	108.81	113.19
4	37-A	204	NAP	O2A-PA-O5B	-2.18	97.82	108.14
4	68-A	204	NAP	O2A-PA-O5B	-2.18	97.84	108.14
4	33-A	204	NAP	O7N-C7N-N7N	-2.18	119.48	122.58
2	157-A	201	FOL	C6-N5-C4A	-2.18	115.83	118.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	65-A	204	NAP	C2B-C3B-C4B	-2.18	96.99	101.95
2	103-A	201	FOL	CB-CA-CT	-2.18	109.12	112.28
4	116-A	204	NAP	N3A-C2A-N1A	-2.18	126.96	128.86
2	61-A	201	FOL	CB-CA-CT	-2.18	109.12	112.28
4	22-A	204	NAP	O7N-C7N-N7N	-2.18	119.49	122.58
4	1-A	204	NAP	O2N-PN-O5D	-2.17	97.87	108.14
4	107-A	204	NAP	O2A-PA-O5B	-2.17	97.88	108.14
4	154-A	204	NAP	N3A-C2A-N1A	-2.17	126.97	128.86
2	55-A	201	FOL	C13-C14-N10	-2.17	116.67	121.03
2	15-A	201	FOL	C9-C6-C7	-2.17	117.71	121.38
2	12-A	201	FOL	CB-CA-CT	-2.15	109.16	112.28
4	106-A	204	NAP	O2A-PA-O5B	-2.15	97.98	108.14
2	6-A	201	FOL	C9-C6-C7	-2.15	117.74	121.38
2	100-A	201	FOL	C6-N5-C4A	-2.15	115.86	118.44
4	105-A	204	NAP	O2A-PA-O5B	-2.15	98.00	108.14
2	82-A	201	FOL	O-C-N	-2.15	118.54	122.46
4	102-A	204	NAP	O2A-PA-O5B	-2.14	98.02	108.14
2	58-A	201	FOL	C7-C6-N5	-2.14	119.39	120.80
2	79-A	201	FOL	NA2-C2-N3	-2.14	117.64	120.26
2	147-A	201	FOL	CB-CA-CT	-2.14	109.18	112.28
4	71-A	204	NAP	O2A-PA-O5B	-2.14	98.04	108.14
2	106-A	201	FOL	O-C-N	-2.14	118.55	122.46
4	109-A	204	NAP	N3A-C2A-N1A	-2.14	127.00	128.86
2	110-A	201	FOL	C13-C14-N10	-2.14	116.73	121.03
4	77-A	204	NAP	N3A-C2A-N1A	-2.13	127.00	128.86
2	109-A	201	FOL	CG-CB-CA	-2.13	108.93	113.19
4	18-A	204	NAP	O2A-PA-O5B	-2.13	98.08	108.14
2	52-A	201	FOL	C7-C6-N5	-2.12	119.41	120.80
2	111-A	201	FOL	CA-N-C	-2.12	119.24	122.15
2	31-A	201	FOL	C16-C11-C12	-2.11	115.65	118.58
4	86-A	204	NAP	O3D-C3D-C2D	-2.11	105.06	111.83
2	144-A	201	FOL	C7-C6-N5	-2.11	119.41	120.80
2	136-A	201	FOL	C13-C14-N10	-2.11	116.77	121.03
2	48-A	201	FOL	C7-C6-N5	-2.10	119.42	120.80
4	120-A	204	NAP	O3D-C3D-C2D	-2.10	105.09	111.83
4	124-A	204	NAP	N3A-C2A-N1A	-2.10	127.03	128.86
2	116-A	201	FOL	C13-C14-N10	-2.10	116.81	121.03
4	38-A	204	NAP	O3D-C3D-C2D	-2.10	105.11	111.83
2	42-A	201	FOL	C9-C6-C7	-2.09	117.85	121.38
2	77-A	201	FOL	NA2-C2-N3	-2.09	117.71	120.26
4	135-A	204	NAP	N3A-C2A-N1A	-2.08	127.04	128.86
2	13-A	201	FOL	NA2-C2-N3	-2.08	117.71	120.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	38-A	204	NAP	O2A-PA-O5B	-2.08	98.31	108.14
2	158-A	201	FOL	NA2-C2-N3	-2.08	117.72	120.26
2	128-A	201	FOL	C7-C6-N5	-2.08	119.43	120.80
2	88-A	201	FOL	O-C-C11	-2.08	117.25	120.94
2	121-A	201	FOL	NA2-C2-N3	-2.08	117.72	120.26
4	121-A	204	NAP	O2A-PA-O5B	-2.08	98.34	108.14
2	103-A	201	FOL	C7-C6-N5	-2.08	119.44	120.80
2	116-A	201	FOL	NA2-C2-N3	-2.07	117.72	120.26
2	163-A	201	FOL	C7-C6-N5	-2.07	119.44	120.80
4	14-A	204	NAP	O3D-C3D-C2D	-2.07	105.19	111.83
2	74-A	201	FOL	C6-N5-C4A	-2.07	115.96	118.44
2	67-A	201	FOL	CB-CA-CT	-2.07	109.28	112.28
4	21-A	204	NAP	N3A-C2A-N1A	-2.07	127.06	128.86
2	9-A	201	FOL	CG-CB-CA	-2.07	109.06	113.19
2	34-A	201	FOL	C16-C11-C12	-2.06	115.72	118.58
2	91-A	201	FOL	C11-C-N	-2.06	113.16	116.97
2	32-A	201	FOL	C13-C14-N10	-2.06	116.88	121.03
2	5-A	201	FOL	O-C-N	-2.06	118.69	122.46
2	155-A	201	FOL	C16-C11-C12	-2.06	115.73	118.58
4	146-A	204	NAP	O2A-PA-O5B	-2.05	98.45	108.14
4	88-A	204	NAP	N3A-C2A-N1A	-2.05	127.07	128.86
2	63-A	201	FOL	C7-C6-N5	-2.05	119.45	120.80
2	57-A	201	FOL	C9-C6-C7	-2.05	117.91	121.38
2	35-A	201	FOL	C13-C14-N10	-2.04	116.91	121.03
2	151-A	201	FOL	O-C-N	-2.04	118.73	122.46
2	31-A	201	FOL	C7-C6-N5	-2.04	119.46	120.80
4	19-A	204	NAP	O2A-PA-O5B	-2.04	98.51	108.14
2	6-A	201	FOL	C6-N5-C4A	-2.04	116.00	118.44
2	147-A	201	FOL	O-C-C11	-2.04	117.33	120.94
2	47-A	201	FOL	C6-N5-C4A	-2.03	116.00	118.44
4	134-A	204	NAP	C2A-N1A-C6A	-2.03	115.22	118.77
2	112-A	201	FOL	CA-N-C	-2.03	119.37	122.15
4	29-A	204	NAP	C1B-N9A-C4A	-2.03	123.14	126.64
2	78-A	201	FOL	NA2-C2-N3	-2.03	117.78	120.26
2	53-A	201	FOL	CB-CA-CT	-2.02	109.34	112.28
4	83-A	204	NAP	N6A-C6A-N1A	-2.02	114.75	118.77
2	120-A	201	FOL	C7-C6-N5	-2.02	119.47	120.80
4	6-A	204	NAP	C2B-C3B-C4B	-2.01	97.37	101.95
4	86-A	204	NAP	N3A-C2A-N1A	-2.01	127.10	128.86
4	32-A	204	NAP	C2A-N1A-C6A	-2.01	115.25	118.77
2	62-A	201	FOL	CB-CA-CT	-2.01	109.37	112.28
4	72-A	204	NAP	O7N-C7N-N7N	-2.01	119.73	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	156-A	201	FOL	NA2-C2-N3	-2.01	117.81	120.26
4	92-A	204	NAP	C2D-C3D-C4D	2.00	106.52	102.62
4	97-A	204	NAP	O3B-C3B-C2B	2.00	116.87	111.18
4	106-A	204	NAP	O2A-PA-O1A	2.00	122.64	112.28
2	97-A	201	FOL	CG-CB-CA	2.00	117.19	113.19
2	121-A	201	FOL	C9-N10-C14	2.00	127.44	122.25
4	51-A	204	NAP	O5B-PA-O1A	2.01	117.34	109.25
4	89-A	204	NAP	C2D-C3D-C4D	2.01	106.53	102.62
2	45-A	201	FOL	C8A-C4A-N5	2.01	122.90	120.59
2	164-A	201	FOL	C9-N10-C14	2.01	127.45	122.25
4	10-A	204	NAP	O3B-C3B-C2B	2.01	116.89	111.18
2	45-A	201	FOL	C9-N10-C14	2.01	127.45	122.25
4	69-A	204	NAP	O3B-C3B-C2B	2.01	116.89	111.18
2	61-A	201	FOL	CB-CA-N	2.01	113.28	110.22
4	86-A	204	NAP	O3X-P2B-O2X	2.01	115.72	107.61
4	51-A	204	NAP	C2N-C3N-C4N	2.01	120.55	118.26
2	71-A	201	FOL	C4-C4A-N5	2.01	120.88	118.68
2	158-A	201	FOL	C9-N10-C14	2.01	127.46	122.25
4	40-A	204	NAP	C4B-O4B-C1B	2.01	111.91	109.77
4	92-A	204	NAP	O3B-C3B-C2B	2.01	116.90	111.18
2	3-A	201	FOL	C8A-C4A-N5	2.01	122.91	120.59
2	38-A	201	FOL	C7-N8-C8A	2.01	119.55	116.70
4	2-A	204	NAP	C2N-C3N-C4N	2.01	120.56	118.26
4	72-A	204	NAP	C2N-C3N-C4N	2.01	120.56	118.26
4	163-A	204	NAP	C2N-C3N-C4N	2.01	120.56	118.26
2	83-A	201	FOL	N1-C8A-N8	2.01	119.97	116.42
4	58-A	204	NAP	O3B-C3B-C2B	2.02	116.91	111.18
2	141-A	201	FOL	C4-C4A-N5	2.02	120.89	118.68
4	23-A	204	NAP	C2N-C3N-C4N	2.02	120.56	118.26
2	84-A	201	FOL	C8A-C4A-N5	2.02	122.91	120.59
2	152-A	201	FOL	C4-C4A-N5	2.02	120.89	118.68
4	11-A	204	NAP	O7N-C7N-C3N	2.02	121.98	119.62
4	13-A	204	NAP	C2N-C3N-C4N	2.02	120.56	118.26
4	104-A	204	NAP	O3B-C3B-C2B	2.02	116.92	111.18
4	10-A	204	NAP	O5B-PA-O1A	2.02	117.40	109.25
2	56-A	201	FOL	C9-N10-C14	2.02	127.48	122.25
2	100-A	201	FOL	C4-C4A-N5	2.02	120.90	118.68
2	36-A	201	FOL	C9-N10-C14	2.02	127.49	122.25
2	94-A	201	FOL	C11-C-N	2.02	120.70	116.97
2	151-A	201	FOL	C4-C4A-N5	2.02	120.90	118.68
2	137-A	201	FOL	C9-N10-C14	2.02	127.49	122.25
4	143-A	204	NAP	C2N-C3N-C4N	2.02	120.57	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	91-A	201	FOL	C9-N10-C14	2.02	127.50	122.25
4	156-A	204	NAP	C2D-C3D-C4D	2.03	106.56	102.62
2	28-A	201	FOL	N1-C8A-N8	2.03	119.99	116.42
4	155-A	204	NAP	O2A-PA-O1A	2.03	122.77	112.28
4	131-A	204	NAP	C2N-C3N-C4N	2.03	120.57	118.26
2	92-A	201	FOL	C8A-C4A-N5	2.03	122.93	120.59
2	31-A	201	FOL	C9-N10-C14	2.03	127.51	122.25
4	112-A	204	NAP	C2D-C3D-C4D	2.03	106.57	102.62
2	106-A	201	FOL	C8A-C4A-N5	2.03	122.93	120.59
2	31-A	201	FOL	CB-CA-N	2.03	113.31	110.22
2	159-A	201	FOL	C6-C9-N10	2.03	117.69	113.15
4	138-A	204	NAP	C5A-C6A-N6A	2.03	124.61	120.47
4	11-A	204	NAP	O5B-PA-O1A	2.03	117.45	109.25
4	27-A	204	NAP	C4B-O4B-C1B	2.03	111.93	109.77
2	22-A	201	FOL	C4-C4A-N5	2.03	120.91	118.68
4	86-A	204	NAP	O3B-C3B-C2B	2.03	116.96	111.18
4	1-A	204	NAP	C4B-O4B-C1B	2.03	111.93	109.77
2	19-A	201	FOL	C9-N10-C14	2.03	127.52	122.25
2	167-A	201	FOL	N1-C8A-N8	2.03	120.00	116.42
2	66-A	201	FOL	C9-N10-C14	2.03	127.52	122.25
4	4-A	204	NAP	C4B-O4B-C1B	2.04	111.94	109.77
2	160-A	201	FOL	C9-N10-C14	2.04	127.53	122.25
4	155-A	204	NAP	O5B-PA-O1A	2.04	117.46	109.25
2	147-A	201	FOL	CB-CA-N	2.04	113.32	110.22
2	106-A	201	FOL	O-C-C11	2.04	124.56	120.94
4	36-A	204	NAP	C4B-O4B-C1B	2.04	111.94	109.77
4	55-A	204	NAP	O3B-C3B-C2B	2.04	116.98	111.18
2	142-A	201	FOL	C9-N10-C14	2.04	127.54	122.25
4	6-A	204	NAP	O2X-P2B-O1X	2.04	118.49	110.50
2	20-A	201	FOL	C9-N10-C14	2.04	127.55	122.25
2	164-A	201	FOL	CA-N-C	2.05	124.95	122.15
4	33-A	204	NAP	O5B-PA-O1A	2.05	117.50	109.25
4	100-A	204	NAP	C2N-C3N-C4N	2.05	120.59	118.26
4	41-A	204	NAP	C4B-O4B-C1B	2.05	111.95	109.77
4	93-A	204	NAP	C2D-C3D-C4D	2.05	106.61	102.62
2	121-A	201	FOL	C4-C4A-N5	2.05	120.92	118.68
2	4-A	201	FOL	C15-C16-C11	2.05	123.08	120.79
2	164-A	201	FOL	C4-C4A-N5	2.05	120.93	118.68
4	159-A	204	NAP	O5B-PA-O1A	2.05	117.52	109.25
4	76-A	204	NAP	C2N-C3N-C4N	2.05	120.60	118.26
2	71-A	201	FOL	C9-N10-C14	2.05	127.57	122.25
4	21-A	204	NAP	O5B-PA-O1A	2.05	117.53	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	201	FOL	CB-CA-N	2.05	113.34	110.22
4	142-A	204	NAP	O3X-P2B-O2X	2.05	115.90	107.61
2	120-A	201	FOL	C4-C4A-N5	2.05	120.93	118.68
2	167-A	201	FOL	C4-C4A-N5	2.06	120.93	118.68
2	144-A	201	FOL	C9-N10-C14	2.06	127.58	122.25
2	137-A	201	FOL	C8A-C4A-N5	2.06	122.96	120.59
2	120-A	201	FOL	C15-C14-N10	2.06	125.18	121.03
4	125-A	204	NAP	C2N-C3N-C4N	2.06	120.61	118.26
2	164-A	201	FOL	N1-C8A-N8	2.06	120.05	116.42
4	105-A	204	NAP	C3N-C7N-N7N	2.06	120.13	117.77
2	65-A	201	FOL	N1-C8A-N8	2.06	120.05	116.42
4	68-A	204	NAP	O5B-PA-O1A	2.06	117.56	109.25
2	147-A	201	FOL	O-C-N	2.06	126.23	122.46
4	70-A	204	NAP	C2N-C3N-C4N	2.06	120.61	118.26
2	65-A	201	FOL	C6-C7-N8	2.06	125.18	123.09
4	119-A	204	NAP	O2A-PA-O1A	2.06	122.96	112.28
4	122-A	204	NAP	N6A-C6A-N1A	2.07	122.86	118.77
4	65-A	204	NAP	O3B-C3B-C2B	2.07	117.07	111.18
4	4-A	204	NAP	O3B-C3B-C2B	2.07	117.07	111.18
4	16-A	204	NAP	C4B-O4B-C1B	2.07	111.97	109.77
4	9-A	204	NAP	O2A-PA-O1A	2.07	123.00	112.28
4	107-A	204	NAP	O2A-PA-O1A	2.07	123.01	112.28
4	47-A	204	NAP	C2D-C3D-C4D	2.07	106.66	102.62
4	34-A	204	NAP	C2D-C3D-C4D	2.07	106.66	102.62
2	55-A	201	FOL	C9-N10-C14	2.07	127.62	122.25
2	105-A	201	FOL	CG-CB-CA	2.07	117.33	113.19
4	159-A	204	NAP	O2A-PA-O1A	2.08	123.03	112.28
2	155-A	201	FOL	C8A-C4A-N5	2.08	122.98	120.59
4	116-A	204	NAP	O5B-PA-O1A	2.08	117.64	109.25
4	118-A	204	NAP	C2N-C3N-C4N	2.08	120.63	118.26
4	134-A	204	NAP	O3B-C3B-C2B	2.08	117.09	111.18
2	97-A	201	FOL	CA-N-C	2.08	125.00	122.15
4	94-A	204	NAP	O3B-C3B-C2B	2.08	117.10	111.18
2	52-A	201	FOL	O-C-C11	2.08	124.63	120.94
2	64-A	201	FOL	C9-N10-C14	2.08	127.64	122.25
4	78-A	204	NAP	C2N-C3N-C4N	2.08	120.64	118.26
4	21-A	204	NAP	O2A-PA-O1A	2.08	123.06	112.28
4	33-A	204	NAP	O2N-PN-O1N	2.08	123.07	112.28
4	43-A	204	NAP	C2D-C3D-C4D	2.09	106.68	102.62
2	10-A	201	FOL	C6-C9-N10	2.09	117.82	113.15
2	45-A	201	FOL	C11-C-N	2.09	120.82	116.97
2	134-A	201	FOL	C9-N10-C14	2.09	127.66	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2-A	204	NAP	O5B-PA-O1A	2.09	117.68	109.25
4	149-A	204	NAP	O5B-PA-O1A	2.09	117.69	109.25
4	121-A	204	NAP	O2A-PA-O1A	2.09	123.11	112.28
4	41-A	204	NAP	O3B-C3B-C2B	2.09	117.13	111.18
4	157-A	204	NAP	C2N-C3N-C4N	2.09	120.65	118.26
2	36-A	201	FOL	C15-C16-C11	2.09	123.13	120.79
4	72-A	204	NAP	O3B-C3B-C2B	2.09	117.14	111.18
4	146-A	204	NAP	C2D-C3D-C4D	2.10	106.70	102.62
4	37-A	204	NAP	O5B-PA-O1A	2.10	117.71	109.25
2	19-A	201	FOL	C4-C4A-N5	2.10	120.98	118.68
2	48-A	201	FOL	C9-C6-N5	2.10	120.53	116.58
2	69-A	201	FOL	C4-C4A-N5	2.10	120.98	118.68
2	93-A	201	FOL	C8A-C4A-N5	2.10	123.01	120.59
4	19-A	204	NAP	O3X-P2B-O2X	2.10	116.08	107.61
4	71-A	204	NAP	O5B-PA-O1A	2.10	117.72	109.25
2	55-A	201	FOL	CA-N-C	2.10	125.03	122.15
2	67-A	201	FOL	C8A-C4A-N5	2.10	123.01	120.59
2	80-A	201	FOL	C6-C7-N8	2.10	125.22	123.09
4	65-A	204	NAP	O5B-PA-O1A	2.10	117.72	109.25
2	95-A	201	FOL	O-C-C11	2.10	124.67	120.94
4	49-A	204	NAP	O5B-C5B-C4B	2.10	116.45	109.00
4	136-A	204	NAP	O3X-P2B-O2X	2.10	116.09	107.61
4	105-A	204	NAP	O3B-C3B-C2B	2.10	117.16	111.18
2	64-A	201	FOL	C4-C4A-N5	2.10	120.99	118.68
4	149-A	204	NAP	C2N-C3N-C4N	2.11	120.66	118.26
4	113-A	204	NAP	C2D-C3D-C4D	2.11	106.72	102.62
2	86-A	201	FOL	CB-CA-N	2.11	113.42	110.22
4	98-A	204	NAP	O3B-C3B-C2B	2.11	117.17	111.18
2	147-A	201	FOL	CA-N-C	2.11	125.04	122.15
4	106-A	204	NAP	O5B-PA-O1A	2.11	117.75	109.25
2	87-A	201	FOL	C8A-C4A-N5	2.11	123.02	120.59
2	76-A	201	FOL	C7-C6-N5	2.11	122.19	120.80
4	39-A	204	NAP	O5B-PA-O1A	2.11	117.77	109.25
4	151-A	204	NAP	O5B-PA-O1A	2.11	117.77	109.25
4	114-A	204	NAP	C2N-C3N-C4N	2.11	120.67	118.26
4	82-A	204	NAP	C2N-C3N-C4N	2.11	120.67	118.26
2	13-A	201	FOL	C7-N8-C8A	2.11	119.69	116.70
4	47-A	204	NAP	C2N-C3N-C4N	2.11	120.67	118.26
4	12-A	204	NAP	C2N-C3N-C4N	2.11	120.67	118.26
2	37-A	201	FOL	C7-N8-C8A	2.11	119.69	116.70
2	68-A	201	FOL	C9-N10-C14	2.12	127.73	122.25
4	100-A	204	NAP	O5B-PA-O1A	2.12	117.79	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	114-A	204	NAP	C2D-C3D-C4D	2.12	106.74	102.62
2	88-A	201	FOL	C9-N10-C14	2.12	127.74	122.25
4	131-A	204	NAP	O2N-PN-O1N	2.12	123.24	112.28
2	63-A	201	FOL	C11-C-N	2.12	120.88	116.97
4	91-A	204	NAP	C2N-C3N-C4N	2.12	120.68	118.26
4	138-A	204	NAP	C2N-C3N-C4N	2.12	120.68	118.26
4	44-A	204	NAP	C2N-C3N-C4N	2.12	120.68	118.26
4	142-A	204	NAP	C2N-C3N-C4N	2.13	120.69	118.26
4	85-A	204	NAP	O5B-PA-O1A	2.13	117.83	109.25
4	93-A	204	NAP	O3B-C3B-C2B	2.13	117.23	111.18
4	3-A	204	NAP	O3B-C3B-C2B	2.13	117.23	111.18
2	139-A	201	FOL	C8A-C4A-N5	2.13	123.04	120.59
2	102-A	201	FOL	C11-C-N	2.13	120.90	116.97
4	48-A	204	NAP	O5B-PA-O1A	2.13	117.84	109.25
2	80-A	201	FOL	C8A-C4A-N5	2.13	123.05	120.59
4	147-A	204	NAP	O3B-C3B-C2B	2.13	117.24	111.18
2	73-A	201	FOL	C9-N10-C14	2.13	127.78	122.25
4	22-A	204	NAP	O3B-C3B-C2B	2.13	117.25	111.18
4	125-A	204	NAP	O5B-PA-O1A	2.13	117.86	109.25
2	34-A	201	FOL	C6-C9-N10	2.14	117.93	113.15
4	145-A	204	NAP	C2N-C3N-C4N	2.14	120.70	118.26
2	50-A	201	FOL	C9-N10-C14	2.14	127.78	122.25
4	90-A	204	NAP	C4B-O4B-C1B	2.14	112.04	109.77
4	1-A	204	NAP	C2D-C3D-C4D	2.14	106.78	102.62
4	34-A	204	NAP	O3B-C3B-C2B	2.14	117.27	111.18
4	17-A	204	NAP	O5B-PA-O1A	2.14	117.89	109.25
2	69-A	201	FOL	C11-C-N	2.14	120.92	116.97
4	106-A	204	NAP	C2N-C3N-C4N	2.14	120.70	118.26
2	116-A	201	FOL	CB-CA-N	2.14	113.48	110.22
4	59-A	204	NAP	O2A-PA-O1A	2.14	123.37	112.28
4	73-A	204	NAP	O3B-C3B-C2B	2.14	117.28	111.18
4	6-A	204	NAP	O2N-PN-O1N	2.14	123.38	112.28
4	8-A	204	NAP	O2N-PN-O1N	2.14	123.38	112.28
4	155-A	204	NAP	O3B-C3B-C2B	2.15	117.28	111.18
4	127-A	204	NAP	C4B-O4B-C1B	2.15	112.05	109.77
2	160-A	201	FOL	CG-CB-CA	2.15	117.47	113.19
2	154-A	201	FOL	N1-C8A-N8	2.15	120.20	116.42
2	128-A	201	FOL	C8A-C4A-N5	2.15	123.06	120.59
4	110-A	204	NAP	C2N-C3N-C4N	2.15	120.71	118.26
4	72-A	204	NAP	O2A-PA-O1A	2.15	123.40	112.28
2	89-A	201	FOL	C4-C4A-N5	2.15	121.04	118.68
2	124-A	201	FOL	C9-N10-C14	2.15	127.82	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	14-A	204	NAP	C2N-C3N-C4N	2.15	120.72	118.26
4	71-A	204	NAP	O3B-C3B-C2B	2.15	117.31	111.18
4	145-A	204	NAP	O5B-PA-O1A	2.15	117.94	109.25
4	26-A	204	NAP	O3B-C3B-C2B	2.15	117.31	111.18
4	87-A	204	NAP	O3B-C3B-C2B	2.16	117.31	111.18
2	24-A	201	FOL	C8A-C4A-N5	2.16	123.08	120.59
2	61-A	201	FOL	C8A-C4A-N5	2.16	123.08	120.59
2	33-A	201	FOL	C4-C4A-N5	2.16	121.05	118.68
4	74-A	204	NAP	C2N-C3N-C4N	2.16	120.72	118.26
4	99-A	204	NAP	C5A-C6A-N6A	2.16	124.87	120.47
4	106-A	204	NAP	O3B-C3B-C2B	2.16	117.32	111.18
4	162-A	204	NAP	O3B-C3B-C2B	2.16	117.32	111.18
4	88-A	204	NAP	C5A-C6A-N6A	2.16	124.87	120.47
4	142-A	204	NAP	O3B-C3B-C2B	2.16	117.33	111.18
4	18-A	204	NAP	O5B-PA-O1A	2.16	117.97	109.25
4	67-A	204	NAP	C4B-O4B-C1B	2.16	112.07	109.77
2	83-A	201	FOL	CG-CB-CA	2.16	117.51	113.19
2	118-A	201	FOL	O-C-C11	2.16	124.78	120.94
4	146-A	204	NAP	O2A-PA-O1A	2.16	123.48	112.28
4	64-A	204	NAP	O5B-PA-O1A	2.16	117.98	109.25
2	48-A	201	FOL	C6-C9-N10	2.17	118.00	113.15
4	62-A	204	NAP	C2N-C3N-C4N	2.17	120.73	118.26
4	118-A	204	NAP	O3B-C3B-C2B	2.17	117.34	111.18
2	78-A	201	FOL	C15-C14-N10	2.17	125.40	121.03
4	34-A	204	NAP	O2A-PA-O1A	2.17	123.50	112.28
4	4-A	204	NAP	C2D-C3D-C4D	2.17	106.84	102.62
4	83-A	204	NAP	O2N-PN-O1N	2.17	123.51	112.28
4	112-A	204	NAP	O2A-PA-O1A	2.17	123.52	112.28
4	144-A	204	NAP	O2A-PA-O1A	2.17	123.52	112.28
4	45-A	204	NAP	C2N-C3N-C4N	2.17	120.74	118.26
2	141-A	201	FOL	C9-N10-C14	2.17	127.88	122.25
4	113-A	204	NAP	O3B-C3B-C2B	2.17	117.36	111.18
4	53-A	204	NAP	O5B-PA-O1A	2.17	118.02	109.25
4	108-A	204	NAP	O2X-P2B-O1X	2.17	119.01	110.50
4	54-A	204	NAP	C4B-O4B-C1B	2.17	112.08	109.77
4	30-A	204	NAP	O5B-PA-O1A	2.17	118.02	109.25
2	114-A	201	FOL	C4-C4A-N5	2.18	121.06	118.68
4	77-A	204	NAP	C2N-C3N-C4N	2.18	120.74	118.26
4	12-A	204	NAP	C2D-C3D-C4D	2.18	106.86	102.62
4	127-A	204	NAP	O3B-C3B-C2B	2.18	117.37	111.18
2	1-A	201	FOL	C8A-C4A-N5	2.18	123.10	120.59
2	2-A	201	FOL	CB-CA-N	2.18	113.53	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	62-A	204	NAP	C4B-O4B-C1B	2.18	112.09	109.77
4	137-A	204	NAP	O3B-C3B-C2B	2.18	117.38	111.18
2	136-A	201	FOL	C4-C4A-N5	2.18	121.07	118.68
2	139-A	201	FOL	N1-C8A-N8	2.18	120.26	116.42
4	69-A	204	NAP	O5B-PA-O1A	2.18	118.05	109.25
4	8-A	204	NAP	C2N-C3N-C4N	2.18	120.75	118.26
4	89-A	204	NAP	O2A-PA-O1A	2.19	123.59	112.28
4	61-A	204	NAP	C2N-C3N-C4N	2.19	120.75	118.26
4	66-A	204	NAP	O3B-C3B-C2B	2.19	117.40	111.18
4	70-A	204	NAP	O3B-C3B-C2B	2.19	117.40	111.18
4	85-A	204	NAP	C2D-C3D-C4D	2.19	106.88	102.62
2	94-A	201	FOL	C4-C4A-N5	2.19	121.08	118.68
2	75-A	201	FOL	C8A-C4A-N5	2.19	123.11	120.59
4	40-A	204	NAP	C2N-C3N-C4N	2.19	120.76	118.26
4	145-A	204	NAP	O2A-PA-O1A	2.19	123.62	112.28
2	91-A	201	FOL	CA-N-C	2.19	125.15	122.15
4	85-A	204	NAP	O3B-C3B-C2B	2.19	117.42	111.18
4	39-A	204	NAP	O3B-C3B-C2B	2.19	117.42	111.18
4	66-A	204	NAP	O5B-PA-O1A	2.19	118.09	109.25
4	160-A	204	NAP	O3B-C3B-C2B	2.19	117.42	111.18
2	115-A	201	FOL	CG-CB-CA	2.20	117.57	113.19
4	92-A	204	NAP	O5B-PA-O1A	2.20	118.11	109.25
2	129-A	201	FOL	N1-C8A-N8	2.20	120.29	116.42
4	63-A	204	NAP	C2N-C3N-C4N	2.20	120.77	118.26
2	88-A	201	FOL	C8A-C4A-N5	2.20	123.12	120.59
2	24-A	201	FOL	C4-C4A-N5	2.20	121.09	118.68
4	116-A	204	NAP	C3N-C7N-N7N	2.20	120.28	117.77
4	146-A	204	NAP	O5B-PA-O1A	2.20	118.12	109.25
4	21-A	204	NAP	C2D-C3D-C4D	2.20	106.90	102.62
4	30-A	204	NAP	C2D-C3D-C4D	2.20	106.90	102.62
4	37-A	204	NAP	O2N-PN-O1N	2.20	123.67	112.28
4	151-A	204	NAP	C2D-C3D-C4D	2.20	106.91	102.62
2	119-A	201	FOL	N1-C8A-N8	2.20	120.30	116.42
4	72-A	204	NAP	O5B-PA-O1A	2.20	118.13	109.25
4	156-A	204	NAP	O2A-PA-O1A	2.20	123.68	112.28
2	18-A	201	FOL	C4-C4A-N5	2.20	121.10	118.68
4	27-A	204	NAP	C2N-C3N-C4N	2.20	120.78	118.26
4	9-A	204	NAP	C2N-C3N-C4N	2.20	120.78	118.26
4	91-A	204	NAP	O3B-C3B-C2B	2.20	117.45	111.18
4	24-A	204	NAP	O5B-PA-O1A	2.21	118.15	109.25
4	67-A	204	NAP	O5B-PA-O1A	2.21	118.16	109.25
4	71-A	204	NAP	O2A-PA-O1A	2.21	123.71	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	46-A	204	NAP	O3B-C3B-C2B	2.21	117.46	111.18
4	108-A	204	NAP	O2N-PN-O1N	2.21	123.72	112.28
2	128-A	201	FOL	C11-C-N	2.21	121.05	116.97
2	25-A	201	FOL	CA-N-C	2.21	125.18	122.15
4	107-A	204	NAP	C2N-C3N-C4N	2.21	120.79	118.26
4	109-A	204	NAP	O3B-C3B-C2B	2.22	117.48	111.18
4	41-A	204	NAP	C2D-C3D-C4D	2.22	106.93	102.62
2	5-A	201	FOL	C9-N10-C14	2.22	127.99	122.25
4	20-A	204	NAP	O2A-PA-O1A	2.22	123.75	112.28
4	111-A	204	NAP	O3B-C3B-C2B	2.22	117.48	111.18
4	40-A	204	NAP	O3B-C3B-C2B	2.22	117.49	111.18
4	55-A	204	NAP	C2N-C3N-C4N	2.22	120.79	118.26
4	147-A	204	NAP	O5B-PA-O1A	2.22	118.20	109.25
2	129-A	201	FOL	CG-CB-CA	2.22	117.62	113.19
4	82-A	204	NAP	O2N-PN-O1N	2.22	123.77	112.28
2	20-A	201	FOL	CB-CA-N	2.22	113.60	110.22
2	79-A	201	FOL	C8A-C4A-N5	2.22	123.15	120.59
4	101-A	204	NAP	O5B-PA-O1A	2.22	118.22	109.25
4	24-A	204	NAP	O2N-PN-O1N	2.22	123.79	112.28
4	139-A	204	NAP	O3B-C3B-C2B	2.22	117.50	111.18
4	114-A	204	NAP	O5B-PA-O1A	2.22	118.22	109.25
4	141-A	204	NAP	O3B-C3B-C2B	2.22	117.51	111.18
4	52-A	204	NAP	O2A-PA-O1A	2.22	123.80	112.28
2	105-A	201	FOL	C9-N10-C14	2.23	128.02	122.25
2	33-A	201	FOL	C6-C9-N10	2.23	118.13	113.15
4	88-A	204	NAP	O2A-PA-O1A	2.23	123.81	112.28
4	46-A	204	NAP	O5B-PA-O1A	2.23	118.24	109.25
2	124-A	201	FOL	N1-C8A-N8	2.23	120.35	116.42
4	66-A	204	NAP	C2N-C3N-C4N	2.23	120.80	118.26
4	122-A	204	NAP	O3B-C3B-C2B	2.23	117.53	111.18
4	121-A	204	NAP	O5B-PA-O1A	2.23	118.25	109.25
4	2-A	204	NAP	O3B-C3B-C2B	2.23	117.53	111.18
2	152-A	201	FOL	N1-C8A-N8	2.23	120.35	116.42
4	166-A	204	NAP	O3B-C3B-C2B	2.23	117.53	111.18
2	159-A	201	FOL	C8A-C4A-N5	2.23	123.16	120.59
4	105-A	204	NAP	O5B-PA-O1A	2.23	118.26	109.25
2	118-A	201	FOL	CG-CB-CA	2.23	117.65	113.19
4	97-A	204	NAP	C2N-C3N-C4N	2.23	120.81	118.26
2	60-A	201	FOL	C8A-C4A-N5	2.24	123.17	120.59
2	57-A	201	FOL	C15-C16-C11	2.24	123.29	120.79
4	102-A	204	NAP	O3B-C3B-C2B	2.24	117.54	111.18
4	5-A	204	NAP	O2A-PA-O1A	2.24	123.87	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	70-A	204	NAP	O5B-PA-O1A	2.24	118.28	109.25
2	9-A	201	FOL	CB-CA-N	2.24	113.63	110.22
4	96-A	204	NAP	O2A-PA-O1A	2.24	123.88	112.28
4	146-A	204	NAP	O3B-C3B-C2B	2.24	117.56	111.18
2	17-A	201	FOL	C8A-C4A-N5	2.24	123.17	120.59
4	92-A	204	NAP	C2N-C3N-C4N	2.24	120.82	118.26
2	118-A	201	FOL	C12-C13-C14	2.24	122.92	120.30
4	19-A	204	NAP	C2N-C3N-C4N	2.24	120.82	118.26
4	118-A	204	NAP	O2A-PA-O1A	2.24	123.90	112.28
2	24-A	201	FOL	C15-C14-N10	2.25	125.56	121.03
2	90-A	201	FOL	CB-CA-N	2.25	113.63	110.22
4	124-A	204	NAP	C2N-C3N-C4N	2.25	120.82	118.26
4	7-A	204	NAP	O3B-C3B-C2B	2.25	117.58	111.18
4	70-A	204	NAP	O2A-PA-O1A	2.25	123.93	112.28
4	159-A	204	NAP	C2N-C3N-C4N	2.25	120.83	118.26
4	20-A	204	NAP	C2N-C3N-C4N	2.25	120.83	118.26
4	164-A	204	NAP	O3B-C3B-C2B	2.25	117.59	111.18
4	18-A	204	NAP	O2A-PA-O1A	2.25	123.94	112.28
2	134-A	201	FOL	C8A-C4A-N5	2.25	123.19	120.59
2	63-A	201	FOL	C8A-C4A-N5	2.25	123.19	120.59
2	59-A	201	FOL	C6-C7-N8	2.25	125.37	123.09
2	112-A	201	FOL	C9-N10-C14	2.25	128.09	122.25
4	88-A	204	NAP	O3B-C3B-C2B	2.26	117.59	111.18
4	63-A	204	NAP	O2A-PA-O1A	2.26	123.95	112.28
4	16-A	204	NAP	O5B-PA-O1A	2.26	118.35	109.25
4	160-A	204	NAP	O2A-PA-O1A	2.26	123.96	112.28
4	95-A	204	NAP	C2D-C3D-C4D	2.26	107.01	102.62
4	43-A	204	NAP	O2A-PA-O1A	2.26	123.97	112.28
4	71-A	204	NAP	C2D-C3D-C4D	2.26	107.02	102.62
4	101-A	204	NAP	C2N-C3N-C4N	2.26	120.84	118.26
4	161-A	204	NAP	O3B-C3B-C2B	2.26	117.61	111.18
4	134-A	204	NAP	O2N-PN-O1N	2.26	123.98	112.28
2	143-A	201	FOL	N1-C8A-N8	2.26	120.41	116.42
2	54-A	201	FOL	CA-N-C	2.26	125.25	122.15
4	144-A	204	NAP	O5B-PA-O1A	2.26	118.38	109.25
4	4-A	204	NAP	C2N-C3N-C4N	2.27	120.84	118.26
4	121-A	204	NAP	O3B-C3B-C2B	2.27	117.62	111.18
4	153-A	204	NAP	O5B-PA-O1A	2.27	118.39	109.25
2	74-A	201	FOL	C8A-C4A-N5	2.27	123.20	120.59
2	133-A	201	FOL	N1-C8A-N8	2.27	120.42	116.42
4	112-A	204	NAP	C2N-C3N-C4N	2.27	120.85	118.26
4	123-A	204	NAP	O3B-C3B-C2B	2.27	117.63	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	156-A	204	NAP	O3B-C3B-C2B	2.27	117.64	111.18
4	162-A	204	NAP	O2A-PA-O1A	2.27	124.03	112.28
4	40-A	204	NAP	C2D-C3D-C4D	2.27	107.04	102.62
4	120-A	204	NAP	O5B-PA-O1A	2.27	118.41	109.25
2	95-A	201	FOL	C8A-C4A-N5	2.27	123.21	120.59
4	111-A	204	NAP	C2N-C3N-C4N	2.27	120.85	118.26
2	37-A	201	FOL	N1-C8A-N8	2.27	120.42	116.42
4	12-A	204	NAP	C4B-O4B-C1B	2.27	112.19	109.77
2	143-A	201	FOL	C9-N10-C14	2.27	128.14	122.25
4	129-A	204	NAP	C4B-O4B-C1B	2.27	112.19	109.77
4	98-A	204	NAP	C2N-C3N-C4N	2.27	120.86	118.26
4	44-A	204	NAP	O2A-PA-O1A	2.27	124.05	112.28
2	78-A	201	FOL	C8A-C4A-N5	2.27	123.21	120.59
4	22-A	204	NAP	O2A-PA-O1A	2.28	124.06	112.28
2	23-A	201	FOL	C4-N3-C2	2.28	119.60	116.17
2	19-A	201	FOL	N1-C8A-N8	2.28	120.43	116.42
4	107-A	204	NAP	O2N-PN-O1N	2.28	124.06	112.28
4	148-A	204	NAP	O5B-PA-O1A	2.28	118.43	109.25
2	6-A	201	FOL	CA-N-C	2.28	125.27	122.15
4	28-A	204	NAP	C4B-O4B-C1B	2.28	112.19	109.77
4	118-A	204	NAP	C4B-O4B-C1B	2.28	112.19	109.77
4	117-A	204	NAP	O3B-C3B-C2B	2.28	117.66	111.18
4	45-A	204	NAP	O3B-C3B-C2B	2.28	117.66	111.18
4	105-A	204	NAP	O2A-PA-O1A	2.28	124.06	112.28
2	62-A	201	FOL	C8A-C4A-N5	2.28	123.22	120.59
2	107-A	201	FOL	C9-N10-C14	2.28	128.16	122.25
4	47-A	204	NAP	O2A-PA-O1A	2.28	124.08	112.28
2	99-A	201	FOL	C9-N10-C14	2.28	128.16	122.25
4	84-A	204	NAP	O2A-PA-O1A	2.28	124.09	112.28
2	6-A	201	FOL	C9-C6-N5	2.28	120.88	116.58
4	25-A	204	NAP	C4B-O4B-C1B	2.28	112.20	109.77
2	107-A	201	FOL	C4-C4A-N5	2.28	121.18	118.68
4	91-A	204	NAP	O5B-PA-O1A	2.28	118.46	109.25
4	140-A	204	NAP	O2A-PA-O1A	2.28	124.11	112.28
4	11-A	204	NAP	C2D-C3D-C4D	2.29	107.07	102.62
4	109-A	204	NAP	O2N-PN-O1N	2.29	124.11	112.28
4	50-A	204	NAP	C2N-C3N-C4N	2.29	120.87	118.26
2	108-A	201	FOL	C8A-C4A-N5	2.29	123.23	120.59
4	115-A	204	NAP	C5A-C6A-N6A	2.29	125.14	120.47
4	152-A	204	NAP	O5B-PA-O1A	2.29	118.49	109.25
4	143-A	204	NAP	O5B-PA-O1A	2.29	118.49	109.25
4	115-A	204	NAP	O5B-PA-O1A	2.29	118.49	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	17-A	204	NAP	O3B-C3B-C2B	2.29	117.70	111.18
4	79-A	204	NAP	C2D-C3D-C4D	2.29	107.08	102.62
2	8-A	201	FOL	N1-C8A-N8	2.29	120.46	116.42
4	151-A	204	NAP	O3B-C3B-C2B	2.29	117.70	111.18
4	90-A	204	NAP	O2A-PA-O1A	2.29	124.16	112.28
4	3-A	204	NAP	C4B-O4B-C1B	2.30	112.21	109.77
4	102-A	204	NAP	C4B-O4B-C1B	2.30	112.21	109.77
4	74-A	204	NAP	O5B-PA-O1A	2.30	118.51	109.25
4	157-A	204	NAP	O3B-C3B-C2B	2.30	117.71	111.18
2	57-A	201	FOL	N1-C8A-N8	2.30	120.47	116.42
2	76-A	201	FOL	C9-C6-N5	2.30	120.91	116.58
2	131-A	201	FOL	CG-CB-CA	2.30	117.78	113.19
2	5-A	201	FOL	CB-CA-N	2.30	113.72	110.22
4	62-A	204	NAP	O2A-PA-O1A	2.30	124.19	112.28
4	25-A	204	NAP	O5B-PA-O1A	2.30	118.54	109.25
2	129-A	201	FOL	C9-N10-C14	2.30	128.22	122.25
2	29-A	201	FOL	C9-N10-C14	2.31	128.22	122.25
4	1-A	204	NAP	O5B-PA-O1A	2.31	118.55	109.25
4	47-A	204	NAP	O5B-PA-O1A	2.31	118.55	109.25
2	53-A	201	FOL	N1-C8A-N8	2.31	120.49	116.42
2	57-A	201	FOL	C9-C6-N5	2.31	120.93	116.58
4	141-A	204	NAP	O2A-PA-O1A	2.31	124.25	112.28
2	158-A	201	FOL	C6-C7-N8	2.31	125.43	123.09
4	102-A	204	NAP	C2N-C3N-C4N	2.31	120.90	118.26
4	150-A	204	NAP	O3B-C3B-C2B	2.31	117.76	111.18
4	10-A	204	NAP	O2A-PA-O1A	2.31	124.26	112.28
2	26-A	201	FOL	N1-C8A-N8	2.32	120.50	116.42
4	77-A	204	NAP	O5B-PA-O1A	2.32	118.59	109.25
2	121-A	201	FOL	N1-C8A-N8	2.32	120.50	116.42
4	41-A	204	NAP	O5B-PA-O1A	2.32	118.60	109.25
2	140-A	201	FOL	C9-N10-C14	2.32	128.26	122.25
4	147-A	204	NAP	O2A-PA-O1A	2.32	124.28	112.28
2	18-A	201	FOL	CB-CA-N	2.32	113.75	110.22
4	135-A	204	NAP	O3B-C3B-C2B	2.32	117.78	111.18
2	38-A	201	FOL	C8A-C4A-N5	2.32	123.26	120.59
2	97-A	201	FOL	C8A-C4A-N5	2.32	123.26	120.59
4	115-A	204	NAP	O3B-C3B-C2B	2.32	117.78	111.18
2	24-A	201	FOL	C9-N10-C14	2.32	128.26	122.25
4	124-A	204	NAP	O3B-C3B-C2B	2.32	117.79	111.18
4	26-A	204	NAP	O2A-PA-O1A	2.32	124.31	112.28
4	113-A	204	NAP	C2N-C3N-C4N	2.32	120.91	118.26
2	99-A	201	FOL	O-C-C11	2.32	125.07	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	142-A	201	FOL	CG-CB-CA	2.32	117.83	113.19
4	143-A	204	NAP	O3B-C3B-C2B	2.33	117.80	111.18
2	136-A	201	FOL	C15-C14-N10	2.33	125.72	121.03
4	116-A	204	NAP	O3B-C3B-C2B	2.33	117.81	111.18
4	23-A	204	NAP	O5B-PA-O1A	2.33	118.65	109.25
4	18-A	204	NAP	O3B-C3B-C2B	2.33	117.81	111.18
4	109-A	204	NAP	O2A-PA-O1A	2.33	124.34	112.28
4	36-A	204	NAP	O5B-PA-O1A	2.33	118.65	109.25
2	153-A	201	FOL	C8A-C4A-N5	2.33	123.28	120.59
4	124-A	204	NAP	O5B-PA-O1A	2.33	118.65	109.25
4	39-A	204	NAP	C2N-C3N-C4N	2.33	120.92	118.26
2	42-A	201	FOL	CG-CB-CA	2.33	117.84	113.19
4	19-A	204	NAP	O2A-PA-O1A	2.33	124.35	112.28
4	126-A	204	NAP	O5B-PA-O1A	2.33	118.67	109.25
4	76-A	204	NAP	O5B-PA-O1A	2.34	118.67	109.25
4	107-A	204	NAP	O5B-PA-O1A	2.34	118.68	109.25
4	100-A	204	NAP	O3B-C3B-C2B	2.34	117.83	111.18
4	105-A	204	NAP	O2N-PN-O1N	2.34	124.38	112.28
4	44-A	204	NAP	O2N-PN-O1N	2.34	124.38	112.28
4	114-A	204	NAP	O2A-PA-O1A	2.34	124.39	112.28
4	35-A	204	NAP	O5B-PA-O1A	2.34	118.69	109.25
4	12-A	204	NAP	O5B-PA-O1A	2.34	118.69	109.25
2	116-A	201	FOL	CB-CA-CT	2.34	115.69	112.28
4	158-A	204	NAP	O3B-C3B-C2B	2.34	117.84	111.18
2	70-A	201	FOL	C4-C4A-N5	2.34	121.25	118.68
4	106-A	204	NAP	O2N-PN-O1N	2.34	124.41	112.28
4	142-A	204	NAP	C5A-C6A-N6A	2.34	125.25	120.47
4	60-A	204	NAP	C2N-C3N-C4N	2.35	120.94	118.26
4	115-A	204	NAP	C2D-C3D-C4D	2.35	107.19	102.62
2	66-A	201	FOL	CB-CA-N	2.35	113.79	110.22
2	157-A	201	FOL	C6-C7-N8	2.35	125.47	123.09
2	117-A	201	FOL	N1-C8A-N8	2.35	120.56	116.42
4	24-A	204	NAP	C4B-O4B-C1B	2.35	112.27	109.77
4	141-A	204	NAP	O5B-PA-O1A	2.35	118.73	109.25
4	96-A	204	NAP	O5B-PA-O1A	2.35	118.73	109.25
4	164-A	204	NAP	O5B-PA-O1A	2.35	118.73	109.25
2	122-A	201	FOL	C4-C4A-N5	2.35	121.26	118.68
2	138-A	201	FOL	CB-CA-N	2.35	113.79	110.22
4	9-A	204	NAP	O2N-PN-O1N	2.35	124.45	112.28
4	55-A	204	NAP	O5B-PA-O1A	2.35	118.75	109.25
4	142-A	204	NAP	O2A-PA-O1A	2.36	124.48	112.28
4	163-A	204	NAP	O2A-PA-O1A	2.36	124.48	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	21-A	204	NAP	C4B-O4B-C1B	2.36	112.28	109.77
4	22-A	204	NAP	O5B-PA-O1A	2.36	118.76	109.25
4	81-A	204	NAP	O3B-C3B-C2B	2.36	117.89	111.18
4	143-A	204	NAP	O2A-PA-O1A	2.36	124.49	112.28
4	46-A	204	NAP	O2A-PA-O1A	2.36	124.49	112.28
4	75-A	204	NAP	C2N-C3N-C4N	2.36	120.95	118.26
4	13-A	204	NAP	O2A-PA-O1A	2.36	124.50	112.28
4	97-A	204	NAP	O2A-PA-O1A	2.36	124.50	112.28
4	155-A	204	NAP	C2N-C3N-C4N	2.36	120.95	118.26
4	95-A	204	NAP	O2N-PN-O1N	2.36	124.50	112.28
4	38-A	204	NAP	C2D-C3D-C4D	2.36	107.22	102.62
4	158-A	204	NAP	C5A-C6A-N6A	2.36	125.28	120.47
4	9-A	204	NAP	O3B-C3B-C2B	2.36	117.90	111.18
2	83-A	201	FOL	C15-C16-C11	2.36	123.43	120.79
4	45-A	204	NAP	O2A-PA-O1A	2.36	124.52	112.28
2	107-A	201	FOL	N1-C8A-N8	2.37	120.59	116.42
2	79-A	201	FOL	CG-CB-CA	2.37	117.91	113.19
4	73-A	204	NAP	C2N-C3N-C4N	2.37	120.96	118.26
4	20-A	204	NAP	C4B-O4B-C1B	2.37	112.29	109.77
4	37-A	204	NAP	C2N-C3N-C4N	2.37	120.96	118.26
4	21-A	204	NAP	O3B-C3B-C2B	2.37	117.91	111.18
4	86-A	204	NAP	O5B-PA-O1A	2.37	118.80	109.25
4	60-A	204	NAP	O3B-C3B-C2B	2.37	117.91	111.18
4	150-A	204	NAP	O5B-PA-O1A	2.37	118.80	109.25
4	38-A	204	NAP	O3B-C3B-C2B	2.37	117.92	111.18
4	31-A	204	NAP	O3X-P2B-O2B	2.37	116.77	106.00
4	89-A	204	NAP	O3B-C3B-C2B	2.37	117.92	111.18
4	136-A	204	NAP	O3B-C3B-C2B	2.37	117.92	111.18
4	11-A	204	NAP	O2A-PA-O1A	2.37	124.55	112.28
4	81-A	204	NAP	O2N-PN-O1N	2.37	124.55	112.28
4	55-A	204	NAP	O2A-PA-O1A	2.37	124.55	112.28
4	22-A	204	NAP	O2N-PN-O1N	2.37	124.56	112.28
4	87-A	204	NAP	O2A-PA-O1A	2.37	124.56	112.28
4	84-A	204	NAP	O3B-C3B-C2B	2.37	117.93	111.18
4	115-A	204	NAP	O2A-PA-O1A	2.37	124.56	112.28
4	34-A	204	NAP	O2N-PN-O1N	2.37	124.56	112.28
2	21-A	201	FOL	C11-C-N	2.37	121.35	116.97
4	11-A	204	NAP	O3B-C3B-C2B	2.38	117.94	111.18
4	35-A	204	NAP	O3B-C3B-C2B	2.38	117.94	111.18
4	37-A	204	NAP	O3B-C3B-C2B	2.38	117.94	111.18
2	11-A	201	FOL	C8A-C4A-N5	2.38	123.33	120.59
2	63-A	201	FOL	C9-C6-N5	2.38	121.06	116.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	96-A	201	FOL	CB-CA-N	2.38	113.84	110.22
4	117-A	204	NAP	C2N-C3N-C4N	2.38	120.97	118.26
4	110-A	204	NAP	O5B-PA-O1A	2.38	118.84	109.25
4	111-A	204	NAP	O2A-PA-O1A	2.38	124.59	112.28
4	105-A	204	NAP	C2N-C3N-C4N	2.38	120.97	118.26
4	15-A	204	NAP	O5B-PA-O1A	2.38	118.85	109.25
2	132-A	201	FOL	C8A-C4A-N5	2.38	123.33	120.59
4	91-A	204	NAP	O2N-PN-O1N	2.38	124.61	112.28
4	44-A	204	NAP	O3B-C3B-C2B	2.38	117.96	111.18
2	160-A	201	FOL	C4-C4A-N5	2.39	121.30	118.68
4	14-A	204	NAP	O2A-PA-O1A	2.39	124.63	112.28
4	136-A	204	NAP	O5B-PA-O1A	2.39	118.88	109.25
4	90-A	204	NAP	O2N-PN-O1N	2.39	124.64	112.28
4	36-A	204	NAP	O2A-PA-O1A	2.39	124.64	112.28
4	87-A	204	NAP	O2N-PN-O1N	2.39	124.66	112.28
2	151-A	201	FOL	CB-CA-N	2.39	113.86	110.22
4	49-A	204	NAP	O2A-PA-O1A	2.39	124.66	112.28
2	29-A	201	FOL	C11-C-N	2.39	121.38	116.97
4	161-A	204	NAP	O2A-PA-O1A	2.39	124.66	112.28
2	42-A	201	FOL	N1-C8A-N8	2.39	120.64	116.42
4	35-A	204	NAP	O2A-PA-O1A	2.39	124.67	112.28
4	50-A	204	NAP	O5B-PA-O1A	2.39	118.91	109.25
4	61-A	204	NAP	O2A-PA-O1A	2.39	124.67	112.28
2	136-A	201	FOL	C9-N10-C14	2.40	128.46	122.25
4	104-A	204	NAP	C2N-C3N-C4N	2.40	120.99	118.26
4	75-A	204	NAP	O3B-C3B-C2B	2.40	117.99	111.18
4	12-A	204	NAP	O2A-PA-O1A	2.40	124.68	112.28
4	114-A	204	NAP	O3B-C3B-C2B	2.40	118.00	111.18
2	4-A	201	FOL	C9-N10-C14	2.40	128.47	122.25
4	141-A	204	NAP	O2N-PN-O1N	2.40	124.70	112.28
4	161-A	204	NAP	O2N-PN-O1N	2.40	124.70	112.28
2	96-A	201	FOL	C4-C4A-N5	2.40	121.31	118.68
2	46-A	201	FOL	C4-C4A-N5	2.40	121.31	118.68
4	135-A	204	NAP	O2A-PA-O1A	2.40	124.70	112.28
4	113-A	204	NAP	O2N-PN-O1N	2.40	124.71	112.28
4	73-A	204	NAP	O5B-PA-O1A	2.40	118.94	109.25
4	80-A	204	NAP	O3B-C3B-C2B	2.40	118.02	111.18
2	141-A	201	FOL	C11-C-N	2.40	121.41	116.97
4	14-A	204	NAP	O3B-C3B-C2B	2.41	118.02	111.18
4	95-A	204	NAP	O2A-PA-O1A	2.41	124.74	112.28
4	45-A	204	NAP	O5B-PA-O1A	2.41	118.96	109.25
2	31-A	201	FOL	C8A-C4A-N5	2.41	123.36	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	55-A	204	NAP	O2N-PN-O1N	2.41	124.76	112.28
4	16-A	204	NAP	C2N-C3N-C4N	2.41	121.02	118.26
2	91-A	201	FOL	C8A-C4A-N5	2.41	123.37	120.59
4	40-A	204	NAP	O2A-PA-O1A	2.42	124.78	112.28
4	37-A	204	NAP	O2A-PA-O1A	2.42	124.78	112.28
4	167-A	204	NAP	O3B-C3B-C2B	2.42	118.05	111.18
2	62-A	201	FOL	C9-N10-C14	2.42	128.51	122.25
4	23-A	204	NAP	C4B-O4B-C1B	2.42	112.34	109.77
2	74-A	201	FOL	N1-C8A-N8	2.42	120.68	116.42
4	96-A	204	NAP	O2N-PN-O1N	2.42	124.79	112.28
2	80-A	201	FOL	O-C-C11	2.42	125.23	120.94
2	59-A	201	FOL	C8A-C4A-N5	2.42	123.38	120.59
2	79-A	201	FOL	C9-N10-C14	2.42	128.52	122.25
4	80-A	204	NAP	C4B-O4B-C1B	2.42	112.34	109.77
4	163-A	204	NAP	O5B-PA-O1A	2.42	119.01	109.25
4	38-A	204	NAP	O2N-PN-O1N	2.42	124.81	112.28
4	60-A	204	NAP	O5B-PA-O1A	2.42	119.02	109.25
2	130-A	201	FOL	C9-N10-C14	2.42	128.53	122.25
4	60-A	204	NAP	O2A-PA-O1A	2.43	124.84	112.28
4	142-A	204	NAP	O2N-PN-O1N	2.43	124.85	112.28
4	48-A	204	NAP	O3B-C3B-C2B	2.43	118.09	111.18
4	14-A	204	NAP	O5B-PA-O1A	2.43	119.05	109.25
4	64-A	204	NAP	O2A-PA-O1A	2.43	124.85	112.28
4	70-A	204	NAP	C2D-C3D-C4D	2.43	107.35	102.62
4	155-A	204	NAP	O2N-PN-O1N	2.43	124.86	112.28
4	110-A	204	NAP	O2N-PN-O1N	2.43	124.87	112.28
2	1-A	201	FOL	O-C-N	2.43	126.91	122.46
4	68-A	204	NAP	O2A-PA-O1A	2.43	124.88	112.28
4	78-A	204	NAP	O5B-PA-O1A	2.44	119.08	109.25
4	23-A	204	NAP	O3B-C3B-C2B	2.44	118.12	111.18
4	113-A	204	NAP	O2A-PA-O1A	2.44	124.90	112.28
4	38-A	204	NAP	O2A-PA-O1A	2.44	124.91	112.28
4	94-A	204	NAP	O2A-PA-O1A	2.44	124.92	112.28
4	137-A	204	NAP	O2A-PA-O1A	2.44	124.92	112.28
4	144-A	204	NAP	O3B-C3B-C2B	2.44	118.13	111.18
2	142-A	201	FOL	CB-CA-N	2.44	113.93	110.22
4	160-A	204	NAP	O5B-PA-O1A	2.44	119.11	109.25
4	80-A	204	NAP	O2A-PA-O1A	2.44	124.94	112.28
4	140-A	204	NAP	O5B-PA-O1A	2.45	119.11	109.25
4	97-A	204	NAP	O2N-PN-O1N	2.45	124.94	112.28
4	84-A	204	NAP	O2N-PN-O1N	2.45	124.94	112.28
2	6-A	201	FOL	C4-C4A-N5	2.45	121.36	118.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	158-A	204	NAP	C2N-C3N-C4N	2.45	121.05	118.26
4	5-A	204	NAP	O3B-C3B-C2B	2.45	118.14	111.18
4	36-A	204	NAP	C2N-C3N-C4N	2.45	121.05	118.26
4	110-A	204	NAP	O3B-C3B-C2B	2.45	118.14	111.18
4	153-A	204	NAP	O2A-PA-O1A	2.45	124.96	112.28
4	98-A	204	NAP	O2N-PN-O1N	2.45	124.97	112.28
2	66-A	201	FOL	N1-C8A-N8	2.45	120.74	116.42
4	125-A	204	NAP	O2N-PN-O1N	2.45	124.98	112.28
2	144-A	201	FOL	C15-C14-N10	2.45	125.98	121.03
4	139-A	204	NAP	O5B-PA-O1A	2.46	119.15	109.25
2	154-A	201	FOL	C4-C4A-N5	2.46	121.37	118.68
4	133-A	204	NAP	O3B-C3B-C2B	2.46	118.17	111.18
4	8-A	204	NAP	O3B-C3B-C2B	2.46	118.17	111.18
4	73-A	204	NAP	O2A-PA-O1A	2.46	125.00	112.28
2	157-A	201	FOL	C4-N3-C2	2.46	119.87	116.17
4	167-A	204	NAP	O5B-PA-O1A	2.46	119.17	109.25
4	42-A	204	NAP	C2N-C3N-C4N	2.46	121.07	118.26
4	151-A	204	NAP	O2N-PN-O1N	2.46	125.03	112.28
4	145-A	204	NAP	O3B-C3B-C2B	2.47	118.19	111.18
4	162-A	204	NAP	O5B-PA-O1A	2.47	119.20	109.25
2	54-A	201	FOL	CG-CB-CA	2.47	118.11	113.19
2	30-A	201	FOL	N1-C8A-N8	2.47	120.77	116.42
2	134-A	201	FOL	N1-C8A-N8	2.47	120.77	116.42
2	78-A	201	FOL	C9-N10-C14	2.47	128.64	122.25
4	33-A	204	NAP	C4B-O4B-C1B	2.47	112.40	109.77
4	167-A	204	NAP	O2A-PA-O1A	2.47	125.07	112.28
4	151-A	204	NAP	O2A-PA-O1A	2.47	125.08	112.28
4	26-A	204	NAP	C2N-C3N-C4N	2.47	121.08	118.26
4	73-A	204	NAP	C5A-C6A-N6A	2.47	125.51	120.47
2	55-A	201	FOL	CB-CA-N	2.47	113.98	110.22
4	147-A	204	NAP	O2N-PN-O1N	2.47	125.08	112.28
4	66-A	204	NAP	C4B-O4B-C1B	2.47	112.40	109.77
2	140-A	201	FOL	C8A-C4A-N5	2.48	123.44	120.59
4	98-A	204	NAP	O5B-PA-O1A	2.48	119.24	109.25
4	117-A	204	NAP	O5B-PA-O1A	2.48	119.24	109.25
4	160-A	204	NAP	C2N-C3N-C4N	2.48	121.09	118.26
4	63-A	204	NAP	O3B-C3B-C2B	2.48	118.22	111.18
4	10-A	204	NAP	C2N-C3N-C4N	2.48	121.09	118.26
2	15-A	201	FOL	C7-C6-N5	2.48	122.43	120.80
4	142-A	204	NAP	O5B-PA-O1A	2.48	119.25	109.25
2	100-A	201	FOL	N1-C8A-N8	2.48	120.79	116.42
4	15-A	204	NAP	O3B-C3B-C2B	2.48	118.23	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	58-A	201	FOL	C8A-C4A-N5	2.48	123.44	120.59
2	149-A	201	FOL	CB-CA-CT	2.48	115.89	112.28
4	52-A	204	NAP	O3B-C3B-C2B	2.48	118.23	111.18
4	50-A	204	NAP	O2A-PA-O1A	2.48	125.12	112.28
4	126-A	204	NAP	O2A-PA-O1A	2.48	125.12	112.28
4	160-A	204	NAP	O2N-PN-O1N	2.48	125.13	112.28
4	24-A	204	NAP	C2N-C3N-C4N	2.48	121.09	118.26
4	144-A	204	NAP	C2N-C3N-C4N	2.48	121.09	118.26
4	43-A	204	NAP	O5B-PA-O1A	2.48	119.27	109.25
4	132-A	204	NAP	O3B-C3B-C2B	2.48	118.25	111.18
4	1-A	204	NAP	O2A-PA-O1A	2.49	125.14	112.28
4	138-A	204	NAP	O2A-PA-O1A	2.49	125.15	112.28
2	152-A	201	FOL	C15-C16-C11	2.49	123.57	120.79
4	136-A	204	NAP	O2A-PA-O1A	2.49	125.16	112.28
2	162-A	201	FOL	C8A-C4A-N5	2.49	123.45	120.59
4	26-A	204	NAP	O5B-PA-O1A	2.49	119.28	109.25
4	30-A	204	NAP	C2N-C3N-C4N	2.49	121.10	118.26
4	51-A	204	NAP	O2A-PA-O1A	2.49	125.16	112.28
4	164-A	204	NAP	O7N-C7N-C3N	2.49	122.53	119.62
4	43-A	204	NAP	O3B-C3B-C2B	2.49	118.26	111.18
4	97-A	204	NAP	O5B-PA-O1A	2.49	119.29	109.25
4	94-A	204	NAP	O2N-PN-O1N	2.49	125.17	112.28
2	153-A	201	FOL	C4-N3-C2	2.49	119.92	116.17
2	57-A	201	FOL	C9-N10-C14	2.49	128.70	122.25
4	149-A	204	NAP	O2A-PA-O1A	2.49	125.17	112.28
4	130-A	204	NAP	O3B-C3B-C2B	2.49	118.27	111.18
4	139-A	204	NAP	O2N-PN-O1N	2.49	125.18	112.28
4	138-A	204	NAP	O3B-C3B-C2B	2.49	118.27	111.18
4	109-A	204	NAP	O2X-P2B-O1X	2.49	120.26	110.50
2	136-A	201	FOL	CG-CB-CA	2.49	118.17	113.19
2	159-A	201	FOL	C6-C7-N8	2.50	125.62	123.09
2	103-A	201	FOL	C8A-C4A-N5	2.50	123.47	120.59
2	162-A	201	FOL	C6-C7-N8	2.50	125.62	123.09
4	117-A	204	NAP	O2A-PA-O1A	2.50	125.22	112.28
4	83-A	204	NAP	C2D-C3D-C4D	2.50	107.49	102.62
4	27-A	204	NAP	O2A-PA-O1A	2.50	125.23	112.28
4	65-A	204	NAP	O2A-PA-O1A	2.50	125.23	112.28
4	69-A	204	NAP	O2N-PN-O1N	2.50	125.23	112.28
4	119-A	204	NAP	O5B-PA-O1A	2.50	119.35	109.25
4	162-A	204	NAP	O2N-PN-O1N	2.50	125.24	112.28
4	39-A	204	NAP	O2A-PA-O1A	2.50	125.24	112.28
2	131-A	201	FOL	C4-N3-C2	2.50	119.94	116.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	23-A	201	FOL	C8A-C4A-N5	2.50	123.47	120.59
4	150-A	204	NAP	O7N-C7N-C3N	2.50	122.55	119.62
2	118-A	201	FOL	C15-C14-N10	2.51	126.08	121.03
2	163-A	201	FOL	CB-CA-CT	2.51	115.93	112.28
4	148-A	204	NAP	O2N-PN-O1N	2.51	125.27	112.28
4	16-A	204	NAP	O2N-PN-O1N	2.51	125.27	112.28
4	109-A	204	NAP	C2D-C3D-C4D	2.51	107.51	102.62
2	123-A	201	FOL	N1-C8A-N8	2.52	120.85	116.42
4	161-A	204	NAP	O5B-PA-O1A	2.52	119.40	109.25
2	127-A	201	FOL	C4-C4A-N5	2.52	121.44	118.68
4	40-A	204	NAP	O2N-PN-O1N	2.52	125.31	112.28
2	8-A	201	FOL	CA-N-C	2.52	125.60	122.15
4	59-A	204	NAP	C2D-C3D-C4D	2.52	107.53	102.62
4	124-A	204	NAP	O2N-PN-O1N	2.52	125.34	112.28
4	90-A	204	NAP	O5B-PA-O1A	2.52	119.43	109.25
4	139-A	204	NAP	O2A-PA-O1A	2.53	125.35	112.28
4	16-A	204	NAP	O3B-C3B-C2B	2.53	118.37	111.18
4	159-A	204	NAP	O3B-C3B-C2B	2.53	118.37	111.18
4	161-A	204	NAP	C2D-C3D-C4D	2.53	107.54	102.62
4	148-A	204	NAP	O3B-C3B-C2B	2.53	118.37	111.18
4	13-A	204	NAP	O5B-PA-O1A	2.53	119.45	109.25
2	124-A	201	FOL	O-C-N	2.53	127.09	122.46
4	33-A	204	NAP	O3B-C3B-C2B	2.53	118.37	111.18
4	166-A	204	NAP	O2A-PA-O1A	2.53	125.37	112.28
4	89-A	204	NAP	O5B-PA-O1A	2.53	119.46	109.25
4	165-A	204	NAP	O5B-PA-O1A	2.53	119.46	109.25
4	7-A	204	NAP	C2N-C3N-C4N	2.53	121.15	118.26
4	51-A	204	NAP	O3B-C3B-C2B	2.53	118.38	111.18
4	138-A	204	NAP	O5B-PA-O1A	2.53	119.47	109.25
2	19-A	201	FOL	CB-CA-N	2.54	114.08	110.22
2	28-A	201	FOL	C4-C4A-N5	2.54	121.46	118.68
2	128-A	201	FOL	CB-CA-N	2.54	114.08	110.22
2	136-A	201	FOL	N1-C8A-N8	2.54	120.89	116.42
2	158-A	201	FOL	N1-C8A-N8	2.54	120.90	116.42
4	88-A	204	NAP	O5B-PA-O1A	2.54	119.50	109.25
2	91-A	201	FOL	O-C-C11	2.54	125.45	120.94
4	86-A	204	NAP	O2A-PA-O1A	2.54	125.45	112.28
4	68-A	204	NAP	O2N-PN-O1N	2.55	125.46	112.28
4	95-A	204	NAP	O5B-PA-O1A	2.55	119.52	109.25
4	23-A	204	NAP	O2A-PA-O1A	2.55	125.47	112.28
2	25-A	201	FOL	C4-C4A-N5	2.55	121.47	118.68
4	13-A	204	NAP	O2N-PN-O1N	2.55	125.47	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	135-A	204	NAP	O2N-PN-O1N	2.55	125.48	112.28
2	50-A	201	FOL	N1-C8A-N8	2.55	120.91	116.42
4	93-A	204	NAP	O2N-PN-O1N	2.55	125.49	112.28
4	146-A	204	NAP	O2N-PN-O1N	2.55	125.49	112.28
4	144-A	204	NAP	O2N-PN-O1N	2.55	125.49	112.28
4	163-A	204	NAP	O2N-PN-O1N	2.55	125.49	112.28
4	137-A	204	NAP	O5B-PA-O1A	2.55	119.55	109.25
4	111-A	204	NAP	O5B-PA-O1A	2.55	119.55	109.25
4	126-A	204	NAP	O2N-PN-O1N	2.56	125.51	112.28
4	39-A	204	NAP	C2D-C3D-C4D	2.56	107.60	102.62
2	12-A	201	FOL	CA-N-C	2.56	125.66	122.15
4	98-A	204	NAP	O2A-PA-O1A	2.56	125.54	112.28
4	12-A	204	NAP	O3B-C3B-C2B	2.56	118.47	111.18
4	46-A	204	NAP	C2N-C3N-C4N	2.56	121.18	118.26
4	88-A	204	NAP	O2N-PN-O1N	2.56	125.55	112.28
4	132-A	204	NAP	C2N-C3N-C4N	2.56	121.19	118.26
4	92-A	204	NAP	O2N-PN-O1N	2.56	125.55	112.28
4	30-A	204	NAP	O2A-PA-O1A	2.56	125.55	112.28
4	113-A	204	NAP	O5B-PA-O1A	2.57	119.60	109.25
2	58-A	201	FOL	C9-N10-C14	2.57	128.90	122.25
2	157-A	201	FOL	C9-N10-C14	2.57	128.91	122.25
4	130-A	204	NAP	O2A-PA-O1A	2.57	125.57	112.28
2	77-A	201	FOL	C8A-C4A-N5	2.57	123.55	120.59
2	48-A	201	FOL	C11-C-N	2.57	121.71	116.97
4	56-A	204	NAP	C2N-C3N-C4N	2.57	121.19	118.26
2	111-A	201	FOL	C4-C4A-N5	2.57	121.50	118.68
4	85-A	204	NAP	O2N-PN-O1N	2.57	125.60	112.28
4	145-A	204	NAP	O2N-PN-O1N	2.57	125.60	112.28
4	24-A	204	NAP	O2A-PA-O1A	2.57	125.61	112.28
2	110-A	201	FOL	N1-C8A-N8	2.57	120.96	116.42
4	85-A	204	NAP	O2A-PA-O1A	2.58	125.61	112.28
4	133-A	204	NAP	C5A-C6A-N6A	2.58	125.72	120.47
2	49-A	201	FOL	C8A-C4A-N5	2.58	123.56	120.59
4	61-A	204	NAP	O5B-PA-O1A	2.58	119.65	109.25
4	16-A	204	NAP	O2A-PA-O1A	2.58	125.62	112.28
4	61-A	204	NAP	O3B-C3B-C2B	2.58	118.51	111.18
4	99-A	204	NAP	O5B-PA-O1A	2.58	119.66	109.25
4	35-A	204	NAP	O7N-C7N-C3N	2.58	122.64	119.62
2	80-A	201	FOL	C6-C9-N10	2.58	118.92	113.15
2	57-A	201	FOL	C6-C7-N8	2.58	125.70	123.09
4	54-A	204	NAP	O2N-PN-O1N	2.58	125.64	112.28
2	158-A	201	FOL	C4-N3-C2	2.58	120.06	116.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	117-A	204	NAP	C3N-C7N-N7N	2.58	120.72	117.77
4	25-A	204	NAP	O2N-PN-O1N	2.58	125.66	112.28
4	71-A	204	NAP	C2N-C3N-C4N	2.59	121.21	118.26
4	39-A	204	NAP	O2N-PN-O1N	2.59	125.68	112.28
4	12-A	204	NAP	O2N-PN-O1N	2.59	125.68	112.28
2	140-A	201	FOL	CG-CB-CA	2.59	118.36	113.19
4	112-A	204	NAP	O5B-PA-O1A	2.59	119.70	109.25
4	64-A	204	NAP	O3B-C3B-C2B	2.59	118.55	111.18
2	141-A	201	FOL	N1-C8A-N8	2.59	120.99	116.42
4	17-A	204	NAP	O2A-PA-O1A	2.59	125.71	112.28
4	41-A	204	NAP	O2A-PA-O1A	2.60	125.72	112.28
2	108-A	201	FOL	C9-N10-C14	2.60	128.98	122.25
2	21-A	201	FOL	CA-N-C	2.60	125.71	122.15
4	11-A	204	NAP	O2N-PN-O1N	2.60	125.73	112.28
4	75-A	204	NAP	O5B-PA-O1A	2.60	119.74	109.25
4	143-A	204	NAP	O2N-PN-O1N	2.60	125.75	112.28
4	150-A	204	NAP	O2N-PN-O1N	2.60	125.75	112.28
4	165-A	204	NAP	O2N-PN-O1N	2.60	125.75	112.28
4	167-A	204	NAP	O2N-PN-O1N	2.60	125.76	112.28
4	101-A	204	NAP	O3B-C3B-C2B	2.60	118.59	111.18
4	116-A	204	NAP	O2N-PN-O1N	2.60	125.76	112.28
4	49-A	204	NAP	O3B-C3B-C2B	2.61	118.59	111.18
4	127-A	204	NAP	O2A-PA-O1A	2.61	125.78	112.28
4	17-A	204	NAP	O2N-PN-O1N	2.61	125.78	112.28
4	104-A	204	NAP	O2A-PA-O1A	2.61	125.78	112.28
4	63-A	204	NAP	O5B-PA-O1A	2.61	119.77	109.25
2	126-A	201	FOL	C9-C6-N5	2.61	121.50	116.58
4	131-A	204	NAP	O3B-C3B-C2B	2.61	118.60	111.18
2	96-A	201	FOL	N1-C8A-N8	2.61	121.02	116.42
4	164-A	204	NAP	O2A-PA-O1A	2.61	125.78	112.28
4	69-A	204	NAP	O2A-PA-O1A	2.61	125.79	112.28
4	125-A	204	NAP	O3B-C3B-C2B	2.61	118.61	111.18
4	101-A	204	NAP	O2A-PA-O1A	2.61	125.80	112.28
2	138-A	201	FOL	C15-C14-N10	2.61	126.30	121.03
2	21-A	201	FOL	C9-C6-N5	2.62	121.51	116.58
4	152-A	204	NAP	O2A-PA-O1A	2.62	125.82	112.28
2	130-A	201	FOL	N1-C8A-N8	2.62	121.03	116.42
2	87-A	201	FOL	CA-N-C	2.62	125.73	122.15
2	94-A	201	FOL	N1-C8A-N8	2.62	121.03	116.42
4	62-A	204	NAP	O5B-PA-O1A	2.62	119.81	109.25
4	32-A	204	NAP	C2N-C3N-C4N	2.62	121.25	118.26
2	64-A	201	FOL	C15-C14-N10	2.62	126.31	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	90-A	204	NAP	O3B-C3B-C2B	2.62	118.63	111.18
4	66-A	204	NAP	O2N-PN-O1N	2.62	125.84	112.28
2	12-A	201	FOL	CG-CB-CA	2.62	118.42	113.19
4	45-A	204	NAP	O2N-PN-O1N	2.62	125.84	112.28
4	2-A	204	NAP	O2A-PA-O1A	2.62	125.85	112.28
4	130-A	204	NAP	O5B-PA-O1A	2.62	119.83	109.25
4	1-A	204	NAP	O3B-C3B-C2B	2.62	118.64	111.18
4	90-A	204	NAP	O7N-C7N-C3N	2.62	122.69	119.62
2	26-A	201	FOL	C11-C-N	2.62	121.81	116.97
4	86-A	204	NAP	O2N-PN-O1N	2.62	125.86	112.28
2	22-A	201	FOL	CA-N-C	2.63	125.75	122.15
4	91-A	204	NAP	O2A-PA-O1A	2.63	125.88	112.28
4	76-A	204	NAP	O2A-PA-O1A	2.63	125.88	112.28
4	111-A	204	NAP	O2N-PN-O1N	2.63	125.89	112.28
4	102-A	204	NAP	O2A-PA-O1A	2.63	125.89	112.28
4	41-A	204	NAP	O2N-PN-O1N	2.63	125.90	112.28
4	148-A	204	NAP	O2A-PA-O1A	2.63	125.90	112.28
2	94-A	201	FOL	C9-C6-N5	2.63	121.54	116.58
4	122-A	204	NAP	O2A-PA-O1A	2.63	125.90	112.28
4	20-A	204	NAP	O3B-C3B-C2B	2.63	118.67	111.18
2	4-A	201	FOL	N1-C8A-N8	2.64	121.06	116.42
4	44-A	204	NAP	O5B-PA-O1A	2.64	119.88	109.25
2	13-A	201	FOL	N1-C8A-N8	2.64	121.07	116.42
4	110-A	204	NAP	O2A-PA-O1A	2.64	125.94	112.28
2	78-A	201	FOL	CA-N-C	2.64	125.76	122.15
4	43-A	204	NAP	O2N-PN-O1N	2.64	125.94	112.28
4	36-A	204	NAP	O2N-PN-O1N	2.64	125.95	112.28
4	42-A	204	NAP	O2N-PN-O1N	2.64	125.95	112.28
4	92-A	204	NAP	O2A-PA-O1A	2.64	125.97	112.28
4	62-A	204	NAP	C5A-C6A-N6A	2.65	125.86	120.47
2	126-A	201	FOL	CB-CA-N	2.65	114.24	110.22
2	66-A	201	FOL	C4-C4A-N5	2.65	121.58	118.68
2	167-A	201	FOL	C15-C14-N10	2.65	126.36	121.03
4	75-A	204	NAP	O2A-PA-O1A	2.65	125.98	112.28
4	36-A	204	NAP	O3B-C3B-C2B	2.65	118.71	111.18
2	85-A	201	FOL	N1-C8A-N8	2.65	121.09	116.42
4	25-A	204	NAP	O2A-PA-O1A	2.65	126.00	112.28
4	5-A	204	NAP	C2N-C3N-C4N	2.65	121.28	118.26
4	67-A	204	NAP	O2A-PA-O1A	2.65	126.00	112.28
4	48-A	204	NAP	O2A-PA-O1A	2.65	126.00	112.28
4	112-A	204	NAP	O2N-PN-O1N	2.65	126.01	112.28
4	17-A	204	NAP	C2N-C3N-C4N	2.65	121.29	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	10-A	204	NAP	O2N-PN-O1N	2.66	126.02	112.28
4	153-A	204	NAP	O2N-PN-O1N	2.66	126.04	112.28
4	66-A	204	NAP	O2A-PA-O1A	2.66	126.04	112.28
4	13-A	204	NAP	O3B-C3B-C2B	2.66	118.75	111.18
4	99-A	204	NAP	O3B-C3B-C2B	2.66	118.75	111.18
4	67-A	204	NAP	O2N-PN-O1N	2.66	126.06	112.28
2	127-A	201	FOL	C11-C-N	2.66	121.88	116.97
4	35-A	204	NAP	O2N-PN-O1N	2.66	126.07	112.28
2	58-A	201	FOL	C12-C13-C14	2.66	123.41	120.30
4	62-A	204	NAP	O2N-PN-O1N	2.67	126.08	112.28
2	74-A	201	FOL	CA-N-C	2.67	125.80	122.15
4	53-A	204	NAP	O2A-PA-O1A	2.67	126.08	112.28
4	127-A	204	NAP	O2N-PN-O1N	2.67	126.08	112.28
4	99-A	204	NAP	O2N-PN-O1N	2.67	126.09	112.28
4	6-A	204	NAP	O3B-C3B-C2B	2.67	118.77	111.18
4	23-A	204	NAP	O5D-PN-O1N	2.67	120.02	109.25
4	73-A	204	NAP	O2N-PN-O1N	2.68	126.13	112.28
4	130-A	204	NAP	C2N-C3N-C4N	2.68	121.31	118.26
2	74-A	201	FOL	C15-C16-C11	2.68	123.78	120.79
2	131-A	201	FOL	CB-CA-CT	2.68	116.17	112.28
2	15-A	201	FOL	C4-C4A-N5	2.68	121.62	118.68
2	12-A	201	FOL	C4-C4A-N5	2.68	121.62	118.68
4	152-A	204	NAP	O2N-PN-O1N	2.69	126.19	112.28
2	108-A	201	FOL	C15-C14-N10	2.69	126.45	121.03
4	140-A	204	NAP	O3B-C3B-C2B	2.69	118.82	111.18
4	149-A	204	NAP	O2N-PN-O1N	2.69	126.20	112.28
4	15-A	204	NAP	O2A-PA-O1A	2.69	126.20	112.28
2	31-A	201	FOL	CG-CB-CA	2.69	118.56	113.19
4	5-A	204	NAP	O5B-PA-O1A	2.69	120.11	109.25
2	40-A	201	FOL	C4-C4A-N5	2.69	121.63	118.68
4	47-A	204	NAP	O2N-PN-O1N	2.69	126.22	112.28
4	4-A	204	NAP	O2A-PA-O1A	2.69	126.22	112.28
4	156-A	204	NAP	O5B-PA-O1A	2.69	120.12	109.25
4	166-A	204	NAP	O5B-PA-O1A	2.70	120.12	109.25
4	21-A	204	NAP	O2N-PN-O1N	2.70	126.23	112.28
4	75-A	204	NAP	O2N-PN-O1N	2.70	126.23	112.28
4	122-A	204	NAP	O5B-PA-O1A	2.70	120.13	109.25
2	153-A	201	FOL	CB-CA-N	2.70	114.32	110.22
2	102-A	201	FOL	C8A-C4A-N5	2.70	123.70	120.59
4	102-A	204	NAP	O2N-PN-O1N	2.70	126.26	112.28
4	135-A	204	NAP	C5A-C6A-N6A	2.70	125.98	120.47
4	126-A	204	NAP	O3B-C3B-C2B	2.70	118.87	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	59-A	201	FOL	CB-CA-N	2.70	114.33	110.22
4	63-A	204	NAP	O2N-PN-O1N	2.71	126.28	112.28
2	104-A	201	FOL	CB-CA-N	2.71	114.33	110.22
2	119-A	201	FOL	C4-C4A-N5	2.71	121.65	118.68
4	3-A	204	NAP	O5B-PA-O1A	2.71	120.17	109.25
4	166-A	204	NAP	O2N-PN-O1N	2.71	126.29	112.28
2	104-A	201	FOL	C8A-C4A-N5	2.71	123.71	120.59
4	62-A	204	NAP	O3B-C3B-C2B	2.71	118.89	111.18
4	30-A	204	NAP	O2N-PN-O1N	2.71	126.31	112.28
2	100-A	201	FOL	C9-C6-N5	2.71	121.69	116.58
2	139-A	201	FOL	CA-N-C	2.71	125.86	122.15
4	123-A	204	NAP	O5B-PA-O1A	2.71	120.19	109.25
2	162-A	201	FOL	C4-N3-C2	2.71	120.26	116.17
4	25-A	204	NAP	O3B-C3B-C2B	2.71	118.90	111.18
2	34-A	201	FOL	C8A-C4A-N5	2.72	123.72	120.59
2	48-A	201	FOL	C4-C4A-N5	2.72	121.66	118.68
2	165-A	201	FOL	C4-N3-C2	2.72	120.27	116.17
2	20-A	201	FOL	C4-N3-C2	2.72	120.27	116.17
4	61-A	204	NAP	O2N-PN-O1N	2.72	126.36	112.28
2	27-A	201	FOL	C4-C4A-N5	2.72	121.67	118.68
4	19-A	204	NAP	O2N-PN-O1N	2.72	126.38	112.28
4	136-A	204	NAP	O2N-PN-O1N	2.73	126.39	112.28
4	154-A	204	NAP	O5B-PA-O1A	2.73	120.25	109.25
2	62-A	201	FOL	CA-N-C	2.73	125.88	122.15
4	42-A	204	NAP	O2A-PA-O1A	2.73	126.39	112.28
4	24-A	204	NAP	O3B-C3B-C2B	2.73	118.95	111.18
4	79-A	204	NAP	O5B-PA-O1A	2.73	120.28	109.25
2	154-A	201	FOL	CA-N-C	2.73	125.89	122.15
4	100-A	204	NAP	O2A-PA-O1A	2.74	126.44	112.28
4	49-A	204	NAP	O5B-PA-O1A	2.74	120.29	109.25
4	26-A	204	NAP	O2N-PN-O1N	2.74	126.47	112.28
4	116-A	204	NAP	O2A-PA-O1A	2.74	126.48	112.28
4	103-A	204	NAP	O2A-PA-O1A	2.74	126.48	112.28
4	93-A	204	NAP	O2A-PA-O1A	2.74	126.48	112.28
4	5-A	204	NAP	O2N-PN-O1N	2.74	126.49	112.28
4	18-A	204	NAP	O2N-PN-O1N	2.75	126.50	112.28
4	19-A	204	NAP	O3B-C3B-C2B	2.75	118.99	111.18
2	137-A	201	FOL	N1-C8A-N8	2.75	121.26	116.42
4	74-A	204	NAP	O2N-PN-O1N	2.75	126.51	112.28
4	29-A	204	NAP	O5B-PA-O1A	2.75	120.35	109.25
4	27-A	204	NAP	O2N-PN-O1N	2.75	126.53	112.28
4	140-A	204	NAP	O2N-PN-O1N	2.75	126.53	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	89-A	201	FOL	N1-C8A-N8	2.75	121.27	116.42
2	52-A	201	FOL	C15-C14-N10	2.76	126.58	121.03
4	165-A	204	NAP	O2A-PA-O1A	2.76	126.55	112.28
4	65-A	204	NAP	O2N-PN-O1N	2.76	126.55	112.28
4	59-A	204	NAP	O3B-C3B-C2B	2.76	119.02	111.18
2	26-A	201	FOL	C9-C6-N5	2.76	121.78	116.58
4	59-A	204	NAP	O2N-PN-O1N	2.76	126.56	112.28
4	115-A	204	NAP	O2N-PN-O1N	2.76	126.56	112.28
2	9-A	201	FOL	C4-N3-C2	2.76	120.33	116.17
4	87-A	204	NAP	O5B-PA-O1A	2.76	120.39	109.25
4	104-A	204	NAP	O5B-PA-O1A	2.77	120.41	109.25
4	15-A	204	NAP	C2N-C3N-C4N	2.77	121.42	118.26
4	115-A	204	NAP	O7N-C7N-C3N	2.77	122.86	119.62
4	50-A	204	NAP	O2N-PN-O1N	2.77	126.63	112.28
2	59-A	201	FOL	C4-N3-C2	2.77	120.35	116.17
2	34-A	201	FOL	O-C-C11	2.78	125.87	120.94
4	56-A	204	NAP	O5D-PN-O1N	2.78	120.46	109.25
2	129-A	201	FOL	C15-C16-C11	2.78	123.90	120.79
4	50-A	204	NAP	C4B-O4B-C1B	2.78	112.73	109.77
4	14-A	204	NAP	O2N-PN-O1N	2.78	126.67	112.28
4	137-A	204	NAP	O2N-PN-O1N	2.78	126.68	112.28
2	42-A	201	FOL	C9-C6-N5	2.78	121.82	116.58
2	65-A	201	FOL	C4-C4A-N5	2.78	121.73	118.68
2	83-A	201	FOL	C6-C7-N8	2.78	125.91	123.09
2	115-A	201	FOL	C9-N10-C14	2.79	129.47	122.25
4	164-A	204	NAP	O2N-PN-O1N	2.79	126.70	112.28
4	118-A	204	NAP	O5B-PA-O1A	2.79	120.50	109.25
4	114-A	204	NAP	O2N-PN-O1N	2.79	126.72	112.28
2	146-A	201	FOL	N1-C8A-N8	2.79	121.34	116.42
4	123-A	204	NAP	O2N-PN-O1N	2.79	126.72	112.28
4	123-A	204	NAP	O2A-PA-O1A	2.79	126.73	112.28
4	79-A	204	NAP	O2A-PA-O1A	2.79	126.75	112.28
4	149-A	204	NAP	O3B-C3B-C2B	2.79	119.13	111.18
4	28-A	204	NAP	O5B-PA-O1A	2.80	120.53	109.25
2	7-A	201	FOL	N1-C8A-N8	2.80	121.35	116.42
2	37-A	201	FOL	C9-C6-N5	2.80	121.86	116.58
4	42-A	204	NAP	O5B-PA-O1A	2.80	120.56	109.25
4	77-A	204	NAP	O2A-PA-O1A	2.80	126.80	112.28
2	56-A	201	FOL	N1-C8A-N8	2.81	121.36	116.42
4	99-A	204	NAP	O2A-PA-O1A	2.81	126.82	112.28
2	9-A	201	FOL	N1-C8A-N8	2.81	121.37	116.42
2	115-A	201	FOL	N1-C8A-N8	2.81	121.37	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	34-A	201	FOL	C4-N3-C2	2.81	120.41	116.17
2	65-A	201	FOL	C9-C6-N5	2.82	121.89	116.58
4	42-A	204	NAP	C4B-O4B-C1B	2.82	112.77	109.77
2	113-A	201	FOL	N1-C8A-N8	2.82	121.39	116.42
4	103-A	204	NAP	O5B-PA-O1A	2.82	120.63	109.25
4	74-A	204	NAP	O2A-PA-O1A	2.82	126.89	112.28
2	156-A	201	FOL	CA-N-C	2.82	126.02	122.15
4	89-A	204	NAP	O2N-PN-O1N	2.82	126.90	112.28
2	146-A	201	FOL	CB-CA-N	2.82	114.51	110.22
4	19-A	204	NAP	C4B-O4B-C1B	2.83	112.78	109.77
4	23-A	204	NAP	O2N-PN-O1N	2.83	126.90	112.28
2	82-A	201	FOL	C11-C-N	2.83	122.19	116.97
4	3-A	204	NAP	O2N-PN-O1N	2.83	126.92	112.28
4	4-A	204	NAP	O2N-PN-O1N	2.83	126.94	112.28
2	34-A	201	FOL	C15-C16-C11	2.83	123.96	120.79
2	158-A	201	FOL	C8A-C4A-N5	2.84	123.86	120.59
4	70-A	204	NAP	O2N-PN-O1N	2.84	126.96	112.28
2	75-A	201	FOL	CG-CB-CA	2.84	118.85	113.19
4	104-A	204	NAP	O2N-PN-O1N	2.84	126.99	112.28
4	50-A	204	NAP	O3B-C3B-C2B	2.85	119.27	111.18
2	64-A	201	FOL	O-C-N	2.85	127.67	122.46
2	114-A	201	FOL	CG-CB-CA	2.85	118.87	113.19
4	80-A	204	NAP	O5B-PA-O1A	2.85	120.73	109.25
2	129-A	201	FOL	C4-C4A-N5	2.85	121.80	118.68
2	54-A	201	FOL	C15-C14-N10	2.85	126.78	121.03
2	71-A	201	FOL	N1-C8A-N8	2.85	121.44	116.42
2	125-A	201	FOL	CB-CA-N	2.85	114.55	110.22
4	3-A	204	NAP	O2A-PA-O1A	2.85	127.04	112.28
2	2-A	201	FOL	N1-C8A-N8	2.85	121.45	116.42
4	94-A	204	NAP	O5B-PA-O1A	2.85	120.76	109.25
4	140-A	204	NAP	C5A-C6A-N6A	2.86	126.29	120.47
4	71-A	204	NAP	O2N-PN-O1N	2.86	127.07	112.28
2	51-A	201	FOL	N1-C8A-N8	2.86	121.46	116.42
2	70-A	201	FOL	N1-C8A-N8	2.86	121.46	116.42
4	156-A	204	NAP	O2N-PN-O1N	2.86	127.09	112.28
2	165-A	201	FOL	CG-CB-CA	2.86	118.90	113.19
4	154-A	204	NAP	O2A-PA-O1A	2.86	127.11	112.28
4	64-A	204	NAP	O2N-PN-O1N	2.87	127.11	112.28
4	124-A	204	NAP	O2A-PA-O1A	2.87	127.12	112.28
4	20-A	204	NAP	O2N-PN-O1N	2.87	127.13	112.28
4	130-A	204	NAP	O2N-PN-O1N	2.87	127.14	112.28
2	155-A	201	FOL	N1-C8A-N8	2.88	121.49	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	93-A	204	NAP	O5B-PA-O1A	2.88	120.86	109.25
4	60-A	204	NAP	O2N-PN-O1N	2.88	127.19	112.28
4	72-A	204	NAP	O2N-PN-O1N	2.88	127.19	112.28
4	127-A	204	NAP	O5B-PA-O1A	2.88	120.87	109.25
4	29-A	204	NAP	O2N-PN-O1N	2.88	127.20	112.28
2	50-A	201	FOL	CA-N-C	2.88	126.10	122.15
4	80-A	204	NAP	O2N-PN-O1N	2.89	127.22	112.28
4	76-A	204	NAP	O2N-PN-O1N	2.89	127.23	112.28
2	140-A	201	FOL	CB-CA-N	2.89	114.61	110.22
2	149-A	201	FOL	C4-N3-C2	2.90	120.54	116.17
2	73-A	201	FOL	C4-N3-C2	2.90	120.54	116.17
2	98-A	201	FOL	C4-C4A-N5	2.90	121.86	118.68
4	28-A	204	NAP	O2N-PN-O1N	2.91	127.32	112.28
4	78-A	204	NAP	O2A-PA-O1A	2.91	127.34	112.28
2	117-A	201	FOL	C4-N3-C2	2.91	120.56	116.17
2	122-A	201	FOL	N1-C8A-N8	2.91	121.55	116.42
2	16-A	201	FOL	C4-N3-C2	2.92	120.56	116.17
2	118-A	201	FOL	C9-N10-C14	2.92	129.81	122.25
4	155-A	204	NAP	O3X-P2B-O2X	2.92	119.38	107.61
4	54-A	204	NAP	O5B-PA-O1A	2.92	121.02	109.25
2	107-A	201	FOL	CA-N-C	2.92	126.15	122.15
2	89-A	201	FOL	C4-N3-C2	2.92	120.57	116.17
4	46-A	204	NAP	O2N-PN-O1N	2.92	127.40	112.28
2	25-A	201	FOL	N1-C8A-N8	2.92	121.57	116.42
4	27-A	204	NAP	O5B-PA-O1A	2.92	121.04	109.25
4	128-A	204	NAP	O2A-PA-O1A	2.92	127.41	112.28
4	121-A	204	NAP	O2N-PN-O1N	2.92	127.41	112.28
2	132-A	201	FOL	N1-C8A-N8	2.93	121.58	116.42
2	61-A	201	FOL	CG-CB-CA	2.93	119.05	113.19
4	122-A	204	NAP	O2N-PN-O1N	2.94	127.47	112.28
2	159-A	201	FOL	C4-N3-C2	2.94	120.59	116.17
2	68-A	201	FOL	N1-C8A-N8	2.94	121.59	116.42
4	154-A	204	NAP	O2N-PN-O1N	2.94	127.50	112.28
4	4-A	204	NAP	O5B-PA-O1A	2.94	121.12	109.25
4	138-A	204	NAP	O2N-PN-O1N	2.94	127.51	112.28
4	2-A	204	NAP	O2N-PN-O1N	2.94	127.52	112.28
4	150-A	204	NAP	O2A-PA-O1A	2.94	127.52	112.28
2	42-A	201	FOL	C4-C4A-N5	2.95	121.91	118.68
4	125-A	204	NAP	O2A-PA-O1A	2.95	127.53	112.28
4	58-A	204	NAP	O2N-PN-O1N	2.95	127.53	112.28
2	166-A	201	FOL	N1-C8A-N8	2.95	121.62	116.42
2	105-A	201	FOL	N1-C8A-N8	2.95	121.62	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	54-A	204	NAP	O2A-PA-O1A	2.95	127.56	112.28
4	51-A	204	NAP	O2N-PN-O1N	2.95	127.56	112.28
2	118-A	201	FOL	N1-C8A-N8	2.96	121.63	116.42
2	59-A	201	FOL	CB-CA-CT	2.96	116.59	112.28
2	13-A	201	FOL	C4-C4A-N5	2.96	121.93	118.68
4	29-A	204	NAP	O2A-PA-O1A	2.97	127.63	112.28
2	125-A	201	FOL	N1-C8A-N8	2.97	121.65	116.42
2	109-A	201	FOL	CA-N-C	2.98	126.22	122.15
4	53-A	204	NAP	O2N-PN-O1N	2.98	127.69	112.28
2	58-A	201	FOL	C15-C14-N10	2.98	127.04	121.03
4	129-A	204	NAP	O2N-PN-O1N	2.98	127.72	112.28
2	10-A	201	FOL	C8A-C4A-N5	3.00	124.04	120.59
2	147-A	201	FOL	C4-N3-C2	3.00	120.69	116.17
4	77-A	204	NAP	C5A-C6A-N6A	3.00	126.59	120.47
4	107-A	204	NAP	C2D-C3D-C4D	3.00	108.47	102.62
4	15-A	204	NAP	O2N-PN-O1N	3.01	127.83	112.28
2	119-A	201	FOL	CB-CA-N	3.02	114.81	110.22
4	128-A	204	NAP	O2N-PN-O1N	3.02	127.92	112.28
2	101-A	201	FOL	C4-N3-C2	3.02	120.72	116.17
2	131-A	201	FOL	C8A-C4A-N5	3.03	124.08	120.59
2	26-A	201	FOL	C4-C4A-N5	3.03	122.01	118.68
2	82-A	201	FOL	CB-CA-CT	3.03	116.69	112.28
2	103-A	201	FOL	CB-CA-N	3.04	114.84	110.22
2	43-A	201	FOL	C4-N3-C2	3.04	120.75	116.17
4	100-A	204	NAP	O2N-PN-O1N	3.04	128.02	112.28
4	28-A	204	NAP	O2A-PA-O1A	3.04	128.03	112.28
2	155-A	201	FOL	C9-N10-C14	3.04	130.14	122.25
2	18-A	201	FOL	N1-C8A-N8	3.05	121.79	116.42
4	101-A	204	NAP	O2N-PN-O1N	3.05	128.06	112.28
2	24-A	201	FOL	N1-C8A-N8	3.05	121.80	116.42
2	113-A	201	FOL	CA-N-C	3.06	126.34	122.15
2	92-A	201	FOL	N1-C8A-N8	3.06	121.82	116.42
4	77-A	204	NAP	O2N-PN-O1N	3.07	128.16	112.28
2	138-A	201	FOL	CG-CB-CA	3.07	119.32	113.19
2	87-A	201	FOL	N1-C8A-N8	3.07	121.83	116.42
4	79-A	204	NAP	O2N-PN-O1N	3.08	128.22	112.28
4	1-A	204	NAP	O2N-PN-O1N	3.08	128.23	112.28
4	129-A	204	NAP	O2A-PA-O1A	3.10	128.31	112.28
2	114-A	201	FOL	N1-C8A-N8	3.10	121.88	116.42
2	34-A	201	FOL	C9-N10-C14	3.10	130.29	122.25
2	40-A	201	FOL	N1-C8A-N8	3.10	121.89	116.42
4	103-A	204	NAP	O2N-PN-O1N	3.11	128.36	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	138-A	201	FOL	C9-N10-C14	3.11	130.31	122.25
2	166-A	201	FOL	C4-N3-C2	3.11	120.86	116.17
4	52-A	204	NAP	O2N-PN-O1N	3.11	128.39	112.28
2	84-A	201	FOL	N1-C8A-N8	3.12	121.91	116.42
2	126-A	201	FOL	C11-C-N	3.12	122.72	116.97
2	162-A	201	FOL	N1-C8A-N8	3.12	121.91	116.42
2	10-A	201	FOL	C4-N3-C2	3.12	120.87	116.17
4	48-A	204	NAP	O2N-PN-O1N	3.13	128.47	112.28
2	113-A	201	FOL	CB-CA-N	3.13	114.98	110.22
2	14-A	201	FOL	N1-C8A-N8	3.14	121.94	116.42
2	32-A	201	FOL	N1-C8A-N8	3.14	121.95	116.42
2	57-A	201	FOL	C8A-C4A-N5	3.14	124.21	120.59
2	5-A	201	FOL	C4-N3-C2	3.15	120.91	116.17
2	114-A	201	FOL	C4-N3-C2	3.15	120.91	116.17
2	17-A	201	FOL	N1-C8A-N8	3.15	121.97	116.42
4	128-A	204	NAP	O5B-PA-O1A	3.15	121.96	109.25
2	35-A	201	FOL	C4-N3-C2	3.15	120.92	116.17
4	49-A	204	NAP	O2N-PN-O1N	3.16	128.63	112.28
2	11-A	201	FOL	N1-C8A-N8	3.17	122.00	116.42
2	47-A	201	FOL	C4-C4A-N5	3.17	122.16	118.68
2	86-A	201	FOL	N1-C8A-N8	3.18	122.02	116.42
2	48-A	201	FOL	C4-N3-C2	3.18	120.96	116.17
2	36-A	201	FOL	N1-C8A-N8	3.18	122.02	116.42
2	44-A	201	FOL	N1-C8A-N8	3.18	122.03	116.42
2	69-A	201	FOL	N1-C8A-N8	3.19	122.03	116.42
2	72-A	201	FOL	N1-C8A-N8	3.19	122.03	116.42
2	52-A	201	FOL	C4-N3-C2	3.19	120.97	116.17
2	55-A	201	FOL	N1-C8A-N8	3.19	122.04	116.42
2	156-A	201	FOL	N1-C8A-N8	3.19	122.04	116.42
4	129-A	204	NAP	O5B-PA-O1A	3.19	122.12	109.25
2	33-A	201	FOL	N1-C8A-N8	3.19	122.05	116.42
2	22-A	201	FOL	N1-C8A-N8	3.20	122.06	116.42
2	158-A	201	FOL	CA-N-C	3.20	126.53	122.15
2	150-A	201	FOL	N1-C8A-N8	3.21	122.08	116.42
2	144-A	201	FOL	C4-N3-C2	3.22	121.02	116.17
4	78-A	204	NAP	O2N-PN-O1N	3.22	128.97	112.28
2	33-A	201	FOL	C4-N3-C2	3.22	121.03	116.17
2	42-A	201	FOL	CA-N-C	3.22	126.57	122.15
2	1-A	201	FOL	N1-C8A-N8	3.23	122.11	116.42
2	108-A	201	FOL	C4-N3-C2	3.23	121.04	116.17
2	18-A	201	FOL	CA-N-C	3.24	126.58	122.15
2	81-A	201	FOL	C8A-C4A-N5	3.24	124.32	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	90-A	201	FOL	C4-N3-C2	3.24	121.05	116.17
2	120-A	201	FOL	C4-N3-C2	3.25	121.06	116.17
4	120-A	204	NAP	O2N-PN-O1N	3.25	129.09	112.28
2	102-A	201	FOL	C4-N3-C2	3.25	121.07	116.17
2	135-A	201	FOL	N1-C8A-N8	3.26	122.16	116.42
2	124-A	201	FOL	CA-N-C	3.26	126.62	122.15
2	92-A	201	FOL	C4-N3-C2	3.26	121.08	116.17
2	139-A	201	FOL	C4-C4A-N5	3.27	122.26	118.68
2	46-A	201	FOL	CB-CA-N	3.27	115.19	110.22
4	49-A	204	NAP	O7N-C7N-C3N	3.27	123.45	119.62
2	140-A	201	FOL	N1-C8A-N8	3.28	122.19	116.42
2	32-A	201	FOL	C4-N3-C2	3.28	121.11	116.17
2	109-A	201	FOL	N1-C8A-N8	3.28	122.20	116.42
2	28-A	201	FOL	CA-N-C	3.29	126.65	122.15
2	32-A	201	FOL	CA-N-C	3.30	126.67	122.15
2	30-A	201	FOL	CA-N-C	3.30	126.67	122.15
2	153-A	201	FOL	C11-C-N	3.31	123.07	116.97
2	157-A	201	FOL	C8A-C4A-N5	3.31	124.40	120.59
2	3-A	201	FOL	N1-C8A-N8	3.31	122.25	116.42
2	45-A	201	FOL	N1-C8A-N8	3.31	122.25	116.42
2	79-A	201	FOL	N1-C8A-N8	3.31	122.25	116.42
4	139-A	204	NAP	O7N-C7N-C3N	3.31	123.50	119.62
2	83-A	201	FOL	C8A-C4A-N5	3.31	124.41	120.59
2	145-A	201	FOL	N1-C8A-N8	3.31	122.26	116.42
2	61-A	201	FOL	N1-C8A-N8	3.32	122.27	116.42
2	63-A	201	FOL	N1-C8A-N8	3.33	122.28	116.42
2	66-A	201	FOL	C15-C14-N10	3.33	127.74	121.03
2	109-A	201	FOL	CB-CA-N	3.33	115.28	110.22
2	144-A	201	FOL	CB-CA-N	3.33	115.28	110.22
2	39-A	201	FOL	C4-N3-C2	3.34	121.20	116.17
2	34-A	201	FOL	C15-C14-N10	3.34	127.77	121.03
2	82-A	201	FOL	N1-C8A-N8	3.34	122.31	116.42
2	88-A	201	FOL	N1-C8A-N8	3.36	122.33	116.42
2	99-A	201	FOL	CG-CB-CA	3.38	119.93	113.19
2	155-A	201	FOL	CA-N-C	3.38	126.78	122.15
2	17-A	201	FOL	C4-N3-C2	3.38	121.26	116.17
4	83-A	204	NAP	C5A-C6A-N6A	3.39	127.38	120.47
2	142-A	201	FOL	C4-N3-C2	3.39	121.28	116.17
2	157-A	201	FOL	N1-C8A-N8	3.40	122.42	116.42
2	12-A	201	FOL	C4-N3-C2	3.41	121.30	116.17
2	147-A	201	FOL	N1-C8A-N8	3.41	122.42	116.42
2	152-A	201	FOL	C4-N3-C2	3.41	121.31	116.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	122-A	201	FOL	CA-N-C	3.41	126.83	122.15
2	103-A	201	FOL	CA-N-C	3.42	126.83	122.15
2	90-A	201	FOL	N1-C8A-N8	3.42	122.45	116.42
2	86-A	201	FOL	C4-N3-C2	3.43	121.34	116.17
2	14-A	201	FOL	CA-N-C	3.43	126.85	122.15
2	4-A	201	FOL	CB-CA-N	3.43	115.44	110.22
2	39-A	201	FOL	N1-C8A-N8	3.44	122.48	116.42
4	104-A	204	NAP	C2D-C3D-C4D	3.44	109.32	102.62
2	45-A	201	FOL	C4-N3-C2	3.44	121.36	116.17
2	14-A	201	FOL	CG-CB-CA	3.44	120.06	113.19
2	87-A	201	FOL	C4-N3-C2	3.45	121.36	116.17
2	77-A	201	FOL	N1-C8A-N8	3.45	122.49	116.42
4	119-A	204	NAP	C4B-O4B-C1B	3.45	113.44	109.77
2	67-A	201	FOL	N1-C8A-N8	3.45	122.50	116.42
2	62-A	201	FOL	N1-C8A-N8	3.45	122.50	116.42
2	37-A	201	FOL	C4-C4A-N5	3.46	122.47	118.68
2	109-A	201	FOL	C4-N3-C2	3.46	121.39	116.17
2	94-A	201	FOL	C4-N3-C2	3.47	121.39	116.17
2	40-A	201	FOL	C4-N3-C2	3.47	121.40	116.17
2	31-A	201	FOL	N1-C8A-N8	3.47	122.54	116.42
2	24-A	201	FOL	CG-CB-CA	3.48	120.13	113.19
2	95-A	201	FOL	C4-N3-C2	3.49	121.42	116.17
2	152-A	201	FOL	CA-N-C	3.49	126.93	122.15
2	34-A	201	FOL	N1-C8A-N8	3.49	122.57	116.42
2	2-A	201	FOL	C4-N3-C2	3.50	121.44	116.17
2	159-A	201	FOL	N1-C8A-N8	3.50	122.58	116.42
2	53-A	201	FOL	CA-N-C	3.50	126.94	122.15
2	129-A	201	FOL	CB-CA-N	3.51	115.55	110.22
2	103-A	201	FOL	C4-N3-C2	3.51	121.46	116.17
2	64-A	201	FOL	N1-C8A-N8	3.51	122.61	116.42
2	21-A	201	FOL	C4-C4A-N5	3.52	122.54	118.68
2	112-A	201	FOL	C4-N3-C2	3.53	121.48	116.17
2	60-A	201	FOL	N1-C8A-N8	3.53	122.64	116.42
2	83-A	201	FOL	CA-N-C	3.53	126.99	122.15
2	153-A	201	FOL	N1-C8A-N8	3.53	122.65	116.42
2	97-A	201	FOL	N1-C8A-N8	3.53	122.65	116.42
2	148-A	201	FOL	N1-C8A-N8	3.54	122.65	116.42
2	99-A	201	FOL	N1-C8A-N8	3.54	122.66	116.42
4	33-A	204	NAP	O7N-C7N-C3N	3.54	123.77	119.62
2	54-A	201	FOL	N1-C8A-N8	3.57	122.70	116.42
2	41-A	201	FOL	C4-N3-C2	3.57	121.55	116.17
2	127-A	201	FOL	N1-C8A-N8	3.58	122.72	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	91-A	201	FOL	C4-N3-C2	3.58	121.57	116.17
2	96-A	201	FOL	C4-N3-C2	3.59	121.58	116.17
2	23-A	201	FOL	CA-N-C	3.59	127.07	122.15
2	163-A	201	FOL	N1-C8A-N8	3.59	122.75	116.42
2	80-A	201	FOL	C4-N3-C2	3.59	121.58	116.17
2	145-A	201	FOL	CB-CA-N	3.60	115.68	110.22
2	124-A	201	FOL	C4-N3-C2	3.60	121.59	116.17
2	26-A	201	FOL	CB-CA-CT	3.60	117.51	112.28
2	78-A	201	FOL	CG-CB-CA	3.61	120.39	113.19
2	135-A	201	FOL	C4-N3-C2	3.61	121.61	116.17
2	140-A	201	FOL	C4-N3-C2	3.61	121.61	116.17
2	120-A	201	FOL	N1-C8A-N8	3.62	122.80	116.42
2	116-A	201	FOL	N1-C8A-N8	3.62	122.80	116.42
2	64-A	201	FOL	C4-N3-C2	3.63	121.64	116.17
2	93-A	201	FOL	C4-N3-C2	3.63	121.64	116.17
2	62-A	201	FOL	C4-N3-C2	3.63	121.64	116.17
2	60-A	201	FOL	C4-N3-C2	3.64	121.65	116.17
2	85-A	201	FOL	C4-N3-C2	3.64	121.66	116.17
2	46-A	201	FOL	N1-C8A-N8	3.64	122.84	116.42
2	67-A	201	FOL	CB-CA-N	3.66	115.78	110.22
2	137-A	201	FOL	C4-N3-C2	3.66	121.69	116.17
2	116-A	201	FOL	C4-N3-C2	3.67	121.69	116.17
2	149-A	201	FOL	N1-C8A-N8	3.68	122.90	116.42
2	54-A	201	FOL	C4-N3-C2	3.68	121.71	116.17
2	81-A	201	FOL	C4-N3-C2	3.69	121.72	116.17
2	127-A	201	FOL	CB-CA-N	3.69	115.83	110.22
2	30-A	201	FOL	C4-N3-C2	3.69	121.73	116.17
2	89-A	201	FOL	CB-CA-N	3.69	115.83	110.22
4	18-A	204	NAP	O7N-C7N-C3N	3.70	123.95	119.62
2	112-A	201	FOL	N1-C8A-N8	3.70	122.94	116.42
2	93-A	201	FOL	CA-N-C	3.72	127.24	122.15
2	95-A	201	FOL	N1-C8A-N8	3.72	122.97	116.42
2	55-A	201	FOL	C4-N3-C2	3.73	121.78	116.17
2	148-A	201	FOL	C4-N3-C2	3.73	121.78	116.17
2	129-A	201	FOL	C4-N3-C2	3.73	121.80	116.17
4	81-A	204	NAP	C5A-C6A-N6A	3.73	128.08	120.47
2	127-A	201	FOL	C4-N3-C2	3.76	121.83	116.17
2	156-A	201	FOL	C4-N3-C2	3.76	121.83	116.17
2	144-A	201	FOL	N1-C8A-N8	3.76	123.05	116.42
2	138-A	201	FOL	C4-N3-C2	3.77	121.84	116.17
2	24-A	201	FOL	C4-N3-C2	3.77	121.85	116.17
2	47-A	201	FOL	C4-N3-C2	3.77	121.86	116.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	20-A	201	FOL	N1-C8A-N8	3.78	123.08	116.42
2	35-A	201	FOL	N1-C8A-N8	3.78	123.08	116.42
2	165-A	201	FOL	N1-C8A-N8	3.79	123.09	116.42
4	108-A	204	NAP	O3D-C3D-C4D	3.79	122.16	111.09
2	150-A	201	FOL	C4-N3-C2	3.79	121.89	116.17
2	18-A	201	FOL	CG-CB-CA	3.79	120.76	113.19
2	36-A	201	FOL	C4-N3-C2	3.80	121.89	116.17
2	31-A	201	FOL	C4-N3-C2	3.80	121.89	116.17
2	73-A	201	FOL	N1-C8A-N8	3.80	123.12	116.42
2	3-A	201	FOL	C4-N3-C2	3.80	121.90	116.17
2	115-A	201	FOL	C4-N3-C2	3.81	121.91	116.17
2	89-A	201	FOL	CA-N-C	3.81	127.37	122.15
2	99-A	201	FOL	C4-N3-C2	3.82	121.92	116.17
2	84-A	201	FOL	C4-N3-C2	3.82	121.92	116.17
2	42-A	201	FOL	C4-N3-C2	3.82	121.93	116.17
2	138-A	201	FOL	N1-C8A-N8	3.82	123.16	116.42
2	7-A	201	FOL	C4-N3-C2	3.82	121.93	116.17
2	59-A	201	FOL	N1-C8A-N8	3.84	123.18	116.42
2	162-A	201	FOL	CB-CA-N	3.84	116.06	110.22
2	13-A	201	FOL	CG-CB-CA	3.84	120.86	113.19
2	161-A	201	FOL	N1-C8A-N8	3.85	123.20	116.42
2	81-A	201	FOL	N1-C8A-N8	3.85	123.20	116.42
2	132-A	201	FOL	CG-CB-CA	3.85	120.88	113.19
2	29-A	201	FOL	C4-N3-C2	3.86	121.98	116.17
2	132-A	201	FOL	C4-N3-C2	3.86	121.98	116.17
2	141-A	201	FOL	C4-N3-C2	3.87	122.00	116.17
2	93-A	201	FOL	N1-C8A-N8	3.87	123.23	116.42
2	83-A	201	FOL	C4-N3-C2	3.87	122.00	116.17
2	118-A	201	FOL	C4-N3-C2	3.88	122.01	116.17
2	78-A	201	FOL	N1-C8A-N8	3.88	123.25	116.42
2	15-A	201	FOL	C4-N3-C2	3.88	122.02	116.17
2	1-A	201	FOL	C4-N3-C2	3.89	122.03	116.17
2	68-A	201	FOL	C4-N3-C2	3.89	122.03	116.17
2	58-A	201	FOL	C4-N3-C2	3.89	122.03	116.17
2	161-A	201	FOL	C4-N3-C2	3.90	122.04	116.17
2	21-A	201	FOL	C4-N3-C2	3.91	122.06	116.17
2	23-A	201	FOL	N1-C8A-N8	3.91	123.31	116.42
2	146-A	201	FOL	C4-N3-C2	3.91	122.07	116.17
2	50-A	201	FOL	C4-N3-C2	3.92	122.08	116.17
2	5-A	201	FOL	N1-C8A-N8	3.94	123.36	116.42
2	122-A	201	FOL	C4-N3-C2	3.94	122.10	116.17
2	52-A	201	FOL	N1-C8A-N8	3.95	123.38	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	101-A	201	FOL	N1-C8A-N8	3.95	123.38	116.42
2	111-A	201	FOL	CB-CA-N	3.95	116.22	110.22
2	93-A	201	FOL	CB-CA-N	3.95	116.23	110.22
2	106-A	201	FOL	N1-C8A-N8	3.96	123.40	116.42
2	74-A	201	FOL	C4-N3-C2	3.96	122.14	116.17
2	56-A	201	FOL	CB-CA-N	3.97	116.25	110.22
2	58-A	201	FOL	N1-C8A-N8	3.97	123.42	116.42
2	38-A	201	FOL	C4-N3-C2	3.97	122.15	116.17
2	130-A	201	FOL	C4-N3-C2	3.97	122.15	116.17
2	56-A	201	FOL	CG-CB-CA	3.98	121.14	113.19
2	163-A	201	FOL	CA-N-C	3.98	127.61	122.15
2	91-A	201	FOL	N1-C8A-N8	3.98	123.44	116.42
2	76-A	201	FOL	C4-C4A-N5	3.99	123.06	118.68
2	1-A	201	FOL	CB-CA-N	4.00	116.31	110.22
2	44-A	201	FOL	C4-N3-C2	4.00	122.20	116.17
2	78-A	201	FOL	C4-N3-C2	4.01	122.22	116.17
2	145-A	201	FOL	C4-N3-C2	4.02	122.22	116.17
2	80-A	201	FOL	N1-C8A-N8	4.02	123.51	116.42
2	40-A	201	FOL	CB-CA-N	4.03	116.34	110.22
2	155-A	201	FOL	C4-N3-C2	4.04	122.25	116.17
2	104-A	201	FOL	C4-N3-C2	4.04	122.25	116.17
2	103-A	201	FOL	N1-C8A-N8	4.05	123.56	116.42
2	118-A	201	FOL	CB-CA-N	4.05	116.38	110.22
2	108-A	201	FOL	N1-C8A-N8	4.05	123.56	116.42
2	70-A	201	FOL	C4-N3-C2	4.05	122.28	116.17
2	113-A	201	FOL	C4-N3-C2	4.05	122.28	116.17
2	44-A	201	FOL	CB-CA-N	4.06	116.40	110.22
2	49-A	201	FOL	C4-N3-C2	4.07	122.30	116.17
2	110-A	201	FOL	CG-CB-CA	4.07	121.31	113.19
2	79-A	201	FOL	C4-N3-C2	4.07	122.30	116.17
2	134-A	201	FOL	C11-C-N	4.08	124.50	116.97
2	57-A	201	FOL	CB-CA-N	4.08	116.42	110.22
2	136-A	201	FOL	CA-N-C	4.09	127.75	122.15
2	82-A	201	FOL	C4-N3-C2	4.09	122.34	116.17
2	80-A	201	FOL	CB-CA-N	4.10	116.45	110.22
2	48-A	201	FOL	N1-C8A-N8	4.10	123.64	116.42
2	29-A	201	FOL	N1-C8A-N8	4.10	123.64	116.42
2	16-A	201	FOL	N1-C8A-N8	4.10	123.64	116.42
2	26-A	201	FOL	C4-N3-C2	4.11	122.36	116.17
2	75-A	201	FOL	C4-N3-C2	4.11	122.36	116.17
2	126-A	201	FOL	C4-C4A-N5	4.12	123.19	118.68
2	121-A	201	FOL	C4-N3-C2	4.12	122.37	116.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-A	201	FOL	C4-N3-C2	4.12	122.38	116.17
2	3-A	201	FOL	CB-CA-CT	4.13	118.29	112.28
2	65-A	201	FOL	C4-N3-C2	4.14	122.40	116.17
2	11-A	201	FOL	C4-N3-C2	4.15	122.42	116.17
2	46-A	201	FOL	C4-N3-C2	4.15	122.42	116.17
2	100-A	201	FOL	C4-N3-C2	4.15	122.42	116.17
2	67-A	201	FOL	C4-N3-C2	4.15	122.42	116.17
2	108-A	201	FOL	CB-CA-N	4.15	116.53	110.22
2	119-A	201	FOL	C4-N3-C2	4.16	122.44	116.17
2	88-A	201	FOL	C4-N3-C2	4.16	122.44	116.17
2	31-A	201	FOL	CA-N-C	4.17	127.86	122.15
2	163-A	201	FOL	C4-N3-C2	4.18	122.47	116.17
2	165-A	201	FOL	CA-N-C	4.18	127.88	122.15
2	6-A	201	FOL	C4-N3-C2	4.19	122.48	116.17
2	30-A	201	FOL	C4-C4A-N5	4.19	123.28	118.68
2	97-A	201	FOL	C4-N3-C2	4.20	122.49	116.17
2	139-A	201	FOL	C4-N3-C2	4.20	122.49	116.17
2	105-A	201	FOL	C4-N3-C2	4.20	122.50	116.17
2	75-A	201	FOL	N1-C8A-N8	4.21	123.83	116.42
2	106-A	201	FOL	C4-N3-C2	4.21	122.51	116.17
2	71-A	201	FOL	C4-N3-C2	4.21	122.51	116.17
2	167-A	201	FOL	CB-CA-CT	4.22	118.41	112.28
2	49-A	201	FOL	N1-C8A-N8	4.22	123.86	116.42
2	33-A	201	FOL	CB-CA-CT	4.22	118.42	112.28
2	28-A	201	FOL	C4-N3-C2	4.22	122.53	116.17
2	128-A	201	FOL	N1-C8A-N8	4.23	123.86	116.42
2	142-A	201	FOL	N1-C8A-N8	4.23	123.87	116.42
2	160-A	201	FOL	CB-CA-N	4.24	116.66	110.22
2	124-A	201	FOL	CB-CA-N	4.24	116.67	110.22
2	51-A	201	FOL	C4-N3-C2	4.25	122.58	116.17
2	57-A	201	FOL	C4-N3-C2	4.26	122.59	116.17
2	61-A	201	FOL	C4-N3-C2	4.26	122.59	116.17
2	77-A	201	FOL	C4-N3-C2	4.27	122.60	116.17
2	19-A	201	FOL	C4-N3-C2	4.27	122.60	116.17
2	18-A	201	FOL	C4-N3-C2	4.27	122.61	116.17
2	37-A	201	FOL	C4-N3-C2	4.29	122.64	116.17
2	128-A	201	FOL	C4-N3-C2	4.30	122.64	116.17
2	69-A	201	FOL	C4-N3-C2	4.32	122.68	116.17
2	143-A	201	FOL	C4-N3-C2	4.32	122.68	116.17
2	41-A	201	FOL	N1-C8A-N8	4.34	124.07	116.42
2	24-A	201	FOL	CB-CA-N	4.35	116.83	110.22
2	123-A	201	FOL	C4-N3-C2	4.36	122.74	116.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	102-A	201	FOL	N1-C8A-N8	4.37	124.12	116.42
2	151-A	201	FOL	C4-N3-C2	4.38	122.76	116.17
2	70-A	201	FOL	CA-N-C	4.38	128.15	122.15
2	104-A	201	FOL	N1-C8A-N8	4.39	124.15	116.42
2	160-A	201	FOL	C4-N3-C2	4.39	122.79	116.17
2	22-A	201	FOL	C4-N3-C2	4.39	122.79	116.17
2	34-A	201	FOL	C12-C13-C14	4.40	125.44	120.30
2	10-A	201	FOL	N1-C8A-N8	4.40	124.17	116.42
2	125-A	201	FOL	C4-N3-C2	4.42	122.83	116.17
2	110-A	201	FOL	C4-N3-C2	4.43	122.85	116.17
2	165-A	201	FOL	CB-CA-N	4.44	116.96	110.22
2	38-A	201	FOL	N1-C8A-N8	4.44	124.25	116.42
4	117-A	204	NAP	O2N-PN-O1N	4.46	135.38	112.28
2	63-A	201	FOL	CA-N-C	4.48	128.28	122.15
2	154-A	201	FOL	C4-N3-C2	4.49	122.93	116.17
2	131-A	201	FOL	N1-C8A-N8	4.51	124.37	116.42
2	43-A	201	FOL	N1-C8A-N8	4.51	124.37	116.42
2	158-A	201	FOL	CB-CA-N	4.54	117.12	110.22
2	10-A	201	FOL	CB-CA-N	4.55	117.13	110.22
2	63-A	201	FOL	C4-N3-C2	4.56	123.04	116.17
2	148-A	201	FOL	CB-CA-CT	4.57	118.93	112.28
2	87-A	201	FOL	CB-CA-N	4.58	117.19	110.22
2	66-A	201	FOL	C4-N3-C2	4.60	123.09	116.17
2	23-A	201	FOL	CB-CA-N	4.60	117.21	110.22
2	110-A	201	FOL	CA-N-C	4.60	128.45	122.15
2	81-A	201	FOL	CB-CA-N	4.62	117.24	110.22
2	60-A	201	FOL	CB-CA-N	4.66	117.30	110.22
2	69-A	201	FOL	CB-CA-N	4.68	117.33	110.22
2	56-A	201	FOL	C4-N3-C2	4.68	123.22	116.17
2	11-A	201	FOL	CB-CA-N	4.69	117.34	110.22
2	128-A	201	FOL	CB-CA-CT	4.69	119.10	112.28
2	134-A	201	FOL	C4-N3-C2	4.69	123.24	116.17
2	82-A	201	FOL	CB-CA-N	4.70	117.36	110.22
2	107-A	201	FOL	C4-N3-C2	4.71	123.27	116.17
2	164-A	201	FOL	C4-N3-C2	4.71	123.27	116.17
2	27-A	201	FOL	C4-N3-C2	4.73	123.29	116.17
2	43-A	201	FOL	CG-CB-CA	4.73	122.63	113.19
2	25-A	201	FOL	C4-N3-C2	4.73	123.30	116.17
2	13-A	201	FOL	CA-N-C	4.75	128.66	122.15
2	53-A	201	FOL	C4-N3-C2	4.77	123.35	116.17
2	111-A	201	FOL	C4-N3-C2	4.78	123.37	116.17
2	63-A	201	FOL	CB-CA-N	4.79	117.51	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	136-A	201	FOL	C4-N3-C2	4.81	123.41	116.17
2	153-A	201	FOL	CG-CB-CA	4.83	122.84	113.19
2	70-A	201	FOL	CG-CB-CA	4.84	122.85	113.19
2	126-A	201	FOL	CG-CB-CA	4.87	122.91	113.19
2	62-A	201	FOL	CB-CA-N	4.89	117.65	110.22
2	14-A	201	FOL	C4-N3-C2	4.92	123.58	116.17
2	72-A	201	FOL	C4-N3-C2	5.00	123.70	116.17
2	8-A	201	FOL	C4-N3-C2	5.01	123.72	116.17
2	70-A	201	FOL	CB-CA-N	5.09	117.96	110.22
2	48-A	201	FOL	CB-CA-CT	5.14	119.75	112.28
2	7-A	201	FOL	CA-N-C	5.15	129.20	122.15
2	167-A	201	FOL	C4-N3-C2	5.17	123.95	116.17
2	52-A	201	FOL	CB-CA-CT	5.19	119.82	112.28
2	15-A	201	FOL	CG-CB-CA	5.28	123.73	113.19
2	126-A	201	FOL	C4-N3-C2	5.36	124.25	116.17
2	26-A	201	FOL	CB-CA-N	5.43	118.47	110.22
2	58-A	201	FOL	CB-CA-CT	5.52	120.30	112.28
2	144-A	201	FOL	CA-N-C	5.54	129.74	122.15
2	98-A	201	FOL	C4-N3-C2	5.57	124.57	116.17
2	139-A	201	FOL	CB-CA-N	5.61	118.74	110.22
2	43-A	201	FOL	CB-CA-N	5.62	118.76	110.22
2	86-A	201	FOL	CA-N-C	5.63	129.86	122.15
2	92-A	201	FOL	CB-CA-N	5.68	118.84	110.22
2	84-A	201	FOL	CB-CA-N	5.69	118.86	110.22
2	76-A	201	FOL	C4-N3-C2	5.82	124.94	116.17
2	133-A	201	FOL	C4-N3-C2	5.99	125.20	116.17
2	13-A	201	FOL	C4-N3-C2	6.04	125.27	116.17
2	144-A	201	FOL	CG-CB-CA	6.07	125.32	113.19
2	129-A	201	FOL	CA-N-C	6.08	130.48	122.15
2	85-A	201	FOL	CB-CA-N	6.26	119.73	110.22
2	138-A	201	FOL	CA-N-C	6.27	130.74	122.15
2	13-A	201	FOL	CB-CA-N	6.28	119.76	110.22
2	14-A	201	FOL	CB-CA-N	6.32	119.83	110.22
2	15-A	201	FOL	CB-CA-CT	6.39	121.56	112.28
2	25-A	201	FOL	CB-CA-N	6.58	120.22	110.22
2	39-A	201	FOL	CA-N-C	6.59	131.18	122.15
2	83-A	201	FOL	CB-CA-N	6.61	120.27	110.22
4	119-A	204	NAP	O2N-PN-O1N	6.66	146.73	112.28
2	39-A	201	FOL	CB-CA-N	7.22	121.19	110.22
2	112-A	201	FOL	CB-CA-N	7.35	121.38	110.22
2	110-A	201	FOL	CB-CA-N	7.93	122.27	110.22
2	115-A	201	FOL	CB-CA-N	8.06	122.46	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	114-A	201	FOL	CB-CA-N	8.17	122.64	110.22
4	56-A	204	NAP	O2N-PN-O1N	8.50	156.26	112.28
2	105-A	201	FOL	CB-CA-CT	8.50	124.64	112.28
4	118-A	204	NAP	O2N-PN-O1N	10.62	167.26	112.28
4	57-A	204	NAP	O2N-PN-O1N	11.81	173.38	112.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.