



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 08:27 PM UTC

PDB ID : 7D49 / pdb_00007d49
Title : X-ray crystal Structure of E.coli Dihydrofolate Reductase complexed with folate and NADP+ at pH4.5
Authors : Wan, Q.; Dealwis, C.
Deposited on : 2020-09-23
Resolution : 1.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

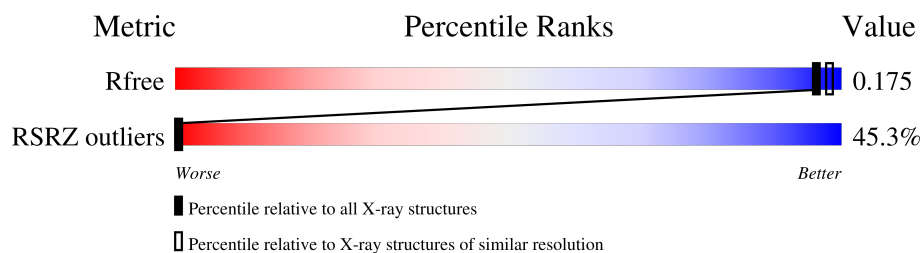
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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))
R_{free}	180053	2563 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 113251 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	2-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	3-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	4-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	5-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	6-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	7-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	8-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	9-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	10-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	11-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	12-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	13-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	14-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	15-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	16-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	17-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	18-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	19-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	20-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	21-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	22-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	23-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	24-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	25-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	26-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	27-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	28-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	29-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	30-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	31-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	32-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	33-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	34-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	35-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	36-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	37-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	38-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	39-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	40-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	41-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	42-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	43-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	44-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	45-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	46-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	47-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	48-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	49-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	50-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	51-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	52-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	53-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	54-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	55-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	56-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	57-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	58-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	59-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	60-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	61-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	62-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	63-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	64-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	65-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	66-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	67-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	68-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	69-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	70-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	71-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	72-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	73-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	74-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	75-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	76-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	77-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	78-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	79-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			

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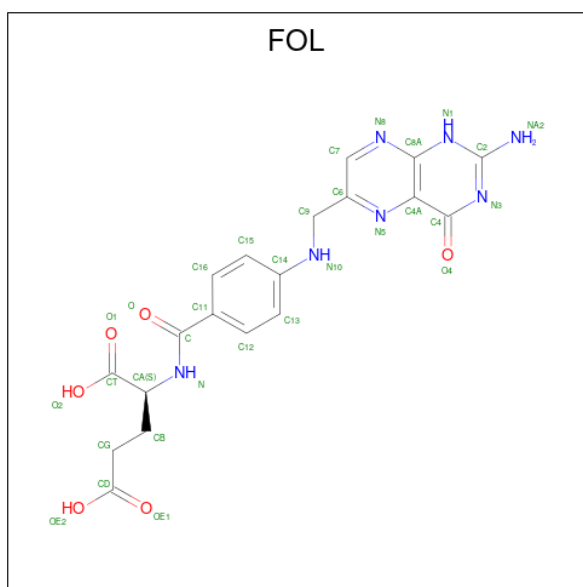
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	80-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASP	ASN	conflict	UNP P0ABQ4

- Molecule 2 is FOLIC ACID (CCD ID: FOL) (formula: $\text{C}_{19}\text{H}_{19}\text{N}_7\text{O}_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1-A	1	Total 32	C 19	N 7	O 6	0	0
2	2-A	1	Total 32	C 19	N 7	O 6	0	0
2	3-A	1	Total 32	C 19	N 7	O 6	0	0
2	4-A	1	Total 32	C 19	N 7	O 6	0	0
2	5-A	1	Total 32	C 19	N 7	O 6	0	0
2	6-A	1	Total 32	C 19	N 7	O 6	0	0
2	7-A	1	Total 32	C 19	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	8-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	9-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	10-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	11-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	12-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	13-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	14-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	15-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	16-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	17-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	18-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	19-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	20-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	21-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	22-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	23-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	24-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	25-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	26-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	27-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	28-A	1	Total	C	N	O	0	0
			32	19	7	6		

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

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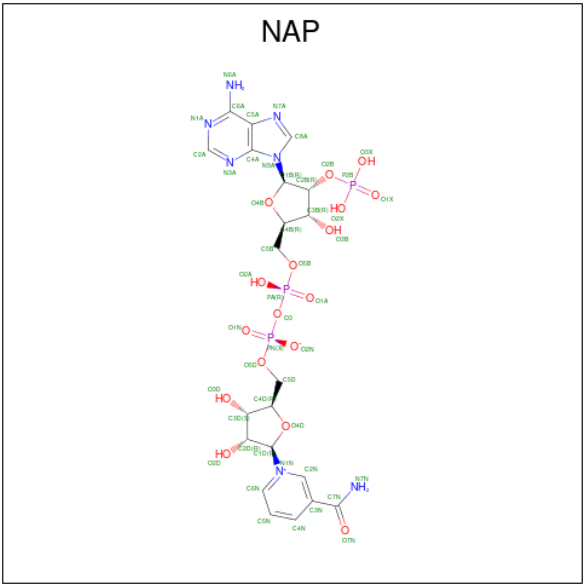
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	50-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	51-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	52-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	53-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	54-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	55-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	56-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	57-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	58-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	59-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	60-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	61-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	62-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	63-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	64-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	65-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	66-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	67-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	68-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	69-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	70-A	1	Total	C	N	O	0	0
			32	19	7	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	71-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	72-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	73-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	74-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	75-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	76-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	77-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	78-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	79-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	80-A	1	Total	C	N	O	0	0
			32	19	7	6		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	2-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	3-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	4-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	5-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	6-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	7-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	8-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	9-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	10-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	11-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	12-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	13-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	14-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	15-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	16-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	17-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	18-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	19-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	20-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	21-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	22-A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	23-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	24-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	25-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	26-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	27-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	28-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	29-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	30-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	31-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	32-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	33-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	34-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	35-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	36-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	37-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	38-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	39-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	40-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	41-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	42-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	43-A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	44-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	45-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	46-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	47-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	48-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	49-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	50-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	51-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	52-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	53-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	54-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	55-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	56-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	57-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	58-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	59-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	60-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	61-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	62-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	63-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	64-A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	65-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	66-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	67-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	68-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	69-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	70-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	71-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	72-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	73-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	74-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	75-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	76-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	77-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	78-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	79-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	80-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	79	Total	O	0	0
			79	79		
4	2-A	68	Total	O	0	0
			68	68		
4	3-A	63	Total	O	0	0
			63	63		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	4-A	67	Total O 67 67	0	0
4	5-A	67	Total O 67 67	0	0
4	6-A	60	Total O 60 60	0	0
4	7-A	61	Total O 61 61	0	0
4	8-A	61	Total O 61 61	0	0
4	9-A	59	Total O 59 59	0	0
4	10-A	57	Total O 57 57	0	0
4	11-A	72	Total O 72 72	0	0
4	12-A	76	Total O 76 76	0	0
4	13-A	75	Total O 75 75	0	0
4	14-A	72	Total O 72 72	0	0
4	15-A	65	Total O 65 65	0	0
4	16-A	64	Total O 64 64	0	0
4	17-A	72	Total O 72 72	0	0
4	18-A	73	Total O 73 73	0	0
4	19-A	76	Total O 76 76	0	0
4	20-A	57	Total O 57 57	0	0
4	21-A	67	Total O 67 67	0	0
4	22-A	69	Total O 69 69	0	0
4	23-A	71	Total O 71 71	0	0
4	24-A	65	Total O 65 65	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	25-A	61	Total O 61 61	0	0
4	26-A	53	Total O 53 53	0	0
4	27-A	67	Total O 67 67	0	0
4	28-A	74	Total O 74 74	0	0
4	29-A	80	Total O 80 80	0	0
4	30-A	72	Total O 72 72	0	0
4	31-A	76	Total O 76 76	0	0
4	32-A	72	Total O 72 72	0	0
4	33-A	70	Total O 70 70	0	0
4	34-A	62	Total O 62 62	0	0
4	35-A	52	Total O 52 52	0	0
4	36-A	62	Total O 62 62	0	0
4	37-A	66	Total O 66 66	0	0
4	38-A	76	Total O 76 76	0	0
4	39-A	72	Total O 72 72	0	0
4	40-A	75	Total O 75 75	0	0
4	41-A	72	Total O 72 72	0	0
4	42-A	66	Total O 66 66	0	0
4	43-A	65	Total O 65 65	0	0
4	44-A	65	Total O 65 65	0	0
4	45-A	69	Total O 69 69	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	46-A	62	Total O 62 62	0	0
4	47-A	63	Total O 63 63	0	0
4	48-A	80	Total O 80 80	0	0
4	49-A	74	Total O 74 74	0	0
4	50-A	70	Total O 70 70	0	0
4	51-A	69	Total O 69 69	0	0
4	52-A	68	Total O 68 68	0	0
4	53-A	63	Total O 63 63	0	0
4	54-A	70	Total O 70 70	0	0
4	55-A	75	Total O 75 75	0	0
4	56-A	76	Total O 76 76	0	0
4	57-A	72	Total O 72 72	0	0
4	58-A	76	Total O 76 76	0	0
4	59-A	71	Total O 71 71	0	0
4	60-A	75	Total O 75 75	0	0
4	61-A	48	Total O 48 48	0	0
4	62-A	52	Total O 52 52	0	0
4	63-A	72	Total O 72 72	0	0
4	64-A	73	Total O 73 73	0	0
4	65-A	74	Total O 74 74	0	0
4	66-A	62	Total O 62 62	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	67-A	56	Total	O	0	0
			56	56		
4	68-A	56	Total	O	0	0
			56	56		
4	69-A	64	Total	O	0	0
			64	64		
4	70-A	69	Total	O	0	0
			69	69		
4	71-A	65	Total	O	0	0
			65	65		
4	72-A	71	Total	O	0	0
			71	71		
4	73-A	65	Total	O	0	0
			65	65		
4	74-A	63	Total	O	0	0
			63	63		
4	75-A	64	Total	O	0	0
			64	64		
4	76-A	61	Total	O	0	0
			61	61		
4	77-A	71	Total	O	0	0
			71	71		
4	78-A	71	Total	O	0	0
			71	71		
4	79-A	76	Total	O	0	0
			76	76		
4	80-A	71	Total	O	0	0
			71	71		

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

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	34.10Å 45.59Å 99.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.31 – 1.65 27.31 – 1.65	Depositor EDS
% Data completeness (in resolution range)	91.8 (27.31-1.65) 91.3 (27.31-1.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 1.65Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.13rc2_2986)	Depositor
R, R_{free}	0.135 , 0.171 0.146 , 0.175	Depositor DCC
R_{free} test set	904 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	113251	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.25% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

160 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	58-A	201	-	34,34,34	1.02	1 (2%)	43,47,47	1.55	7 (16%)
3	NAP	60-A	202	-	50,52,52	3.29	13 (26%)	71,80,80	1.70	13 (18%)
3	NAP	5-A	202	-	50,52,52	3.30	13 (26%)	71,80,80	1.65	14 (19%)
2	FOL	15-A	201	-	34,34,34	1.01	1 (2%)	43,47,47	1.38	6 (13%)
3	NAP	35-A	202	-	50,52,52	3.34	14 (28%)	71,80,80	1.61	13 (18%)
3	NAP	24-A	202	-	50,52,52	3.34	13 (26%)	71,80,80	1.60	13 (18%)
3	NAP	49-A	202	-	50,52,52	3.30	13 (26%)	71,80,80	1.68	16 (22%)
2	FOL	24-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.33	4 (9%)
2	FOL	5-A	201	-	34,34,34	1.08	3 (8%)	43,47,47	1.39	5 (11%)
3	NAP	44-A	202	-	50,52,52	3.32	14 (28%)	71,80,80	1.65	17 (23%)
2	FOL	9-A	201	-	34,34,34	0.97	2 (5%)	43,47,47	1.46	4 (9%)
3	NAP	42-A	202	-	50,52,52	3.29	14 (28%)	71,80,80	1.71	15 (21%)
3	NAP	74-A	202	-	50,52,52	3.33	16 (32%)	71,80,80	1.79	14 (19%)
3	NAP	79-A	202	-	50,52,52	3.28	14 (28%)	71,80,80	1.58	12 (16%)
2	FOL	23-A	201	-	34,34,34	0.94	2 (5%)	43,47,47	1.53	4 (9%)
2	FOL	62-A	201	-	34,34,34	0.97	1 (2%)	43,47,47	1.39	4 (9%)
3	NAP	27-A	202	-	50,52,52	3.30	13 (26%)	71,80,80	1.54	12 (16%)
3	NAP	2-A	202	-	50,52,52	3.33	14 (28%)	71,80,80	1.67	14 (19%)
3	NAP	69-A	202	-	50,52,52	3.26	14 (28%)	71,80,80	1.59	13 (18%)
2	FOL	70-A	201	-	34,34,34	1.23	3 (8%)	43,47,47	1.86	11 (25%)
3	NAP	67-A	202	-	50,52,52	3.27	14 (28%)	71,80,80	1.62	13 (18%)
2	FOL	71-A	201	-	34,34,34	0.99	2 (5%)	43,47,47	1.91	9 (20%)
2	FOL	10-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.38	6 (13%)
2	FOL	65-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.73	9 (20%)
3	NAP	36-A	202	-	50,52,52	3.32	14 (28%)	71,80,80	1.63	16 (22%)
2	FOL	72-A	201	-	34,34,34	1.11	2 (5%)	43,47,47	2.63	17 (39%)
3	NAP	56-A	202	-	50,52,52	3.28	13 (26%)	71,80,80	1.54	11 (15%)
3	NAP	61-A	202	-	50,52,52	3.32	13 (26%)	71,80,80	1.59	14 (19%)
2	FOL	41-A	201	-	34,34,34	0.99	3 (8%)	43,47,47	1.41	3 (6%)
2	FOL	61-A	201	-	34,34,34	1.07	2 (5%)	43,47,47	1.56	6 (13%)
2	FOL	19-A	201	-	34,34,34	1.06	2 (5%)	43,47,47	1.39	4 (9%)
3	NAP	19-A	202	-	50,52,52	3.25	13 (26%)	71,80,80	1.62	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	11-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.23	3 (6%)
2	FOL	64-A	201	-	34,34,34	1.09	1 (2%)	43,47,47	2.08	12 (27%)
3	NAP	1-A	202	-	50,52,52	3.35	14 (28%)	71,80,80	1.64	14 (19%)
2	FOL	28-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.22	2 (4%)
3	NAP	18-A	202	-	50,52,52	3.24	12 (24%)	71,80,80	1.62	12 (16%)
3	NAP	46-A	202	-	50,52,52	3.31	14 (28%)	71,80,80	1.64	13 (18%)
3	NAP	8-A	202	-	50,52,52	3.29	14 (28%)	71,80,80	1.62	13 (18%)
3	NAP	80-A	202	-	50,52,52	3.26	14 (28%)	71,80,80	1.76	16 (22%)
3	NAP	15-A	202	-	50,52,52	3.32	14 (28%)	71,80,80	1.61	12 (16%)
2	FOL	8-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.42	4 (9%)
2	FOL	35-A	201	-	34,34,34	0.96	2 (5%)	43,47,47	1.38	4 (9%)
2	FOL	7-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.32	3 (6%)
2	FOL	4-A	201	-	34,34,34	1.04	1 (2%)	43,47,47	1.37	4 (9%)
3	NAP	47-A	202	-	50,52,52	3.30	14 (28%)	71,80,80	1.67	13 (18%)
3	NAP	33-A	202	-	50,52,52	3.31	14 (28%)	71,80,80	1.58	13 (18%)
3	NAP	57-A	202	-	50,52,52	3.27	14 (28%)	71,80,80	1.63	14 (19%)
3	NAP	32-A	202	-	50,52,52	3.32	14 (28%)	71,80,80	1.58	12 (16%)
3	NAP	22-A	202	-	50,52,52	3.32	13 (26%)	71,80,80	1.63	15 (21%)
3	NAP	45-A	202	-	50,52,52	3.33	14 (28%)	71,80,80	1.62	15 (21%)
3	NAP	70-A	202	-	50,52,52	3.31	13 (26%)	71,80,80	1.59	13 (18%)
2	FOL	75-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.44	4 (9%)
3	NAP	58-A	202	-	50,52,52	3.26	14 (28%)	71,80,80	1.61	15 (21%)
2	FOL	27-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.31	3 (6%)
2	FOL	45-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.41	4 (9%)
3	NAP	29-A	202	-	50,52,52	3.32	13 (26%)	71,80,80	1.63	15 (21%)
3	NAP	50-A	202	-	50,52,52	3.27	13 (26%)	71,80,80	1.65	14 (19%)
3	NAP	40-A	202	-	50,52,52	3.37	14 (28%)	71,80,80	1.70	15 (21%)
2	FOL	21-A	201	-	34,34,34	0.97	2 (5%)	43,47,47	1.21	2 (4%)
3	NAP	38-A	202	-	50,52,52	3.33	14 (28%)	71,80,80	1.59	15 (21%)
2	FOL	67-A	201	-	34,34,34	1.15	2 (5%)	43,47,47	2.06	8 (18%)
2	FOL	78-A	201	-	34,34,34	1.23	3 (8%)	43,47,47	1.85	8 (18%)
2	FOL	39-A	201	-	34,34,34	1.13	1 (2%)	43,47,47	1.54	7 (16%)
2	FOL	42-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.29	2 (4%)
2	FOL	73-A	201	-	34,34,34	1.27	4 (11%)	43,47,47	2.68	17 (39%)
3	NAP	48-A	202	-	50,52,52	3.30	13 (26%)	71,80,80	1.68	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	3-A	202	-	50,52,52	3.36	14 (28%)	71,80,80	1.61	14 (19%)
2	FOL	26-A	201	-	34,34,34	1.01	1 (2%)	43,47,47	1.39	6 (13%)
3	NAP	23-A	202	-	50,52,52	3.31	14 (28%)	71,80,80	1.68	14 (19%)
2	FOL	48-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.55	6 (13%)
3	NAP	20-A	202	-	50,52,52	3.30	13 (26%)	71,80,80	1.57	11 (15%)
3	NAP	17-A	202	-	50,52,52	3.26	13 (26%)	71,80,80	1.59	12 (16%)
3	NAP	14-A	202	-	50,52,52	3.31	12 (24%)	71,80,80	1.57	11 (15%)
3	NAP	76-A	202	-	50,52,52	3.34	14 (28%)	71,80,80	1.59	15 (21%)
2	FOL	2-A	201	-	34,34,34	1.01	1 (2%)	43,47,47	1.29	2 (4%)
2	FOL	22-A	201	-	34,34,34	0.98	2 (5%)	43,47,47	1.39	6 (13%)
2	FOL	69-A	201	-	34,34,34	1.29	3 (8%)	43,47,47	2.26	11 (25%)
3	NAP	71-A	202	-	50,52,52	3.28	13 (26%)	71,80,80	1.67	13 (18%)
2	FOL	46-A	201	-	34,34,34	0.96	2 (5%)	43,47,47	1.46	6 (13%)
2	FOL	43-A	201	-	34,34,34	0.97	1 (2%)	43,47,47	1.44	3 (6%)
3	NAP	21-A	202	-	50,52,52	3.32	13 (26%)	71,80,80	1.58	12 (16%)
2	FOL	17-A	201	-	34,34,34	1.03	2 (5%)	43,47,47	1.34	4 (9%)
2	FOL	49-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.44	5 (11%)
2	FOL	3-A	201	-	34,34,34	1.01	1 (2%)	43,47,47	1.37	4 (9%)
3	NAP	31-A	202	-	50,52,52	3.32	15 (30%)	71,80,80	1.59	13 (18%)
3	NAP	52-A	202	-	50,52,52	3.30	13 (26%)	71,80,80	1.61	14 (19%)
3	NAP	34-A	202	-	50,52,52	3.35	14 (28%)	71,80,80	1.70	14 (19%)
2	FOL	20-A	201	-	34,34,34	1.01	3 (8%)	43,47,47	1.35	4 (9%)
2	FOL	31-A	201	-	34,34,34	0.99	1 (2%)	43,47,47	1.40	4 (9%)
2	FOL	34-A	201	-	34,34,34	0.97	1 (2%)	43,47,47	1.37	3 (6%)
2	FOL	74-A	201	-	34,34,34	1.09	2 (5%)	43,47,47	1.80	8 (18%)
2	FOL	37-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.43	5 (11%)
2	FOL	18-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.36	3 (6%)
2	FOL	55-A	201	-	34,34,34	0.99	1 (2%)	43,47,47	1.48	4 (9%)
2	FOL	29-A	201	-	34,34,34	1.06	2 (5%)	43,47,47	1.53	7 (16%)
3	NAP	53-A	202	-	50,52,52	3.28	13 (26%)	71,80,80	1.63	13 (18%)
2	FOL	14-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.49	7 (16%)
3	NAP	66-A	202	-	50,52,52	3.28	13 (26%)	71,80,80	1.66	14 (19%)
3	NAP	55-A	202	-	50,52,52	3.20	13 (26%)	71,80,80	1.69	13 (18%)
3	NAP	39-A	202	-	50,52,52	3.38	14 (28%)	71,80,80	1.62	15 (21%)
2	FOL	53-A	201	-	34,34,34	0.97	2 (5%)	43,47,47	1.34	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	51-A	201	-	34,34,34	0.96	1 (2%)	43,47,47	1.30	2 (4%)
2	FOL	36-A	201	-	34,34,34	0.98	2 (5%)	43,47,47	1.25	3 (6%)
3	NAP	73-A	202	-	50,52,52	3.33	13 (26%)	71,80,80	1.58	13 (18%)
3	NAP	78-A	202	-	50,52,52	3.30	13 (26%)	71,80,80	1.64	14 (19%)
3	NAP	9-A	202	-	50,52,52	3.32	13 (26%)	71,80,80	1.63	13 (18%)
3	NAP	12-A	202	-	50,52,52	3.29	13 (26%)	71,80,80	1.61	14 (19%)
2	FOL	33-A	201	-	34,34,34	1.03	2 (5%)	43,47,47	1.44	5 (11%)
3	NAP	51-A	202	-	50,52,52	3.26	13 (26%)	71,80,80	1.58	12 (16%)
3	NAP	30-A	202	-	50,52,52	3.31	13 (26%)	71,80,80	1.61	14 (19%)
2	FOL	1-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.37	3 (6%)
3	NAP	13-A	202	-	50,52,52	3.29	13 (26%)	71,80,80	1.60	12 (16%)
3	NAP	62-A	202	-	50,52,52	3.31	13 (26%)	71,80,80	1.62	15 (21%)
2	FOL	47-A	201	-	34,34,34	0.97	1 (2%)	43,47,47	1.49	6 (13%)
2	FOL	40-A	201	-	34,34,34	1.04	1 (2%)	43,47,47	1.72	8 (18%)
2	FOL	32-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.32	5 (11%)
2	FOL	60-A	201	-	34,34,34	1.06	2 (5%)	43,47,47	1.53	5 (11%)
3	NAP	37-A	202	-	50,52,52	3.35	13 (26%)	71,80,80	1.60	14 (19%)
3	NAP	7-A	202	-	50,52,52	3.32	13 (26%)	71,80,80	1.65	14 (19%)
3	NAP	11-A	202	-	50,52,52	3.27	13 (26%)	71,80,80	1.59	13 (18%)
2	FOL	12-A	201	-	34,34,34	1.03	2 (5%)	43,47,47	1.23	2 (4%)
2	FOL	13-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.21	3 (6%)
3	NAP	59-A	202	-	50,52,52	3.31	13 (26%)	71,80,80	1.58	14 (19%)
2	FOL	38-A	201	-	34,34,34	1.14	2 (5%)	43,47,47	1.34	4 (9%)
3	NAP	65-A	202	-	50,52,52	3.29	13 (26%)	71,80,80	1.68	14 (19%)
3	NAP	77-A	202	-	50,52,52	3.31	13 (26%)	71,80,80	1.57	14 (19%)
2	FOL	6-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.31	3 (6%)
3	NAP	41-A	202	-	50,52,52	3.33	14 (28%)	71,80,80	1.65	14 (19%)
2	FOL	50-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.26	3 (6%)
2	FOL	44-A	201	-	34,34,34	0.99	2 (5%)	43,47,47	1.28	3 (6%)
2	FOL	59-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.33	4 (9%)
3	NAP	64-A	202	-	50,52,52	3.34	12 (24%)	71,80,80	1.61	13 (18%)
2	FOL	76-A	201	-	34,34,34	1.11	3 (8%)	43,47,47	1.80	8 (18%)
2	FOL	77-A	201	-	34,34,34	1.07	1 (2%)	43,47,47	1.85	6 (13%)
2	FOL	80-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.62	7 (16%)
3	NAP	63-A	202	-	50,52,52	3.32	13 (26%)	71,80,80	1.62	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	43-A	202	-	50,52,52	3.29	14 (28%)	71,80,80	1.64	14 (19%)
3	NAP	25-A	202	-	50,52,52	3.33	13 (26%)	71,80,80	1.66	16 (22%)
2	FOL	63-A	201	-	34,34,34	1.05	1 (2%)	43,47,47	1.84	8 (18%)
3	NAP	10-A	202	-	50,52,52	3.27	13 (26%)	71,80,80	1.66	14 (19%)
2	FOL	68-A	201	-	34,34,34	1.10	2 (5%)	43,47,47	1.67	9 (20%)
3	NAP	72-A	202	-	50,52,52	3.31	14 (28%)	71,80,80	1.58	12 (16%)
2	FOL	56-A	201	-	34,34,34	0.97	1 (2%)	43,47,47	1.49	6 (13%)
2	FOL	66-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	1.55	6 (13%)
2	FOL	52-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.52	4 (9%)
3	NAP	26-A	202	-	50,52,52	3.31	13 (26%)	71,80,80	1.60	14 (19%)
2	FOL	25-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.68	7 (16%)
3	NAP	4-A	202	-	50,52,52	3.32	14 (28%)	71,80,80	1.64	13 (18%)
2	FOL	79-A	201	-	34,34,34	1.07	2 (5%)	43,47,47	1.79	6 (13%)
3	NAP	75-A	202	-	50,52,52	3.32	15 (30%)	71,80,80	1.63	15 (21%)
3	NAP	54-A	202	-	50,52,52	3.32	15 (30%)	71,80,80	1.67	12 (16%)
2	FOL	30-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.36	3 (6%)
2	FOL	57-A	201	-	34,34,34	0.97	1 (2%)	43,47,47	1.54	7 (16%)
3	NAP	6-A	202	-	50,52,52	3.33	13 (26%)	71,80,80	1.61	13 (18%)
3	NAP	28-A	202	-	50,52,52	3.32	13 (26%)	71,80,80	1.67	13 (18%)
2	FOL	54-A	201	-	34,34,34	0.95	1 (2%)	43,47,47	1.49	5 (11%)
2	FOL	16-A	201	-	34,34,34	0.95	1 (2%)	43,47,47	1.31	2 (4%)
3	NAP	68-A	202	-	50,52,52	3.31	13 (26%)	71,80,80	1.61	14 (19%)
3	NAP	16-A	202	-	50,52,52	3.28	14 (28%)	71,80,80	1.61	14 (19%)

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	58-A	201	-	-	10/22/22/22	0/3/3/3
3	NAP	60-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	5-A	202	-	-	6/35/67/67	0/5/5/5
2	FOL	15-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	35-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	24-A	202	-	-	3/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	49-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	24-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	5-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	44-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	9-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	42-A	202	-	-	2/35/67/67	0/5/5/5
3	NAP	74-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	79-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	23-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	62-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	27-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	2-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	69-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	70-A	201	-	-	10/22/22/22	0/3/3/3
3	NAP	67-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	71-A	201	-	-	16/22/22/22	0/3/3/3
2	FOL	10-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	65-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	36-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	72-A	201	-	-	12/22/22/22	0/3/3/3
3	NAP	56-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	61-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	41-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	61-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	19-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	19-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	11-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	64-A	201	-	-	12/22/22/22	0/3/3/3
3	NAP	1-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	28-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	18-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	46-A	202	-	-	6/35/67/67	0/5/5/5
3	NAP	8-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	80-A	202	-	-	6/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	15-A	202	-	-	6/35/67/67	0/5/5/5
2	FOL	8-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	35-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	7-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	4-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	47-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	33-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	57-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	32-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	22-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	45-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	70-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	75-A	201	-	-	9/22/22/22	0/3/3/3
3	NAP	58-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	27-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	45-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	29-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	50-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	40-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	21-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	38-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	67-A	201	-	-	11/22/22/22	0/3/3/3
2	FOL	78-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	39-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	42-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	73-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	48-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	3-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	26-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	23-A	202	-	-	6/35/67/67	0/5/5/5
2	FOL	48-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	20-A	202	-	-	7/35/67/67	0/5/5/5
3	NAP	17-A	202	-	-	2/35/67/67	0/5/5/5
3	NAP	14-A	202	-	-	4/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	76-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	2-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	22-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	69-A	201	-	-	9/22/22/22	0/3/3/3
3	NAP	71-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	46-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	43-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	21-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	17-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	49-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	3-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	31-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	52-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	34-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	20-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	31-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	34-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	74-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	37-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	18-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	55-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	29-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	53-A	202	-	-	6/35/67/67	0/5/5/5
2	FOL	14-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	66-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	55-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	39-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	53-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	51-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	36-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	73-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	78-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	9-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	12-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	33-A	201	-	-	4/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	51-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	30-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	1-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	13-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	62-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	47-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	40-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	32-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	60-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	37-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	7-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	11-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	12-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	13-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	59-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	38-A	201	-	-	8/22/22/22	0/3/3/3
3	NAP	65-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	77-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	6-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	41-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	50-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	44-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	59-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	64-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	76-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	77-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	80-A	201	-	-	11/22/22/22	0/3/3/3
3	NAP	63-A	202	-	-	6/35/67/67	0/5/5/5
3	NAP	43-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	25-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	63-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	10-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	68-A	201	-	-	9/22/22/22	0/3/3/3
3	NAP	72-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	56-A	201	-	-	7/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	66-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	52-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	26-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	25-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	4-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	79-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	75-A	202	-	-	6/35/67/67	0/5/5/5
3	NAP	54-A	202	-	-	11/35/67/67	0/5/5/5
2	FOL	30-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	57-A	201	-	-	8/22/22/22	0/3/3/3
3	NAP	6-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	28-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	54-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	16-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	68-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	16-A	202	-	-	5/35/67/67	0/5/5/5

All (1223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	39-A	202	NAP	O4D-C1D	14.91	1.60	1.40
3	35-A	202	NAP	O4D-C1D	14.91	1.60	1.40
3	3-A	202	NAP	O4D-C1D	14.86	1.60	1.40
3	44-A	202	NAP	O4D-C1D	14.86	1.60	1.40
3	40-A	202	NAP	O4D-C1D	14.84	1.60	1.40
3	34-A	202	NAP	O4D-C1D	14.81	1.60	1.40
3	37-A	202	NAP	O4D-C1D	14.76	1.60	1.40
3	76-A	202	NAP	O4D-C1D	14.76	1.60	1.40
3	32-A	202	NAP	O4D-C1D	14.74	1.60	1.40
3	77-A	202	NAP	O4D-C1D	14.73	1.60	1.40
3	36-A	202	NAP	O4D-C1D	14.72	1.60	1.40
3	7-A	202	NAP	O4D-C1D	14.72	1.60	1.40
3	41-A	202	NAP	O4D-C1D	14.71	1.60	1.40
3	29-A	202	NAP	O4D-C1D	14.71	1.60	1.40
3	31-A	202	NAP	O4D-C1D	14.70	1.60	1.40
3	1-A	202	NAP	O4D-C1D	14.68	1.60	1.40
3	24-A	202	NAP	O4D-C1D	14.67	1.60	1.40
3	25-A	202	NAP	O4D-C1D	14.65	1.60	1.40
3	78-A	202	NAP	O4D-C1D	14.64	1.60	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6-A	202	NAP	O4D-C1D	14.61	1.60	1.40
3	45-A	202	NAP	O4D-C1D	14.60	1.60	1.40
3	43-A	202	NAP	O4D-C1D	14.57	1.60	1.40
3	75-A	202	NAP	O4D-C1D	14.55	1.60	1.40
3	73-A	202	NAP	O4D-C1D	14.53	1.60	1.40
3	23-A	202	NAP	O4D-C1D	14.53	1.60	1.40
3	26-A	202	NAP	O4D-C1D	14.53	1.60	1.40
3	52-A	202	NAP	O4D-C1D	14.52	1.60	1.40
3	15-A	202	NAP	O4D-C1D	14.51	1.59	1.40
3	4-A	202	NAP	O4D-C1D	14.51	1.59	1.40
3	33-A	202	NAP	O4D-C1D	14.51	1.59	1.40
3	5-A	202	NAP	O4D-C1D	14.51	1.59	1.40
3	9-A	202	NAP	O4D-C1D	14.50	1.59	1.40
3	13-A	202	NAP	O4D-C1D	14.49	1.59	1.40
3	72-A	202	NAP	O4D-C1D	14.47	1.59	1.40
3	53-A	202	NAP	O4D-C1D	14.47	1.59	1.40
3	30-A	202	NAP	O4D-C1D	14.45	1.59	1.40
3	46-A	202	NAP	O4D-C1D	14.44	1.59	1.40
3	38-A	202	NAP	O4D-C1D	14.43	1.59	1.40
3	54-A	202	NAP	O4D-C1D	14.42	1.59	1.40
3	61-A	202	NAP	O4D-C1D	14.42	1.59	1.40
3	12-A	202	NAP	O4D-C1D	14.42	1.59	1.40
3	22-A	202	NAP	O4D-C1D	14.41	1.59	1.40
3	8-A	202	NAP	O4D-C1D	14.41	1.59	1.40
3	74-A	202	NAP	O4D-C1D	14.40	1.59	1.40
3	62-A	202	NAP	O4D-C1D	14.38	1.59	1.40
3	20-A	202	NAP	O4D-C1D	14.38	1.59	1.40
3	2-A	202	NAP	O4D-C1D	14.37	1.59	1.40
3	47-A	202	NAP	O4D-C1D	14.37	1.59	1.40
3	16-A	202	NAP	O4D-C1D	14.36	1.59	1.40
3	64-A	202	NAP	O4D-C1D	14.36	1.59	1.40
3	27-A	202	NAP	O4D-C1D	14.35	1.59	1.40
3	14-A	202	NAP	O4D-C1D	14.35	1.59	1.40
3	21-A	202	NAP	O4D-C1D	14.33	1.59	1.40
3	70-A	202	NAP	O4D-C1D	14.32	1.59	1.40
3	28-A	202	NAP	O4D-C1D	14.31	1.59	1.40
3	71-A	202	NAP	O4D-C1D	14.28	1.59	1.40
3	42-A	202	NAP	O4D-C1D	14.27	1.59	1.40
3	79-A	202	NAP	O4D-C1D	14.27	1.59	1.40
3	63-A	202	NAP	O4D-C1D	14.26	1.59	1.40
3	19-A	202	NAP	O4D-C1D	14.24	1.59	1.40
3	48-A	202	NAP	O4D-C1D	14.20	1.59	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	49-A	202	NAP	O4D-C1D	14.20	1.59	1.40
3	68-A	202	NAP	O4D-C1D	14.19	1.59	1.40
3	59-A	202	NAP	O4D-C1D	14.19	1.59	1.40
3	10-A	202	NAP	O4D-C1D	14.17	1.59	1.40
3	17-A	202	NAP	O4D-C1D	14.17	1.59	1.40
3	80-A	202	NAP	O4D-C1D	14.17	1.59	1.40
3	60-A	202	NAP	O4D-C1D	14.17	1.59	1.40
3	11-A	202	NAP	O4D-C1D	14.17	1.59	1.40
3	56-A	202	NAP	O4D-C1D	14.16	1.59	1.40
3	50-A	202	NAP	O4D-C1D	14.13	1.59	1.40
3	57-A	202	NAP	O4D-C1D	14.07	1.59	1.40
3	58-A	202	NAP	O4D-C1D	14.06	1.59	1.40
3	66-A	202	NAP	O4D-C1D	14.05	1.59	1.40
3	18-A	202	NAP	O4D-C1D	14.01	1.59	1.40
3	51-A	202	NAP	O4D-C1D	14.01	1.59	1.40
3	55-A	202	NAP	O4D-C1D	13.98	1.59	1.40
3	65-A	202	NAP	O4D-C1D	13.89	1.59	1.40
3	69-A	202	NAP	O4D-C1D	13.84	1.59	1.40
3	67-A	202	NAP	O4D-C1D	13.78	1.59	1.40
3	74-A	202	NAP	C2B-C1B	-8.87	1.31	1.53
3	64-A	202	NAP	C2B-C1B	-8.62	1.31	1.53
3	71-A	202	NAP	C2B-C1B	-8.57	1.32	1.53
3	28-A	202	NAP	C2B-C1B	-8.57	1.32	1.53
3	80-A	202	NAP	C2B-C1B	-8.55	1.32	1.53
3	9-A	202	NAP	C2B-C1B	-8.51	1.32	1.53
3	4-A	202	NAP	C2B-C1B	-8.51	1.32	1.53
3	54-A	202	NAP	O4B-C1B	8.50	1.61	1.42
3	43-A	202	NAP	C2B-C1B	-8.50	1.32	1.53
3	67-A	202	NAP	C2B-C1B	-8.50	1.32	1.53
3	66-A	202	NAP	C2B-C1B	-8.48	1.32	1.53
3	60-A	202	NAP	C2B-C1B	-8.48	1.32	1.53
3	15-A	202	NAP	C2B-C1B	-8.47	1.32	1.53
3	5-A	202	NAP	C2B-C1B	-8.44	1.32	1.53
3	65-A	202	NAP	C2B-C1B	-8.43	1.32	1.53
3	76-A	202	NAP	C2B-C1B	-8.42	1.32	1.53
3	63-A	202	NAP	C2B-C1B	-8.42	1.32	1.53
3	2-A	202	NAP	C2B-C1B	-8.41	1.32	1.53
3	38-A	202	NAP	O4B-C1B	8.40	1.61	1.42
3	12-A	202	NAP	C2B-C1B	-8.40	1.32	1.53
3	16-A	202	NAP	C2B-C1B	-8.39	1.32	1.53
3	7-A	202	NAP	C2B-C1B	-8.39	1.32	1.53
3	40-A	202	NAP	C2B-C1B	-8.39	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	39-A	202	NAP	O4B-C1B	8.38	1.61	1.42
3	18-A	202	NAP	C2B-C1B	-8.37	1.32	1.53
3	1-A	202	NAP	C2B-C1B	-8.37	1.32	1.53
3	69-A	202	NAP	C2B-C1B	-8.37	1.32	1.53
3	6-A	202	NAP	C2B-C1B	-8.37	1.32	1.53
3	77-A	202	NAP	C2B-C1B	-8.37	1.32	1.53
3	61-A	202	NAP	C2B-C1B	-8.37	1.32	1.53
3	13-A	202	NAP	C2B-C1B	-8.35	1.32	1.53
3	31-A	202	NAP	C2B-C1B	-8.35	1.32	1.53
3	62-A	202	NAP	C2B-C1B	-8.35	1.32	1.53
3	25-A	202	NAP	C2B-C1B	-8.34	1.32	1.53
3	52-A	202	NAP	C2B-C1B	-8.32	1.32	1.53
3	42-A	202	NAP	C2B-C1B	-8.32	1.32	1.53
3	75-A	202	NAP	O4B-C1B	8.32	1.61	1.42
3	70-A	202	NAP	C2B-C1B	-8.31	1.32	1.53
3	79-A	202	NAP	C2B-C1B	-8.31	1.32	1.53
3	22-A	202	NAP	C2B-C1B	-8.31	1.32	1.53
3	68-A	202	NAP	C2B-C1B	-8.31	1.32	1.53
3	37-A	202	NAP	O4B-C1B	8.31	1.61	1.42
3	10-A	202	NAP	C2B-C1B	-8.30	1.32	1.53
3	35-A	202	NAP	O4B-C1B	8.30	1.61	1.42
3	34-A	202	NAP	O4B-C1B	8.30	1.61	1.42
3	73-A	202	NAP	C2B-C1B	-8.30	1.32	1.53
3	3-A	202	NAP	C2B-C1B	-8.29	1.32	1.53
3	47-A	202	NAP	C2B-C1B	-8.29	1.32	1.53
3	11-A	202	NAP	C2B-C1B	-8.28	1.32	1.53
3	48-A	202	NAP	C2B-C1B	-8.28	1.32	1.53
3	78-A	202	NAP	C2B-C1B	-8.28	1.32	1.53
3	29-A	202	NAP	C2B-C1B	-8.28	1.32	1.53
3	35-A	202	NAP	C2B-C1B	-8.28	1.32	1.53
3	53-A	202	NAP	C2B-C1B	-8.27	1.32	1.53
3	8-A	202	NAP	C2B-C1B	-8.27	1.32	1.53
3	58-A	202	NAP	O4B-C1B	8.26	1.61	1.42
3	56-A	202	NAP	C2B-C1B	-8.26	1.32	1.53
3	59-A	202	NAP	O4B-C1B	8.26	1.61	1.42
3	75-A	202	NAP	C2B-C1B	-8.25	1.32	1.53
3	32-A	202	NAP	C2B-C1B	-8.25	1.32	1.53
3	59-A	202	NAP	C2B-C1B	-8.25	1.32	1.53
3	26-A	202	NAP	C2B-C1B	-8.24	1.32	1.53
3	40-A	202	NAP	O4B-C1B	8.24	1.61	1.42
3	57-A	202	NAP	O4B-C1B	8.24	1.61	1.42
3	57-A	202	NAP	C2B-C1B	-8.23	1.32	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	65-A	202	NAP	O4B-C1B	8.23	1.61	1.42
3	14-A	202	NAP	C2B-C1B	-8.23	1.32	1.53
3	34-A	202	NAP	C2B-C1B	-8.23	1.32	1.53
3	62-A	202	NAP	O4B-C1B	8.23	1.61	1.42
3	36-A	202	NAP	C2B-C1B	-8.23	1.32	1.53
3	33-A	202	NAP	O4B-C1B	8.22	1.61	1.42
3	24-A	202	NAP	C2B-C1B	-8.22	1.32	1.53
3	60-A	202	NAP	O4B-C1B	8.22	1.61	1.42
3	28-A	202	NAP	O4B-C1B	8.21	1.61	1.42
3	41-A	202	NAP	O4B-C1B	8.21	1.61	1.42
3	44-A	202	NAP	C2B-C1B	-8.21	1.32	1.53
3	72-A	202	NAP	C2B-C1B	-8.20	1.32	1.53
3	39-A	202	NAP	C2B-C1B	-8.20	1.32	1.53
3	33-A	202	NAP	C2B-C1B	-8.20	1.32	1.53
3	27-A	202	NAP	O4B-C1B	8.20	1.61	1.42
3	76-A	202	NAP	O4B-C1B	8.20	1.60	1.42
3	30-A	202	NAP	C2B-C1B	-8.19	1.32	1.53
3	45-A	202	NAP	C2B-C1B	-8.19	1.32	1.53
3	17-A	202	NAP	C2B-C1B	-8.19	1.32	1.53
3	38-A	202	NAP	C2B-C1B	-8.18	1.33	1.53
3	23-A	202	NAP	C2B-C1B	-8.18	1.33	1.53
3	32-A	202	NAP	O4B-C1B	8.18	1.60	1.42
3	26-A	202	NAP	O4B-C1B	8.18	1.60	1.42
3	30-A	202	NAP	O4B-C1B	8.18	1.60	1.42
3	63-A	202	NAP	O4B-C1B	8.18	1.60	1.42
3	2-A	202	NAP	O4B-C1B	8.17	1.60	1.42
3	14-A	202	NAP	O4B-C1B	8.17	1.60	1.42
3	36-A	202	NAP	O4B-C1B	8.16	1.60	1.42
3	46-A	202	NAP	C2B-C1B	-8.16	1.33	1.53
3	21-A	202	NAP	C2B-C1B	-8.16	1.33	1.53
3	49-A	202	NAP	C2B-C1B	-8.16	1.33	1.53
3	37-A	202	NAP	C2B-C1B	-8.15	1.33	1.53
3	31-A	202	NAP	O4B-C1B	8.15	1.60	1.42
3	27-A	202	NAP	C2B-C1B	-8.15	1.33	1.53
3	72-A	202	NAP	O4B-C1B	8.15	1.60	1.42
3	50-A	202	NAP	C2B-C1B	-8.14	1.33	1.53
3	20-A	202	NAP	C2B-C1B	-8.14	1.33	1.53
3	49-A	202	NAP	O4B-C1B	8.14	1.60	1.42
3	41-A	202	NAP	C2B-C1B	-8.13	1.33	1.53
3	29-A	202	NAP	O4B-C1B	8.13	1.60	1.42
3	78-A	202	NAP	O4B-C1B	8.13	1.60	1.42
3	66-A	202	NAP	O4B-C1B	8.12	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	54-A	202	NAP	C2B-C1B	-8.12	1.33	1.53
3	69-A	202	NAP	O4B-C1B	8.11	1.60	1.42
3	25-A	202	NAP	O4B-C1B	8.11	1.60	1.42
3	70-A	202	NAP	O4B-C1B	8.11	1.60	1.42
3	61-A	202	NAP	O4B-C1B	8.11	1.60	1.42
3	46-A	202	NAP	O4B-C1B	8.11	1.60	1.42
3	10-A	202	NAP	O4B-C1B	8.10	1.60	1.42
3	15-A	202	NAP	O4B-C1B	8.10	1.60	1.42
3	68-A	202	NAP	O4B-C1B	8.10	1.60	1.42
3	55-A	202	NAP	C2B-C1B	-8.10	1.33	1.53
3	45-A	202	NAP	O4B-C1B	8.09	1.60	1.42
3	58-A	202	NAP	C2B-C1B	-8.09	1.33	1.53
3	42-A	202	NAP	O4B-C1B	8.09	1.60	1.42
3	52-A	202	NAP	O4B-C1B	8.09	1.60	1.42
3	67-A	202	NAP	O4B-C1B	8.08	1.60	1.42
3	7-A	202	NAP	O4B-C1B	8.08	1.60	1.42
3	73-A	202	NAP	O4B-C1B	8.08	1.60	1.42
3	19-A	202	NAP	C2B-C1B	-8.07	1.33	1.53
3	56-A	202	NAP	O4B-C1B	8.07	1.60	1.42
3	6-A	202	NAP	O4B-C1B	8.07	1.60	1.42
3	9-A	202	NAP	O4B-C1B	8.07	1.60	1.42
3	21-A	202	NAP	O4B-C1B	8.07	1.60	1.42
3	1-A	202	NAP	O4B-C1B	8.06	1.60	1.42
3	12-A	202	NAP	O4B-C1B	8.06	1.60	1.42
3	64-A	202	NAP	O4B-C1B	8.06	1.60	1.42
3	77-A	202	NAP	O4B-C1B	8.06	1.60	1.42
3	13-A	202	NAP	O4B-C1B	8.05	1.60	1.42
3	51-A	202	NAP	C2B-C1B	-8.04	1.33	1.53
3	23-A	202	NAP	O4B-C1B	8.04	1.60	1.42
3	3-A	202	NAP	O4B-C1B	8.04	1.60	1.42
3	4-A	202	NAP	O4B-C1B	8.04	1.60	1.42
3	22-A	202	NAP	O4B-C1B	8.04	1.60	1.42
3	71-A	202	NAP	O4B-C1B	8.04	1.60	1.42
3	74-A	202	NAP	O4B-C1B	8.03	1.60	1.42
3	24-A	202	NAP	O4B-C1B	8.03	1.60	1.42
3	17-A	202	NAP	O4B-C1B	8.02	1.60	1.42
3	55-A	202	NAP	O4B-C1B	8.02	1.60	1.42
3	5-A	202	NAP	O4B-C1B	8.02	1.60	1.42
3	48-A	202	NAP	O4B-C1B	8.01	1.60	1.42
3	11-A	202	NAP	O4B-C1B	8.01	1.60	1.42
3	51-A	202	NAP	O4B-C1B	8.00	1.60	1.42
3	50-A	202	NAP	O4B-C1B	8.00	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	53-A	202	NAP	O4B-C1B	7.98	1.60	1.42
3	20-A	202	NAP	O4B-C1B	7.97	1.60	1.42
3	47-A	202	NAP	O4B-C1B	7.97	1.60	1.42
3	79-A	202	NAP	O4B-C1B	7.93	1.60	1.42
3	16-A	202	NAP	O4B-C1B	7.93	1.60	1.42
3	44-A	202	NAP	O4B-C1B	7.93	1.60	1.42
3	8-A	202	NAP	O4B-C1B	7.88	1.60	1.42
3	19-A	202	NAP	O4B-C1B	7.88	1.60	1.42
3	43-A	202	NAP	O4B-C1B	7.83	1.60	1.42
3	18-A	202	NAP	O4B-C1B	7.74	1.59	1.42
3	80-A	202	NAP	O4B-C1B	7.55	1.59	1.42
3	63-A	202	NAP	PN-O3	6.41	1.66	1.59
3	3-A	202	NAP	PN-O3	6.36	1.66	1.59
3	68-A	202	NAP	PN-O3	6.33	1.66	1.59
3	64-A	202	NAP	PN-O3	6.23	1.66	1.59
3	54-A	202	NAP	PN-O3	6.22	1.66	1.59
3	48-A	202	NAP	PN-O3	6.21	1.66	1.59
3	21-A	202	NAP	PN-O3	6.20	1.66	1.59
3	40-A	202	NAP	PN-O3	6.18	1.66	1.59
3	2-A	202	NAP	PN-O3	6.17	1.66	1.59
3	39-A	202	NAP	PN-O3	6.14	1.66	1.59
3	61-A	202	NAP	PN-O3	6.14	1.66	1.59
3	34-A	202	NAP	PN-O3	6.09	1.66	1.59
3	27-A	202	NAP	PN-O3	6.05	1.66	1.59
3	38-A	202	NAP	PN-O3	6.05	1.66	1.59
3	4-A	202	NAP	PN-O3	6.05	1.66	1.59
3	70-A	202	NAP	PN-O3	6.05	1.66	1.59
3	24-A	202	NAP	PN-O3	6.04	1.66	1.59
3	26-A	202	NAP	PN-O3	6.00	1.66	1.59
3	1-A	202	NAP	PN-O3	5.99	1.66	1.59
3	28-A	202	NAP	PN-O3	5.98	1.66	1.59
3	79-A	202	NAP	PN-O3	5.97	1.65	1.59
3	37-A	202	NAP	PN-O3	5.95	1.65	1.59
3	49-A	202	NAP	PN-O3	5.95	1.65	1.59
3	59-A	202	NAP	PN-O3	5.95	1.65	1.59
3	47-A	202	NAP	PN-O3	5.93	1.65	1.59
3	66-A	202	NAP	PN-O3	5.93	1.65	1.59
3	9-A	202	NAP	PN-O3	5.89	1.65	1.59
3	45-A	202	NAP	PN-O3	5.88	1.65	1.59
3	62-A	202	NAP	PN-O3	5.87	1.65	1.59
3	67-A	202	NAP	PN-O3	5.87	1.65	1.59
3	75-A	202	NAP	PN-O3	5.87	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	73-A	202	NAP	PN-O3	5.85	1.65	1.59
3	15-A	202	NAP	PN-O3	5.85	1.65	1.59
3	80-A	202	NAP	PN-O3	5.84	1.65	1.59
3	51-A	202	NAP	PN-O3	5.83	1.65	1.59
3	23-A	202	NAP	PN-O3	5.83	1.65	1.59
3	65-A	202	NAP	PN-O3	5.83	1.65	1.59
3	60-A	202	NAP	PN-O3	5.82	1.65	1.59
3	72-A	202	NAP	PN-O3	5.82	1.65	1.59
3	25-A	202	NAP	PN-O3	5.81	1.65	1.59
3	14-A	202	NAP	PN-O3	5.80	1.65	1.59
3	6-A	202	NAP	PN-O3	5.79	1.65	1.59
3	56-A	202	NAP	PN-O3	5.79	1.65	1.59
3	50-A	202	NAP	PN-O3	5.79	1.65	1.59
3	74-A	202	NAP	PN-O3	5.78	1.65	1.59
3	20-A	202	NAP	PN-O3	5.77	1.65	1.59
3	69-A	202	NAP	PN-O3	5.77	1.65	1.59
3	73-A	202	NAP	C7N-N7N	5.76	1.43	1.33
3	6-A	202	NAP	C7N-N7N	5.74	1.43	1.33
3	80-A	202	NAP	O4B-C4B	-5.73	1.32	1.45
3	33-A	202	NAP	PN-O3	5.73	1.65	1.59
3	22-A	202	NAP	PN-O3	5.72	1.65	1.59
3	8-A	202	NAP	PN-O3	5.71	1.65	1.59
3	24-A	202	NAP	C7N-N7N	5.70	1.43	1.33
3	20-A	202	NAP	O4D-C4D	-5.69	1.32	1.45
3	30-A	202	NAP	PN-O3	5.69	1.65	1.59
3	46-A	202	NAP	PN-O3	5.68	1.65	1.59
3	7-A	202	NAP	PN-O3	5.67	1.65	1.59
3	51-A	202	NAP	C7N-N7N	5.66	1.43	1.33
3	27-A	202	NAP	O4B-C4B	-5.66	1.32	1.45
3	37-A	202	NAP	O4D-C4D	-5.66	1.32	1.45
3	65-A	202	NAP	C7N-N7N	5.65	1.43	1.33
3	41-A	202	NAP	O4B-C4B	-5.65	1.32	1.45
3	19-A	202	NAP	O4D-C4D	-5.65	1.32	1.45
3	46-A	202	NAP	C7N-N7N	5.64	1.43	1.33
3	24-A	202	NAP	O4B-C4B	-5.64	1.32	1.45
3	29-A	202	NAP	PN-O3	5.64	1.65	1.59
3	46-A	202	NAP	O4B-C4B	-5.63	1.32	1.45
3	69-A	202	NAP	C7N-N7N	5.63	1.43	1.33
3	70-A	202	NAP	C7N-N7N	5.63	1.43	1.33
3	42-A	202	NAP	PN-O3	5.62	1.65	1.59
3	32-A	202	NAP	PN-O3	5.61	1.65	1.59
3	38-A	202	NAP	O4B-C4B	-5.61	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	76-A	202	NAP	C7N-N7N	5.61	1.43	1.33
3	8-A	202	NAP	C7N-N7N	5.61	1.43	1.33
3	75-A	202	NAP	C7N-N7N	5.60	1.43	1.33
3	18-A	202	NAP	C7N-N7N	5.60	1.43	1.33
3	23-A	202	NAP	O4B-C4B	-5.59	1.32	1.45
3	14-A	202	NAP	O4D-C4D	-5.58	1.32	1.45
3	59-A	202	NAP	C7N-N7N	5.57	1.43	1.33
3	39-A	202	NAP	O4B-C4B	-5.57	1.32	1.45
3	10-A	202	NAP	PN-O3	5.57	1.65	1.59
3	22-A	202	NAP	O4B-C4B	-5.57	1.32	1.45
3	50-A	202	NAP	C7N-N7N	5.57	1.43	1.33
3	16-A	202	NAP	C7N-N7N	5.57	1.43	1.33
3	57-A	202	NAP	C7N-N7N	5.56	1.43	1.33
3	5-A	202	NAP	PN-O3	5.56	1.65	1.59
3	11-A	202	NAP	O4B-C4B	-5.55	1.32	1.45
3	43-A	202	NAP	O4B-C4B	-5.55	1.32	1.45
3	12-A	202	NAP	C7N-N7N	5.55	1.43	1.33
3	67-A	202	NAP	C7N-N7N	5.55	1.43	1.33
3	25-A	202	NAP	C7N-N7N	5.55	1.43	1.33
3	48-A	202	NAP	C7N-N7N	5.55	1.43	1.33
3	55-A	202	NAP	C7N-N7N	5.54	1.43	1.33
3	72-A	202	NAP	C7N-N7N	5.54	1.43	1.33
3	8-A	202	NAP	O4B-C4B	-5.54	1.32	1.45
3	7-A	202	NAP	C7N-N7N	5.54	1.43	1.33
3	36-A	202	NAP	PN-O3	5.54	1.65	1.59
3	41-A	202	NAP	PN-O3	5.54	1.65	1.59
3	58-A	202	NAP	PN-O3	5.53	1.65	1.59
3	64-A	202	NAP	O4B-C4B	-5.53	1.32	1.45
3	45-A	202	NAP	O4B-C4B	-5.52	1.32	1.45
3	59-A	202	NAP	O4B-C4B	-5.52	1.32	1.45
3	17-A	202	NAP	C7N-N7N	5.52	1.43	1.33
3	30-A	202	NAP	C7N-N7N	5.52	1.43	1.33
3	23-A	202	NAP	C7N-N7N	5.52	1.43	1.33
3	5-A	202	NAP	C7N-N7N	5.51	1.43	1.33
3	49-A	202	NAP	C7N-N7N	5.51	1.43	1.33
3	53-A	202	NAP	C7N-N7N	5.51	1.43	1.33
3	38-A	202	NAP	O4D-C4D	-5.51	1.32	1.45
3	39-A	202	NAP	O4D-C4D	-5.51	1.32	1.45
3	1-A	202	NAP	C7N-N7N	5.51	1.43	1.33
3	78-A	202	NAP	O4B-C4B	-5.50	1.32	1.45
3	57-A	202	NAP	O4B-C4B	-5.50	1.32	1.45
3	2-A	202	NAP	C7N-N7N	5.50	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	67-A	202	NAP	O4D-C4D	-5.49	1.32	1.45
3	14-A	202	NAP	C7N-N7N	5.49	1.43	1.33
3	28-A	202	NAP	O4B-C4B	-5.49	1.32	1.45
3	40-A	202	NAP	O4B-C4B	-5.49	1.32	1.45
3	65-A	202	NAP	O4B-C4B	-5.49	1.32	1.45
3	74-A	202	NAP	O4B-C4B	-5.49	1.32	1.45
3	21-A	202	NAP	O4D-C4D	-5.49	1.32	1.45
3	26-A	202	NAP	O4B-C4B	-5.49	1.32	1.45
3	61-A	202	NAP	C7N-N7N	5.49	1.43	1.33
3	29-A	202	NAP	O4B-C4B	-5.49	1.32	1.45
3	20-A	202	NAP	O4B-C4B	-5.49	1.32	1.45
3	42-A	202	NAP	C7N-N7N	5.48	1.43	1.33
3	29-A	202	NAP	O4D-C4D	-5.48	1.32	1.45
3	40-A	202	NAP	O4D-C4D	-5.48	1.32	1.45
3	18-A	202	NAP	O4B-C4B	-5.48	1.32	1.45
3	52-A	202	NAP	O4B-C4B	-5.48	1.32	1.45
3	61-A	202	NAP	O4B-C4B	-5.47	1.32	1.45
3	54-A	202	NAP	O4B-C4B	-5.47	1.32	1.45
3	74-A	202	NAP	C7N-N7N	5.47	1.43	1.33
3	64-A	202	NAP	C7N-N7N	5.47	1.43	1.33
3	10-A	202	NAP	O4B-C4B	-5.47	1.32	1.45
3	7-A	202	NAP	O4B-C4B	-5.47	1.32	1.45
3	35-A	202	NAP	O4D-C4D	-5.47	1.32	1.45
3	29-A	202	NAP	C7N-N7N	5.47	1.43	1.33
3	53-A	202	NAP	O4B-C4B	-5.47	1.32	1.45
3	52-A	202	NAP	C7N-N7N	5.46	1.43	1.33
3	44-A	202	NAP	O4B-C4B	-5.46	1.32	1.45
3	73-A	202	NAP	O4B-C4B	-5.46	1.32	1.45
3	72-A	202	NAP	O4B-C4B	-5.46	1.32	1.45
3	19-A	202	NAP	O4B-C4B	-5.46	1.32	1.45
3	58-A	202	NAP	O4B-C4B	-5.45	1.32	1.45
3	78-A	202	NAP	C7N-N7N	5.45	1.43	1.33
3	7-A	202	NAP	O4D-C4D	-5.45	1.32	1.45
3	25-A	202	NAP	O4B-C4B	-5.45	1.32	1.45
3	22-A	202	NAP	O4D-C4D	-5.44	1.32	1.45
3	42-A	202	NAP	O4B-C4B	-5.44	1.32	1.45
3	11-A	202	NAP	PN-O3	5.44	1.65	1.59
3	12-A	202	NAP	O4B-C4B	-5.44	1.32	1.45
3	71-A	202	NAP	PN-O3	5.43	1.65	1.59
3	60-A	202	NAP	O4B-C4B	-5.43	1.32	1.45
3	10-A	202	NAP	C7N-N7N	5.43	1.43	1.33
3	31-A	202	NAP	O4B-C4B	-5.43	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	16-A	202	NAP	O4B-C4B	-5.43	1.32	1.45
3	1-A	202	NAP	O4B-C4B	-5.43	1.32	1.45
3	12-A	202	NAP	PN-O3	5.43	1.65	1.59
3	57-A	202	NAP	PN-O3	5.43	1.65	1.59
3	4-A	202	NAP	O4D-C4D	-5.43	1.32	1.45
3	32-A	202	NAP	O4B-C4B	-5.43	1.32	1.45
3	15-A	202	NAP	C7N-N7N	5.43	1.43	1.33
3	47-A	202	NAP	O4B-C4B	-5.42	1.32	1.45
3	58-A	202	NAP	C7N-N7N	5.42	1.42	1.33
3	21-A	202	NAP	O4B-C4B	-5.42	1.32	1.45
3	51-A	202	NAP	O4B-C4B	-5.42	1.32	1.45
3	21-A	202	NAP	C7N-N7N	5.42	1.42	1.33
3	48-A	202	NAP	O4B-C4B	-5.41	1.33	1.45
3	71-A	202	NAP	C7N-N7N	5.41	1.42	1.33
3	33-A	202	NAP	O4B-C4B	-5.41	1.33	1.45
3	13-A	202	NAP	O4D-C4D	-5.41	1.33	1.45
3	34-A	202	NAP	O4D-C4D	-5.41	1.33	1.45
3	37-A	202	NAP	O4B-C4B	-5.41	1.33	1.45
3	77-A	202	NAP	O4B-C4B	-5.41	1.33	1.45
3	3-A	202	NAP	O4B-C4B	-5.41	1.33	1.45
3	76-A	202	NAP	O4B-C4B	-5.40	1.33	1.45
3	20-A	202	NAP	C7N-N7N	5.40	1.42	1.33
3	5-A	202	NAP	O4B-C4B	-5.40	1.33	1.45
3	14-A	202	NAP	O4B-C4B	-5.40	1.33	1.45
3	13-A	202	NAP	C7N-N7N	5.40	1.42	1.33
3	17-A	202	NAP	O4B-C4B	-5.40	1.33	1.45
3	11-A	202	NAP	C7N-N7N	5.40	1.42	1.33
3	9-A	202	NAP	O4B-C4B	-5.40	1.33	1.45
3	66-A	202	NAP	O4D-C4D	-5.40	1.33	1.45
3	6-A	202	NAP	O4D-C4D	-5.39	1.33	1.45
3	68-A	202	NAP	O4D-C4D	-5.39	1.33	1.45
3	69-A	202	NAP	O4B-C4B	-5.39	1.33	1.45
3	31-A	202	NAP	PN-O3	5.39	1.65	1.59
3	44-A	202	NAP	PN-O3	5.39	1.65	1.59
3	79-A	202	NAP	O4B-C4B	-5.39	1.33	1.45
3	18-A	202	NAP	PN-O3	5.39	1.65	1.59
3	54-A	202	NAP	C7N-N7N	5.39	1.42	1.33
3	28-A	202	NAP	O4D-C4D	-5.39	1.33	1.45
3	49-A	202	NAP	O4D-C4D	-5.39	1.33	1.45
3	56-A	202	NAP	O4B-C4B	-5.38	1.33	1.45
3	30-A	202	NAP	O4B-C4B	-5.38	1.33	1.45
3	63-A	202	NAP	C7N-N7N	5.38	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	70-A	202	NAP	O4B-C4B	-5.38	1.33	1.45
3	2-A	202	NAP	O4D-C4D	-5.38	1.33	1.45
3	47-A	202	NAP	O4D-C4D	-5.38	1.33	1.45
3	16-A	202	NAP	O4D-C4D	-5.38	1.33	1.45
3	18-A	202	NAP	O4D-C4D	-5.38	1.33	1.45
3	47-A	202	NAP	C7N-N7N	5.37	1.42	1.33
3	6-A	202	NAP	O4B-C4B	-5.37	1.33	1.45
3	50-A	202	NAP	O4D-C4D	-5.37	1.33	1.45
3	22-A	202	NAP	C7N-N7N	5.37	1.42	1.33
3	56-A	202	NAP	C7N-N7N	5.37	1.42	1.33
3	30-A	202	NAP	O4D-C4D	-5.36	1.33	1.45
3	62-A	202	NAP	O4B-C4B	-5.36	1.33	1.45
3	9-A	202	NAP	C7N-N7N	5.36	1.42	1.33
3	60-A	202	NAP	C7N-N7N	5.36	1.42	1.33
3	50-A	202	NAP	O4B-C4B	-5.36	1.33	1.45
3	45-A	202	NAP	C7N-N7N	5.36	1.42	1.33
3	76-A	202	NAP	PN-O3	5.35	1.65	1.59
3	77-A	202	NAP	PN-O3	5.35	1.65	1.59
3	36-A	202	NAP	O4B-C4B	-5.35	1.33	1.45
3	19-A	202	NAP	PN-O3	5.35	1.65	1.59
3	52-A	202	NAP	O4D-C4D	-5.35	1.33	1.45
3	2-A	202	NAP	O4B-C4B	-5.34	1.33	1.45
3	1-A	202	NAP	O4D-C4D	-5.34	1.33	1.45
3	77-A	202	NAP	O4D-C4D	-5.34	1.33	1.45
3	76-A	202	NAP	O4D-C4D	-5.34	1.33	1.45
3	65-A	202	NAP	O4D-C4D	-5.34	1.33	1.45
3	15-A	202	NAP	O4B-C4B	-5.34	1.33	1.45
3	64-A	202	NAP	O4D-C4D	-5.34	1.33	1.45
3	71-A	202	NAP	O4B-C4B	-5.34	1.33	1.45
3	68-A	202	NAP	C7N-N7N	5.33	1.42	1.33
3	42-A	202	NAP	O4D-C4D	-5.33	1.33	1.45
3	8-A	202	NAP	O4D-C4D	-5.33	1.33	1.45
3	17-A	202	NAP	O4D-C4D	-5.33	1.33	1.45
3	41-A	202	NAP	O4D-C4D	-5.33	1.33	1.45
3	70-A	202	NAP	O4D-C4D	-5.33	1.33	1.45
3	67-A	202	NAP	O4B-C4B	-5.33	1.33	1.45
3	44-A	202	NAP	O4D-C4D	-5.33	1.33	1.45
3	36-A	202	NAP	O4D-C4D	-5.33	1.33	1.45
3	13-A	202	NAP	O4B-C4B	-5.33	1.33	1.45
3	53-A	202	NAP	O4D-C4D	-5.33	1.33	1.45
3	35-A	202	NAP	PN-O3	5.33	1.65	1.59
3	4-A	202	NAP	O4B-C4B	-5.32	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	27-A	202	NAP	O4D-C4D	-5.32	1.33	1.45
3	35-A	202	NAP	O4B-C4B	-5.31	1.33	1.45
3	38-A	202	NAP	C7N-N7N	5.31	1.42	1.33
3	48-A	202	NAP	O4D-C4D	-5.31	1.33	1.45
3	66-A	202	NAP	O4B-C4B	-5.31	1.33	1.45
3	33-A	202	NAP	O4D-C4D	-5.31	1.33	1.45
3	71-A	202	NAP	O4D-C4D	-5.31	1.33	1.45
3	49-A	202	NAP	O4B-C4B	-5.31	1.33	1.45
3	62-A	202	NAP	C7N-N7N	5.31	1.42	1.33
3	35-A	202	NAP	C7N-N7N	5.31	1.42	1.33
3	68-A	202	NAP	O4B-C4B	-5.30	1.33	1.45
3	75-A	202	NAP	O4B-C4B	-5.30	1.33	1.45
3	4-A	202	NAP	C7N-N7N	5.30	1.42	1.33
3	28-A	202	NAP	C7N-N7N	5.30	1.42	1.33
3	66-A	202	NAP	C7N-N7N	5.30	1.42	1.33
3	13-A	202	NAP	PN-O3	5.30	1.65	1.59
3	46-A	202	NAP	O4D-C4D	-5.30	1.33	1.45
3	79-A	202	NAP	O4D-C4D	-5.30	1.33	1.45
3	31-A	202	NAP	C7N-N7N	5.29	1.42	1.33
3	32-A	202	NAP	O4D-C4D	-5.29	1.33	1.45
3	63-A	202	NAP	O4D-C4D	-5.29	1.33	1.45
3	51-A	202	NAP	O4D-C4D	-5.29	1.33	1.45
3	33-A	202	NAP	C7N-N7N	5.28	1.42	1.33
3	19-A	202	NAP	C7N-N7N	5.28	1.42	1.33
3	15-A	202	NAP	O4D-C4D	-5.28	1.33	1.45
3	34-A	202	NAP	O4B-C4B	-5.28	1.33	1.45
3	80-A	202	NAP	C7N-N7N	5.28	1.42	1.33
3	9-A	202	NAP	O4D-C4D	-5.27	1.33	1.45
3	57-A	202	NAP	O4D-C4D	-5.27	1.33	1.45
3	78-A	202	NAP	PN-O3	5.27	1.65	1.59
3	3-A	202	NAP	O4D-C4D	-5.26	1.33	1.45
3	55-A	202	NAP	O4B-C4B	-5.25	1.33	1.45
3	45-A	202	NAP	O4D-C4D	-5.25	1.33	1.45
3	56-A	202	NAP	O4D-C4D	-5.25	1.33	1.45
3	78-A	202	NAP	O4D-C4D	-5.25	1.33	1.45
3	31-A	202	NAP	O4D-C4D	-5.25	1.33	1.45
3	3-A	202	NAP	C7N-N7N	5.25	1.42	1.33
3	36-A	202	NAP	C7N-N7N	5.25	1.42	1.33
3	26-A	202	NAP	O4D-C4D	-5.24	1.33	1.45
3	53-A	202	NAP	PN-O3	5.24	1.65	1.59
3	63-A	202	NAP	O4B-C4B	-5.24	1.33	1.45
3	11-A	202	NAP	O4D-C4D	-5.24	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	72-A	202	NAP	O4D-C4D	-5.24	1.33	1.45
3	5-A	202	NAP	O4D-C4D	-5.24	1.33	1.45
3	59-A	202	NAP	O4D-C4D	-5.23	1.33	1.45
3	27-A	202	NAP	C7N-N7N	5.23	1.42	1.33
3	75-A	202	NAP	O4D-C4D	-5.23	1.33	1.45
3	77-A	202	NAP	C7N-N7N	5.23	1.42	1.33
3	34-A	202	NAP	C7N-N7N	5.23	1.42	1.33
3	52-A	202	NAP	PN-O3	5.23	1.65	1.59
3	43-A	202	NAP	PN-O3	5.23	1.65	1.59
3	37-A	202	NAP	C7N-N7N	5.22	1.42	1.33
3	55-A	202	NAP	O4D-C4D	-5.21	1.33	1.45
3	79-A	202	NAP	C7N-N7N	5.21	1.42	1.33
3	80-A	202	NAP	O4D-C4D	-5.21	1.33	1.45
3	54-A	202	NAP	O4D-C4D	-5.20	1.33	1.45
3	40-A	202	NAP	C7N-N7N	5.20	1.42	1.33
3	25-A	202	NAP	O4D-C4D	-5.20	1.33	1.45
3	26-A	202	NAP	C7N-N7N	5.20	1.42	1.33
3	43-A	202	NAP	O4D-C4D	-5.19	1.33	1.45
3	16-A	202	NAP	PN-O3	5.19	1.65	1.59
3	69-A	202	NAP	O4D-C4D	-5.19	1.33	1.45
3	62-A	202	NAP	O4D-C4D	-5.19	1.33	1.45
3	17-A	202	NAP	PN-O3	5.18	1.65	1.59
3	24-A	202	NAP	O4D-C4D	-5.17	1.33	1.45
3	23-A	202	NAP	O4D-C4D	-5.15	1.33	1.45
3	60-A	202	NAP	O4D-C4D	-5.15	1.33	1.45
3	58-A	202	NAP	O4D-C4D	-5.15	1.33	1.45
3	41-A	202	NAP	C7N-N7N	5.15	1.42	1.33
3	61-A	202	NAP	O4D-C4D	-5.14	1.33	1.45
3	12-A	202	NAP	O4D-C4D	-5.13	1.33	1.45
3	10-A	202	NAP	O4D-C4D	-5.13	1.33	1.45
3	73-A	202	NAP	O4D-C4D	-5.11	1.33	1.45
3	44-A	202	NAP	C7N-N7N	5.10	1.42	1.33
3	43-A	202	NAP	C7N-N7N	5.09	1.42	1.33
3	74-A	202	NAP	O4D-C4D	-5.08	1.33	1.45
3	32-A	202	NAP	C7N-N7N	5.04	1.42	1.33
3	39-A	202	NAP	C7N-N7N	4.99	1.42	1.33
3	55-A	202	NAP	PN-O3	4.92	1.64	1.59
2	69-A	201	FOL	C8A-N1	-4.43	1.32	1.38
3	35-A	202	NAP	O2D-C2D	3.71	1.52	1.43
3	36-A	202	NAP	O2D-C2D	3.64	1.52	1.43
3	31-A	202	NAP	O2D-C2D	3.62	1.51	1.43
3	41-A	202	NAP	O2D-C2D	3.60	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	30-A	202	NAP	O2D-C2D	3.60	1.51	1.43
2	66-A	201	FOL	C8A-N1	-3.59	1.33	1.38
3	19-A	202	NAP	O2D-C2D	3.58	1.51	1.43
3	37-A	202	NAP	O2D-C2D	3.58	1.51	1.43
3	20-A	202	NAP	O2D-C2D	3.57	1.51	1.43
3	52-A	202	NAP	O2D-C2D	3.56	1.51	1.43
2	38-A	201	FOL	C8A-N1	-3.56	1.33	1.38
2	78-A	201	FOL	C8A-N1	-3.53	1.33	1.38
2	11-A	201	FOL	C8A-N1	-3.52	1.33	1.38
3	73-A	202	NAP	O2D-C2D	3.52	1.51	1.43
3	21-A	202	NAP	O2D-C2D	3.52	1.51	1.43
3	9-A	202	NAP	O2D-C2D	3.51	1.51	1.43
3	39-A	202	NAP	O2D-C2D	3.50	1.51	1.43
3	13-A	202	NAP	O2D-C2D	3.50	1.51	1.43
2	29-A	201	FOL	C8A-N1	-3.48	1.33	1.38
2	4-A	201	FOL	C8A-N1	-3.47	1.33	1.38
3	29-A	202	NAP	O2D-C2D	3.47	1.51	1.43
3	60-A	202	NAP	O2D-C2D	3.46	1.51	1.43
3	58-A	202	NAP	O2D-C2D	3.45	1.51	1.43
3	17-A	202	NAP	O2D-C2D	3.45	1.51	1.43
3	2-A	202	NAP	O2D-C2D	3.44	1.51	1.43
2	13-A	201	FOL	C8A-N1	-3.43	1.33	1.38
3	44-A	202	NAP	O2D-C2D	3.43	1.51	1.43
2	37-A	201	FOL	C8A-N1	-3.42	1.33	1.38
3	59-A	202	NAP	O2D-C2D	3.41	1.51	1.43
3	1-A	202	NAP	O2D-C2D	3.41	1.51	1.43
2	70-A	201	FOL	C8A-N1	-3.40	1.33	1.38
2	5-A	201	FOL	C8A-N1	-3.39	1.33	1.38
3	32-A	202	NAP	O2D-C2D	3.39	1.51	1.43
3	56-A	202	NAP	O2D-C2D	3.39	1.51	1.43
2	32-A	201	FOL	C8A-N1	-3.39	1.33	1.38
3	12-A	202	NAP	O2D-C2D	3.39	1.51	1.43
3	38-A	202	NAP	O2D-C2D	3.39	1.51	1.43
3	65-A	202	NAP	O2D-C2D	3.39	1.51	1.43
2	25-A	201	FOL	C8A-N1	-3.39	1.33	1.38
3	67-A	202	NAP	O2D-C2D	3.38	1.51	1.43
2	39-A	201	FOL	C8A-N1	-3.38	1.33	1.38
3	66-A	202	NAP	O2D-C2D	3.37	1.51	1.43
3	11-A	202	NAP	O2D-C2D	3.37	1.51	1.43
2	19-A	201	FOL	C8A-N1	-3.36	1.33	1.38
3	23-A	202	NAP	O2D-C2D	3.36	1.51	1.43
3	28-A	202	NAP	O2D-C2D	3.36	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	16-A	202	NAP	O2D-C2D	3.36	1.51	1.43
2	24-A	201	FOL	C8A-N1	-3.36	1.33	1.38
2	50-A	201	FOL	C8A-N1	-3.36	1.33	1.38
3	72-A	202	NAP	O2D-C2D	3.35	1.51	1.43
3	61-A	202	NAP	O2D-C2D	3.35	1.51	1.43
3	57-A	202	NAP	O2D-C2D	3.34	1.51	1.43
3	3-A	202	NAP	O2D-C2D	3.34	1.51	1.43
3	5-A	202	NAP	O2D-C2D	3.34	1.51	1.43
3	62-A	202	NAP	O2D-C2D	3.34	1.51	1.43
3	4-A	202	NAP	O2D-C2D	3.34	1.51	1.43
3	40-A	202	NAP	O2D-C2D	3.34	1.51	1.43
2	33-A	201	FOL	C8A-N1	-3.33	1.33	1.38
3	34-A	202	NAP	O2D-C2D	3.33	1.51	1.43
3	51-A	202	NAP	O2D-C2D	3.33	1.51	1.43
2	68-A	201	FOL	C8A-N1	-3.33	1.33	1.38
3	53-A	202	NAP	O2D-C2D	3.33	1.51	1.43
3	76-A	202	NAP	O2D-C2D	3.32	1.51	1.43
2	26-A	201	FOL	C8A-N1	-3.32	1.33	1.38
3	25-A	202	NAP	O2D-C2D	3.32	1.51	1.43
3	22-A	202	NAP	O2D-C2D	3.32	1.51	1.43
3	24-A	202	NAP	O2D-C2D	3.31	1.51	1.43
3	63-A	202	NAP	O2D-C2D	3.30	1.51	1.43
3	45-A	202	NAP	O2D-C2D	3.30	1.51	1.43
3	70-A	202	NAP	O2D-C2D	3.30	1.51	1.43
2	8-A	201	FOL	C8A-N1	-3.30	1.33	1.38
3	68-A	202	NAP	O2D-C2D	3.30	1.51	1.43
3	69-A	202	NAP	O2D-C2D	3.29	1.51	1.43
3	79-A	202	NAP	O2D-C2D	3.29	1.51	1.43
2	15-A	201	FOL	C8A-N1	-3.28	1.33	1.38
2	77-A	201	FOL	C8A-N1	-3.28	1.33	1.38
3	27-A	202	NAP	O2D-C2D	3.28	1.51	1.43
3	78-A	202	NAP	O2D-C2D	3.27	1.51	1.43
3	7-A	202	NAP	O2D-C2D	3.27	1.51	1.43
3	14-A	202	NAP	O2D-C2D	3.25	1.51	1.43
3	42-A	202	NAP	O2D-C2D	3.25	1.51	1.43
3	71-A	202	NAP	O2D-C2D	3.25	1.51	1.43
3	15-A	202	NAP	O2D-C2D	3.24	1.51	1.43
3	6-A	202	NAP	O2D-C2D	3.24	1.51	1.43
2	12-A	201	FOL	C8A-N1	-3.24	1.34	1.38
2	49-A	201	FOL	C8A-N1	-3.24	1.34	1.38
3	77-A	202	NAP	O2D-C2D	3.23	1.51	1.43
3	64-A	202	NAP	O2D-C2D	3.22	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	18-A	201	FOL	C8A-N1	-3.22	1.34	1.38
3	10-A	202	NAP	O2D-C2D	3.22	1.50	1.43
2	6-A	201	FOL	C8A-N1	-3.21	1.34	1.38
3	26-A	202	NAP	O2D-C2D	3.21	1.50	1.43
2	7-A	201	FOL	C8A-N1	-3.20	1.34	1.38
3	43-A	202	NAP	O2D-C2D	3.20	1.50	1.43
3	49-A	202	NAP	O2D-C2D	3.20	1.50	1.43
3	33-A	202	NAP	O2D-C2D	3.19	1.50	1.43
3	18-A	202	NAP	O2D-C2D	3.19	1.50	1.43
2	14-A	201	FOL	C8A-N1	-3.19	1.34	1.38
3	75-A	202	NAP	O2D-C2D	3.18	1.50	1.43
2	27-A	201	FOL	C8A-N1	-3.18	1.34	1.38
2	3-A	201	FOL	C8A-N1	-3.17	1.34	1.38
3	74-A	202	NAP	O2D-C2D	3.17	1.50	1.43
2	17-A	201	FOL	C8A-N1	-3.16	1.34	1.38
2	65-A	201	FOL	C8A-N1	-3.16	1.34	1.38
3	50-A	202	NAP	O2D-C2D	3.15	1.50	1.43
3	8-A	202	NAP	O2D-C2D	3.14	1.50	1.43
2	70-A	201	FOL	C14-N10	-3.13	1.29	1.38
3	55-A	202	NAP	O3B-C3B	-3.12	1.35	1.43
2	79-A	201	FOL	C8A-N1	-3.12	1.34	1.38
3	1-A	202	NAP	O3B-C3B	-3.11	1.35	1.43
3	80-A	202	NAP	O2D-C2D	3.11	1.50	1.43
2	76-A	201	FOL	C8A-N1	-3.11	1.34	1.38
2	55-A	201	FOL	C8A-N1	-3.11	1.34	1.38
2	42-A	201	FOL	C8A-N1	-3.10	1.34	1.38
2	61-A	201	FOL	C8A-N1	-3.10	1.34	1.38
3	54-A	202	NAP	O2D-C2D	3.09	1.50	1.43
3	47-A	202	NAP	O2D-C2D	3.09	1.50	1.43
2	2-A	201	FOL	C8A-N1	-3.08	1.34	1.38
3	49-A	202	NAP	O7N-C7N	-3.08	1.18	1.24
2	45-A	201	FOL	C8A-N1	-3.07	1.34	1.38
3	22-A	202	NAP	O3B-C3B	-3.07	1.35	1.43
3	48-A	202	NAP	O2D-C2D	3.06	1.50	1.43
2	30-A	201	FOL	C8A-N1	-3.05	1.34	1.38
2	36-A	201	FOL	C8A-N1	-3.05	1.34	1.38
3	46-A	202	NAP	O2D-C2D	3.05	1.50	1.43
2	28-A	201	FOL	C8A-N1	-3.05	1.34	1.38
2	57-A	201	FOL	C8A-N1	-3.04	1.34	1.38
2	31-A	201	FOL	C8A-N1	-3.03	1.34	1.38
2	48-A	201	FOL	C8A-N1	-3.03	1.34	1.38
2	58-A	201	FOL	C8A-N1	-3.02	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	50-A	202	NAP	O7N-C7N	-3.01	1.18	1.24
2	63-A	201	FOL	C8A-N1	-3.01	1.34	1.38
3	25-A	202	NAP	O3B-C3B	-3.00	1.35	1.43
3	18-A	202	NAP	O3B-C3B	-2.98	1.35	1.43
3	24-A	202	NAP	O3B-C3B	-2.98	1.35	1.43
2	34-A	201	FOL	C8A-N1	-2.98	1.34	1.38
3	73-A	202	NAP	O3B-C3B	-2.98	1.35	1.43
3	75-A	202	NAP	O3B-C3B	-2.97	1.35	1.43
2	59-A	201	FOL	C8A-N1	-2.96	1.34	1.38
3	54-A	202	NAP	O3B-C3B	-2.95	1.35	1.43
2	10-A	201	FOL	C8A-N1	-2.95	1.34	1.38
2	22-A	201	FOL	C8A-N1	-2.94	1.34	1.38
2	78-A	201	FOL	CB-CA	-2.94	1.46	1.53
2	40-A	201	FOL	C8A-N1	-2.94	1.34	1.38
2	60-A	201	FOL	C8A-N1	-2.93	1.34	1.38
3	64-A	202	NAP	O3B-C3B	-2.93	1.35	1.43
3	14-A	202	NAP	O3B-C3B	-2.92	1.35	1.43
2	20-A	201	FOL	C8A-N1	-2.92	1.34	1.38
3	17-A	202	NAP	O3B-C3B	-2.92	1.35	1.43
3	72-A	202	NAP	O3B-C3B	-2.91	1.35	1.43
3	41-A	202	NAP	O3B-C3B	-2.91	1.35	1.43
2	51-A	201	FOL	C8A-N1	-2.91	1.34	1.38
3	46-A	202	NAP	O7N-C7N	-2.90	1.18	1.24
3	16-A	202	NAP	O3B-C3B	-2.90	1.35	1.43
2	75-A	201	FOL	C8A-N1	-2.90	1.34	1.38
2	47-A	201	FOL	C8A-N1	-2.89	1.34	1.38
3	60-A	202	NAP	O3B-C3B	-2.89	1.35	1.43
3	2-A	202	NAP	O3B-C3B	-2.89	1.35	1.43
3	63-A	202	NAP	O3B-C3B	-2.89	1.35	1.43
3	15-A	202	NAP	O3B-C3B	-2.88	1.35	1.43
3	76-A	202	NAP	O3B-C3B	-2.88	1.35	1.43
2	56-A	201	FOL	C8A-N1	-2.88	1.34	1.38
3	21-A	202	NAP	O3B-C3B	-2.87	1.35	1.43
2	80-A	201	FOL	C8A-N1	-2.87	1.34	1.38
3	44-A	202	NAP	O3B-C3B	-2.87	1.35	1.43
3	49-A	202	NAP	O3B-C3B	-2.86	1.35	1.43
3	42-A	202	NAP	O3B-C3B	-2.85	1.35	1.43
3	59-A	202	NAP	O7N-C7N	-2.85	1.18	1.24
3	20-A	202	NAP	O3B-C3B	-2.85	1.35	1.43
2	16-A	201	FOL	C8A-N1	-2.85	1.34	1.38
3	65-A	202	NAP	O3B-C3B	-2.85	1.35	1.43
3	27-A	202	NAP	O3B-C3B	-2.85	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	21-A	201	FOL	C8A-N1	-2.84	1.34	1.38
3	12-A	202	NAP	O3B-C3B	-2.84	1.35	1.43
3	59-A	202	NAP	O3B-C3B	-2.84	1.35	1.43
3	8-A	202	NAP	O3B-C3B	-2.84	1.35	1.43
3	19-A	202	NAP	O3B-C3B	-2.84	1.35	1.43
3	79-A	202	NAP	O3B-C3B	-2.84	1.35	1.43
3	41-A	202	NAP	O7N-C7N	-2.83	1.18	1.24
2	74-A	201	FOL	C8A-N1	-2.83	1.34	1.38
3	5-A	202	NAP	O3B-C3B	-2.83	1.35	1.43
3	28-A	202	NAP	O3B-C3B	-2.83	1.35	1.43
3	52-A	202	NAP	O7N-C7N	-2.83	1.18	1.24
3	11-A	202	NAP	O3B-C3B	-2.82	1.36	1.43
3	47-A	202	NAP	O3B-C3B	-2.82	1.36	1.43
2	80-A	201	FOL	OE2-CD	-2.82	1.21	1.30
3	48-A	202	NAP	O3B-C3B	-2.82	1.36	1.43
2	35-A	201	FOL	C8A-N1	-2.82	1.34	1.38
3	68-A	202	NAP	O3B-C3B	-2.82	1.36	1.43
3	74-A	202	NAP	O3B-C3B	-2.81	1.36	1.43
3	7-A	202	NAP	O3B-C3B	-2.81	1.36	1.43
3	9-A	202	NAP	O3B-C3B	-2.81	1.36	1.43
3	43-A	202	NAP	O3B-C3B	-2.80	1.36	1.43
3	3-A	202	NAP	O3B-C3B	-2.80	1.36	1.43
3	62-A	202	NAP	O3B-C3B	-2.80	1.36	1.43
2	62-A	201	FOL	C8A-N1	-2.79	1.34	1.38
3	33-A	202	NAP	O3B-C3B	-2.79	1.36	1.43
3	23-A	202	NAP	O3B-C3B	-2.79	1.36	1.43
3	6-A	202	NAP	O3B-C3B	-2.79	1.36	1.43
2	52-A	201	FOL	C8A-N1	-2.78	1.34	1.38
3	53-A	202	NAP	O3B-C3B	-2.78	1.36	1.43
3	61-A	202	NAP	O3B-C3B	-2.78	1.36	1.43
2	54-A	201	FOL	C8A-N1	-2.78	1.34	1.38
3	66-A	202	NAP	O3B-C3B	-2.78	1.36	1.43
2	53-A	201	FOL	C8A-N1	-2.78	1.34	1.38
3	21-A	202	NAP	O7N-C7N	-2.77	1.19	1.24
3	70-A	202	NAP	O3B-C3B	-2.77	1.36	1.43
3	51-A	202	NAP	O3B-C3B	-2.77	1.36	1.43
3	40-A	202	NAP	O3B-C3B	-2.76	1.36	1.43
2	44-A	201	FOL	C8A-N1	-2.76	1.34	1.38
3	4-A	202	NAP	O3B-C3B	-2.76	1.36	1.43
3	77-A	202	NAP	O3B-C3B	-2.76	1.36	1.43
3	45-A	202	NAP	O3B-C3B	-2.76	1.36	1.43
3	31-A	202	NAP	O3B-C3B	-2.75	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	45-A	202	NAP	O7N-C7N	-2.75	1.19	1.24
3	2-A	202	NAP	O7N-C7N	-2.75	1.19	1.24
3	1-A	202	NAP	O7N-C7N	-2.75	1.19	1.24
3	52-A	202	NAP	O3B-C3B	-2.74	1.36	1.43
3	36-A	202	NAP	O3B-C3B	-2.74	1.36	1.43
3	69-A	202	NAP	O3B-C3B	-2.74	1.36	1.43
3	17-A	202	NAP	O7N-C7N	-2.74	1.19	1.24
3	22-A	202	NAP	O7N-C7N	-2.74	1.19	1.24
3	23-A	202	NAP	O7N-C7N	-2.74	1.19	1.24
3	26-A	202	NAP	O3B-C3B	-2.74	1.36	1.43
3	78-A	202	NAP	O3B-C3B	-2.74	1.36	1.43
3	20-A	202	NAP	O7N-C7N	-2.73	1.19	1.24
3	57-A	202	NAP	O3B-C3B	-2.73	1.36	1.43
3	74-A	202	NAP	C8A-N7A	2.73	1.36	1.31
3	71-A	202	NAP	O3B-C3B	-2.73	1.36	1.43
2	43-A	201	FOL	C8A-N1	-2.72	1.34	1.38
3	39-A	202	NAP	O3B-C3B	-2.72	1.36	1.43
2	41-A	201	FOL	C8A-N1	-2.72	1.34	1.38
2	1-A	201	FOL	C8A-N1	-2.72	1.34	1.38
3	25-A	202	NAP	O7N-C7N	-2.71	1.19	1.24
3	51-A	202	NAP	O7N-C7N	-2.71	1.19	1.24
2	23-A	201	FOL	C8A-N1	-2.71	1.34	1.38
3	18-A	202	NAP	O7N-C7N	-2.70	1.19	1.24
3	30-A	202	NAP	O3B-C3B	-2.69	1.36	1.43
3	46-A	202	NAP	O3B-C3B	-2.69	1.36	1.43
2	9-A	201	FOL	C8A-N1	-2.69	1.34	1.38
3	14-A	202	NAP	O7N-C7N	-2.69	1.19	1.24
3	47-A	202	NAP	O7N-C7N	-2.69	1.19	1.24
3	16-A	202	NAP	O7N-C7N	-2.68	1.19	1.24
3	37-A	202	NAP	O3B-C3B	-2.68	1.36	1.43
3	50-A	202	NAP	O3B-C3B	-2.67	1.36	1.43
3	67-A	202	NAP	O3B-C3B	-2.67	1.36	1.43
3	35-A	202	NAP	O3B-C3B	-2.67	1.36	1.43
3	11-A	202	NAP	O7N-C7N	-2.67	1.19	1.24
3	10-A	202	NAP	O3B-C3B	-2.67	1.36	1.43
3	56-A	202	NAP	O3B-C3B	-2.67	1.36	1.43
3	48-A	202	NAP	O7N-C7N	-2.66	1.19	1.24
3	36-A	202	NAP	O7N-C7N	-2.66	1.19	1.24
3	80-A	202	NAP	C8A-N7A	2.66	1.36	1.31
3	37-A	202	NAP	O7N-C7N	-2.66	1.19	1.24
3	34-A	202	NAP	O7N-C7N	-2.65	1.19	1.24
3	65-A	202	NAP	O7N-C7N	-2.65	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	10-A	202	NAP	C8A-N7A	2.65	1.36	1.31
3	13-A	202	NAP	O3B-C3B	-2.64	1.36	1.43
3	80-A	202	NAP	O3B-C3B	-2.64	1.36	1.43
3	30-A	202	NAP	O7N-C7N	-2.64	1.19	1.24
3	58-A	202	NAP	O3B-C3B	-2.64	1.36	1.43
3	63-A	202	NAP	C8A-N7A	2.64	1.36	1.31
3	34-A	202	NAP	O3B-C3B	-2.64	1.36	1.43
3	39-A	202	NAP	O7N-C7N	-2.64	1.19	1.24
3	32-A	202	NAP	O3B-C3B	-2.63	1.36	1.43
3	64-A	202	NAP	O7N-C7N	-2.63	1.19	1.24
3	29-A	202	NAP	O3B-C3B	-2.62	1.36	1.43
3	38-A	202	NAP	O3B-C3B	-2.62	1.36	1.43
3	71-A	202	NAP	O7N-C7N	-2.62	1.19	1.24
3	62-A	202	NAP	O7N-C7N	-2.61	1.19	1.24
3	13-A	202	NAP	C8A-N7A	2.61	1.36	1.31
3	61-A	202	NAP	O7N-C7N	-2.61	1.19	1.24
3	66-A	202	NAP	O7N-C7N	-2.61	1.19	1.24
2	46-A	201	FOL	C8A-N1	-2.61	1.34	1.38
3	32-A	202	NAP	O7N-C7N	-2.60	1.19	1.24
3	38-A	202	NAP	O7N-C7N	-2.60	1.19	1.24
3	48-A	202	NAP	C8A-N7A	2.60	1.36	1.31
3	23-A	202	NAP	C8A-N7A	2.59	1.36	1.31
3	69-A	202	NAP	C8A-N7A	2.58	1.36	1.31
3	76-A	202	NAP	O7N-C7N	-2.58	1.19	1.24
3	28-A	202	NAP	C8A-N7A	2.57	1.36	1.31
3	24-A	202	NAP	O7N-C7N	-2.57	1.19	1.24
3	44-A	202	NAP	O7N-C7N	-2.57	1.19	1.24
3	57-A	202	NAP	C8A-N7A	2.57	1.36	1.31
3	56-A	202	NAP	O7N-C7N	-2.57	1.19	1.24
3	8-A	202	NAP	C8A-N7A	2.56	1.36	1.31
3	74-A	202	NAP	O7N-C7N	-2.56	1.19	1.24
3	53-A	202	NAP	O7N-C7N	-2.55	1.19	1.24
3	4-A	202	NAP	C8A-N7A	2.55	1.36	1.31
3	13-A	202	NAP	O7N-C7N	-2.54	1.19	1.24
3	50-A	202	NAP	C8A-N7A	2.54	1.36	1.31
3	67-A	202	NAP	O3D-C3D	-2.54	1.36	1.43
3	9-A	202	NAP	C8A-N7A	2.54	1.36	1.31
3	22-A	202	NAP	C8A-N7A	2.53	1.36	1.31
3	26-A	202	NAP	O7N-C7N	-2.53	1.19	1.24
3	6-A	202	NAP	O7N-C7N	-2.53	1.19	1.24
3	51-A	202	NAP	C8A-N7A	2.53	1.36	1.31
3	64-A	202	NAP	C8A-N7A	2.53	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	20-A	202	NAP	C8A-N7A	2.53	1.36	1.31
3	12-A	202	NAP	C8A-N7A	2.52	1.36	1.31
3	11-A	202	NAP	C8A-N7A	2.52	1.36	1.31
3	19-A	202	NAP	O7N-C7N	-2.52	1.19	1.24
3	75-A	202	NAP	C8A-N7A	2.52	1.36	1.31
3	33-A	202	NAP	O7N-C7N	-2.52	1.19	1.24
3	73-A	202	NAP	C8A-N7A	2.52	1.36	1.31
3	43-A	202	NAP	O7N-C7N	-2.51	1.19	1.24
3	1-A	202	NAP	C8A-N7A	2.51	1.36	1.31
3	3-A	202	NAP	O3D-C3D	-2.51	1.36	1.43
3	52-A	202	NAP	C8A-N7A	2.51	1.36	1.31
3	58-A	202	NAP	O7N-C7N	-2.50	1.19	1.24
3	42-A	202	NAP	C8A-N7A	2.50	1.36	1.31
3	46-A	202	NAP	C8A-N7A	2.50	1.36	1.31
3	66-A	202	NAP	C8A-N7A	2.49	1.36	1.31
3	60-A	202	NAP	O7N-C7N	-2.49	1.19	1.24
3	68-A	202	NAP	O7N-C7N	-2.49	1.19	1.24
3	21-A	202	NAP	C8A-N7A	2.49	1.36	1.31
3	16-A	202	NAP	C8A-N7A	2.49	1.36	1.31
3	31-A	202	NAP	O7N-C7N	-2.49	1.19	1.24
3	71-A	202	NAP	C8A-N7A	2.49	1.36	1.31
3	74-A	202	NAP	O3D-C3D	-2.48	1.36	1.43
3	53-A	202	NAP	C8A-N7A	2.48	1.36	1.31
3	66-A	202	NAP	O3D-C3D	-2.48	1.36	1.43
3	3-A	202	NAP	O7N-C7N	-2.48	1.19	1.24
3	5-A	202	NAP	C8A-N7A	2.48	1.36	1.31
3	70-A	202	NAP	C8A-N7A	2.48	1.36	1.31
2	73-A	201	FOL	C9-C6	2.48	1.56	1.50
2	75-A	201	FOL	OE2-CD	-2.48	1.22	1.30
3	55-A	202	NAP	O7N-C7N	-2.48	1.19	1.24
3	49-A	202	NAP	C8A-N7A	2.48	1.36	1.31
3	56-A	202	NAP	C8A-N7A	2.48	1.36	1.31
3	62-A	202	NAP	C8A-N7A	2.47	1.36	1.31
3	61-A	202	NAP	O3D-C3D	-2.47	1.36	1.43
3	77-A	202	NAP	O7N-C7N	-2.47	1.19	1.24
3	72-A	202	NAP	O7N-C7N	-2.46	1.19	1.24
3	2-A	202	NAP	C8A-N7A	2.46	1.36	1.31
3	3-A	202	NAP	C8A-N7A	2.46	1.36	1.31
3	42-A	202	NAP	O7N-C7N	-2.46	1.19	1.24
3	7-A	202	NAP	C8A-N7A	2.46	1.36	1.31
3	47-A	202	NAP	C8A-N7A	2.46	1.36	1.31
3	10-A	202	NAP	O7N-C7N	-2.46	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	40-A	202	NAP	O7N-C7N	-2.46	1.19	1.24
3	75-A	202	NAP	O7N-C7N	-2.46	1.19	1.24
3	27-A	202	NAP	O7N-C7N	-2.44	1.19	1.24
3	73-A	202	NAP	O3D-C3D	-2.44	1.36	1.43
2	73-A	201	FOL	C13-C12	2.44	1.42	1.38
3	14-A	202	NAP	C8A-N7A	2.43	1.36	1.31
3	30-A	202	NAP	O3D-C3D	-2.43	1.36	1.43
3	54-A	202	NAP	C8A-N7A	2.43	1.36	1.31
3	25-A	202	NAP	C8A-N7A	2.43	1.36	1.31
3	19-A	202	NAP	C8A-N7A	2.43	1.36	1.31
3	28-A	202	NAP	O3D-C3D	-2.43	1.36	1.43
3	60-A	202	NAP	C8A-N7A	2.42	1.36	1.31
3	26-A	202	NAP	C8A-N7A	2.42	1.36	1.31
3	5-A	202	NAP	O7N-C7N	-2.42	1.19	1.24
3	15-A	202	NAP	C8A-N7A	2.42	1.36	1.31
3	9-A	202	NAP	O7N-C7N	-2.42	1.19	1.24
3	17-A	202	NAP	C8A-N7A	2.41	1.36	1.31
3	78-A	202	NAP	C8A-N7A	2.41	1.36	1.31
2	37-A	201	FOL	C4-N3	-2.41	1.33	1.38
3	41-A	202	NAP	C8A-N7A	2.41	1.36	1.31
3	79-A	202	NAP	C8A-N7A	2.41	1.36	1.31
3	40-A	202	NAP	C8A-N7A	2.40	1.36	1.31
3	68-A	202	NAP	C8A-N7A	2.40	1.36	1.31
3	72-A	202	NAP	C8A-N7A	2.39	1.36	1.31
3	78-A	202	NAP	O7N-C7N	-2.39	1.19	1.24
3	44-A	202	NAP	C8A-N7A	2.39	1.36	1.31
3	32-A	202	NAP	O3D-C3D	-2.39	1.37	1.43
3	12-A	202	NAP	O7N-C7N	-2.39	1.19	1.24
3	76-A	202	NAP	C8A-N7A	2.39	1.36	1.31
3	59-A	202	NAP	C8A-N7A	2.38	1.36	1.31
3	4-A	202	NAP	O7N-C7N	-2.38	1.19	1.24
3	67-A	202	NAP	O7N-C7N	-2.38	1.19	1.24
3	70-A	202	NAP	O7N-C7N	-2.37	1.19	1.24
3	6-A	202	NAP	C8A-N7A	2.37	1.36	1.31
3	54-A	202	NAP	O7N-C7N	-2.37	1.19	1.24
3	69-A	202	NAP	O3D-C3D	-2.37	1.37	1.43
3	29-A	202	NAP	O7N-C7N	-2.37	1.19	1.24
3	65-A	202	NAP	O3D-C3D	-2.36	1.37	1.43
3	24-A	202	NAP	C8A-N7A	2.36	1.36	1.31
3	35-A	202	NAP	O7N-C7N	-2.36	1.19	1.24
3	69-A	202	NAP	O7N-C7N	-2.35	1.19	1.24
3	57-A	202	NAP	O3D-C3D	-2.35	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	27-A	202	NAP	O3D-C3D	-2.35	1.37	1.43
3	37-A	202	NAP	O3D-C3D	-2.35	1.37	1.43
2	72-A	201	FOL	C8A-N1	-2.35	1.35	1.38
3	76-A	202	NAP	O3D-C3D	-2.35	1.37	1.43
3	52-A	202	NAP	O3D-C3D	-2.35	1.37	1.43
3	77-A	202	NAP	C8A-N7A	2.34	1.36	1.31
3	60-A	202	NAP	O3D-C3D	-2.34	1.37	1.43
3	58-A	202	NAP	C8A-N7A	2.34	1.36	1.31
3	18-A	202	NAP	C8A-N7A	2.34	1.36	1.31
3	68-A	202	NAP	O3D-C3D	-2.34	1.37	1.43
3	71-A	202	NAP	O3D-C3D	-2.34	1.37	1.43
3	34-A	202	NAP	C8A-N7A	2.34	1.36	1.31
3	65-A	202	NAP	C8A-N7A	2.34	1.36	1.31
3	46-A	202	NAP	O3D-C3D	-2.34	1.37	1.43
3	39-A	202	NAP	O3D-C3D	-2.34	1.37	1.43
3	67-A	202	NAP	C8A-N7A	2.33	1.36	1.31
3	47-A	202	NAP	O3D-C3D	-2.33	1.37	1.43
3	43-A	202	NAP	C8A-N7A	2.33	1.36	1.31
3	45-A	202	NAP	C8A-N7A	2.33	1.36	1.31
3	1-A	202	NAP	O3D-C3D	-2.33	1.37	1.43
3	31-A	202	NAP	O3D-C3D	-2.33	1.37	1.43
3	35-A	202	NAP	O3D-C3D	-2.33	1.37	1.43
3	36-A	202	NAP	O3D-C3D	-2.32	1.37	1.43
3	4-A	202	NAP	O3D-C3D	-2.32	1.37	1.43
3	7-A	202	NAP	O7N-C7N	-2.32	1.19	1.24
3	11-A	202	NAP	O3D-C3D	-2.32	1.37	1.43
3	34-A	202	NAP	C5N-C4N	-2.32	1.34	1.38
3	57-A	202	NAP	O7N-C7N	-2.32	1.19	1.24
3	29-A	202	NAP	O3D-C3D	-2.32	1.37	1.43
3	75-A	202	NAP	O3D-C3D	-2.32	1.37	1.43
3	70-A	202	NAP	O3D-C3D	-2.32	1.37	1.43
3	27-A	202	NAP	C8A-N7A	2.31	1.36	1.31
3	29-A	202	NAP	C8A-N7A	2.31	1.36	1.31
3	63-A	202	NAP	O7N-C7N	-2.31	1.19	1.24
3	39-A	202	NAP	C8A-N7A	2.31	1.36	1.31
3	38-A	202	NAP	O3D-C3D	-2.31	1.37	1.43
3	51-A	202	NAP	O3D-C3D	-2.31	1.37	1.43
2	32-A	201	FOL	C4-N3	-2.30	1.34	1.38
3	61-A	202	NAP	C8A-N7A	2.30	1.36	1.31
3	80-A	202	NAP	O7N-C7N	-2.30	1.19	1.24
3	59-A	202	NAP	O3D-C3D	-2.30	1.37	1.43
3	31-A	202	NAP	C8A-N7A	2.30	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	79-A	202	NAP	O7N-C7N	-2.30	1.19	1.24
2	69-A	201	FOL	C14-N10	-2.30	1.32	1.38
3	38-A	202	NAP	C8A-N7A	2.30	1.36	1.31
3	33-A	202	NAP	C8A-N7A	2.29	1.36	1.31
3	35-A	202	NAP	C5N-C4N	-2.29	1.35	1.38
3	72-A	202	NAP	O3D-C3D	-2.29	1.37	1.43
3	2-A	202	NAP	O3D-C3D	-2.29	1.37	1.43
2	64-A	201	FOL	C4-N3	-2.29	1.34	1.38
2	22-A	201	FOL	C4-N3	-2.29	1.34	1.38
2	71-A	201	FOL	C8A-N1	-2.28	1.35	1.38
3	8-A	202	NAP	O3D-C3D	-2.28	1.37	1.43
3	50-A	202	NAP	O3D-C3D	-2.28	1.37	1.43
2	23-A	201	FOL	C4-N3	-2.28	1.34	1.38
3	77-A	202	NAP	C5N-C4N	-2.28	1.35	1.38
3	64-A	202	NAP	O3D-C3D	-2.28	1.37	1.43
3	35-A	202	NAP	C8A-N7A	2.28	1.36	1.31
3	30-A	202	NAP	C8A-N7A	2.27	1.36	1.31
2	73-A	201	FOL	C16-C15	-2.27	1.35	1.38
3	53-A	202	NAP	O3D-C3D	-2.27	1.37	1.43
3	62-A	202	NAP	O3D-C3D	-2.27	1.37	1.43
3	55-A	202	NAP	C8A-N7A	2.27	1.36	1.31
3	26-A	202	NAP	O3D-C3D	-2.27	1.37	1.43
3	32-A	202	NAP	C8A-N7A	2.27	1.36	1.31
2	71-A	201	FOL	C4-N3	-2.26	1.34	1.38
3	36-A	202	NAP	C8A-N7A	2.26	1.36	1.31
3	23-A	202	NAP	O3D-C3D	-2.26	1.37	1.43
2	73-A	201	FOL	C4-N3	-2.26	1.34	1.38
3	38-A	202	NAP	C6A-N6A	2.26	1.40	1.34
3	15-A	202	NAP	O7N-C7N	-2.26	1.19	1.24
2	67-A	201	FOL	C8A-N1	-2.25	1.35	1.38
3	49-A	202	NAP	O3D-C3D	-2.25	1.37	1.43
3	55-A	202	NAP	O2D-C2D	2.25	1.48	1.43
3	12-A	202	NAP	O3D-C3D	-2.25	1.37	1.43
2	30-A	201	FOL	C4-N3	-2.24	1.34	1.38
3	37-A	202	NAP	C8A-N7A	2.24	1.36	1.31
3	43-A	202	NAP	O3D-C3D	-2.24	1.37	1.43
3	45-A	202	NAP	C5N-C4N	-2.24	1.35	1.38
2	72-A	201	FOL	CA-N	2.23	1.50	1.45
3	41-A	202	NAP	O3D-C3D	-2.23	1.37	1.43
3	42-A	202	NAP	O3D-C3D	-2.23	1.37	1.43
3	50-A	202	NAP	C6A-N6A	2.23	1.39	1.34
3	34-A	202	NAP	O3D-C3D	-2.23	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	33-A	202	NAP	O3D-C3D	-2.23	1.37	1.43
3	45-A	202	NAP	C6A-N6A	2.23	1.39	1.34
3	45-A	202	NAP	O3D-C3D	-2.23	1.37	1.43
2	25-A	201	FOL	C4-N3	-2.23	1.34	1.38
3	13-A	202	NAP	O3D-C3D	-2.22	1.37	1.43
3	19-A	202	NAP	O3D-C3D	-2.22	1.37	1.43
2	19-A	201	FOL	C4-N3	-2.22	1.34	1.38
2	29-A	201	FOL	C4-N3	-2.22	1.34	1.38
2	42-A	201	FOL	C4-N3	-2.22	1.34	1.38
2	45-A	201	FOL	C4-N3	-2.22	1.34	1.38
3	48-A	202	NAP	O3D-C3D	-2.22	1.37	1.43
3	8-A	202	NAP	O7N-C7N	-2.21	1.20	1.24
2	24-A	201	FOL	C4-N3	-2.21	1.34	1.38
3	44-A	202	NAP	C5N-C4N	-2.21	1.35	1.38
2	20-A	201	FOL	C4-N3	-2.21	1.34	1.38
2	38-A	201	FOL	C4-N3	-2.21	1.34	1.38
3	10-A	202	NAP	O3D-C3D	-2.21	1.37	1.43
3	37-A	202	NAP	C6A-N6A	2.20	1.39	1.34
3	25-A	202	NAP	O3D-C3D	-2.20	1.37	1.43
3	34-A	202	NAP	C6A-N6A	2.20	1.39	1.34
3	7-A	202	NAP	O3D-C3D	-2.20	1.37	1.43
2	46-A	201	FOL	C4-N3	-2.20	1.34	1.38
3	21-A	202	NAP	C6A-N6A	2.20	1.39	1.34
3	32-A	202	NAP	C6A-N6A	2.20	1.39	1.34
3	63-A	202	NAP	O3D-C3D	-2.19	1.37	1.43
3	22-A	202	NAP	O3D-C3D	-2.19	1.37	1.43
3	78-A	202	NAP	C5N-C4N	-2.19	1.35	1.38
3	2-A	202	NAP	C5N-C4N	-2.19	1.35	1.38
2	61-A	201	FOL	C4-N3	-2.19	1.34	1.38
3	51-A	202	NAP	C6A-N6A	2.18	1.39	1.34
3	44-A	202	NAP	O3D-C3D	-2.18	1.37	1.43
3	43-A	202	NAP	C5N-C4N	-2.18	1.35	1.38
3	5-A	202	NAP	O3D-C3D	-2.18	1.37	1.43
3	3-A	202	NAP	C5N-C4N	-2.18	1.35	1.38
3	24-A	202	NAP	O3D-C3D	-2.17	1.37	1.43
3	22-A	202	NAP	C6A-N6A	2.17	1.39	1.34
3	3-A	202	NAP	C6A-N6A	2.17	1.39	1.34
3	23-A	202	NAP	C6A-N6A	2.17	1.39	1.34
3	41-A	202	NAP	C5N-C4N	-2.17	1.35	1.38
3	16-A	202	NAP	C5N-C4N	-2.16	1.35	1.38
3	76-A	202	NAP	C5N-C4N	-2.16	1.35	1.38
2	41-A	201	FOL	OE2-CD	-2.16	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	80-A	202	NAP	C5N-C4N	-2.16	1.35	1.38
3	69-A	202	NAP	C5N-C4N	-2.16	1.35	1.38
3	16-A	202	NAP	C6A-N6A	2.16	1.39	1.34
3	60-A	202	NAP	C6A-N6A	2.16	1.39	1.34
3	79-A	202	NAP	O3D-C3D	-2.15	1.37	1.43
3	65-A	202	NAP	C6A-N6A	2.15	1.39	1.34
3	78-A	202	NAP	O3D-C3D	-2.15	1.37	1.43
3	75-A	202	NAP	C6A-N6A	2.15	1.39	1.34
3	54-A	202	NAP	O3D-C3D	-2.14	1.37	1.43
2	69-A	201	FOL	C4A-C8A	2.14	1.48	1.42
3	7-A	202	NAP	C6A-N6A	2.14	1.39	1.34
3	49-A	202	NAP	C6A-N6A	2.14	1.39	1.34
2	67-A	201	FOL	C4-N3	-2.14	1.34	1.38
3	56-A	202	NAP	O3D-C3D	-2.14	1.37	1.43
2	12-A	201	FOL	C4-N3	-2.14	1.34	1.38
3	75-A	202	NAP	C5N-C4N	-2.14	1.35	1.38
3	79-A	202	NAP	C5N-C4N	-2.14	1.35	1.38
2	35-A	201	FOL	C4-N3	-2.13	1.34	1.38
3	5-A	202	NAP	C6A-N6A	2.13	1.39	1.34
3	39-A	202	NAP	C5N-C4N	-2.13	1.35	1.38
3	59-A	202	NAP	C6A-N6A	2.13	1.39	1.34
3	21-A	202	NAP	O3D-C3D	-2.13	1.37	1.43
3	43-A	202	NAP	C6A-N6A	2.13	1.39	1.34
3	28-A	202	NAP	O7N-C7N	-2.13	1.20	1.24
3	20-A	202	NAP	C6A-N6A	2.13	1.39	1.34
3	46-A	202	NAP	C6A-N6A	2.13	1.39	1.34
3	14-A	202	NAP	O3D-C3D	-2.13	1.37	1.43
3	80-A	202	NAP	O3D-C3D	-2.12	1.37	1.43
2	50-A	201	FOL	C4-N3	-2.12	1.34	1.38
3	58-A	202	NAP	C6A-N6A	2.12	1.39	1.34
3	72-A	202	NAP	C6A-N6A	2.12	1.39	1.34
3	40-A	202	NAP	O3D-C3D	-2.12	1.37	1.43
3	41-A	202	NAP	C6A-N6A	2.12	1.39	1.34
3	77-A	202	NAP	O3D-C3D	-2.12	1.37	1.43
3	10-A	202	NAP	C6A-N6A	2.12	1.39	1.34
2	7-A	201	FOL	C4-N3	-2.12	1.34	1.38
3	2-A	202	NAP	C6A-N6A	2.12	1.39	1.34
3	63-A	202	NAP	C6A-N6A	2.11	1.39	1.34
3	28-A	202	NAP	C6A-N6A	2.11	1.39	1.34
3	36-A	202	NAP	C6A-N6A	2.11	1.39	1.34
3	1-A	202	NAP	C5N-C4N	-2.11	1.35	1.38
3	47-A	202	NAP	C6A-N6A	2.11	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	40-A	202	NAP	C5N-C4N	-2.11	1.35	1.38
2	18-A	201	FOL	C4-N3	-2.10	1.34	1.38
3	33-A	202	NAP	C5N-C4N	-2.10	1.35	1.38
3	61-A	202	NAP	C6A-N6A	2.10	1.39	1.34
3	20-A	202	NAP	O3D-C3D	-2.10	1.37	1.43
3	79-A	202	NAP	C6A-N6A	2.10	1.39	1.34
3	15-A	202	NAP	C5N-C4N	-2.10	1.35	1.38
3	73-A	202	NAP	O7N-C7N	-2.10	1.20	1.24
2	78-A	201	FOL	C4-N3	-2.10	1.34	1.38
2	60-A	201	FOL	C4-N3	-2.10	1.34	1.38
3	42-A	202	NAP	C5N-C4N	-2.10	1.35	1.38
3	74-A	202	NAP	C5N-C4N	-2.10	1.35	1.38
3	74-A	202	NAP	C1B-N9A	-2.10	1.40	1.46
2	44-A	201	FOL	C4-N3	-2.09	1.34	1.38
2	33-A	201	FOL	C4-N3	-2.09	1.34	1.38
3	48-A	202	NAP	C6A-N6A	2.09	1.39	1.34
2	76-A	201	FOL	CA-N	2.09	1.50	1.45
3	70-A	202	NAP	C6A-N6A	2.09	1.39	1.34
3	4-A	202	NAP	C6A-N6A	2.09	1.39	1.34
3	54-A	202	NAP	C2A-N3A	2.09	1.37	1.33
3	71-A	202	NAP	C5N-C4N	-2.09	1.35	1.38
3	42-A	202	NAP	C6A-N6A	2.09	1.39	1.34
2	28-A	201	FOL	C4-N3	-2.09	1.34	1.38
3	62-A	202	NAP	C6A-N6A	2.09	1.39	1.34
3	33-A	202	NAP	C6A-N6A	2.09	1.39	1.34
2	21-A	201	FOL	C4-N3	-2.09	1.34	1.38
3	16-A	202	NAP	O3D-C3D	-2.09	1.37	1.43
2	68-A	201	FOL	C4-N3	-2.08	1.34	1.38
2	74-A	201	FOL	C4-N3	-2.08	1.34	1.38
3	9-A	202	NAP	O3D-C3D	-2.08	1.37	1.43
2	36-A	201	FOL	C4-N3	-2.08	1.34	1.38
3	72-A	202	NAP	C5N-C4N	-2.08	1.35	1.38
3	23-A	202	NAP	C5N-C4N	-2.08	1.35	1.38
3	27-A	202	NAP	C6A-N6A	2.08	1.39	1.34
3	31-A	202	NAP	C6A-N6A	2.08	1.39	1.34
3	6-A	202	NAP	O3D-C3D	-2.08	1.37	1.43
3	58-A	202	NAP	O3D-C3D	-2.08	1.37	1.43
2	13-A	201	FOL	C4-N3	-2.08	1.34	1.38
2	65-A	201	FOL	C4-N3	-2.08	1.34	1.38
2	17-A	201	FOL	C4-N3	-2.07	1.34	1.38
3	1-A	202	NAP	C6A-N6A	2.07	1.39	1.34
3	67-A	202	NAP	C6A-N6A	2.07	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6-A	202	NAP	C6A-N6A	2.07	1.39	1.34
2	70-A	201	FOL	C15-C14	-2.07	1.35	1.39
3	12-A	202	NAP	C6A-N6A	2.07	1.39	1.34
3	57-A	202	NAP	C6A-N6A	2.07	1.39	1.34
3	36-A	202	NAP	C5N-C4N	-2.07	1.35	1.38
3	55-A	202	NAP	C6A-N6A	2.07	1.39	1.34
2	48-A	201	FOL	C4-N3	-2.07	1.34	1.38
3	80-A	202	NAP	C6A-N6A	2.07	1.39	1.34
3	47-A	202	NAP	C5N-C4N	-2.07	1.35	1.38
3	15-A	202	NAP	C6A-N6A	2.07	1.39	1.34
2	59-A	201	FOL	C4-N3	-2.06	1.34	1.38
3	25-A	202	NAP	C6A-N6A	2.06	1.39	1.34
3	66-A	202	NAP	C6A-N6A	2.06	1.39	1.34
3	68-A	202	NAP	C6A-N6A	2.06	1.39	1.34
3	40-A	202	NAP	C6A-N6A	2.06	1.39	1.34
3	4-A	202	NAP	C5N-C4N	-2.06	1.35	1.38
3	44-A	202	NAP	C6A-N6A	2.06	1.39	1.34
2	5-A	201	FOL	O2-CT	-2.05	1.24	1.30
2	6-A	201	FOL	C4-N3	-2.05	1.34	1.38
2	10-A	201	FOL	C4-N3	-2.05	1.34	1.38
3	19-A	202	NAP	C6A-N6A	2.05	1.39	1.34
2	53-A	201	FOL	C4-N3	-2.05	1.34	1.38
3	38-A	202	NAP	C5N-C4N	-2.05	1.35	1.38
3	30-A	202	NAP	C6A-N6A	2.05	1.39	1.34
3	74-A	202	NAP	C6A-N6A	2.05	1.39	1.34
3	35-A	202	NAP	C6A-N6A	2.05	1.39	1.34
3	17-A	202	NAP	C6A-N6A	2.05	1.39	1.34
3	24-A	202	NAP	C6A-N6A	2.04	1.39	1.34
2	41-A	201	FOL	C4-N3	-2.04	1.34	1.38
2	8-A	201	FOL	C4-N3	-2.04	1.34	1.38
3	29-A	202	NAP	C6A-N6A	2.04	1.39	1.34
2	1-A	201	FOL	C4-N3	-2.04	1.34	1.38
2	66-A	201	FOL	O2-CT	-2.04	1.24	1.30
3	54-A	202	NAP	C6A-N6A	2.04	1.39	1.34
2	5-A	201	FOL	C4-N3	-2.04	1.34	1.38
3	11-A	202	NAP	C6A-N6A	2.04	1.39	1.34
2	11-A	201	FOL	C4-N3	-2.04	1.34	1.38
3	58-A	202	NAP	C5N-C4N	-2.04	1.35	1.38
2	9-A	201	FOL	C4-N3	-2.04	1.34	1.38
3	74-A	202	NAP	C5A-C4A	-2.04	1.35	1.39
3	46-A	202	NAP	C5N-C4N	-2.03	1.35	1.38
3	73-A	202	NAP	C6A-N6A	2.03	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	75-A	202	NAP	C2A-N3A	2.03	1.37	1.33
3	13-A	202	NAP	C6A-N6A	2.03	1.39	1.34
3	53-A	202	NAP	C6A-N6A	2.03	1.39	1.34
3	31-A	202	NAP	C2A-N3A	2.03	1.37	1.33
3	26-A	202	NAP	C6A-N6A	2.03	1.39	1.34
3	52-A	202	NAP	C6A-N6A	2.02	1.39	1.34
2	27-A	201	FOL	C4-N3	-2.02	1.34	1.38
3	69-A	202	NAP	C6A-N6A	2.02	1.39	1.34
3	9-A	202	NAP	C6A-N6A	2.02	1.39	1.34
2	79-A	201	FOL	C4-N3	-2.02	1.34	1.38
3	8-A	202	NAP	C5N-C4N	-2.02	1.35	1.38
3	55-A	202	NAP	C5N-C4N	-2.02	1.35	1.38
3	54-A	202	NAP	C5N-C4N	-2.02	1.35	1.38
3	15-A	202	NAP	O3D-C3D	-2.01	1.38	1.43
3	39-A	202	NAP	C6A-N6A	2.01	1.39	1.34
3	18-A	202	NAP	O3D-C3D	-2.01	1.38	1.43
3	56-A	202	NAP	C5N-C4N	-2.01	1.35	1.38
3	8-A	202	NAP	C5A-C4A	-2.01	1.35	1.39
3	32-A	202	NAP	C5N-C4N	-2.01	1.35	1.38
3	17-A	202	NAP	O3D-C3D	-2.01	1.38	1.43
3	67-A	202	NAP	C5N-C4N	-2.01	1.35	1.38
2	76-A	201	FOL	OE2-CD	-2.00	1.24	1.30
2	14-A	201	FOL	C4-N3	-2.00	1.34	1.38
3	76-A	202	NAP	C2A-N3A	2.00	1.37	1.33
2	66-A	201	FOL	C4-N3	-2.00	1.34	1.38
3	31-A	202	NAP	C5N-C4N	-2.00	1.35	1.38
3	57-A	202	NAP	C5N-C4N	-2.00	1.35	1.38
2	20-A	201	FOL	O2-CT	-2.00	1.24	1.30

All (1518) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	73-A	201	FOL	C7-C6-N5	-7.80	115.81	120.87
2	72-A	201	FOL	CA-N-C	7.66	139.95	121.56
2	73-A	201	FOL	N1-C8A-N8	7.41	127.44	116.38
2	72-A	201	FOL	CG-CB-CA	7.08	126.21	113.16
2	67-A	201	FOL	N1-C8A-N8	6.99	126.81	116.38
2	78-A	201	FOL	CG-CB-CA	-6.75	100.71	113.16
2	64-A	201	FOL	N1-C8A-N8	6.55	126.16	116.38
2	67-A	201	FOL	C7-C6-N5	-6.42	116.71	120.87
2	79-A	201	FOL	CT-CA-N	6.26	125.10	110.57
2	77-A	201	FOL	CG-CB-CA	-5.96	102.17	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	71-A	201	FOL	N1-C8A-N8	5.82	125.07	116.38
2	76-A	201	FOL	CT-CA-N	5.76	123.93	110.57
2	69-A	201	FOL	C8A-C4A-C4	-5.75	115.83	119.56
3	52-A	202	NAP	N3A-C2A-N1A	-5.64	120.04	128.58
2	79-A	201	FOL	CG-CB-CA	-5.63	102.79	113.16
2	73-A	201	FOL	C9-N10-C14	5.63	139.91	121.87
3	71-A	202	NAP	N3A-C2A-N1A	-5.58	120.13	128.58
3	35-A	202	NAP	N3A-C2A-N1A	-5.57	120.15	128.58
3	70-A	202	NAP	N3A-C2A-N1A	-5.56	120.16	128.58
3	80-A	202	NAP	N3A-C2A-N1A	-5.50	120.26	128.58
3	2-A	202	NAP	N3A-C2A-N1A	-5.49	120.28	128.58
3	43-A	202	NAP	N3A-C2A-N1A	-5.49	120.28	128.58
2	69-A	201	FOL	C9-C6-C7	-5.48	111.52	121.38
2	23-A	201	FOL	C8A-C4A-C4	-5.48	116.01	119.56
2	72-A	201	FOL	N1-C8A-N8	5.46	124.53	116.38
3	22-A	202	NAP	N3A-C2A-N1A	-5.45	120.33	128.58
3	1-A	202	NAP	N3A-C2A-N1A	-5.44	120.35	128.58
3	64-A	202	NAP	N3A-C2A-N1A	-5.44	120.35	128.58
2	63-A	201	FOL	C8A-C4A-C4	-5.44	116.03	119.56
2	31-A	201	FOL	C8A-C4A-C4	-5.43	116.04	119.56
3	15-A	202	NAP	N3A-C2A-N1A	-5.43	120.36	128.58
3	54-A	202	NAP	N3A-C2A-N1A	-5.43	120.36	128.58
3	34-A	202	NAP	N3A-C2A-N1A	-5.43	120.37	128.58
3	79-A	202	NAP	N3A-C2A-N1A	-5.42	120.37	128.58
3	28-A	202	NAP	N3A-C2A-N1A	-5.42	120.38	128.58
3	33-A	202	NAP	N3A-C2A-N1A	-5.42	120.38	128.58
3	47-A	202	NAP	N3A-C2A-N1A	-5.41	120.39	128.58
3	56-A	202	NAP	N3A-C2A-N1A	-5.41	120.40	128.58
3	55-A	202	NAP	N3A-C2A-N1A	-5.40	120.41	128.58
3	3-A	202	NAP	N3A-C2A-N1A	-5.39	120.43	128.58
3	44-A	202	NAP	N3A-C2A-N1A	-5.38	120.44	128.58
2	68-A	201	FOL	C6-C9-N10	-5.38	101.31	113.13
3	19-A	202	NAP	N3A-C2A-N1A	-5.38	120.44	128.58
3	69-A	202	NAP	N3A-C2A-N1A	-5.37	120.45	128.58
2	69-A	201	FOL	C9-C6-N5	5.37	126.71	116.56
3	51-A	202	NAP	N3A-C2A-N1A	-5.37	120.46	128.58
3	24-A	202	NAP	N3A-C2A-N1A	-5.36	120.47	128.58
2	73-A	201	FOL	C9-C6-C7	5.35	131.00	121.38
3	8-A	202	NAP	N3A-C2A-N1A	-5.35	120.48	128.58
3	23-A	202	NAP	N3A-C2A-N1A	-5.35	120.48	128.58
3	49-A	202	NAP	N3A-C2A-N1A	-5.34	120.50	128.58
3	4-A	202	NAP	N3A-C2A-N1A	-5.33	120.51	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-A	202	NAP	N3A-C2A-N1A	-5.32	120.53	128.58
3	37-A	202	NAP	N3A-C2A-N1A	-5.32	120.54	128.58
3	67-A	202	NAP	N3A-C2A-N1A	-5.31	120.54	128.58
3	31-A	202	NAP	N3A-C2A-N1A	-5.31	120.54	128.58
3	74-A	202	NAP	N3A-C2A-N1A	-5.31	120.55	128.58
3	9-A	202	NAP	N3A-C2A-N1A	-5.29	120.58	128.58
3	48-A	202	NAP	N3A-C2A-N1A	-5.29	120.58	128.58
3	60-A	202	NAP	N3A-C2A-N1A	-5.29	120.58	128.58
3	18-A	202	NAP	N3A-C2A-N1A	-5.28	120.58	128.58
3	10-A	202	NAP	N3A-C2A-N1A	-5.28	120.59	128.58
3	32-A	202	NAP	N3A-C2A-N1A	-5.28	120.59	128.58
3	61-A	202	NAP	N3A-C2A-N1A	-5.28	120.59	128.58
3	7-A	202	NAP	N3A-C2A-N1A	-5.27	120.60	128.58
3	66-A	202	NAP	N3A-C2A-N1A	-5.26	120.61	128.58
3	42-A	202	NAP	N3A-C2A-N1A	-5.26	120.61	128.58
3	40-A	202	NAP	N3A-C2A-N1A	-5.26	120.63	128.58
2	80-A	201	FOL	C8A-C4A-C4	-5.25	116.15	119.56
3	53-A	202	NAP	N3A-C2A-N1A	-5.25	120.63	128.58
3	41-A	202	NAP	N3A-C2A-N1A	-5.24	120.65	128.58
3	13-A	202	NAP	N3A-C2A-N1A	-5.24	120.65	128.58
3	11-A	202	NAP	N3A-C2A-N1A	-5.23	120.66	128.58
3	39-A	202	NAP	N3A-C2A-N1A	-5.23	120.66	128.58
3	36-A	202	NAP	N3A-C2A-N1A	-5.23	120.66	128.58
3	14-A	202	NAP	N3A-C2A-N1A	-5.23	120.66	128.58
3	21-A	202	NAP	N3A-C2A-N1A	-5.22	120.67	128.58
3	77-A	202	NAP	N3A-C2A-N1A	-5.22	120.68	128.58
3	72-A	202	NAP	N3A-C2A-N1A	-5.22	120.68	128.58
3	17-A	202	NAP	N3A-C2A-N1A	-5.22	120.68	128.58
3	50-A	202	NAP	N3A-C2A-N1A	-5.21	120.70	128.58
2	66-A	201	FOL	C8A-C4A-C4	-5.20	116.19	119.56
3	27-A	202	NAP	N3A-C2A-N1A	-5.18	120.74	128.58
3	73-A	202	NAP	N3A-C2A-N1A	-5.18	120.74	128.58
3	26-A	202	NAP	N3A-C2A-N1A	-5.18	120.74	128.58
3	68-A	202	NAP	N3A-C2A-N1A	-5.18	120.74	128.58
2	74-A	201	FOL	CT-CA-N	5.18	122.58	110.57
3	12-A	202	NAP	N3A-C2A-N1A	-5.18	120.75	128.58
3	30-A	202	NAP	N3A-C2A-N1A	-5.17	120.75	128.58
3	54-A	202	NAP	C5A-C4A-N3A	-5.16	119.61	126.72
3	29-A	202	NAP	N3A-C2A-N1A	-5.15	120.78	128.58
3	20-A	202	NAP	N3A-C2A-N1A	-5.15	120.78	128.58
2	23-A	201	FOL	N1-C8A-N8	5.14	124.05	116.38
2	78-A	201	FOL	CT-CA-N	5.11	122.43	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	25-A	202	NAP	N3A-C2A-N1A	-5.11	120.85	128.58
3	57-A	202	NAP	N3A-C2A-N1A	-5.11	120.85	128.58
3	46-A	202	NAP	N3A-C2A-N1A	-5.10	120.86	128.58
3	58-A	202	NAP	N3A-C2A-N1A	-5.10	120.86	128.58
3	45-A	202	NAP	N3A-C2A-N1A	-5.09	120.88	128.58
3	62-A	202	NAP	N3A-C2A-N1A	-5.08	120.89	128.58
2	57-A	201	FOL	C8A-C4A-C4	-5.08	116.27	119.56
3	65-A	202	NAP	N3A-C2A-N1A	-5.07	120.90	128.58
2	40-A	201	FOL	C11-C-N	5.06	126.43	117.04
3	78-A	202	NAP	N3A-C2A-N1A	-5.05	120.93	128.58
3	45-A	202	NAP	C5A-C4A-N3A	-5.02	119.81	126.72
3	75-A	202	NAP	N3A-C2A-N1A	-5.01	121.00	128.58
2	45-A	201	FOL	C8A-C4A-C4	-5.01	116.31	119.56
3	5-A	202	NAP	N3A-C2A-N1A	-5.00	121.02	128.58
2	63-A	201	FOL	CA-N-C	5.00	133.55	121.56
3	46-A	202	NAP	C5A-C4A-N3A	-4.98	119.86	126.72
3	38-A	202	NAP	N3A-C2A-N1A	-4.97	121.05	128.58
3	63-A	202	NAP	N3A-C2A-N1A	-4.97	121.05	128.58
3	16-A	202	NAP	N3A-C2A-N1A	-4.96	121.08	128.58
3	75-A	202	NAP	C5A-C4A-N3A	-4.95	119.90	126.72
3	59-A	202	NAP	N3A-C2A-N1A	-4.95	121.09	128.58
2	55-A	201	FOL	C8A-C4A-C4	-4.94	116.35	119.56
2	70-A	201	FOL	C8A-C4A-C4	-4.94	116.36	119.56
3	63-A	202	NAP	C5A-C4A-N3A	-4.93	119.93	126.72
3	40-A	202	NAP	C5A-C4A-N3A	-4.93	119.93	126.72
3	42-A	202	NAP	C5A-C4A-N3A	-4.89	119.98	126.72
2	9-A	201	FOL	C8A-C4A-C4	-4.89	116.39	119.56
2	37-A	201	FOL	C8A-C4A-C4	-4.89	116.39	119.56
3	39-A	202	NAP	C5A-C4A-N3A	-4.88	120.00	126.72
3	74-A	202	NAP	N9A-C8A-N7A	-4.87	107.02	113.94
2	68-A	201	FOL	N1-C8A-N8	4.87	123.65	116.38
3	76-A	202	NAP	N3A-C2A-N1A	-4.87	121.22	128.58
3	78-A	202	NAP	C5A-C4A-N3A	-4.85	120.04	126.72
2	69-A	201	FOL	C13-C12-C11	-4.83	115.64	120.80
3	23-A	202	NAP	C5A-C4A-N3A	-4.81	120.09	126.72
3	62-A	202	NAP	C5A-C4A-N3A	-4.81	120.09	126.72
3	32-A	202	NAP	C5A-C4A-N3A	-4.80	120.10	126.72
3	34-A	202	NAP	C5A-C4A-N3A	-4.79	120.12	126.72
2	64-A	201	FOL	C7-C6-N5	-4.79	117.76	120.87
2	53-A	201	FOL	C8A-C4A-C4	-4.78	116.46	119.56
3	76-A	202	NAP	C5A-C4A-N3A	-4.76	120.17	126.72
3	21-A	202	NAP	C5A-C4A-N3A	-4.75	120.18	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	26-A	202	NAP	C5A-C4A-N3A	-4.75	120.18	126.72
3	25-A	202	NAP	C5A-C4A-N3A	-4.75	120.18	126.72
3	31-A	202	NAP	C5A-C4A-N3A	-4.74	120.19	126.72
3	30-A	202	NAP	C5A-C4A-N3A	-4.74	120.19	126.72
3	29-A	202	NAP	C5A-C4A-N3A	-4.73	120.20	126.72
3	22-A	202	NAP	C5A-C4A-N3A	-4.72	120.22	126.72
2	77-A	201	FOL	CB-CG-CD	-4.71	99.93	112.49
2	14-A	201	FOL	C8A-C4A-C4	-4.70	116.51	119.56
3	59-A	202	NAP	C5A-C4A-N3A	-4.68	120.27	126.72
2	77-A	201	FOL	C8A-C4A-C4	-4.68	116.53	119.56
3	27-A	202	NAP	C5A-C4A-N3A	-4.67	120.29	126.72
3	33-A	202	NAP	C5A-C4A-N3A	-4.67	120.29	126.72
3	14-A	202	NAP	C5A-C4A-N3A	-4.67	120.29	126.72
3	35-A	202	NAP	C5A-C4A-N3A	-4.65	120.31	126.72
3	65-A	202	NAP	C5A-C4A-N3A	-4.65	120.31	126.72
3	11-A	202	NAP	C5A-C4A-N3A	-4.65	120.32	126.72
3	38-A	202	NAP	C5A-C4A-N3A	-4.63	120.35	126.72
3	58-A	202	NAP	C5A-C4A-N3A	-4.62	120.35	126.72
3	73-A	202	NAP	C5A-C4A-N3A	-4.62	120.36	126.72
3	24-A	202	NAP	C5A-C4A-N3A	-4.61	120.37	126.72
3	47-A	202	NAP	C5A-C4A-N3A	-4.61	120.37	126.72
2	56-A	201	FOL	C8A-C4A-C4	-4.60	116.58	119.56
3	72-A	202	NAP	C5A-C4A-N3A	-4.59	120.39	126.72
3	36-A	202	NAP	C5A-C4A-N3A	-4.59	120.40	126.72
3	50-A	202	NAP	C5A-C4A-N3A	-4.59	120.40	126.72
3	57-A	202	NAP	C5A-C4A-N3A	-4.59	120.40	126.72
3	12-A	202	NAP	C5A-C4A-N3A	-4.58	120.41	126.72
2	43-A	201	FOL	CG-CB-CA	-4.57	104.74	113.16
2	65-A	201	FOL	CG-CB-CA	4.55	121.55	113.16
3	60-A	202	NAP	C5A-C4A-N3A	-4.54	120.46	126.72
3	61-A	202	NAP	C5A-C4A-N3A	-4.54	120.47	126.72
3	51-A	202	NAP	C5A-C4A-N3A	-4.54	120.47	126.72
2	26-A	201	FOL	C8A-C4A-C4	-4.53	116.62	119.56
3	20-A	202	NAP	C5A-C4A-N3A	-4.52	120.49	126.72
3	41-A	202	NAP	C5A-C4A-N3A	-4.52	120.49	126.72
2	69-A	201	FOL	C6-C9-N10	4.51	123.03	113.13
3	13-A	202	NAP	C5A-C4A-N3A	-4.50	120.52	126.72
2	35-A	201	FOL	N1-C8A-N8	4.50	123.10	116.38
2	52-A	201	FOL	C8A-C4A-C4	-4.50	116.64	119.56
3	17-A	202	NAP	C5A-C4A-N3A	-4.50	120.52	126.72
2	15-A	201	FOL	C8A-C4A-C4	-4.49	116.64	119.56
3	74-A	202	NAP	C5A-C4A-N3A	-4.49	120.53	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-A	201	FOL	C8A-C4A-C4	-4.49	116.65	119.56
3	9-A	202	NAP	C5A-C4A-N3A	-4.48	120.54	126.72
3	69-A	202	NAP	C5A-C4A-N3A	-4.48	120.55	126.72
2	22-A	201	FOL	C8A-C4A-C4	-4.48	116.66	119.56
3	68-A	202	NAP	C5A-C4A-N3A	-4.47	120.56	126.72
3	55-A	202	NAP	C5A-C4A-N3A	-4.47	120.56	126.72
2	47-A	201	FOL	C8A-C4A-C4	-4.47	116.66	119.56
3	49-A	202	NAP	C5A-C4A-N3A	-4.47	120.56	126.72
3	10-A	202	NAP	C5A-C4A-N3A	-4.47	120.57	126.72
3	6-A	202	NAP	C5A-C4A-N3A	-4.46	120.57	126.72
2	71-A	201	FOL	CG-CB-CA	4.46	121.39	113.16
3	15-A	202	NAP	C5A-C4A-N3A	-4.46	120.58	126.72
3	53-A	202	NAP	C5A-C4A-N3A	-4.45	120.58	126.72
2	54-A	201	FOL	N1-C8A-N8	4.45	123.03	116.38
3	4-A	202	NAP	C5A-C4A-N3A	-4.45	120.59	126.72
3	5-A	202	NAP	C5A-C4A-N3A	-4.44	120.60	126.72
3	44-A	202	NAP	C5A-C4A-N3A	-4.44	120.60	126.72
2	19-A	201	FOL	C8A-C4A-C4	-4.44	116.68	119.56
3	43-A	202	NAP	C5A-C4A-N3A	-4.43	120.62	126.72
2	79-A	201	FOL	C8A-C4A-C4	-4.42	116.69	119.56
3	77-A	202	NAP	C5A-C4A-N3A	-4.41	120.64	126.72
3	37-A	202	NAP	C5A-C4A-N3A	-4.40	120.65	126.72
3	79-A	202	NAP	C5A-C4A-N3A	-4.40	120.65	126.72
3	48-A	202	NAP	C5A-C4A-N3A	-4.40	120.66	126.72
2	17-A	201	FOL	N1-C8A-N8	4.40	122.95	116.38
2	43-A	201	FOL	C8A-C4A-C4	-4.40	116.71	119.56
2	18-A	201	FOL	N1-C8A-N8	4.38	122.91	116.38
2	54-A	201	FOL	C8A-C4A-C4	-4.37	116.72	119.56
3	28-A	202	NAP	C5A-C4A-N3A	-4.37	120.71	126.72
3	3-A	202	NAP	C5A-C4A-N3A	-4.36	120.71	126.72
2	41-A	201	FOL	C8A-C4A-C4	-4.36	116.73	119.56
2	34-A	201	FOL	N1-C8A-N8	4.35	122.88	116.38
3	41-A	202	NAP	C4D-O4D-C1D	-4.35	105.94	109.92
3	16-A	202	NAP	C5A-C4A-N3A	-4.34	120.74	126.72
2	46-A	201	FOL	C8A-C4A-C4	-4.34	116.75	119.56
2	40-A	201	FOL	N1-C8A-N8	4.34	122.85	116.38
2	63-A	201	FOL	C11-C-N	-4.34	109.00	117.04
3	1-A	202	NAP	C5A-C4A-N3A	-4.34	120.75	126.72
2	10-A	201	FOL	N1-C8A-N8	4.33	122.85	116.38
2	36-A	201	FOL	N1-C8A-N8	4.33	122.85	116.38
2	25-A	201	FOL	CG-CB-CA	4.33	121.15	113.16
2	21-A	201	FOL	N1-C8A-N8	4.33	122.84	116.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	28-A	202	NAP	N9A-C8A-N7A	-4.33	107.79	113.94
2	61-A	201	FOL	C8A-C4A-C4	-4.32	116.76	119.56
3	7-A	202	NAP	C5A-C4A-N3A	-4.32	120.77	126.72
3	70-A	202	NAP	C5A-C4A-N3A	-4.32	120.77	126.72
2	35-A	201	FOL	C8A-C4A-C4	-4.31	116.76	119.56
2	58-A	201	FOL	N1-C8A-N8	4.31	122.81	116.38
3	5-A	202	NAP	N9A-C8A-N7A	-4.31	107.83	113.94
3	66-A	202	NAP	C5A-C4A-N3A	-4.30	120.79	126.72
2	41-A	201	FOL	N1-C8A-N8	4.30	122.80	116.38
2	46-A	201	FOL	N1-C8A-N8	4.30	122.79	116.38
2	11-A	201	FOL	C8A-C4A-C4	-4.29	116.77	119.56
3	40-A	202	NAP	N6A-C6A-N1A	-4.29	108.81	118.38
3	80-A	202	NAP	N9A-C8A-N7A	-4.29	107.85	113.94
2	32-A	201	FOL	N1-C8A-N8	4.29	122.78	116.38
3	74-A	202	NAP	C4A-N9A-C1B	-4.29	116.61	126.63
3	2-A	202	NAP	N9A-C8A-N7A	-4.27	107.88	113.94
2	42-A	201	FOL	C8A-C4A-C4	-4.27	116.79	119.56
3	2-A	202	NAP	C5A-C4A-N3A	-4.27	120.84	126.72
2	9-A	201	FOL	N1-C8A-N8	4.25	122.73	116.38
3	74-A	202	NAP	N6A-C6A-N1A	-4.25	108.91	118.38
3	18-A	202	NAP	C5A-C4A-N3A	-4.25	120.87	126.72
2	74-A	201	FOL	C8A-C4A-C4	-4.24	116.81	119.56
3	71-A	202	NAP	C5A-C4A-N3A	-4.24	120.88	126.72
3	23-A	202	NAP	N6A-C6A-N1A	-4.24	108.93	118.38
2	31-A	201	FOL	N1-C8A-N8	4.24	122.71	116.38
3	28-A	202	NAP	N6A-C6A-N1A	-4.24	108.94	118.38
3	60-A	202	NAP	N6A-C6A-N1A	-4.24	108.94	118.38
2	3-A	201	FOL	C8A-C4A-C4	-4.24	116.81	119.56
3	67-A	202	NAP	C5A-C4A-N3A	-4.24	120.89	126.72
2	51-A	201	FOL	N1-C8A-N8	4.23	122.69	116.38
2	39-A	201	FOL	C11-C-N	4.22	124.86	117.04
2	1-A	201	FOL	N1-C8A-N8	4.22	122.68	116.38
3	1-A	202	NAP	N9A-C8A-N7A	-4.21	107.96	113.94
2	16-A	201	FOL	N1-C8A-N8	4.21	122.66	116.38
3	13-A	202	NAP	N6A-C6A-N1A	-4.21	109.01	118.38
2	72-A	201	FOL	C9-N10-C14	4.20	135.34	121.87
3	34-A	202	NAP	N6A-C6A-N1A	-4.20	109.03	118.38
3	8-A	202	NAP	C5A-C4A-N3A	-4.20	120.94	126.72
2	6-A	201	FOL	C8A-C4A-C4	-4.20	116.84	119.56
2	64-A	201	FOL	C9-C6-C7	4.19	128.92	121.38
2	2-A	201	FOL	C8A-C4A-C4	-4.19	116.84	119.56
2	48-A	201	FOL	N1-C8A-N8	4.19	122.64	116.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	74-A	201	FOL	N1-C8A-N8	4.19	122.64	116.38
3	25-A	202	NAP	N9A-C8A-N7A	-4.18	108.00	113.94
3	47-A	202	NAP	N9A-C8A-N7A	-4.17	108.01	113.94
2	16-A	201	FOL	C8A-C4A-C4	-4.17	116.85	119.56
2	65-A	201	FOL	C8A-C4A-C4	-4.17	116.85	119.56
2	14-A	201	FOL	N1-C8A-N8	4.17	122.61	116.38
2	61-A	201	FOL	N1-C8A-N8	4.17	122.60	116.38
2	30-A	201	FOL	N1-C8A-N8	4.17	122.60	116.38
2	75-A	201	FOL	C8A-C4A-C4	-4.16	116.86	119.56
3	75-A	202	NAP	N6A-C6A-N1A	-4.16	109.10	118.38
2	27-A	201	FOL	N1-C8A-N8	4.16	122.59	116.38
3	78-A	202	NAP	N6A-C6A-N1A	-4.15	109.12	118.38
3	10-A	202	NAP	N9A-C8A-N7A	-4.15	108.05	113.94
3	42-A	202	NAP	N6A-C6A-N1A	-4.15	109.13	118.38
2	72-A	201	FOL	CB-CA-N	4.15	119.12	110.91
2	50-A	201	FOL	C8A-C4A-C4	-4.15	116.87	119.56
3	11-A	202	NAP	N6A-C6A-N1A	-4.15	109.13	118.38
3	64-A	202	NAP	C5A-C4A-N3A	-4.15	121.00	126.72
2	75-A	201	FOL	N1-C8A-N8	4.14	122.57	116.38
2	33-A	201	FOL	C8A-C4A-C4	-4.14	116.88	119.56
3	80-A	202	NAP	C5A-C4A-N3A	-4.13	121.03	126.72
3	12-A	202	NAP	N6A-C6A-N1A	-4.13	109.18	118.38
3	71-A	202	NAP	N9A-C8A-N7A	-4.13	108.08	113.94
2	7-A	201	FOL	N1-C8A-N8	4.13	122.54	116.38
3	18-A	202	NAP	N9A-C8A-N7A	-4.13	108.08	113.94
3	19-A	202	NAP	C5A-C4A-N3A	-4.12	121.04	126.72
2	29-A	201	FOL	C8A-C4A-C4	-4.12	116.89	119.56
2	40-A	201	FOL	CB-CA-N	4.12	119.06	110.91
2	12-A	201	FOL	C8A-C4A-C4	-4.12	116.89	119.56
3	60-A	202	NAP	N9A-C8A-N7A	-4.12	108.10	113.94
3	7-A	202	NAP	N6A-C6A-N1A	-4.11	109.22	118.38
3	54-A	202	NAP	N6A-C6A-N1A	-4.11	109.22	118.38
2	22-A	201	FOL	N1-C8A-N8	4.11	122.52	116.38
3	80-A	202	NAP	N6A-C6A-N1A	-4.11	109.23	118.38
3	9-A	202	NAP	N9A-C8A-N7A	-4.11	108.11	113.94
2	6-A	201	FOL	N1-C8A-N8	4.11	122.51	116.38
3	66-A	202	NAP	N6A-C6A-N1A	-4.10	109.24	118.38
2	44-A	201	FOL	N1-C8A-N8	4.09	122.49	116.38
2	3-A	201	FOL	N1-C8A-N8	4.09	122.48	116.38
2	20-A	201	FOL	N1-C8A-N8	4.08	122.48	116.38
3	44-A	202	NAP	N9A-C8A-N7A	-4.08	108.14	113.94
3	72-A	202	NAP	N6A-C6A-N1A	-4.08	109.29	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	56-A	202	NAP	C5A-C4A-N3A	-4.08	121.10	126.72
2	13-A	201	FOL	N1-C8A-N8	4.08	122.47	116.38
2	76-A	201	FOL	C8A-C4A-C4	-4.08	116.91	119.56
2	8-A	201	FOL	CG-CB-CA	-4.08	105.64	113.16
3	39-A	202	NAP	N6A-C6A-N1A	-4.08	109.30	118.38
3	63-A	202	NAP	N6A-C6A-N1A	-4.07	109.31	118.38
3	4-A	202	NAP	N9A-C8A-N7A	-4.06	108.17	113.94
2	48-A	201	FOL	C11-C-N	4.06	124.56	117.04
2	43-A	201	FOL	N1-C8A-N8	4.06	122.44	116.38
3	71-A	202	NAP	N6A-C6A-N1A	-4.05	109.35	118.38
3	10-A	202	NAP	N6A-C6A-N1A	-4.05	109.35	118.38
2	78-A	201	FOL	C8A-C4A-C4	-4.05	116.93	119.56
2	66-A	201	FOL	C9-N10-C14	4.05	134.85	121.87
2	4-A	201	FOL	C8A-C4A-C4	-4.04	116.94	119.56
3	42-A	202	NAP	N9A-C8A-N7A	-4.04	108.20	113.94
3	67-A	202	NAP	N9A-C8A-N7A	-4.04	108.20	113.94
3	57-A	202	NAP	N6A-C6A-N1A	-4.04	109.38	118.38
3	40-A	202	NAP	N9A-C8A-N7A	-4.04	108.21	113.94
2	77-A	201	FOL	N1-C8A-N8	4.03	122.40	116.38
2	8-A	201	FOL	N1-C8A-N8	4.03	122.39	116.38
2	62-A	201	FOL	N1-C8A-N8	4.03	122.39	116.38
3	17-A	202	NAP	N6A-C6A-N1A	-4.02	109.41	118.38
3	37-A	202	NAP	N6A-C6A-N1A	-4.02	109.42	118.38
3	69-A	202	NAP	N6A-C6A-N1A	-4.02	109.42	118.38
3	16-A	202	NAP	N6A-C6A-N1A	-4.02	109.43	118.38
3	9-A	202	NAP	N6A-C6A-N1A	-4.02	109.43	118.38
2	52-A	201	FOL	N1-C8A-N8	4.01	122.37	116.38
3	29-A	202	NAP	N9A-C8A-N7A	-4.01	108.24	113.94
3	15-A	202	NAP	N6A-C6A-N1A	-4.01	109.44	118.38
2	15-A	201	FOL	N1-C8A-N8	4.01	122.37	116.38
3	34-A	202	NAP	N9A-C8A-N7A	-4.00	108.26	113.94
2	73-A	201	FOL	CA-N-C	4.00	131.16	121.56
2	24-A	201	FOL	N1-C8A-N8	4.00	122.35	116.38
2	25-A	201	FOL	C8A-C4A-C4	-4.00	116.97	119.56
3	55-A	202	NAP	N6A-C6A-N1A	-4.00	109.47	118.38
3	53-A	202	NAP	N6A-C6A-N1A	-4.00	109.48	118.38
3	5-A	202	NAP	N6A-C6A-N1A	-3.99	109.48	118.38
2	56-A	201	FOL	N1-C8A-N8	3.99	122.34	116.38
3	65-A	202	NAP	N9A-C8A-N7A	-3.99	108.27	113.94
3	64-A	202	NAP	N9A-C8A-N7A	-3.99	108.27	113.94
3	12-A	202	NAP	N9A-C8A-N7A	-3.98	108.29	113.94
3	52-A	202	NAP	C5A-C4A-N3A	-3.98	121.23	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	30-A	202	NAP	N6A-C6A-N1A	-3.98	109.51	118.38
3	8-A	202	NAP	N9A-C8A-N7A	-3.98	108.29	113.94
3	38-A	202	NAP	N6A-C6A-N1A	-3.98	109.52	118.38
3	76-A	202	NAP	N6A-C6A-N1A	-3.97	109.53	118.38
3	43-A	202	NAP	N9A-C8A-N7A	-3.97	108.30	113.94
3	15-A	202	NAP	N9A-C8A-N7A	-3.97	108.31	113.94
3	66-A	202	NAP	N9A-C8A-N7A	-3.97	108.31	113.94
2	33-A	201	FOL	N1-C8A-N8	3.96	122.30	116.38
3	35-A	202	NAP	N6A-C6A-N1A	-3.96	109.56	118.38
2	28-A	201	FOL	N1-C8A-N8	3.96	122.29	116.38
3	48-A	202	NAP	N9A-C8A-N7A	-3.95	108.33	113.94
2	76-A	201	FOL	N1-C8A-N8	3.95	122.28	116.38
3	19-A	202	NAP	N9A-C8A-N7A	-3.95	108.34	113.94
3	22-A	202	NAP	N6A-C6A-N1A	-3.95	109.59	118.38
2	18-A	201	FOL	C8A-C4A-C4	-3.94	117.00	119.56
2	34-A	201	FOL	C8A-C4A-C4	-3.94	117.00	119.56
2	25-A	201	FOL	N1-C8A-N8	3.94	122.26	116.38
3	3-A	202	NAP	N9A-C8A-N7A	-3.94	108.35	113.94
3	68-A	202	NAP	N9A-C8A-N7A	-3.94	108.35	113.94
2	1-A	201	FOL	C8A-C4A-C4	-3.94	117.01	119.56
2	20-A	201	FOL	C8A-C4A-C4	-3.94	117.01	119.56
3	1-A	202	NAP	N6A-C6A-N1A	-3.93	109.61	118.38
3	29-A	202	NAP	N6A-C6A-N1A	-3.93	109.62	118.38
3	36-A	202	NAP	N6A-C6A-N1A	-3.93	109.63	118.38
3	59-A	202	NAP	N6A-C6A-N1A	-3.93	109.63	118.38
2	2-A	201	FOL	N1-C8A-N8	3.93	122.24	116.38
3	73-A	202	NAP	N6A-C6A-N1A	-3.92	109.64	118.38
2	28-A	201	FOL	C8A-C4A-C4	-3.92	117.02	119.56
2	42-A	201	FOL	N1-C8A-N8	3.91	122.22	116.38
2	27-A	201	FOL	C8A-C4A-C4	-3.91	117.02	119.56
2	65-A	201	FOL	N1-C8A-N8	3.91	122.22	116.38
3	45-A	202	NAP	N6A-C6A-N1A	-3.91	109.67	118.38
2	60-A	201	FOL	N1-C8A-N8	3.90	122.20	116.38
3	22-A	202	NAP	N9A-C8A-N7A	-3.90	108.41	113.94
3	18-A	202	NAP	N6A-C6A-N1A	-3.90	109.70	118.38
2	62-A	201	FOL	C8A-C4A-C4	-3.89	117.03	119.56
3	41-A	202	NAP	N9A-C8A-N7A	-3.89	108.42	113.94
3	62-A	202	NAP	N6A-C6A-N1A	-3.89	109.72	118.38
3	55-A	202	NAP	N9A-C8A-N7A	-3.89	108.42	113.94
3	23-A	202	NAP	N9A-C8A-N7A	-3.88	108.42	113.94
3	50-A	202	NAP	N6A-C6A-N1A	-3.88	109.73	118.38
3	49-A	202	NAP	N9A-C8A-N7A	-3.88	108.43	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	49-A	202	NAP	N6A-C6A-N1A	-3.88	109.74	118.38
3	4-A	202	NAP	N6A-C6A-N1A	-3.88	109.75	118.38
3	80-A	202	NAP	C4A-N9A-C1B	-3.87	117.58	126.63
2	25-A	201	FOL	CB-CA-N	3.87	118.57	110.91
2	59-A	201	FOL	N1-C8A-N8	3.87	122.16	116.38
2	44-A	201	FOL	C8A-C4A-C4	-3.87	117.05	119.56
3	44-A	202	NAP	N6A-C6A-N1A	-3.87	109.76	118.38
3	25-A	202	NAP	N6A-C6A-N1A	-3.87	109.77	118.38
2	67-A	201	FOL	C16-C15-C14	3.87	124.75	120.30
2	13-A	201	FOL	C8A-C4A-C4	-3.86	117.05	119.56
3	65-A	202	NAP	N6A-C6A-N1A	-3.86	109.77	118.38
3	6-A	202	NAP	N9A-C8A-N7A	-3.86	108.46	113.94
2	12-A	201	FOL	N1-C8A-N8	3.86	122.14	116.38
2	69-A	201	FOL	C16-C15-C14	-3.86	115.86	120.30
3	70-A	202	NAP	N9A-C8A-N7A	-3.85	108.47	113.94
3	70-A	202	NAP	N6A-C6A-N1A	-3.85	109.81	118.38
3	21-A	202	NAP	N6A-C6A-N1A	-3.84	109.81	118.38
2	49-A	201	FOL	N1-C8A-N8	3.84	122.11	116.38
3	58-A	202	NAP	N9A-C8A-N7A	-3.84	108.49	113.94
3	47-A	202	NAP	N6A-C6A-N1A	-3.84	109.83	118.38
3	7-A	202	NAP	N9A-C8A-N7A	-3.84	108.50	113.94
2	4-A	201	FOL	N1-C8A-N8	3.83	122.10	116.38
2	55-A	201	FOL	N1-C8A-N8	3.83	122.10	116.38
2	10-A	201	FOL	C8A-C4A-C4	-3.83	117.08	119.56
3	57-A	202	NAP	N9A-C8A-N7A	-3.83	108.51	113.94
2	53-A	201	FOL	N1-C8A-N8	3.83	122.09	116.38
3	13-A	202	NAP	N9A-C8A-N7A	-3.82	108.51	113.94
2	7-A	201	FOL	C8A-C4A-C4	-3.82	117.08	119.56
3	19-A	202	NAP	N6A-C6A-N1A	-3.82	109.87	118.38
3	20-A	202	NAP	N6A-C6A-N1A	-3.82	109.87	118.38
3	78-A	202	NAP	N9A-C8A-N7A	-3.81	108.52	113.94
2	30-A	201	FOL	C8A-C4A-C4	-3.81	117.09	119.56
3	2-A	202	NAP	N6A-C6A-N1A	-3.81	109.88	118.38
3	17-A	202	NAP	N9A-C8A-N7A	-3.81	108.53	113.94
3	61-A	202	NAP	N6A-C6A-N1A	-3.81	109.89	118.38
3	46-A	202	NAP	N9A-C8A-N7A	-3.81	108.54	113.94
2	58-A	201	FOL	CB-CA-N	3.80	118.44	110.91
3	36-A	202	NAP	N9A-C8A-N7A	-3.80	108.55	113.94
3	46-A	202	NAP	N6A-C6A-N1A	-3.79	109.93	118.38
3	14-A	202	NAP	N6A-C6A-N1A	-3.79	109.93	118.38
3	64-A	202	NAP	N6A-C6A-N1A	-3.79	109.93	118.38
2	47-A	201	FOL	N1-C8A-N8	3.79	122.03	116.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	31-A	202	NAP	N9A-C8A-N7A	-3.79	108.56	113.94
3	52-A	202	NAP	N9A-C8A-N7A	-3.79	108.57	113.94
3	79-A	202	NAP	N9A-C8A-N7A	-3.78	108.57	113.94
3	8-A	202	NAP	C4D-O4D-C1D	-3.78	106.46	109.92
2	71-A	201	FOL	CA-N-C	3.78	130.63	121.56
3	16-A	202	NAP	N9A-C8A-N7A	-3.78	108.58	113.94
2	73-A	201	FOL	C15-C16-C11	3.78	124.83	120.80
3	7-A	202	NAP	C4D-O4D-C1D	-3.77	106.47	109.92
2	59-A	201	FOL	C8A-C4A-C4	-3.77	117.12	119.56
2	48-A	201	FOL	C8A-C4A-C4	-3.75	117.12	119.56
3	20-A	202	NAP	N9A-C8A-N7A	-3.75	108.62	113.94
3	26-A	202	NAP	N9A-C8A-N7A	-3.75	108.62	113.94
2	78-A	201	FOL	N1-C8A-N8	3.75	121.97	116.38
3	48-A	202	NAP	N6A-C6A-N1A	-3.74	110.05	118.38
2	72-A	201	FOL	C8A-C4A-C4	-3.74	117.13	119.56
3	48-A	202	NAP	C4D-O4D-C1D	-3.74	106.50	109.92
3	11-A	202	NAP	N9A-C8A-N7A	-3.73	108.64	113.94
3	67-A	202	NAP	N6A-C6A-N1A	-3.73	110.07	118.38
3	49-A	202	NAP	C4D-O4D-C1D	-3.73	106.51	109.92
3	62-A	202	NAP	N9A-C8A-N7A	-3.72	108.66	113.94
3	6-A	202	NAP	N6A-C6A-N1A	-3.72	110.10	118.38
3	76-A	202	NAP	N9A-C8A-N7A	-3.72	108.67	113.94
3	56-A	202	NAP	N9A-C8A-N7A	-3.71	108.67	113.94
3	58-A	202	NAP	N6A-C6A-N1A	-3.71	110.11	118.38
3	41-A	202	NAP	N6A-C6A-N1A	-3.71	110.11	118.38
3	26-A	202	NAP	N6A-C6A-N1A	-3.71	110.12	118.38
3	30-A	202	NAP	N9A-C8A-N7A	-3.70	108.69	113.94
2	8-A	201	FOL	C8A-C4A-C4	-3.70	117.16	119.56
3	69-A	202	NAP	N9A-C8A-N7A	-3.70	108.69	113.94
2	5-A	201	FOL	N1-C8A-N8	3.69	121.89	116.38
2	74-A	201	FOL	CA-N-C	3.69	130.41	121.56
2	60-A	201	FOL	C8A-C4A-C4	-3.69	117.17	119.56
2	21-A	201	FOL	C8A-C4A-C4	-3.69	117.17	119.56
3	32-A	202	NAP	N6A-C6A-N1A	-3.68	110.17	118.38
3	24-A	202	NAP	N6A-C6A-N1A	-3.68	110.17	118.38
2	37-A	201	FOL	N1-C8A-N8	3.68	121.88	116.38
3	63-A	202	NAP	N9A-C8A-N7A	-3.68	108.72	113.94
2	72-A	201	FOL	CT-CA-N	3.68	119.10	110.57
3	77-A	202	NAP	N9A-C8A-N7A	-3.67	108.72	113.94
3	79-A	202	NAP	N6A-C6A-N1A	-3.67	110.20	118.38
2	77-A	201	FOL	CT-CA-N	3.67	119.09	110.57
3	52-A	202	NAP	N6A-C6A-N1A	-3.67	110.20	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	64-A	201	FOL	C9-N10-C14	3.67	133.64	121.87
2	60-A	201	FOL	CB-CA-N	-3.66	103.66	110.91
3	31-A	202	NAP	N6A-C6A-N1A	-3.66	110.22	118.38
2	19-A	201	FOL	N1-C8A-N8	3.66	121.84	116.38
3	33-A	202	NAP	N6A-C6A-N1A	-3.66	110.23	118.38
3	61-A	202	NAP	N9A-C8A-N7A	-3.65	108.75	113.94
3	21-A	202	NAP	N9A-C8A-N7A	-3.65	108.76	113.94
3	56-A	202	NAP	N6A-C6A-N1A	-3.65	110.25	118.38
3	8-A	202	NAP	C4A-N9A-C1B	-3.65	118.10	126.63
2	11-A	201	FOL	N1-C8A-N8	3.65	121.82	116.38
2	38-A	201	FOL	C8A-C4A-C4	-3.65	117.19	119.56
2	57-A	201	FOL	N1-C8A-N8	3.64	121.82	116.38
3	43-A	202	NAP	N6A-C6A-N1A	-3.64	110.27	118.38
2	39-A	201	FOL	N1-C8A-N8	3.64	121.81	116.38
3	51-A	202	NAP	N6A-C6A-N1A	-3.64	110.28	118.38
2	17-A	201	FOL	C8A-C4A-C4	-3.64	117.20	119.56
3	14-A	202	NAP	N9A-C8A-N7A	-3.63	108.79	113.94
2	36-A	201	FOL	C8A-C4A-C4	-3.63	117.21	119.56
3	14-A	202	NAP	C4D-O4D-C1D	-3.62	106.61	109.92
3	33-A	202	NAP	N9A-C8A-N7A	-3.62	108.80	113.94
3	78-A	202	NAP	C4D-O4D-C1D	-3.61	106.62	109.92
2	40-A	201	FOL	C8A-C4A-C4	-3.61	117.22	119.56
3	73-A	202	NAP	N9A-C8A-N7A	-3.60	108.82	113.94
3	53-A	202	NAP	N9A-C8A-N7A	-3.60	108.83	113.94
3	59-A	202	NAP	N9A-C8A-N7A	-3.60	108.83	113.94
3	28-A	202	NAP	C4A-N9A-C1B	-3.60	118.22	126.63
3	39-A	202	NAP	N9A-C8A-N7A	-3.59	108.84	113.94
3	51-A	202	NAP	C4D-O4D-C1D	-3.59	106.64	109.92
3	50-A	202	NAP	N9A-C8A-N7A	-3.58	108.85	113.94
2	51-A	201	FOL	C8A-C4A-C4	-3.58	117.23	119.56
2	45-A	201	FOL	N1-C8A-N8	3.58	121.73	116.38
2	70-A	201	FOL	C9-C6-C7	-3.58	114.94	121.38
2	32-A	201	FOL	C8A-C4A-C4	-3.58	117.24	119.56
3	77-A	202	NAP	N6A-C6A-N1A	-3.58	110.41	118.38
2	29-A	201	FOL	CB-CA-N	-3.57	103.84	110.91
3	3-A	202	NAP	N6A-C6A-N1A	-3.57	110.43	118.38
3	64-A	202	NAP	C4A-N9A-C1B	-3.55	118.33	126.63
2	49-A	201	FOL	C8A-C4A-C4	-3.55	117.26	119.56
3	65-A	202	NAP	C6N-N1N-C2N	-3.54	118.86	121.88
3	68-A	202	NAP	N6A-C6A-N1A	-3.54	110.50	118.38
3	52-A	202	NAP	C4A-N9A-C1B	-3.53	118.38	126.63
2	41-A	201	FOL	CG-CB-CA	-3.53	106.65	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	35-A	202	NAP	N9A-C8A-N7A	-3.52	108.94	113.94
2	79-A	201	FOL	N1-C8A-N8	3.52	121.63	116.38
3	2-A	202	NAP	C4A-N9A-C1B	-3.51	118.42	126.63
2	70-A	201	FOL	CG-CB-CA	3.51	119.64	113.16
3	71-A	202	NAP	C4A-N9A-C1B	-3.51	118.43	126.63
2	74-A	201	FOL	CB-CA-N	-3.50	103.98	110.91
2	50-A	201	FOL	N1-C8A-N8	3.49	121.60	116.38
3	1-A	202	NAP	C4A-N9A-C1B	-3.49	118.46	126.63
2	29-A	201	FOL	N1-C8A-N8	3.49	121.59	116.38
3	8-A	202	NAP	N6A-C6A-N1A	-3.49	110.60	118.38
2	80-A	201	FOL	N1-C8A-N8	3.49	121.58	116.38
3	24-A	202	NAP	N9A-C8A-N7A	-3.48	108.99	113.94
3	42-A	202	NAP	C4D-O4D-C1D	-3.48	106.73	109.92
2	58-A	201	FOL	CG-CB-CA	3.48	119.58	113.16
2	63-A	201	FOL	N1-C8A-N8	3.48	121.58	116.38
3	27-A	202	NAP	N6A-C6A-N1A	-3.47	110.64	118.38
3	46-A	202	NAP	C4D-O4D-C1D	-3.47	106.75	109.92
3	32-A	202	NAP	N9A-C8A-N7A	-3.47	109.01	113.94
3	19-A	202	NAP	C4A-N9A-C1B	-3.47	118.53	126.63
3	18-A	202	NAP	C4A-N9A-C1B	-3.47	118.53	126.63
2	39-A	201	FOL	C8A-C4A-C4	-3.46	117.31	119.56
3	54-A	202	NAP	C4D-O4D-C1D	-3.45	106.77	109.92
2	70-A	201	FOL	C9-C6-N5	3.44	123.06	116.56
3	47-A	202	NAP	C4D-O4D-C1D	-3.43	106.78	109.92
3	45-A	202	NAP	N9A-C8A-N7A	-3.43	109.08	113.94
3	51-A	202	NAP	N9A-C8A-N7A	-3.41	109.10	113.94
3	4-A	202	NAP	C4A-N9A-C1B	-3.40	118.68	126.63
2	72-A	201	FOL	C7-C6-N5	-3.40	118.66	120.87
2	17-A	201	FOL	C11-C-N	3.39	123.33	117.04
3	2-A	202	NAP	C4D-O4D-C1D	-3.39	106.82	109.92
2	75-A	201	FOL	CG-CB-CA	-3.39	106.91	113.16
3	37-A	202	NAP	N9A-C8A-N7A	-3.38	109.13	113.94
3	24-A	202	NAP	C4D-O4D-C1D	-3.38	106.83	109.92
2	52-A	201	FOL	C11-C-N	3.38	123.31	117.04
3	74-A	202	NAP	C4D-O4D-C1D	-3.38	106.83	109.92
3	60-A	202	NAP	C4A-N9A-C1B	-3.38	118.73	126.63
3	54-A	202	NAP	N9A-C8A-N7A	-3.37	109.16	113.94
2	49-A	201	FOL	CB-CG-CD	-3.37	103.52	112.49
3	48-A	202	NAP	C4A-N9A-C1B	-3.35	118.79	126.63
3	59-A	202	NAP	C4D-O4D-C1D	-3.35	106.86	109.92
2	71-A	201	FOL	C9-N10-C14	3.35	132.60	121.87
3	72-A	202	NAP	N9A-C8A-N7A	-3.34	109.19	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	58-A	201	FOL	C8A-C4A-C4	-3.34	117.39	119.56
3	27-A	202	NAP	N9A-C8A-N7A	-3.34	109.20	113.94
3	75-A	202	NAP	N9A-C8A-N7A	-3.34	109.20	113.94
2	26-A	201	FOL	N1-C8A-N8	3.34	121.36	116.38
3	72-A	202	NAP	C4D-O4D-C1D	-3.31	106.90	109.92
3	54-A	202	NAP	C2A-N3A-C4A	3.30	119.90	111.83
3	50-A	202	NAP	C4D-O4D-C1D	-3.30	106.90	109.92
3	10-A	202	NAP	C4A-N9A-C1B	-3.30	118.92	126.63
3	7-A	202	NAP	C4A-N9A-C1B	-3.30	118.92	126.63
3	71-A	202	NAP	C4D-O4D-C1D	-3.30	106.91	109.92
3	9-A	202	NAP	C4A-N9A-C1B	-3.29	118.93	126.63
3	23-A	202	NAP	C4D-O4D-C1D	-3.29	106.91	109.92
3	5-A	202	NAP	C4A-N9A-C1B	-3.28	118.95	126.63
3	66-A	202	NAP	C4A-N9A-C1B	-3.28	118.96	126.63
3	44-A	202	NAP	C4A-N9A-C1B	-3.27	118.98	126.63
3	16-A	202	NAP	C4A-N9A-C1B	-3.27	118.99	126.63
2	61-A	201	FOL	C11-C-N	3.26	123.09	117.04
3	16-A	202	NAP	C4D-O4D-C1D	-3.26	106.94	109.92
3	70-A	202	NAP	C4A-N9A-C1B	-3.25	119.03	126.63
3	56-A	202	NAP	C4A-N9A-C1B	-3.25	119.04	126.63
3	31-A	202	NAP	C4D-O4D-C1D	-3.24	106.96	109.92
3	74-A	202	NAP	C1B-N9A-C8A	3.24	134.28	127.09
3	49-A	202	NAP	C4A-N9A-C1B	-3.24	119.06	126.63
3	38-A	202	NAP	N9A-C8A-N7A	-3.23	109.35	113.94
3	75-A	202	NAP	C5A-C6A-N6A	3.23	131.28	123.29
3	37-A	202	NAP	C5A-C6A-N6A	3.22	131.27	123.29
3	28-A	202	NAP	C5A-C6A-N6A	3.22	131.25	123.29
3	7-A	202	NAP	C5A-C6A-N6A	3.21	131.24	123.29
3	3-A	202	NAP	C4A-N9A-C1B	-3.21	119.12	126.63
3	74-A	202	NAP	C4A-N9A-C8A	3.20	109.10	105.74
2	38-A	201	FOL	N1-C8A-N8	3.20	121.16	116.38
2	38-A	201	FOL	C11-C-N	3.20	122.97	117.04
3	23-A	202	NAP	C2A-N3A-C4A	3.20	119.64	111.83
3	34-A	202	NAP	C2A-N3A-C4A	3.19	119.63	111.83
3	47-A	202	NAP	C4A-N9A-C1B	-3.19	119.17	126.63
3	6-A	202	NAP	C4A-N9A-C1B	-3.19	119.17	126.63
3	6-A	202	NAP	C4D-O4D-C1D	-3.19	107.00	109.92
3	30-A	202	NAP	C4D-O4D-C1D	-3.19	107.00	109.92
2	25-A	201	FOL	C11-C-N	3.19	122.95	117.04
3	22-A	202	NAP	C2A-N3A-C4A	3.18	119.61	111.83
3	15-A	202	NAP	C4A-N9A-C1B	-3.18	119.19	126.63
3	58-A	202	NAP	C4D-O4D-C1D	-3.18	107.01	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	73-A	201	FOL	C13-C14-N10	3.18	128.14	120.96
3	55-A	202	NAP	C4D-O4D-C1D	-3.18	107.02	109.92
3	25-A	202	NAP	C4A-N9A-C1B	-3.17	119.21	126.63
3	33-A	202	NAP	C4D-O4D-C1D	-3.17	107.02	109.92
3	36-A	202	NAP	C4D-O4D-C1D	-3.17	107.02	109.92
3	35-A	202	NAP	C2A-N3A-C4A	3.17	119.57	111.83
3	40-A	202	NAP	C2A-N3A-C4A	3.17	119.57	111.83
3	79-A	202	NAP	C4A-N9A-C1B	-3.17	119.23	126.63
3	79-A	202	NAP	C4D-O4D-C1D	-3.17	107.03	109.92
3	74-A	202	NAP	C5A-N7A-C8A	3.16	108.41	103.45
3	77-A	202	NAP	C4D-O4D-C1D	-3.16	107.03	109.92
3	40-A	202	NAP	C6N-N1N-C2N	-3.15	119.19	121.88
3	80-A	202	NAP	C4D-O4D-C1D	-3.15	107.04	109.92
2	67-A	201	FOL	C9-C6-C7	3.15	127.04	121.38
3	23-A	202	NAP	C5A-C6A-N6A	3.15	131.09	123.29
2	24-A	201	FOL	C8A-C4A-C4	-3.15	117.52	119.56
3	54-A	202	NAP	O4B-C4B-C3B	-3.15	98.90	105.15
3	57-A	202	NAP	C4A-N9A-C1B	-3.15	119.27	126.63
2	60-A	201	FOL	CB-CA-CT	3.15	117.83	110.35
3	60-A	202	NAP	C4D-O4D-C1D	-3.15	107.04	109.92
3	42-A	202	NAP	C2A-N3A-C4A	3.15	119.52	111.83
3	60-A	202	NAP	C5A-C6A-N6A	3.14	131.07	123.29
3	54-A	202	NAP	N3A-C4A-N9A	3.14	132.51	127.17
2	65-A	201	FOL	C11-C-N	3.14	122.86	117.04
3	38-A	202	NAP	C5A-C6A-N6A	3.14	131.06	123.29
3	47-A	202	NAP	C2A-N3A-C4A	3.14	119.49	111.83
3	72-A	202	NAP	C5A-C6A-N6A	3.13	131.04	123.29
2	10-A	201	FOL	C11-C-N	3.13	122.84	117.04
3	34-A	202	NAP	C4D-O4D-C1D	-3.12	107.06	109.92
3	27-A	202	NAP	C4D-O4D-C1D	-3.12	107.06	109.92
3	55-A	202	NAP	C2A-N3A-C4A	3.12	119.45	111.83
3	34-A	202	NAP	C5A-C6A-N6A	3.12	131.01	123.29
3	26-A	202	NAP	N3A-C4A-N9A	3.12	132.47	127.17
3	42-A	202	NAP	C4A-N9A-C1B	-3.11	119.35	126.63
3	45-A	202	NAP	C2A-N3A-C4A	3.11	119.43	111.83
3	40-A	202	NAP	C5A-C6A-N6A	3.11	130.99	123.29
2	66-A	201	FOL	N1-C8A-N8	3.11	121.02	116.38
3	41-A	202	NAP	C4A-N9A-C1B	-3.11	119.36	126.63
3	12-A	202	NAP	C5A-C6A-N6A	3.11	130.98	123.29
3	60-A	202	NAP	C2A-N3A-C4A	3.11	119.42	111.83
3	80-A	202	NAP	C1B-N9A-C8A	3.10	133.98	127.09
3	80-A	202	NAP	C5A-C6A-N6A	3.10	130.96	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	13-A	202	NAP	C4A-N9A-C1B	-3.10	119.39	126.63
3	69-A	202	NAP	C4A-N9A-C1B	-3.10	119.39	126.63
3	48-A	202	NAP	C6N-N1N-C2N	-3.10	119.24	121.88
2	25-A	201	FOL	CB-CA-CT	-3.10	103.00	110.35
3	66-A	202	NAP	C5A-C6A-N6A	3.10	130.95	123.29
3	78-A	202	NAP	C5A-C6A-N6A	3.09	130.94	123.29
2	71-A	201	FOL	CB-CA-CT	3.09	117.69	110.35
3	16-A	202	NAP	C5A-C6A-N6A	3.09	130.94	123.29
3	45-A	202	NAP	C5A-C6A-N6A	3.09	130.94	123.29
3	51-A	202	NAP	C2A-N3A-C4A	3.09	119.37	111.83
3	26-A	202	NAP	C4D-O4D-C1D	-3.09	107.10	109.92
3	13-A	202	NAP	C5A-C6A-N6A	3.08	130.92	123.29
3	39-A	202	NAP	C2A-N3A-C4A	3.08	119.35	111.83
2	58-A	201	FOL	C11-C-N	3.08	122.74	117.04
3	74-A	202	NAP	C2A-N3A-C4A	3.08	119.34	111.83
3	31-A	202	NAP	N3A-C4A-N9A	3.08	132.40	127.17
3	3-A	202	NAP	C4D-O4D-C1D	-3.07	107.11	109.92
3	63-A	202	NAP	C5A-C6A-N6A	3.07	130.90	123.29
3	38-A	202	NAP	C4D-O4D-C1D	-3.07	107.11	109.92
3	78-A	202	NAP	C2A-N3A-C4A	3.07	119.33	111.83
3	43-A	202	NAP	C4A-N9A-C1B	-3.07	119.45	126.63
3	33-A	202	NAP	C2A-N3A-C4A	3.07	119.33	111.83
3	46-A	202	NAP	C2A-N3A-C4A	3.07	119.33	111.83
3	67-A	202	NAP	C4A-N9A-C1B	-3.07	119.46	126.63
2	76-A	201	FOL	C11-C-N	3.07	122.72	117.04
2	4-A	201	FOL	C11-C-N	3.06	122.72	117.04
2	64-A	201	FOL	C6-C9-N10	-3.06	106.41	113.13
3	4-A	202	NAP	C2A-N3A-C4A	3.06	119.30	111.83
3	32-A	202	NAP	C2A-N3A-C4A	3.06	119.30	111.83
3	21-A	202	NAP	C2A-N3A-C4A	3.06	119.30	111.83
3	17-A	202	NAP	C4A-N9A-C1B	-3.06	119.48	126.63
3	1-A	202	NAP	C2A-N3A-C4A	3.06	119.30	111.83
3	22-A	202	NAP	C4A-N9A-C1B	-3.05	119.49	126.63
3	68-A	202	NAP	C4A-N9A-C1B	-3.05	119.50	126.63
3	30-A	202	NAP	C2A-N3A-C4A	3.05	119.28	111.83
3	75-A	202	NAP	C2A-N3A-C4A	3.05	119.28	111.83
3	42-A	202	NAP	C5A-C6A-N6A	3.05	130.83	123.29
3	63-A	202	NAP	C2A-N3A-C4A	3.04	119.27	111.83
3	31-A	202	NAP	C2A-N3A-C4A	3.04	119.27	111.83
3	50-A	202	NAP	C2A-N3A-C4A	3.04	119.27	111.83
3	40-A	202	NAP	N3A-C4A-N9A	3.04	132.34	127.17
3	11-A	202	NAP	C2A-N3A-C4A	3.04	119.26	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	46-A	202	NAP	N3A-C4A-N9A	3.04	132.34	127.17
3	26-A	202	NAP	C2A-N3A-C4A	3.04	119.25	111.83
3	23-A	202	NAP	C4A-N9A-C1B	-3.04	119.53	126.63
3	25-A	202	NAP	C2A-N3A-C4A	3.03	119.24	111.83
3	53-A	202	NAP	C4A-N9A-C1B	-3.03	119.54	126.63
3	69-A	202	NAP	C2A-N3A-C4A	3.03	119.24	111.83
3	32-A	202	NAP	C4D-O4D-C1D	-3.03	107.15	109.92
3	42-A	202	NAP	C5A-N7A-C8A	3.03	108.22	103.45
3	32-A	202	NAP	N3A-C4A-N9A	3.03	132.32	127.17
3	57-A	202	NAP	C5A-C6A-N6A	3.03	130.79	123.29
3	39-A	202	NAP	N3A-C4A-N9A	3.03	132.32	127.17
3	10-A	202	NAP	C5A-C6A-N6A	3.03	130.79	123.29
3	49-A	202	NAP	C2A-N3A-C4A	3.02	119.22	111.83
3	17-A	202	NAP	C4D-O4D-C1D	-3.02	107.16	109.92
3	14-A	202	NAP	C2A-N3A-C4A	3.02	119.21	111.83
3	71-A	202	NAP	C2A-N3A-C4A	3.02	119.21	111.83
3	11-A	202	NAP	C5A-C6A-N6A	3.02	130.77	123.29
3	34-A	202	NAP	C4A-N9A-C1B	-3.02	119.57	126.63
3	39-A	202	NAP	C5A-C6A-N6A	3.02	130.76	123.29
3	61-A	202	NAP	C2A-N3A-C4A	3.02	119.20	111.83
3	60-A	202	NAP	C5A-N7A-C8A	3.02	108.19	103.45
3	24-A	202	NAP	C2A-N3A-C4A	3.02	119.20	111.83
3	29-A	202	NAP	C2A-N3A-C4A	3.02	119.20	111.83
3	77-A	202	NAP	C4A-N9A-C1B	-3.01	119.58	126.63
3	5-A	202	NAP	C5A-N7A-C8A	3.01	108.19	103.45
3	33-A	202	NAP	N3A-C4A-N9A	3.01	132.29	127.17
3	9-A	202	NAP	C5A-C6A-N6A	3.01	130.75	123.29
3	43-A	202	NAP	C2A-N3A-C4A	3.01	119.19	111.83
3	53-A	202	NAP	C4D-O4D-C1D	-3.01	107.17	109.92
3	76-A	202	NAP	N3A-C4A-N9A	3.01	132.28	127.17
2	37-A	201	FOL	C11-C-N	3.01	122.61	117.04
3	12-A	202	NAP	C4A-N9A-C1B	-3.01	119.60	126.63
3	73-A	202	NAP	C2A-N3A-C4A	3.00	119.17	111.83
2	71-A	201	FOL	C7-C6-N5	-3.00	118.92	120.87
3	15-A	202	NAP	C2A-N3A-C4A	3.00	119.16	111.83
2	72-A	201	FOL	C16-C15-C14	3.00	123.75	120.30
3	27-A	202	NAP	N3A-C4A-N9A	3.00	132.26	127.17
3	53-A	202	NAP	C2A-N3A-C4A	3.00	119.15	111.83
3	36-A	202	NAP	C5A-C6A-N6A	3.00	130.70	123.29
3	19-A	202	NAP	C4D-O4D-C1D	-3.00	107.18	109.92
3	62-A	202	NAP	C2A-N3A-C4A	2.99	119.14	111.83
3	62-A	202	NAP	C5A-C6A-N6A	2.99	130.69	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	17-A	202	NAP	C2A-N3A-C4A	2.99	119.14	111.83
3	28-A	202	NAP	C2A-N3A-C4A	2.99	119.14	111.83
3	70-A	202	NAP	C2A-N3A-C4A	2.99	119.14	111.83
3	72-A	202	NAP	C2A-N3A-C4A	2.99	119.13	111.83
3	79-A	202	NAP	C2A-N3A-C4A	2.99	119.13	111.83
3	9-A	202	NAP	C2A-N3A-C4A	2.99	119.12	111.83
3	69-A	202	NAP	C5A-C6A-N6A	2.98	130.67	123.29
2	47-A	201	FOL	CB-CG-CD	-2.98	104.54	112.49
3	48-A	202	NAP	C2A-N3A-C4A	2.98	119.11	111.83
3	44-A	202	NAP	C2A-N3A-C4A	2.98	119.11	111.83
3	25-A	202	NAP	N3A-C4A-N9A	2.98	132.23	127.17
2	80-A	201	FOL	C11-C-N	2.98	122.56	117.04
3	10-A	202	NAP	C2A-N3A-C4A	2.97	119.10	111.83
3	53-A	202	NAP	C5A-C6A-N6A	2.97	130.65	123.29
2	33-A	201	FOL	CB-CA-N	-2.97	105.03	110.91
3	13-A	202	NAP	C2A-N3A-C4A	2.97	119.09	111.83
3	12-A	202	NAP	C2A-N3A-C4A	2.97	119.08	111.83
3	20-A	202	NAP	C2A-N3A-C4A	2.97	119.08	111.83
3	34-A	202	NAP	C5A-N7A-C8A	2.97	108.12	103.45
3	28-A	202	NAP	C5A-N7A-C8A	2.97	108.11	103.45
3	17-A	202	NAP	C5A-C6A-N6A	2.96	130.63	123.29
3	3-A	202	NAP	C2A-N3A-C4A	2.96	119.07	111.83
3	54-A	202	NAP	C5A-C6A-N6A	2.96	130.62	123.29
3	40-A	202	NAP	C4A-N9A-C1B	-2.96	119.71	126.63
3	2-A	202	NAP	C2A-N3A-C4A	2.96	119.06	111.83
3	6-A	202	NAP	C2A-N3A-C4A	2.96	119.06	111.83
3	5-A	202	NAP	C5A-C6A-N6A	2.96	130.61	123.29
3	64-A	202	NAP	C2A-N3A-C4A	2.96	119.05	111.83
3	55-A	202	NAP	C5A-C6A-N6A	2.96	130.61	123.29
3	2-A	202	NAP	C5A-N7A-C8A	2.96	108.10	103.45
3	30-A	202	NAP	C5A-C6A-N6A	2.96	130.60	123.29
3	76-A	202	NAP	C5A-C6A-N6A	2.95	130.60	123.29
3	59-A	202	NAP	C2A-N3A-C4A	2.95	119.04	111.83
3	15-A	202	NAP	C5A-C6A-N6A	2.95	130.59	123.29
3	44-A	202	NAP	C5A-C6A-N6A	2.95	130.59	123.29
3	8-A	202	NAP	C2A-N3A-C4A	2.95	119.04	111.83
3	8-A	202	NAP	C1B-N9A-C8A	2.95	133.64	127.09
3	45-A	202	NAP	N3A-C4A-N9A	2.95	132.18	127.17
3	65-A	202	NAP	C5A-N7A-C8A	2.95	108.09	103.45
3	26-A	202	NAP	C4A-N9A-C1B	-2.95	119.73	126.63
3	80-A	202	NAP	C2A-N3A-C4A	2.95	119.03	111.83
3	70-A	202	NAP	C5A-C6A-N6A	2.95	130.58	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	47-A	202	NAP	C5A-N7A-C8A	2.95	108.08	103.45
3	41-A	202	NAP	C2A-N3A-C4A	2.94	119.02	111.83
3	35-A	202	NAP	C4A-N9A-C1B	-2.94	119.75	126.63
3	65-A	202	NAP	C2A-N3A-C4A	2.94	119.02	111.83
3	1-A	202	NAP	C4D-O4D-C1D	-2.94	107.23	109.92
3	5-A	202	NAP	C2A-N3A-C4A	2.94	119.02	111.83
3	18-A	202	NAP	C2A-N3A-C4A	2.94	119.01	111.83
3	74-A	202	NAP	C5A-C6A-N6A	2.94	130.56	123.29
2	14-A	201	FOL	CB-CG-CD	-2.94	104.65	112.49
3	52-A	202	NAP	C2A-N3A-C4A	2.94	119.01	111.83
3	49-A	202	NAP	C5A-C6A-N6A	2.94	130.56	123.29
2	62-A	201	FOL	O1-CT-CA	-2.94	112.79	122.26
3	50-A	202	NAP	C4A-N9A-C1B	-2.94	119.77	126.63
3	24-A	202	NAP	N3A-C4A-N9A	2.94	132.16	127.17
3	59-A	202	NAP	C5A-C6A-N6A	2.93	130.54	123.29
3	36-A	202	NAP	C2A-N3A-C4A	2.93	118.99	111.83
3	66-A	202	NAP	C2A-N3A-C4A	2.93	118.99	111.83
3	65-A	202	NAP	N3A-C4A-N9A	2.93	132.15	127.17
2	66-A	201	FOL	C4-C4A-N5	2.93	123.17	118.55
3	35-A	202	NAP	C5A-C6A-N6A	2.93	130.54	123.29
3	71-A	202	NAP	C5A-C6A-N6A	2.93	130.53	123.29
3	15-A	202	NAP	C4D-O4D-C1D	-2.93	107.25	109.92
3	25-A	202	NAP	C5A-N7A-C8A	2.93	108.05	103.45
3	67-A	202	NAP	C4D-O4D-C1D	-2.92	107.25	109.92
3	20-A	202	NAP	C4A-N9A-C1B	-2.92	119.80	126.63
3	33-A	202	NAP	C4A-N9A-C1B	-2.92	119.80	126.63
3	57-A	202	NAP	C2A-N3A-C4A	2.92	118.96	111.83
3	40-A	202	NAP	C5A-N7A-C8A	2.92	108.04	103.45
3	13-A	202	NAP	C4D-O4D-C1D	-2.92	107.25	109.92
3	29-A	202	NAP	N3A-C4A-N9A	2.92	132.13	127.17
3	27-A	202	NAP	C2A-N3A-C4A	2.92	118.95	111.83
3	63-A	202	NAP	C5A-N7A-C8A	2.91	108.03	103.45
3	21-A	202	NAP	C5A-C6A-N6A	2.91	130.49	123.29
3	50-A	202	NAP	C5A-C6A-N6A	2.91	130.49	123.29
3	29-A	202	NAP	C5A-C6A-N6A	2.91	130.49	123.29
3	22-A	202	NAP	C5A-C6A-N6A	2.91	130.48	123.29
3	19-A	202	NAP	C2A-N3A-C4A	2.90	118.92	111.83
3	5-A	202	NAP	C4D-O4D-C1D	-2.90	107.27	109.92
3	34-A	202	NAP	N3A-C4A-N9A	2.90	132.10	127.17
3	57-A	202	NAP	C4D-O4D-C1D	-2.90	107.27	109.92
3	65-A	202	NAP	C5A-C6A-N6A	2.90	130.46	123.29
3	18-A	202	NAP	C5A-C6A-N6A	2.90	130.46	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	22-A	202	NAP	C4D-O4D-C1D	-2.90	107.27	109.92
2	70-A	201	FOL	N1-C8A-N8	2.90	120.70	116.38
2	72-A	201	FOL	C11-C-N	2.89	122.40	117.04
3	76-A	202	NAP	C2A-N3A-C4A	2.89	118.89	111.83
2	72-A	201	FOL	C13-C14-N10	2.89	127.50	120.96
3	55-A	202	NAP	C4A-N9A-C1B	-2.89	119.87	126.63
3	34-A	202	NAP	C6N-N1N-C2N	-2.89	119.42	121.88
3	61-A	202	NAP	C4A-N9A-C1B	-2.89	119.88	126.63
3	37-A	202	NAP	C2A-N3A-C4A	2.88	118.87	111.83
3	38-A	202	NAP	C2A-N3A-C4A	2.88	118.87	111.83
3	12-A	202	NAP	C4D-O4D-C1D	-2.88	107.29	109.92
3	58-A	202	NAP	C2A-N3A-C4A	2.88	118.87	111.83
3	22-A	202	NAP	N3A-C4A-N9A	2.88	132.07	127.17
3	46-A	202	NAP	C5A-N7A-C8A	2.88	107.98	103.45
3	47-A	202	NAP	C5A-C6A-N6A	2.88	130.41	123.29
2	75-A	201	FOL	CT-CA-N	2.88	117.25	110.57
3	78-A	202	NAP	N3A-C4A-N9A	2.88	132.06	127.17
3	62-A	202	NAP	C5A-N7A-C8A	2.88	107.97	103.45
3	51-A	202	NAP	C4A-N9A-C1B	-2.88	119.91	126.63
3	52-A	202	NAP	C4D-O4D-C1D	-2.88	107.29	109.92
3	77-A	202	NAP	C2A-N3A-C4A	2.88	118.85	111.83
3	30-A	202	NAP	N3A-C4A-N9A	2.87	132.06	127.17
2	76-A	201	FOL	CB-CA-CT	-2.87	103.54	110.35
3	44-A	202	NAP	C5A-N7A-C8A	2.87	107.96	103.45
3	73-A	202	NAP	C5A-C6A-N6A	2.87	130.40	123.29
3	46-A	202	NAP	C5A-C6A-N6A	2.87	130.39	123.29
3	80-A	202	NAP	O2D-C2D-C3D	-2.87	102.63	111.82
3	67-A	202	NAP	C2A-N3A-C4A	2.87	118.83	111.83
3	19-A	202	NAP	C5A-C6A-N6A	2.87	130.38	123.29
3	2-A	202	NAP	C5A-C6A-N6A	2.87	130.38	123.29
3	1-A	202	NAP	C5A-C6A-N6A	2.87	130.38	123.29
3	68-A	202	NAP	C2A-N3A-C4A	2.86	118.82	111.83
3	7-A	202	NAP	C2A-N3A-C4A	2.86	118.81	111.83
3	35-A	202	NAP	N3A-C4A-N9A	2.86	132.03	127.17
3	43-A	202	NAP	N3A-C4A-N9A	2.86	132.03	127.17
3	58-A	202	NAP	N3A-C4A-N9A	2.86	132.03	127.17
3	42-A	202	NAP	N3A-C4A-N9A	2.86	132.03	127.17
3	52-A	202	NAP	C1B-N9A-C8A	2.86	133.43	127.09
3	29-A	202	NAP	C5A-N7A-C8A	2.85	107.94	103.45
3	16-A	202	NAP	C2A-N3A-C4A	2.85	118.80	111.83
3	11-A	202	NAP	C4A-N9A-C1B	-2.85	119.96	126.63
3	48-A	202	NAP	C5A-C6A-N6A	2.84	130.33	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	10-A	202	NAP	C5A-N7A-C8A	2.84	107.92	103.45
3	56-A	202	NAP	C2A-N3A-C4A	2.84	118.77	111.83
3	62-A	202	NAP	N3A-C4A-N9A	2.84	132.00	127.17
3	14-A	202	NAP	N3A-C4A-N9A	2.84	131.99	127.17
3	21-A	202	NAP	C4A-N9A-C1B	-2.83	120.01	126.63
3	4-A	202	NAP	C4D-O4D-C1D	-2.83	107.33	109.92
3	36-A	202	NAP	C4A-N9A-C1B	-2.83	120.01	126.63
3	23-A	202	NAP	N3A-C4A-N9A	2.83	131.98	127.17
3	68-A	202	NAP	N3A-C4A-N9A	2.83	131.98	127.17
3	15-A	202	NAP	N3A-C4A-N9A	2.83	131.97	127.17
3	12-A	202	NAP	C5A-N7A-C8A	2.83	107.89	103.45
3	20-A	202	NAP	C5A-C6A-N6A	2.82	130.28	123.29
3	21-A	202	NAP	N3A-C4A-N9A	2.82	131.96	127.17
3	73-A	202	NAP	C4A-N9A-C1B	-2.82	120.04	126.63
3	59-A	202	NAP	C4A-N9A-C1B	-2.82	120.04	126.63
2	69-A	201	FOL	C4-C4A-N5	2.82	122.99	118.55
3	45-A	202	NAP	C5A-N7A-C8A	2.82	107.88	103.45
2	7-A	201	FOL	CG-CB-CA	-2.82	107.96	113.16
3	3-A	202	NAP	N3A-C4A-N9A	2.82	131.96	127.17
2	54-A	201	FOL	C11-C-N	2.82	122.26	117.04
3	61-A	202	NAP	C5A-C6A-N6A	2.81	130.25	123.29
3	25-A	202	NAP	C5A-C6A-N6A	2.81	130.25	123.29
3	23-A	202	NAP	C5A-N7A-C8A	2.81	107.87	103.45
3	9-A	202	NAP	C5A-N7A-C8A	2.81	107.86	103.45
3	66-A	202	NAP	C6N-N1N-C2N	-2.81	119.49	121.88
3	47-A	202	NAP	N3A-C4A-N9A	2.81	131.94	127.17
3	14-A	202	NAP	C4A-N9A-C1B	-2.80	120.07	126.63
3	43-A	202	NAP	C6N-N1N-C2N	-2.80	119.49	121.88
3	63-A	202	NAP	N3A-C4A-N9A	2.80	131.94	127.17
3	17-A	202	NAP	N3A-C4A-N9A	2.80	131.94	127.17
3	67-A	202	NAP	C5A-C6A-N6A	2.80	130.23	123.29
2	24-A	201	FOL	C11-C-N	2.80	122.23	117.04
3	29-A	202	NAP	C4A-N9A-C1B	-2.80	120.08	126.63
2	64-A	201	FOL	CB-CA-N	2.80	116.45	110.91
3	42-A	202	NAP	C6N-N1N-C2N	-2.80	119.50	121.88
3	1-A	202	NAP	C5A-N7A-C8A	2.80	107.85	103.45
3	58-A	202	NAP	C4A-N9A-C1B	-2.80	120.09	126.63
3	80-A	202	NAP	C5A-N7A-C8A	2.80	107.84	103.45
3	58-A	202	NAP	C5A-C6A-N6A	2.80	130.21	123.29
3	37-A	202	NAP	C4A-N9A-C1B	-2.79	120.10	126.63
3	18-A	202	NAP	N3A-C4A-N9A	2.79	131.92	127.17
3	78-A	202	NAP	C5A-N7A-C8A	2.79	107.84	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6-A	202	NAP	N3A-C4A-N9A	2.79	131.92	127.17
3	4-A	202	NAP	C5A-C6A-N6A	2.79	130.20	123.29
3	36-A	202	NAP	C5A-N7A-C8A	2.79	107.84	103.45
2	55-A	201	FOL	C11-C-N	2.79	122.22	117.04
2	65-A	201	FOL	C15-C16-C11	2.79	123.78	120.80
3	55-A	202	NAP	C5A-N7A-C8A	2.79	107.84	103.45
3	41-A	202	NAP	N3A-C4A-N9A	2.79	131.91	127.17
3	31-A	202	NAP	C4A-N9A-C1B	-2.79	120.11	126.63
3	64-A	202	NAP	C1B-N9A-C8A	2.79	133.28	127.09
3	18-A	202	NAP	C4D-O4D-C1D	-2.79	107.37	109.92
3	61-A	202	NAP	N3A-C4A-N9A	2.79	131.91	127.17
3	36-A	202	NAP	N3A-C4A-N9A	2.78	131.90	127.17
3	10-A	202	NAP	C6N-N1N-C2N	-2.78	119.51	121.88
2	71-A	201	FOL	C9-C6-C7	2.78	126.38	121.38
3	1-A	202	NAP	C1B-N9A-C8A	2.78	133.26	127.09
3	58-A	202	NAP	C5A-N7A-C8A	2.78	107.81	103.45
3	2-A	202	NAP	C1B-N9A-C8A	2.77	133.25	127.09
3	57-A	202	NAP	C5A-N7A-C8A	2.77	107.81	103.45
3	38-A	202	NAP	C6N-N1N-C2N	-2.77	119.52	121.88
3	67-A	202	NAP	C6N-N1N-C2N	-2.77	119.52	121.88
3	78-A	202	NAP	C4A-N9A-C1B	-2.77	120.15	126.63
3	19-A	202	NAP	C1B-N9A-C8A	2.77	133.23	127.09
2	63-A	201	FOL	C4-C4A-N5	2.77	122.91	118.55
3	62-A	202	NAP	C4A-N9A-C1B	-2.76	120.17	126.63
3	77-A	202	NAP	N3A-C4A-N9A	2.76	131.86	127.17
3	66-A	202	NAP	C5A-N7A-C8A	2.76	107.79	103.45
3	63-A	202	NAP	C4A-N9A-C1B	-2.76	120.18	126.63
3	75-A	202	NAP	N3A-C4A-N9A	2.76	131.86	127.17
2	20-A	201	FOL	C11-C-N	2.75	122.15	117.04
3	28-A	202	NAP	C1B-N9A-C8A	2.75	133.21	127.09
2	70-A	201	FOL	C4-C4A-N5	2.75	122.89	118.55
3	40-A	202	NAP	C4D-O4D-C1D	-2.75	107.40	109.92
3	7-A	202	NAP	C1B-N9A-C8A	2.75	133.20	127.09
3	32-A	202	NAP	C5A-C6A-N6A	2.75	130.09	123.29
3	56-A	202	NAP	C1B-N9A-C8A	2.75	133.19	127.09
3	64-A	202	NAP	C6N-N1N-C2N	-2.74	119.54	121.88
3	22-A	202	NAP	C5A-N7A-C8A	2.74	107.76	103.45
3	50-A	202	NAP	N3A-C4A-N9A	2.74	131.83	127.17
3	12-A	202	NAP	N3A-C4A-N9A	2.74	131.83	127.17
3	79-A	202	NAP	C5A-C6A-N6A	2.74	130.07	123.29
3	39-A	202	NAP	C6N-N1N-C2N	-2.73	119.55	121.88
3	44-A	202	NAP	C6N-N1N-C2N	-2.73	119.55	121.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	56-A	202	NAP	C4D-O4D-C1D	-2.73	107.42	109.92
3	67-A	202	NAP	N3A-C4A-N9A	2.73	131.81	127.17
3	59-A	202	NAP	N3A-C4A-N9A	2.73	131.81	127.17
2	68-A	201	FOL	C12-C13-C14	2.73	123.44	120.30
2	79-A	201	FOL	CB-CA-N	-2.73	105.51	110.91
3	9-A	202	NAP	N3A-C4A-N9A	2.73	131.80	127.17
3	75-A	202	NAP	C4D-O4D-C1D	-2.73	107.43	109.92
3	4-A	202	NAP	C5A-N7A-C8A	2.73	107.73	103.45
3	4-A	202	NAP	N3A-C4A-N9A	2.72	131.80	127.17
3	41-A	202	NAP	C5A-C6A-N6A	2.72	130.03	123.29
3	21-A	202	NAP	C4D-O4D-C1D	-2.72	107.43	109.92
2	47-A	201	FOL	OE1-CD-CG	-2.72	114.45	123.09
3	60-A	202	NAP	C1B-N9A-C8A	2.72	133.13	127.09
2	40-A	201	FOL	O-C-N	-2.72	117.30	122.47
3	62-A	202	NAP	O2A-PA-O3	2.72	114.62	107.27
3	73-A	202	NAP	N3A-C4A-N9A	2.72	131.79	127.17
2	64-A	201	FOL	C8A-C4A-C4	-2.72	117.80	119.56
3	18-A	202	NAP	C4A-N9A-C8A	2.72	108.59	105.74
3	51-A	202	NAP	N3A-C4A-N9A	2.72	131.78	127.17
3	4-A	202	NAP	C1B-N9A-C8A	2.71	133.12	127.09
3	20-A	202	NAP	N3A-C4A-N9A	2.71	131.78	127.17
3	16-A	202	NAP	C1B-N9A-C8A	2.71	133.11	127.09
3	48-A	202	NAP	C1B-N9A-C8A	2.71	133.10	127.09
3	76-A	202	NAP	C4A-N9A-C1B	-2.70	120.31	126.63
3	29-A	202	NAP	C4D-O4D-C1D	-2.70	107.45	109.92
2	61-A	201	FOL	OE1-CD-CG	-2.70	114.53	123.09
3	74-A	202	NAP	N3A-C4A-N9A	2.70	131.76	127.17
3	49-A	202	NAP	C5A-N7A-C8A	2.70	107.69	103.45
3	14-A	202	NAP	C5A-C6A-N6A	2.69	129.96	123.29
3	35-A	202	NAP	C4D-O4D-C1D	-2.69	107.46	109.92
3	43-A	202	NAP	C5A-N7A-C8A	2.69	107.68	103.45
3	30-A	202	NAP	C5A-N7A-C8A	2.69	107.68	103.45
3	60-A	202	NAP	N3A-C4A-N9A	2.69	131.74	127.17
3	7-A	202	NAP	C5A-N7A-C8A	2.69	107.67	103.45
3	49-A	202	NAP	N3A-C4A-N9A	2.69	131.74	127.17
3	52-A	202	NAP	C5A-C6A-N6A	2.69	129.94	123.29
3	9-A	202	NAP	C4D-O4D-C1D	-2.69	107.47	109.92
3	6-A	202	NAP	C5A-C6A-N6A	2.68	129.93	123.29
2	78-A	201	FOL	CB-CA-CT	2.68	116.72	110.35
3	57-A	202	NAP	N3A-C4A-N9A	2.68	131.73	127.17
3	71-A	202	NAP	C1B-N9A-C8A	2.68	133.04	127.09
3	24-A	202	NAP	C5A-C6A-N6A	2.68	129.92	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	56-A	201	FOL	C11-C-N	2.68	122.01	117.04
3	76-A	202	NAP	C5A-N7A-C8A	2.68	107.66	103.45
3	48-A	202	NAP	N3A-C4A-N9A	2.68	131.72	127.17
3	43-A	202	NAP	C5A-C6A-N6A	2.68	129.91	123.29
3	51-A	202	NAP	C5A-C6A-N6A	2.67	129.90	123.29
3	11-A	202	NAP	N3A-C4A-N9A	2.67	131.71	127.17
3	13-A	202	NAP	N3A-C4A-N9A	2.67	131.70	127.17
3	28-A	202	NAP	C4A-N9A-C8A	2.67	108.54	105.74
3	77-A	202	NAP	C5A-C6A-N6A	2.67	129.89	123.29
3	5-A	202	NAP	N3A-C4A-N9A	2.66	131.69	127.17
3	70-A	202	NAP	C5A-N7A-C8A	2.66	107.63	103.45
3	71-A	202	NAP	N3A-C4A-N9A	2.66	131.69	127.17
3	65-A	202	NAP	C4A-N9A-C1B	-2.66	120.42	126.63
2	70-A	201	FOL	C6-C9-N10	2.65	118.96	113.13
3	31-A	202	NAP	C5A-C6A-N6A	2.65	129.86	123.29
3	24-A	202	NAP	C4A-N9A-C1B	-2.65	120.42	126.63
3	10-A	202	NAP	C1B-N9A-C8A	2.65	132.98	127.09
2	15-A	201	FOL	C11-C-N	2.65	121.95	117.04
3	71-A	202	NAP	C5A-N7A-C8A	2.65	107.61	103.45
3	79-A	202	NAP	N3A-C4A-N9A	2.65	131.67	127.17
3	71-A	202	NAP	C4A-N9A-C8A	2.65	108.52	105.74
3	44-A	202	NAP	N3A-C4A-N9A	2.65	131.67	127.17
3	43-A	202	NAP	C4D-O4D-C1D	-2.65	107.50	109.92
2	70-A	201	FOL	CB-CG-CD	2.64	119.55	112.49
3	75-A	202	NAP	C5A-N7A-C8A	2.64	107.61	103.45
3	41-A	202	NAP	C5A-N7A-C8A	2.64	107.60	103.45
3	38-A	202	NAP	N3A-C4A-N9A	2.64	131.66	127.17
3	72-A	202	NAP	N3A-C4A-N9A	2.64	131.66	127.17
3	67-A	202	NAP	C5A-N7A-C8A	2.64	107.60	103.45
3	18-A	202	NAP	C5A-N7A-C8A	2.64	107.60	103.45
3	9-A	202	NAP	C1B-N9A-C8A	2.64	132.95	127.09
2	70-A	201	FOL	C15-C14-N10	-2.64	115.00	120.96
3	59-A	202	NAP	C5A-N7A-C8A	2.64	107.59	103.45
3	28-A	202	NAP	N3A-C4A-N9A	2.64	131.65	127.17
2	73-A	201	FOL	C12-C11-C	2.64	129.14	120.60
3	30-A	202	NAP	C4A-N9A-C1B	-2.63	120.47	126.63
3	10-A	202	NAP	N3A-C4A-N9A	2.63	131.64	127.17
2	32-A	201	FOL	OE2-CD-CG	2.63	122.31	114.00
2	64-A	201	FOL	CA-N-C	2.63	127.88	121.56
2	49-A	201	FOL	OE1-CD-CG	-2.63	114.75	123.09
3	57-A	202	NAP	C1B-N9A-C8A	2.63	132.93	127.09
3	75-A	202	NAP	C4A-N9A-C1B	-2.63	120.48	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	61-A	202	NAP	C4D-O4D-C1D	-2.63	107.52	109.92
3	61-A	202	NAP	C5A-N7A-C8A	2.63	107.58	103.45
3	41-A	202	NAP	C2N-C3N-C4N	2.63	121.31	118.26
2	39-A	201	FOL	O-C-N	-2.63	117.47	122.47
3	11-A	202	NAP	C5A-N7A-C8A	2.62	107.57	103.45
2	80-A	201	FOL	O-C-C11	-2.62	115.70	120.90
3	70-A	202	NAP	C1B-N9A-C8A	2.62	132.91	127.09
2	69-A	201	FOL	C12-C13-C14	2.62	123.32	120.30
3	66-A	202	NAP	C1B-N9A-C8A	2.62	132.91	127.09
3	48-A	202	NAP	C5A-N7A-C8A	2.62	107.57	103.45
3	76-A	202	NAP	C4D-O4D-C1D	-2.62	107.53	109.92
2	32-A	201	FOL	OE1-CD-CG	-2.61	114.80	123.09
3	56-A	202	NAP	C5A-C6A-N6A	2.61	129.76	123.29
3	73-A	202	NAP	C4D-O4D-C1D	-2.61	107.53	109.92
3	68-A	202	NAP	C5A-C6A-N6A	2.61	129.75	123.29
3	18-A	202	NAP	C1B-N9A-C8A	2.61	132.88	127.09
3	8-A	202	NAP	N3A-C4A-N9A	2.61	131.60	127.17
3	26-A	202	NAP	C5A-C6A-N6A	2.61	129.74	123.29
2	30-A	201	FOL	C11-C-N	2.61	121.87	117.04
3	53-A	202	NAP	N3A-C4A-N9A	2.60	131.59	127.17
3	15-A	202	NAP	C5A-N7A-C8A	2.60	107.54	103.45
3	42-A	202	NAP	C1B-N9A-C8A	2.60	132.87	127.09
2	72-A	201	FOL	O-C-C11	-2.60	115.75	120.90
3	69-A	202	NAP	N3A-C4A-N9A	2.60	131.59	127.17
3	6-A	202	NAP	C5A-N7A-C8A	2.60	107.53	103.45
3	49-A	202	NAP	C1B-N9A-C8A	2.59	132.84	127.09
3	33-A	202	NAP	C5A-C6A-N6A	2.59	129.69	123.29
3	54-A	202	NAP	C5A-N7A-C8A	2.59	107.52	103.45
3	70-A	202	NAP	N3A-C4A-N9A	2.58	131.56	127.17
3	55-A	202	NAP	N3A-C4A-N9A	2.58	131.56	127.17
3	27-A	202	NAP	C5A-C6A-N6A	2.58	129.68	123.29
3	69-A	202	NAP	C1B-N9A-C8A	2.58	132.83	127.09
3	53-A	202	NAP	C1B-N9A-C8A	2.58	132.82	127.09
2	3-A	201	FOL	C9-N10-C14	2.58	130.15	121.87
3	1-A	202	NAP	N3A-C4A-N9A	2.58	131.55	127.17
3	21-A	202	NAP	C5A-N7A-C8A	2.58	107.50	103.45
3	73-A	202	NAP	C5A-N7A-C8A	2.58	107.50	103.45
3	66-A	202	NAP	C4D-O4D-C1D	-2.58	107.56	109.92
3	31-A	202	NAP	C5A-N7A-C8A	2.58	107.50	103.45
2	80-A	201	FOL	CT-CA-N	2.58	116.55	110.57
3	39-A	202	NAP	C4A-N9A-C1B	-2.57	120.61	126.63
3	39-A	202	NAP	C5A-N7A-C8A	2.57	107.50	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	64-A	202	NAP	C5A-C6A-N6A	2.57	129.66	123.29
3	37-A	202	NAP	C4D-O4D-C1D	-2.57	107.57	109.92
3	80-A	202	NAP	C4A-N9A-C8A	2.57	108.44	105.74
3	11-A	202	NAP	C4D-O4D-C1D	-2.57	107.57	109.92
3	79-A	202	NAP	C1B-N9A-C8A	2.56	132.79	127.09
3	32-A	202	NAP	C5A-N7A-C8A	2.56	107.48	103.45
3	45-A	202	NAP	C4A-C5A-N7A	-2.56	107.65	110.58
3	25-A	202	NAP	C4D-O4D-C1D	-2.56	107.58	109.92
3	33-A	202	NAP	C6N-N1N-C2N	-2.56	119.70	121.88
3	16-A	202	NAP	C5A-N7A-C8A	2.56	107.47	103.45
2	78-A	201	FOL	OE1-CD-CG	-2.56	114.97	123.09
3	44-A	202	NAP	C1B-N9A-C8A	2.56	132.78	127.09
3	37-A	202	NAP	N3A-C4A-N9A	2.56	131.52	127.17
3	66-A	202	NAP	N3A-C4A-N9A	2.56	131.52	127.17
3	2-A	202	NAP	N3A-C4A-N9A	2.56	131.52	127.17
3	65-A	202	NAP	C4D-O4D-C1D	-2.56	107.58	109.92
3	62-A	202	NAP	C4D-O4D-C1D	-2.56	107.58	109.92
3	68-A	202	NAP	C5A-N7A-C8A	2.55	107.47	103.45
3	64-A	202	NAP	N3A-C4A-N9A	2.55	131.51	127.17
2	59-A	201	FOL	C13-C12-C11	-2.55	118.07	120.80
3	67-A	202	NAP	C4A-N9A-C8A	2.55	108.42	105.74
3	17-A	202	NAP	C5A-N7A-C8A	2.55	107.45	103.45
3	53-A	202	NAP	O2D-C2D-C3D	-2.55	103.66	111.82
3	73-A	202	NAP	C6N-N1N-C2N	-2.54	119.71	121.88
3	3-A	202	NAP	C5A-N7A-C8A	2.54	107.44	103.45
3	72-A	202	NAP	C5A-N7A-C8A	2.54	107.44	103.45
3	3-A	202	NAP	C5A-C6A-N6A	2.54	129.57	123.29
3	6-A	202	NAP	C1B-N9A-C8A	2.54	132.72	127.09
2	63-A	201	FOL	O-C-C11	2.54	125.92	120.90
3	20-A	202	NAP	C5A-N7A-C8A	2.53	107.43	103.45
3	46-A	202	NAP	C4A-N9A-C1B	-2.53	120.71	126.63
3	47-A	202	NAP	C1B-N9A-C8A	2.53	132.71	127.09
3	41-A	202	NAP	C1B-N9A-C8A	2.53	132.70	127.09
3	63-A	202	NAP	C4A-C5A-N7A	-2.52	107.70	110.58
3	3-A	202	NAP	C6N-N1N-C2N	-2.52	119.73	121.88
3	19-A	202	NAP	C5A-N7A-C8A	2.52	107.41	103.45
3	13-A	202	NAP	C5A-N7A-C8A	2.51	107.40	103.45
3	5-A	202	NAP	C1B-N9A-C8A	2.51	132.67	127.09
2	29-A	201	FOL	CG-CB-CA	2.51	117.79	113.16
3	64-A	202	NAP	C4A-N9A-C8A	2.51	108.38	105.74
3	3-A	202	NAP	C1B-N9A-C8A	2.51	132.67	127.09
3	23-A	202	NAP	C1B-N9A-C8A	2.51	132.67	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	69-A	202	NAP	C5A-N7A-C8A	2.51	107.39	103.45
3	37-A	202	NAP	C5A-N7A-C8A	2.51	107.39	103.45
3	53-A	202	NAP	C5A-N7A-C8A	2.51	107.39	103.45
2	46-A	201	FOL	C11-C-N	2.51	121.69	117.04
3	77-A	202	NAP	C5A-N7A-C8A	2.50	107.39	103.45
3	33-A	202	NAP	C5A-N7A-C8A	2.50	107.39	103.45
3	32-A	202	NAP	C4A-N9A-C1B	-2.50	120.78	126.63
3	19-A	202	NAP	N3A-C4A-N9A	2.50	131.42	127.17
3	26-A	202	NAP	C5A-N7A-C8A	2.50	107.38	103.45
3	64-A	202	NAP	C4D-O4D-C1D	-2.50	107.64	109.92
3	13-A	202	NAP	C1B-N9A-C8A	2.49	132.63	127.09
2	67-A	201	FOL	O4-C4-N3	2.49	124.02	120.23
3	15-A	202	NAP	C4A-N9A-C8A	2.49	108.36	105.74
3	12-A	202	NAP	C6N-N1N-C2N	-2.49	119.76	121.88
3	10-A	202	NAP	C4D-O4D-C1D	-2.49	107.64	109.92
3	22-A	202	NAP	C1B-N9A-C8A	2.49	132.62	127.09
3	72-A	202	NAP	C4A-N9A-C1B	-2.49	120.81	126.63
3	45-A	202	NAP	C6N-N1N-C2N	-2.49	119.76	121.88
3	79-A	202	NAP	C5A-N7A-C8A	2.48	107.35	103.45
2	71-A	201	FOL	C13-C14-N10	2.48	126.56	120.96
2	9-A	201	FOL	C11-C-N	2.48	121.63	117.04
3	35-A	202	NAP	C5A-N7A-C8A	2.48	107.34	103.45
2	72-A	201	FOL	C9-C6-C7	2.48	125.83	121.38
3	50-A	202	NAP	C5A-N7A-C8A	2.48	107.34	103.45
3	75-A	202	NAP	C4A-C5A-N7A	-2.47	107.75	110.58
3	74-A	202	NAP	C4A-C5A-N7A	-2.47	107.75	110.58
3	35-A	202	NAP	C1B-N9A-C8A	2.47	132.57	127.09
3	69-A	202	NAP	C4D-O4D-C1D	-2.46	107.67	109.92
3	25-A	202	NAP	C1B-N9A-C8A	2.46	132.56	127.09
3	55-A	202	NAP	O4B-C1B-N9A	-2.46	103.36	108.09
3	5-A	202	NAP	C4A-N9A-C8A	2.46	108.32	105.74
3	11-A	202	NAP	C6N-N1N-C2N	-2.46	119.79	121.88
3	64-A	202	NAP	C5A-N7A-C8A	2.46	107.31	103.45
3	2-A	202	NAP	C4A-N9A-C8A	2.45	108.31	105.74
2	35-A	201	FOL	C11-C-N	2.45	121.59	117.04
3	51-A	202	NAP	C1B-N9A-C8A	2.45	132.54	127.09
3	43-A	202	NAP	O2A-PA-O3	2.45	113.89	107.27
2	76-A	201	FOL	CA-N-C	2.45	127.43	121.56
3	77-A	202	NAP	C1B-N9A-C8A	2.45	132.53	127.09
3	7-A	202	NAP	N3A-C4A-N9A	2.45	131.33	127.17
2	73-A	201	FOL	C15-C14-N10	-2.44	115.44	120.96
3	52-A	202	NAP	N3A-C4A-N9A	2.44	131.32	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	52-A	201	FOL	CB-CG-CD	-2.44	105.99	112.49
3	16-A	202	NAP	N3A-C4A-N9A	2.44	131.31	127.17
3	50-A	202	NAP	C1B-N9A-C8A	2.44	132.50	127.09
2	74-A	201	FOL	O2-CT-O1	-2.44	118.55	124.08
2	39-A	201	FOL	CB-CA-N	2.44	115.73	110.91
3	4-A	202	NAP	C6N-N1N-C2N	-2.44	119.81	121.88
3	75-A	202	NAP	C6N-N1N-C2N	-2.43	119.81	121.88
2	5-A	201	FOL	C9-N10-C14	2.43	129.68	121.87
3	43-A	202	NAP	C4A-N9A-C8A	2.43	108.29	105.74
2	57-A	201	FOL	C11-C-N	2.43	121.54	117.04
3	34-A	202	NAP	C1B-N9A-C8A	2.43	132.49	127.09
3	60-A	202	NAP	C4A-C5A-N7A	-2.43	107.81	110.58
3	22-A	202	NAP	C2N-C3N-C4N	2.42	121.08	118.26
3	42-A	202	NAP	C4A-C5A-N7A	-2.42	107.81	110.58
3	12-A	202	NAP	C1B-N9A-C8A	2.42	132.47	127.09
3	45-A	202	NAP	C6A-C5A-C4A	2.42	120.48	117.18
3	45-A	202	NAP	C4D-O4D-C1D	-2.42	107.71	109.92
3	58-A	202	NAP	O2A-PA-O3	2.42	113.80	107.27
3	15-A	202	NAP	C1B-N9A-C8A	2.42	132.46	127.09
3	53-A	202	NAP	C6N-N1N-C2N	-2.41	119.82	121.88
3	1-A	202	NAP	C4A-N9A-C8A	2.41	108.27	105.74
3	14-A	202	NAP	C5A-N7A-C8A	2.41	107.24	103.45
3	38-A	202	NAP	C4A-N9A-C1B	-2.41	120.99	126.63
2	29-A	201	FOL	C9-N10-C14	2.41	129.61	121.87
3	11-A	202	NAP	C1B-N9A-C8A	2.41	132.44	127.09
3	21-A	202	NAP	C1B-N9A-C8A	2.41	132.44	127.09
3	20-A	202	NAP	C1B-N9A-C8A	2.41	132.44	127.09
3	8-A	202	NAP	C4A-N9A-C8A	2.40	108.26	105.74
3	62-A	202	NAP	C4A-C5A-N7A	-2.40	107.84	110.58
3	25-A	202	NAP	C6N-N1N-C2N	-2.40	119.84	121.88
3	17-A	202	NAP	C1B-N9A-C8A	2.40	132.42	127.09
2	57-A	201	FOL	CA-N-C	-2.40	115.82	121.56
3	36-A	202	NAP	C6N-N1N-C2N	-2.40	119.84	121.88
3	76-A	202	NAP	C6N-N1N-C2N	-2.40	119.84	121.88
3	74-A	202	NAP	C6N-N1N-C2N	-2.39	119.84	121.88
2	68-A	201	FOL	C9-C6-C7	2.39	125.68	121.38
3	61-A	202	NAP	C6N-N1N-C2N	-2.39	119.84	121.88
3	50-A	202	NAP	C2N-C3N-C4N	2.39	121.04	118.26
2	33-A	201	FOL	CB-CG-CD	-2.39	106.12	112.49
2	73-A	201	FOL	C6-C7-N8	2.39	125.43	123.14
3	80-A	202	NAP	N3A-C4A-N9A	2.39	131.23	127.17
3	19-A	202	NAP	C4A-N9A-C8A	2.38	108.24	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	47-A	201	FOL	CB-CA-CT	-2.38	104.70	110.35
3	38-A	202	NAP	C5A-N7A-C8A	2.38	107.19	103.45
3	44-A	202	NAP	C4A-N9A-C8A	2.38	108.24	105.74
3	37-A	202	NAP	C1B-N9A-C8A	2.38	132.38	127.09
3	63-A	202	NAP	C1B-N9A-C8A	2.38	132.37	127.09
3	27-A	202	NAP	C4A-N9A-C1B	-2.38	121.07	126.63
3	26-A	202	NAP	C6N-N1N-C2N	-2.38	119.86	121.88
3	59-A	202	NAP	C1B-N9A-C8A	2.38	132.37	127.09
2	29-A	201	FOL	CB-CA-CT	2.38	115.99	110.35
3	56-A	202	NAP	C5A-N7A-C8A	2.38	107.18	103.45
3	25-A	202	NAP	C4A-N9A-C8A	2.37	108.23	105.74
2	76-A	201	FOL	CG-CB-CA	-2.37	108.79	113.16
2	59-A	201	FOL	OE1-CD-CG	-2.37	115.58	123.09
3	61-A	202	NAP	C1B-N9A-C8A	2.37	132.35	127.09
3	39-A	202	NAP	C4D-O4D-C1D	-2.37	107.76	109.92
2	67-A	201	FOL	C15-C16-C11	-2.37	118.27	120.80
3	56-A	202	NAP	N3A-C4A-N9A	2.37	131.19	127.17
2	70-A	201	FOL	C15-C16-C11	2.36	123.32	120.80
3	68-A	202	NAP	C1B-N9A-C8A	2.36	132.33	127.09
2	26-A	201	FOL	C13-C12-C11	-2.36	118.28	120.80
3	3-A	202	NAP	C4A-N9A-C8A	2.36	108.21	105.74
3	73-A	202	NAP	C1B-N9A-C8A	2.35	132.32	127.09
3	40-A	202	NAP	C1B-N9A-C8A	2.35	132.32	127.09
3	63-A	202	NAP	C4D-O4D-C1D	-2.35	107.77	109.92
3	69-A	202	NAP	C2N-C3N-C4N	2.35	121.00	118.26
2	61-A	201	FOL	CB-CG-CD	-2.35	106.22	112.49
3	78-A	202	NAP	C4A-C5A-N7A	-2.35	107.89	110.58
3	33-A	202	NAP	C1B-N9A-C8A	2.35	132.31	127.09
3	75-A	202	NAP	C1B-N9A-C8A	2.35	132.31	127.09
3	28-A	202	NAP	C4D-O4D-C1D	-2.35	107.77	109.92
3	46-A	202	NAP	C6A-C5A-C4A	2.35	120.38	117.18
2	56-A	201	FOL	CB-CA-N	2.35	115.55	110.91
3	20-A	202	NAP	C4D-O4D-C1D	-2.35	107.78	109.92
2	40-A	201	FOL	O-C-C11	-2.35	116.25	120.90
3	55-A	202	NAP	C1B-N9A-C8A	2.35	132.30	127.09
2	60-A	201	FOL	CB-CG-CD	2.34	118.74	112.49
3	24-A	202	NAP	C5A-N7A-C8A	2.34	107.12	103.45
3	28-A	202	NAP	C4A-C5A-N7A	-2.34	107.91	110.58
3	4-A	202	NAP	C4A-N9A-C8A	2.33	108.19	105.74
3	34-A	202	NAP	C4A-C5A-N7A	-2.33	107.92	110.58
3	8-A	202	NAP	C5A-C6A-N6A	2.33	129.06	123.29
3	52-A	202	NAP	C4A-N9A-C8A	2.33	108.19	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	68-A	202	NAP	C4D-O4D-C1D	-2.33	107.79	109.92
2	6-A	201	FOL	C9-N10-C14	2.32	129.32	121.87
3	43-A	202	NAP	C1B-N9A-C8A	2.32	132.25	127.09
3	23-A	202	NAP	C2N-C3N-C4N	2.32	120.96	118.26
3	44-A	202	NAP	C4A-C5A-N7A	-2.32	107.93	110.58
2	19-A	201	FOL	C9-N10-C14	2.32	129.31	121.87
3	62-A	202	NAP	C6A-C5A-C4A	2.31	120.34	117.18
3	68-A	202	NAP	C4A-N9A-C8A	2.31	108.17	105.74
3	26-A	202	NAP	C1B-N9A-C8A	2.31	132.23	127.09
2	64-A	201	FOL	OE2-CD-CG	2.31	121.29	114.00
2	26-A	201	FOL	C4-C4A-N5	2.31	122.18	118.55
3	52-A	202	NAP	C5A-N7A-C8A	2.30	107.06	103.45
3	51-A	202	NAP	C5A-N7A-C8A	2.30	107.06	103.45
3	27-A	202	NAP	C5A-N7A-C8A	2.30	107.06	103.45
3	5-A	202	NAP	C4A-C5A-N7A	-2.30	107.95	110.58
3	62-A	202	NAP	C1B-N9A-C8A	2.30	132.19	127.09
3	36-A	202	NAP	C1B-N9A-C8A	2.30	132.19	127.09
2	67-A	201	FOL	C13-C12-C11	2.29	123.25	120.80
2	26-A	201	FOL	OE1-CD-CG	-2.29	115.83	123.09
2	73-A	201	FOL	O4-C4-N3	2.29	123.71	120.23
3	8-A	202	NAP	C5A-N7A-C8A	2.29	107.05	103.45
2	45-A	201	FOL	C4-C4A-N5	2.29	122.15	118.55
2	57-A	201	FOL	CB-CA-N	2.28	115.42	110.91
3	75-A	202	NAP	C6A-C5A-C4A	2.28	120.28	117.18
3	29-A	202	NAP	C4A-N9A-C8A	2.27	108.13	105.74
3	23-A	202	NAP	C4A-C5A-N7A	-2.27	107.98	110.58
3	16-A	202	NAP	C2N-C3N-C4N	2.27	120.90	118.26
3	47-A	202	NAP	C4A-N9A-C8A	2.27	108.12	105.74
2	10-A	201	FOL	O-C-N	-2.27	118.15	122.47
3	14-A	202	NAP	C1B-N9A-C8A	2.27	132.13	127.09
2	54-A	201	FOL	CB-CG-CD	-2.27	106.44	112.49
2	15-A	201	FOL	OE2-CD-CG	2.27	121.16	114.00
3	66-A	202	NAP	C4A-N9A-C8A	2.26	108.11	105.74
3	67-A	202	NAP	C1B-N9A-C8A	2.26	132.11	127.09
3	80-A	202	NAP	O2A-PA-O3	2.26	113.38	107.27
3	60-A	202	NAP	C4A-N9A-C8A	2.26	108.11	105.74
3	45-A	202	NAP	C2N-C3N-C4N	2.26	120.89	118.26
2	58-A	201	FOL	O-C-C11	-2.26	116.43	120.90
3	42-A	202	NAP	C2N-C3N-C4N	2.26	120.88	118.26
3	49-A	202	NAP	O2A-PA-O3	2.26	113.37	107.27
3	9-A	202	NAP	C4A-N9A-C8A	2.25	108.10	105.74
3	48-A	202	NAP	C4A-N9A-C8A	2.25	108.10	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-A	202	NAP	C6N-N1N-C2N	-2.25	119.96	121.88
3	72-A	202	NAP	C4A-C5A-N7A	-2.25	108.01	110.58
3	65-A	202	NAP	C4A-C5A-N7A	-2.24	108.02	110.58
2	69-A	201	FOL	C16-C11-C12	2.24	121.42	118.57
2	80-A	201	FOL	C4-C4A-N5	2.24	122.08	118.55
3	57-A	202	NAP	C4A-C5A-N7A	-2.24	108.02	110.58
3	17-A	202	NAP	C4A-N9A-C8A	2.24	108.09	105.74
3	65-A	202	NAP	C4A-N9A-C8A	2.24	108.09	105.74
3	52-A	202	NAP	C6N-N1N-C2N	-2.24	119.97	121.88
2	76-A	201	FOL	O2-CT-CA	2.23	121.07	113.51
3	6-A	202	NAP	C4A-N9A-C8A	2.23	108.08	105.74
2	72-A	201	FOL	C16-C11-C12	-2.23	115.73	118.57
3	10-A	202	NAP	C4A-N9A-C8A	2.23	108.08	105.74
2	40-A	201	FOL	CB-CG-CD	2.23	118.44	112.49
3	29-A	202	NAP	C4A-C5A-N7A	-2.23	108.03	110.58
3	49-A	202	NAP	C4A-N9A-C8A	2.23	108.08	105.74
2	14-A	201	FOL	OE1-CD-CG	-2.23	116.02	123.09
3	76-A	202	NAP	C6A-C5A-C4A	2.23	120.22	117.18
3	55-A	202	NAP	C4A-C5A-N7A	-2.23	108.03	110.58
2	78-A	201	FOL	OE2-CD-CG	2.23	121.04	114.00
2	34-A	201	FOL	OE2-CD-CG	2.22	121.03	114.00
2	72-A	201	FOL	OE2-CD-CG	2.22	121.03	114.00
3	63-A	202	NAP	C6A-C5A-C4A	2.22	120.22	117.18
3	75-A	202	NAP	C5A-C4A-N9A	2.22	108.23	105.81
3	29-A	202	NAP	C6N-N1N-C2N	-2.22	119.99	121.88
2	73-A	201	FOL	C4A-C8A-N1	-2.22	117.42	120.13
3	46-A	202	NAP	C4A-C5A-N7A	-2.22	108.04	110.58
3	58-A	202	NAP	C6A-C5A-C4A	2.22	120.21	117.18
2	74-A	201	FOL	C13-C14-N10	-2.22	115.94	120.96
3	31-A	202	NAP	C4A-N9A-C8A	2.22	108.07	105.74
3	2-A	202	NAP	C6N-N1N-C2N	-2.22	119.99	121.88
2	9-A	201	FOL	C4-C4A-N5	2.21	122.04	118.55
2	73-A	201	FOL	CT-CA-N	2.21	115.71	110.57
2	56-A	201	FOL	CG-CB-CA	2.21	117.24	113.16
3	78-A	202	NAP	C1B-N9A-C8A	2.21	132.00	127.09
2	78-A	201	FOL	CA-N-C	2.21	126.86	121.56
3	59-A	202	NAP	C4A-C5A-N7A	-2.21	108.06	110.58
2	64-A	201	FOL	CG-CB-CA	2.20	117.23	113.16
3	70-A	202	NAP	C4A-N9A-C8A	2.20	108.05	105.74
2	57-A	201	FOL	C4-C4A-N5	2.20	122.02	118.55
2	48-A	201	FOL	CG-CB-CA	2.20	117.22	113.16
3	2-A	202	NAP	C4A-C5A-N7A	-2.20	108.07	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	7-A	202	NAP	C4A-C5A-N7A	-2.20	108.07	110.58
2	33-A	201	FOL	O2-CT-CA	2.20	120.95	113.51
3	62-A	202	NAP	C6N-N1N-C2N	-2.20	120.01	121.88
3	58-A	202	NAP	C1B-N9A-C8A	2.20	131.97	127.09
3	63-A	202	NAP	C6N-N1N-C2N	-2.19	120.01	121.88
3	30-A	202	NAP	C2N-C3N-C4N	2.19	120.81	118.26
2	68-A	201	FOL	O4-C4-N3	2.19	123.56	120.23
2	63-A	201	FOL	O2-CT-CA	2.19	120.93	113.51
3	57-A	202	NAP	C6N-N1N-C2N	-2.19	120.01	121.88
3	50-A	202	NAP	C6N-N1N-C2N	-2.19	120.01	121.88
3	80-A	202	NAP	C6N-N1N-C2N	-2.19	120.01	121.88
3	40-A	202	NAP	C4A-C5A-N7A	-2.19	108.08	110.58
3	26-A	202	NAP	C4A-N9A-C8A	2.19	108.04	105.74
2	26-A	201	FOL	OE2-CD-CG	2.19	120.91	114.00
2	71-A	201	FOL	C15-C14-N10	-2.19	116.02	120.96
3	27-A	202	NAP	C6A-C5A-C4A	2.19	120.16	117.18
3	51-A	202	NAP	O2A-PA-O3	2.19	113.18	107.27
2	48-A	201	FOL	C9-N10-C14	2.19	128.88	121.87
2	57-A	201	FOL	C9-N10-C14	2.19	128.88	121.87
2	68-A	201	FOL	C15-C16-C11	2.18	123.13	120.80
3	25-A	202	NAP	C2N-C3N-C4N	2.18	120.80	118.26
2	23-A	201	FOL	O4-C4-C4A	-2.18	116.59	120.42
2	5-A	201	FOL	C4-C4A-N5	2.18	121.98	118.55
3	47-A	202	NAP	C4A-C5A-N7A	-2.18	108.09	110.58
2	48-A	201	FOL	O-C-N	-2.18	118.33	122.47
3	30-A	202	NAP	C4A-C5A-N7A	-2.18	108.09	110.58
3	54-A	202	NAP	C6A-C5A-C4A	2.18	120.15	117.18
2	31-A	201	FOL	C4-C4A-N5	2.17	121.98	118.55
2	73-A	201	FOL	C13-C12-C11	-2.17	118.48	120.80
3	49-A	202	NAP	C4A-C5A-N7A	-2.17	108.10	110.58
2	38-A	201	FOL	C9-N10-C14	2.17	128.84	121.87
3	66-A	202	NAP	C4A-C5A-N7A	-2.17	108.10	110.58
2	62-A	201	FOL	O2-CT-CA	2.17	120.85	113.51
2	68-A	201	FOL	C16-C15-C14	-2.17	117.80	120.30
3	44-A	202	NAP	C2N-C3N-C4N	2.17	120.78	118.26
3	6-A	202	NAP	C6N-N1N-C2N	-2.17	120.03	121.88
3	35-A	202	NAP	C6N-N1N-C2N	-2.16	120.04	121.88
3	24-A	202	NAP	C1B-N9A-C8A	2.16	131.90	127.09
3	80-A	202	NAP	C4A-C5A-N7A	-2.16	108.11	110.58
3	16-A	202	NAP	C4A-C5A-N7A	-2.16	108.11	110.58
2	67-A	201	FOL	NA2-C2-N1	2.16	121.31	116.77
3	39-A	202	NAP	O2A-PA-O3	2.16	113.10	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	39-A	201	FOL	C9-N10-C14	2.15	128.78	121.87
2	11-A	201	FOL	C4-C4A-N5	2.15	121.94	118.55
2	80-A	201	FOL	O2-CT-CA	2.15	120.80	113.51
3	1-A	202	NAP	C2N-C3N-C4N	2.15	120.76	118.26
2	65-A	201	FOL	C4-C4A-N5	2.15	121.94	118.55
3	32-A	202	NAP	C6A-C5A-C4A	2.15	120.11	117.18
3	37-A	202	NAP	C4A-C5A-N7A	-2.15	108.12	110.58
3	38-A	202	NAP	C6A-C5A-C4A	2.15	120.11	117.18
2	46-A	201	FOL	OE1-CD-CG	-2.15	116.27	123.09
3	36-A	202	NAP	C4A-C5A-N7A	-2.15	108.13	110.58
3	40-A	202	NAP	C2N-C3N-C4N	2.15	120.75	118.26
3	7-A	202	NAP	C2N-C3N-C4N	2.15	120.75	118.26
2	17-A	201	FOL	O-C-C11	-2.15	116.65	120.90
2	66-A	201	FOL	C13-C14-N10	-2.14	116.12	120.96
3	25-A	202	NAP	C4A-C5A-N7A	-2.14	108.13	110.58
3	79-A	202	NAP	C4A-N9A-C8A	2.14	107.99	105.74
3	58-A	202	NAP	C4A-C5A-N7A	-2.14	108.13	110.58
3	12-A	202	NAP	C4A-C5A-N7A	-2.14	108.13	110.58
3	36-A	202	NAP	C2N-C3N-C4N	2.14	120.75	118.26
3	65-A	202	NAP	C6A-C5A-C4A	2.14	120.10	117.18
3	38-A	202	NAP	O2A-PA-O3	2.14	113.05	107.27
2	72-A	201	FOL	C15-C14-N10	-2.14	116.14	120.96
2	8-A	201	FOL	C13-C12-C11	-2.13	118.52	120.80
3	27-A	202	NAP	C6N-N1N-C2N	-2.13	120.06	121.88
2	66-A	201	FOL	C6-C9-N10	-2.13	108.45	113.13
3	31-A	202	NAP	C1B-N9A-C8A	2.13	131.82	127.09
2	65-A	201	FOL	CT-CA-N	2.13	115.51	110.57
3	39-A	202	NAP	C2N-C3N-C4N	2.13	120.73	118.26
3	13-A	202	NAP	C4A-N9A-C8A	2.13	107.97	105.74
2	55-A	201	FOL	C4-C4A-N5	2.13	121.90	118.55
3	31-A	202	NAP	C6A-C5A-C4A	2.13	120.08	117.18
2	65-A	201	FOL	CA-N-C	2.12	126.66	121.56
3	63-A	202	NAP	C5A-C4A-N9A	2.12	108.12	105.81
3	76-A	202	NAP	C1B-N9A-C8A	2.12	131.81	127.09
2	65-A	201	FOL	O-C-C11	-2.12	116.70	120.90
3	59-A	202	NAP	C6A-C5A-C4A	2.12	120.07	117.18
3	10-A	202	NAP	C4A-C5A-N7A	-2.12	108.16	110.58
3	37-A	202	NAP	C2N-C3N-C4N	2.12	120.72	118.26
3	54-A	202	NAP	C4A-C5A-N7A	-2.11	108.17	110.58
3	29-A	202	NAP	C1B-N9A-C8A	2.11	131.78	127.09
2	4-A	201	FOL	C4-C4A-N5	2.11	121.88	118.55
3	40-A	202	NAP	C4A-N9A-C8A	2.11	107.95	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	69-A	201	FOL	O2-CT-CA	2.11	120.65	113.51
2	25-A	201	FOL	C9-N10-C14	2.11	128.63	121.87
3	25-A	202	NAP	C6A-C5A-C4A	2.11	120.06	117.18
3	72-A	202	NAP	C1B-N9A-C8A	2.11	131.77	127.09
2	23-A	201	FOL	O4-C4-N3	2.11	123.43	120.23
2	29-A	201	FOL	O2-CT-CA	2.11	120.63	113.51
2	14-A	201	FOL	C11-C-N	2.10	120.94	117.04
3	35-A	202	NAP	C2N-C3N-C4N	2.10	120.70	118.26
3	24-A	202	NAP	C2N-C3N-C4N	2.10	120.70	118.26
3	38-A	202	NAP	C1B-N9A-C8A	2.10	131.76	127.09
2	73-A	201	FOL	C11-C-N	-2.10	113.15	117.04
2	14-A	201	FOL	C4-C4A-N5	2.10	121.86	118.55
2	35-A	201	FOL	C9-N10-C14	2.10	128.61	121.87
3	73-A	202	NAP	C4A-C5A-N7A	-2.10	108.18	110.58
2	10-A	201	FOL	C4-C4A-N5	2.10	121.86	118.55
3	70-A	202	NAP	C4A-C5A-N7A	-2.10	108.18	110.58
3	34-A	202	NAP	C4A-N9A-C8A	2.10	107.94	105.74
3	3-A	202	NAP	C2N-C3N-C4N	2.10	120.70	118.26
3	39-A	202	NAP	C1B-N9A-C8A	2.10	131.75	127.09
2	77-A	201	FOL	O1-CT-CA	-2.10	115.49	122.26
3	58-A	202	NAP	C4A-N9A-C8A	2.10	107.94	105.74
3	41-A	202	NAP	O2A-PA-O3	2.10	112.94	107.27
2	53-A	201	FOL	C11-C-N	2.09	120.92	117.04
3	78-A	202	NAP	C6A-C5A-C4A	2.09	120.04	117.18
2	5-A	201	FOL	OE2-CD-CG	2.09	120.62	114.00
3	49-A	202	NAP	C6N-N1N-C2N	-2.09	120.10	121.88
3	30-A	202	NAP	C1B-N9A-C8A	2.09	131.74	127.09
3	21-A	202	NAP	C6A-C5A-C4A	2.09	120.03	117.18
2	74-A	201	FOL	C4-C4A-N5	2.09	121.84	118.55
3	49-A	202	NAP	C2N-C3N-C4N	2.09	120.69	118.26
3	22-A	202	NAP	C6N-N1N-C2N	-2.09	120.10	121.88
2	20-A	201	FOL	O-C-N	-2.09	118.50	122.47
3	12-A	202	NAP	C4A-N9A-C8A	2.09	107.93	105.74
3	41-A	202	NAP	C4A-N9A-C8A	2.09	107.93	105.74
2	22-A	201	FOL	O2-CT-CA	2.09	120.57	113.51
2	58-A	201	FOL	C9-N10-C14	2.08	128.56	121.87
3	71-A	202	NAP	C2N-C3N-C4N	2.08	120.68	118.26
3	8-A	202	NAP	O2A-PA-O3	2.08	112.90	107.27
2	73-A	201	FOL	C15-C14-C13	-2.08	116.28	119.04
2	54-A	201	FOL	OE1-CD-CG	-2.08	116.50	123.09
3	61-A	202	NAP	C2N-C3N-C4N	2.08	120.67	118.26
2	63-A	201	FOL	C16-C11-C	-2.08	113.87	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	49-A	201	FOL	C9-N10-C14	2.08	128.53	121.87
2	56-A	201	FOL	C9-N10-C14	2.08	128.53	121.87
2	39-A	201	FOL	CG-CB-CA	2.08	116.99	113.16
3	24-A	202	NAP	C6N-N1N-C2N	-2.07	120.11	121.88
2	32-A	201	FOL	CB-CG-CD	-2.07	106.96	112.49
3	38-A	202	NAP	C4A-C5A-N7A	-2.07	108.21	110.58
3	45-A	202	NAP	C4A-N9A-C1B	-2.07	121.78	126.63
2	70-A	201	FOL	CT-CA-N	2.07	115.38	110.57
3	29-A	202	NAP	C6A-C5A-C4A	2.07	120.01	117.18
2	1-A	201	FOL	C9-N10-C14	2.07	128.52	121.87
2	64-A	201	FOL	NA2-C2-N1	2.07	121.13	116.77
2	10-A	201	FOL	C9-N10-C14	2.07	128.51	121.87
2	24-A	201	FOL	OE1-CD-CG	-2.07	116.54	123.09
3	37-A	202	NAP	O2A-PA-O3	2.07	112.86	107.27
3	1-A	202	NAP	C4A-C5A-N7A	-2.07	108.22	110.58
2	27-A	201	FOL	C9-N10-C14	2.07	128.50	121.87
3	39-A	202	NAP	C6A-C5A-C4A	2.07	120.00	117.18
2	44-A	201	FOL	C11-C-N	2.06	120.86	117.04
3	68-A	202	NAP	C6A-C5A-C4A	2.06	120.00	117.18
3	44-A	202	NAP	C4D-O4D-C1D	-2.06	108.04	109.92
2	45-A	201	FOL	CG-CB-CA	-2.06	109.36	113.16
3	11-A	202	NAP	C4A-C5A-N7A	-2.06	108.23	110.58
2	47-A	201	FOL	C9-N10-C14	2.06	128.47	121.87
3	42-A	202	NAP	C6A-C5A-C4A	2.06	119.99	117.18
3	46-A	202	NAP	C1B-N9A-C8A	2.06	131.66	127.09
2	72-A	201	FOL	C15-C14-C13	-2.05	116.32	119.04
2	79-A	201	FOL	C4-C4A-N5	2.05	121.78	118.55
2	68-A	201	FOL	C11-C-N	2.05	120.84	117.04
3	23-A	202	NAP	O2A-PA-O3	2.05	112.82	107.27
3	77-A	202	NAP	C4A-N9A-C8A	2.05	107.89	105.74
3	22-A	202	NAP	C4A-C5A-N7A	-2.05	108.24	110.58
2	22-A	201	FOL	CA-N-C	2.05	126.48	121.56
3	52-A	202	NAP	C2N-C3N-C4N	2.05	120.64	118.26
3	70-A	202	NAP	C6N-N1N-C2N	-2.05	120.14	121.88
3	76-A	202	NAP	C4A-C5A-N7A	-2.05	108.24	110.58
3	22-A	202	NAP	C4A-N9A-C8A	2.05	107.89	105.74
3	33-A	202	NAP	C4A-N9A-C8A	2.05	107.89	105.74
2	18-A	201	FOL	C9-N10-C14	2.05	128.44	121.87
3	59-A	202	NAP	O2A-PA-O3	2.05	112.80	107.27
3	76-A	202	NAP	C4A-N9A-C8A	2.04	107.88	105.74
2	50-A	201	FOL	C9-N10-C14	2.04	128.41	121.87
2	3-A	201	FOL	C4-C4A-N5	2.04	121.76	118.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	36-A	202	NAP	O2A-PA-O3	2.04	112.78	107.27
2	19-A	201	FOL	C11-C-N	2.04	120.82	117.04
2	15-A	201	FOL	C4-C4A-N5	2.03	121.76	118.55
3	32-A	202	NAP	C1B-N9A-C8A	2.03	131.61	127.09
2	15-A	201	FOL	C9-N10-C14	2.03	128.39	121.87
2	14-A	201	FOL	OE2-CD-CG	2.03	120.42	114.00
3	77-A	202	NAP	O2A-PA-O3	2.03	112.77	107.27
3	16-A	202	NAP	C4A-N9A-C8A	2.03	107.87	105.74
3	26-A	202	NAP	C6A-C5A-C4A	2.03	119.95	117.18
3	77-A	202	NAP	C6A-C5A-C4A	2.03	119.95	117.18
2	36-A	201	FOL	C9-N10-C14	2.03	128.38	121.87
2	46-A	201	FOL	CB-CG-CD	-2.03	107.08	112.49
3	57-A	202	NAP	C6A-C5A-C4A	2.03	119.95	117.18
2	31-A	201	FOL	C11-C-N	2.03	120.80	117.04
3	69-A	202	NAP	C4A-C5A-N7A	-2.03	108.26	110.58
3	68-A	202	NAP	O7N-C7N-N7N	-2.03	119.69	122.62
2	73-A	201	FOL	OE2-CD-CG	2.03	120.40	114.00
2	64-A	201	FOL	C12-C13-C14	2.03	122.63	120.30
2	22-A	201	FOL	C9-N10-C14	2.03	128.37	121.87
3	50-A	202	NAP	O2A-PA-O3	2.02	112.74	107.27
2	40-A	201	FOL	CA-N-C	-2.02	116.71	121.56
3	9-A	202	NAP	C4A-C5A-N7A	-2.02	108.27	110.58
3	36-A	202	NAP	C6A-C5A-C4A	2.02	119.94	117.18
3	7-A	202	NAP	C4A-N9A-C8A	2.02	107.86	105.74
2	37-A	201	FOL	O-C-N	-2.02	118.63	122.47
2	22-A	201	FOL	C4-C4A-N5	2.02	121.73	118.55
3	61-A	202	NAP	C4A-C5A-N7A	-2.02	108.28	110.58
3	44-A	202	NAP	C6A-C5A-C4A	2.01	119.93	117.18
3	45-A	202	NAP	C5A-C4A-N9A	2.01	108.00	105.81
3	44-A	202	NAP	O2A-PA-O3	2.01	112.71	107.27
2	68-A	201	FOL	C13-C12-C11	-2.01	118.65	120.80
3	30-A	202	NAP	C6A-C5A-C4A	2.01	119.92	117.18
2	61-A	201	FOL	CT-CA-N	2.01	115.22	110.57
2	69-A	201	FOL	C9-N10-C14	2.01	128.31	121.87
2	13-A	201	FOL	C4-C4A-N5	2.01	121.71	118.55
2	46-A	201	FOL	C9-N10-C14	2.00	128.29	121.87
2	37-A	201	FOL	C4-C4A-N5	2.00	121.70	118.55
3	78-A	202	NAP	C4A-N9A-C8A	2.00	107.84	105.74

There are no chirality outliers.

All (717) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2-A	201	FOL	N-CA-CB-CG
2	5-A	201	FOL	CT-CA-CB-CG
2	17-A	201	FOL	N-CA-CB-CG
2	23-A	201	FOL	N-CA-CB-CG
2	25-A	201	FOL	C11-C-N-CA
2	29-A	201	FOL	N-CA-CB-CG
2	29-A	201	FOL	CT-CA-CB-CG
2	32-A	201	FOL	CT-CA-CB-CG
2	38-A	201	FOL	C11-C-N-CA
2	39-A	201	FOL	C11-C-N-CA
2	55-A	201	FOL	C11-C-N-CA
2	55-A	201	FOL	CT-CA-CB-CG
2	56-A	201	FOL	C11-C-N-CA
2	57-A	201	FOL	C11-C-N-CA
2	58-A	201	FOL	C11-C-N-CA
2	58-A	201	FOL	CA-CB-CG-CD
2	61-A	201	FOL	CB-CA-N-C
2	64-A	201	FOL	N-CA-CB-CG
2	65-A	201	FOL	CA-CB-CG-CD
2	67-A	201	FOL	C11-C-N-CA
2	68-A	201	FOL	C6-C9-N10-C14
2	69-A	201	FOL	C6-C9-N10-C14
2	69-A	201	FOL	O-C-N-CA
2	70-A	201	FOL	CA-CB-CG-CD
2	71-A	201	FOL	C11-C-N-CA
2	72-A	201	FOL	C11-C-N-CA
2	73-A	201	FOL	C6-C9-N10-C14
2	78-A	201	FOL	CA-CB-CG-CD
3	1-A	202	NAP	PA-O3-PN-O5D
3	1-A	202	NAP	O4D-C1D-N1N-C6N
3	3-A	202	NAP	O4D-C1D-N1N-C6N
3	4-A	202	NAP	O4D-C1D-N1N-C6N
3	5-A	202	NAP	PA-O3-PN-O5D
3	5-A	202	NAP	O4D-C1D-N1N-C6N
3	6-A	202	NAP	PA-O3-PN-O5D
3	6-A	202	NAP	O4D-C1D-N1N-C6N
3	7-A	202	NAP	O4D-C1D-N1N-C6N
3	8-A	202	NAP	PA-O3-PN-O5D
3	9-A	202	NAP	PA-O3-PN-O5D
3	10-A	202	NAP	O4D-C1D-N1N-C6N
3	11-A	202	NAP	O4D-C1D-N1N-C6N
3	12-A	202	NAP	O4D-C1D-N1N-C6N
3	13-A	202	NAP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	15-A	202	NAP	O4D-C1D-N1N-C2N
3	15-A	202	NAP	O4D-C1D-N1N-C6N
3	15-A	202	NAP	C2D-C1D-N1N-C2N
3	16-A	202	NAP	O4D-C1D-N1N-C6N
3	17-A	202	NAP	O4D-C1D-N1N-C6N
3	18-A	202	NAP	O4D-C1D-N1N-C6N
3	19-A	202	NAP	O4D-C1D-N1N-C6N
3	20-A	202	NAP	O4D-C1D-N1N-C6N
3	21-A	202	NAP	O4D-C1D-N1N-C6N
3	23-A	202	NAP	O4D-C1D-N1N-C6N
3	24-A	202	NAP	PA-O3-PN-O5D
3	24-A	202	NAP	O4D-C1D-N1N-C6N
3	25-A	202	NAP	O4D-C1D-N1N-C6N
3	26-A	202	NAP	PA-O3-PN-O5D
3	26-A	202	NAP	O4D-C1D-N1N-C6N
3	27-A	202	NAP	PA-O3-PN-O5D
3	27-A	202	NAP	O4D-C1D-N1N-C6N
3	28-A	202	NAP	O4D-C1D-N1N-C6N
3	29-A	202	NAP	O4D-C1D-N1N-C6N
3	30-A	202	NAP	O4D-C1D-N1N-C6N
3	31-A	202	NAP	O4D-C1D-N1N-C6N
3	32-A	202	NAP	O4D-C1D-N1N-C2N
3	32-A	202	NAP	O4D-C1D-N1N-C6N
3	33-A	202	NAP	O4D-C1D-N1N-C6N
3	34-A	202	NAP	O4D-C1D-N1N-C6N
3	35-A	202	NAP	O4D-C1D-N1N-C2N
3	35-A	202	NAP	O4D-C1D-N1N-C6N
3	35-A	202	NAP	C2D-C1D-N1N-C2N
3	36-A	202	NAP	PA-O3-PN-O5D
3	36-A	202	NAP	O4D-C1D-N1N-C6N
3	37-A	202	NAP	PA-O3-PN-O5D
3	37-A	202	NAP	O4D-C1D-N1N-C6N
3	38-A	202	NAP	PA-O3-PN-O5D
3	39-A	202	NAP	PA-O3-PN-O5D
3	39-A	202	NAP	O4D-C1D-N1N-C6N
3	40-A	202	NAP	O4D-C1D-N1N-C6N
3	42-A	202	NAP	O4D-C1D-N1N-C6N
3	44-A	202	NAP	O4D-C1D-N1N-C6N
3	45-A	202	NAP	O4D-C1D-N1N-C6N
3	46-A	202	NAP	O4D-C1D-N1N-C6N
3	47-A	202	NAP	O4D-C1D-N1N-C6N
3	48-A	202	NAP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	50-A	202	NAP	O4D-C1D-N1N-C6N
3	51-A	202	NAP	O4D-C1D-N1N-C6N
3	52-A	202	NAP	O4D-C1D-N1N-C6N
3	53-A	202	NAP	O4D-C1D-N1N-C6N
3	54-A	202	NAP	O4D-C1D-N1N-C6N
3	55-A	202	NAP	O4D-C1D-N1N-C2N
3	55-A	202	NAP	O4D-C1D-N1N-C6N
3	55-A	202	NAP	C2D-C1D-N1N-C2N
3	56-A	202	NAP	O4D-C1D-N1N-C6N
3	57-A	202	NAP	PA-O3-PN-O5D
3	57-A	202	NAP	O4D-C1D-N1N-C6N
3	58-A	202	NAP	PA-O3-PN-O5D
3	59-A	202	NAP	PA-O3-PN-O5D
3	59-A	202	NAP	O4D-C1D-N1N-C6N
3	60-A	202	NAP	O4D-C1D-N1N-C6N
3	61-A	202	NAP	O4D-C1D-N1N-C6N
3	62-A	202	NAP	O4D-C1D-N1N-C6N
3	63-A	202	NAP	PA-O3-PN-O5D
3	64-A	202	NAP	O4D-C1D-N1N-C6N
3	65-A	202	NAP	O4D-C1D-N1N-C6N
3	66-A	202	NAP	O4D-C1D-N1N-C6N
3	68-A	202	NAP	PA-O3-PN-O5D
3	68-A	202	NAP	O4D-C1D-N1N-C6N
3	69-A	202	NAP	O4D-C1D-N1N-C6N
3	70-A	202	NAP	O4D-C1D-N1N-C6N
3	71-A	202	NAP	O4D-C1D-N1N-C6N
3	72-A	202	NAP	PA-O3-PN-O5D
3	72-A	202	NAP	O4D-C1D-N1N-C6N
3	73-A	202	NAP	O4D-C1D-N1N-C2N
3	73-A	202	NAP	O4D-C1D-N1N-C6N
3	73-A	202	NAP	C2D-C1D-N1N-C2N
3	74-A	202	NAP	O4D-C1D-N1N-C6N
3	75-A	202	NAP	PA-O3-PN-O5D
3	75-A	202	NAP	O4D-C1D-N1N-C6N
3	76-A	202	NAP	O4D-C1D-N1N-C6N
3	77-A	202	NAP	PA-O3-PN-O5D
3	78-A	202	NAP	O4D-C1D-N1N-C6N
3	79-A	202	NAP	PA-O3-PN-O5D
3	79-A	202	NAP	O4D-C1D-N1N-C6N
3	80-A	202	NAP	PA-O3-PN-O5D
3	80-A	202	NAP	O4D-C1D-N1N-C6N
2	25-A	201	FOL	O-C-N-CA

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Mol	Chain	Res	Type	Atoms
2	38-A	201	FOL	O-C-N-CA
2	39-A	201	FOL	O-C-N-CA
2	55-A	201	FOL	O-C-N-CA
2	56-A	201	FOL	O-C-N-CA
2	57-A	201	FOL	O-C-N-CA
2	58-A	201	FOL	O-C-N-CA
2	61-A	201	FOL	O-C-N-CA
2	67-A	201	FOL	O-C-N-CA
2	68-A	201	FOL	O-C-N-CA
2	70-A	201	FOL	O-C-N-CA
2	72-A	201	FOL	O-C-N-CA
2	75-A	201	FOL	O-C-N-CA
2	78-A	201	FOL	CB-CA-N-C
2	80-A	201	FOL	CB-CA-N-C
2	48-A	201	FOL	C11-C-N-CA
2	61-A	201	FOL	C11-C-N-CA
2	68-A	201	FOL	C11-C-N-CA
2	69-A	201	FOL	C11-C-N-CA
2	70-A	201	FOL	C11-C-N-CA
2	75-A	201	FOL	C11-C-N-CA
2	74-A	201	FOL	CT-CA-N-C
2	74-A	201	FOL	O-C-C11-C12
2	74-A	201	FOL	O-C-C11-C16
2	71-A	201	FOL	N-C-C11-C16
2	74-A	201	FOL	N-C-C11-C12
2	7-A	201	FOL	O-C-N-CA
2	48-A	201	FOL	O-C-N-CA
2	64-A	201	FOL	O-C-N-CA
2	71-A	201	FOL	O-C-N-CA
2	71-A	201	FOL	O-C-C11-C16
2	62-A	201	FOL	CB-CA-N-C
2	7-A	201	FOL	C11-C-N-CA
2	62-A	201	FOL	C11-C-N-CA
2	64-A	201	FOL	C11-C-N-CA
2	74-A	201	FOL	N-C-C11-C16
2	76-A	201	FOL	CT-CA-N-C
2	71-A	201	FOL	N-C-C11-C12
2	71-A	201	FOL	O-C-C11-C12
2	47-A	201	FOL	C11-C-N-CA
2	74-A	201	FOL	C11-C-N-CA
2	72-A	201	FOL	N-C-C11-C12
2	74-A	201	FOL	O-C-N-CA

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Mol	Chain	Res	Type	Atoms
2	75-A	201	FOL	CT-CA-N-C
2	64-A	201	FOL	C13-C14-N10-C9
2	5-A	201	FOL	N-CA-CB-CG
2	8-A	201	FOL	N-CA-CB-CG
2	9-A	201	FOL	N-CA-CB-CG
2	10-A	201	FOL	N-CA-CB-CG
2	25-A	201	FOL	N-CA-CB-CG
2	32-A	201	FOL	N-CA-CB-CG
2	38-A	201	FOL	N-CA-CB-CG
2	42-A	201	FOL	N-CA-CB-CG
2	63-A	201	FOL	N-CA-CB-CG
2	76-A	201	FOL	N-CA-CB-CG
2	78-A	201	FOL	N-CA-CB-CG
2	79-A	201	FOL	N-CA-CB-CG
2	80-A	201	FOL	N-CA-CB-CG
2	47-A	201	FOL	O-C-N-CA
2	62-A	201	FOL	O-C-N-CA
2	56-A	201	FOL	CA-CB-CG-CD
3	54-A	202	NAP	O4B-C4B-C5B-O5B
3	54-A	202	NAP	C3B-C4B-C5B-O5B
2	69-A	201	FOL	C13-C14-N10-C9
2	70-A	201	FOL	C13-C14-N10-C9
2	70-A	201	FOL	C15-C14-N10-C9
2	72-A	201	FOL	N-C-C11-C16
2	64-A	201	FOL	C15-C14-N10-C9
2	66-A	201	FOL	C15-C14-N10-C9
2	67-A	201	FOL	C13-C14-N10-C9
2	69-A	201	FOL	C15-C14-N10-C9
2	72-A	201	FOL	O-C-C11-C12
2	7-A	201	FOL	CB-CA-N-C
2	35-A	201	FOL	N-CA-CB-CG
2	49-A	201	FOL	N-CA-CB-CG
2	66-A	201	FOL	C13-C14-N10-C9
2	67-A	201	FOL	C15-C14-N10-C9
2	8-A	201	FOL	CA-CB-CG-CD
2	62-A	201	FOL	CA-CB-CG-CD
2	76-A	201	FOL	C11-C-N-CA
2	8-A	201	FOL	CT-CA-CB-CG
2	9-A	201	FOL	CT-CA-CB-CG
2	12-A	201	FOL	CT-CA-CB-CG
2	17-A	201	FOL	CT-CA-CB-CG
2	23-A	201	FOL	CT-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	35-A	201	FOL	CT-CA-CB-CG
2	42-A	201	FOL	CT-CA-CB-CG
2	49-A	201	FOL	CT-CA-CB-CG
2	63-A	201	FOL	CT-CA-CB-CG
2	64-A	201	FOL	CT-CA-CB-CG
2	79-A	201	FOL	CT-CA-CB-CG
2	80-A	201	FOL	CT-CA-CB-CG
2	80-A	201	FOL	N-C-C11-C12
2	72-A	201	FOL	O-C-C11-C16
2	55-A	201	FOL	N-CA-CB-CG
2	73-A	201	FOL	C13-C14-N10-C9
2	76-A	201	FOL	O-C-N-CA
2	10-A	201	FOL	C11-C-N-CA
2	73-A	201	FOL	C15-C14-N10-C9
2	40-A	201	FOL	C11-C-N-CA
2	63-A	201	FOL	C6-C9-N10-C14
2	80-A	201	FOL	N-C-C11-C16
2	75-A	201	FOL	N-CA-CT-O2
2	2-A	201	FOL	CT-CA-CB-CG
2	10-A	201	FOL	CT-CA-CB-CG
2	25-A	201	FOL	CT-CA-CB-CG
2	38-A	201	FOL	CT-CA-CB-CG
2	43-A	201	FOL	CT-CA-CB-CG
2	57-A	201	FOL	CT-CA-CB-CG
2	76-A	201	FOL	CT-CA-CB-CG
2	78-A	201	FOL	CT-CA-CB-CG
2	80-A	201	FOL	O-C-C11-C12
2	35-A	201	FOL	CA-CB-CG-CD
2	49-A	201	FOL	CA-CB-CG-CD
2	67-A	201	FOL	CA-CB-CG-CD
2	43-A	201	FOL	N-CA-CB-CG
2	71-A	201	FOL	C15-C14-N10-C9
2	71-A	201	FOL	N-CA-CT-O1
2	71-A	201	FOL	N-CA-CT-O2
2	42-A	201	FOL	CA-CB-CG-CD
2	80-A	201	FOL	O-C-N-CA
2	24-A	201	FOL	N-CA-CB-CG
2	7-A	201	FOL	N-CA-CT-O1
2	75-A	201	FOL	N-CA-CT-O1
2	10-A	201	FOL	O-C-N-CA
2	15-A	201	FOL	CT-CA-CB-CG
3	80-A	202	NAP	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	9-A	201	FOL	CA-CB-CG-CD
2	61-A	201	FOL	CA-CB-CG-CD
2	71-A	201	FOL	C13-C14-N10-C9
2	40-A	201	FOL	O-C-N-CA
2	67-A	201	FOL	CT-CA-N-C
2	28-A	201	FOL	N-CA-CT-O2
2	64-A	201	FOL	N-CA-CT-O2
2	67-A	201	FOL	N-CA-CT-O1
2	72-A	201	FOL	N-CA-CT-O1
2	72-A	201	FOL	N-CA-CT-O2
2	74-A	201	FOL	N-CA-CT-O1
2	31-A	201	FOL	N-CA-CB-CG
2	80-A	201	FOL	O-C-C11-C16
2	35-A	201	FOL	C11-C-N-CA
2	64-A	201	FOL	CB-CA-CT-O1
2	65-A	201	FOL	CB-CA-CT-O1
2	41-A	201	FOL	CA-CB-CG-CD
2	30-A	201	FOL	C11-C-N-CA
2	52-A	201	FOL	C11-C-N-CA
2	11-A	201	FOL	O-C-N-CA
2	24-A	201	FOL	O-C-N-CA
2	35-A	201	FOL	O-C-N-CA
2	11-A	201	FOL	C11-C-N-CA
2	24-A	201	FOL	C11-C-N-CA
2	7-A	201	FOL	N-CA-CT-O2
2	28-A	201	FOL	N-CA-CT-O1
2	64-A	201	FOL	N-CA-CT-O1
2	67-A	201	FOL	N-CA-CT-O2
2	79-A	201	FOL	N-CA-CT-O2
3	23-A	202	NAP	C2B-O2B-P2B-O3X
3	58-A	202	NAP	C2B-O2B-P2B-O3X
2	12-A	201	FOL	N-CA-CB-CG
2	15-A	201	FOL	N-CA-CB-CG
2	48-A	201	FOL	CT-CA-CB-CG
2	66-A	201	FOL	CT-CA-CB-CG
2	77-A	201	FOL	CA-CB-CG-CD
2	57-A	201	FOL	CB-CA-CT-O1
2	64-A	201	FOL	CB-CA-CT-O2
2	65-A	201	FOL	CB-CA-CT-O2
2	52-A	201	FOL	O-C-N-CA
2	58-A	201	FOL	CB-CA-N-C
2	74-A	201	FOL	N-CA-CT-O2

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Mol	Chain	Res	Type	Atoms
2	68-A	201	FOL	O-C-C11-C12
2	57-A	201	FOL	CB-CA-CT-O2
2	30-A	201	FOL	O-C-N-CA
3	2-A	202	NAP	PA-O3-PN-O5D
3	4-A	202	NAP	PA-O3-PN-O5D
3	7-A	202	NAP	PA-O3-PN-O5D
3	14-A	202	NAP	PA-O3-PN-O5D
3	15-A	202	NAP	PA-O3-PN-O5D
3	16-A	202	NAP	PA-O3-PN-O5D
3	18-A	202	NAP	PA-O3-PN-O5D
3	19-A	202	NAP	PA-O3-PN-O5D
3	20-A	202	NAP	PA-O3-PN-O5D
3	21-A	202	NAP	PA-O3-PN-O5D
3	23-A	202	NAP	PA-O3-PN-O5D
3	28-A	202	NAP	PA-O3-PN-O5D
3	30-A	202	NAP	PA-O3-PN-O5D
3	31-A	202	NAP	PA-O3-PN-O5D
3	34-A	202	NAP	PA-O3-PN-O5D
3	35-A	202	NAP	PA-O3-PN-O5D
3	40-A	202	NAP	PA-O3-PN-O5D
3	41-A	202	NAP	PA-O3-PN-O5D
3	43-A	202	NAP	PA-O3-PN-O5D
3	45-A	202	NAP	PA-O3-PN-O5D
3	46-A	202	NAP	PA-O3-PN-O5D
3	47-A	202	NAP	PA-O3-PN-O5D
3	48-A	202	NAP	PA-O3-PN-O5D
3	49-A	202	NAP	PA-O3-PN-O5D
3	50-A	202	NAP	PA-O3-PN-O5D
3	51-A	202	NAP	PA-O3-PN-O5D
3	52-A	202	NAP	PA-O3-PN-O5D
3	54-A	202	NAP	PA-O3-PN-O5D
3	56-A	202	NAP	PA-O3-PN-O5D
3	60-A	202	NAP	PA-O3-PN-O5D
3	61-A	202	NAP	PA-O3-PN-O5D
3	62-A	202	NAP	PA-O3-PN-O5D
3	64-A	202	NAP	PA-O3-PN-O5D
3	65-A	202	NAP	PA-O3-PN-O5D
3	66-A	202	NAP	PA-O3-PN-O5D
3	67-A	202	NAP	PA-O3-PN-O5D
3	70-A	202	NAP	PA-O3-PN-O5D
3	71-A	202	NAP	PA-O3-PN-O5D
3	76-A	202	NAP	PA-O3-PN-O5D

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Mol	Chain	Res	Type	Atoms
2	26-A	201	FOL	CA-CB-CG-CD
2	33-A	201	FOL	CT-CA-CB-CG
2	58-A	201	FOL	CT-CA-CB-CG
2	62-A	201	FOL	CT-CA-CB-CG
2	69-A	201	FOL	CT-CA-CB-CG
2	72-A	201	FOL	CT-CA-CB-CG
2	9-A	201	FOL	C11-C-N-CA
2	80-A	201	FOL	C11-C-N-CA
2	64-A	201	FOL	C6-C9-N10-C14
2	67-A	201	FOL	C6-C9-N10-C14
2	58-A	201	FOL	CB-CA-CT-O1
2	58-A	201	FOL	CB-CA-CT-O2
2	79-A	201	FOL	CB-CA-CT-O2
2	9-A	201	FOL	O-C-N-CA
2	61-A	201	FOL	N-CA-CT-O2
2	79-A	201	FOL	N-CA-CT-O1
2	68-A	201	FOL	N-C-C11-C12
2	77-A	201	FOL	CB-CA-N-C
2	38-A	201	FOL	CB-CA-CT-O2
2	39-A	201	FOL	CB-CA-CT-O1
2	39-A	201	FOL	CB-CA-CT-O2
2	70-A	201	FOL	CB-CA-CT-O1
2	46-A	201	FOL	CA-CB-CG-CD
2	31-A	201	FOL	O-C-N-CA
2	31-A	201	FOL	CT-CA-CB-CG
2	75-A	201	FOL	CT-CA-CB-CG
2	56-A	201	FOL	CB-CA-CT-O1
2	56-A	201	FOL	CB-CA-CT-O2
2	75-A	201	FOL	CB-CA-CT-O2
2	47-A	201	FOL	CA-CB-CG-CD
2	46-A	201	FOL	O-C-N-CA
3	6-A	202	NAP	C5B-O5B-PA-O1A
3	54-A	202	NAP	C5B-O5B-PA-O1A
3	54-A	202	NAP	C5B-O5B-PA-O2A
3	54-A	202	NAP	C5B-O5B-PA-O3
3	58-A	202	NAP	C5B-O5B-PA-O1A
3	75-A	202	NAP	C5B-O5B-PA-O1A
2	70-A	201	FOL	CB-CA-CT-O2
2	71-A	201	FOL	CB-CA-CT-O1
2	54-A	201	FOL	CA-CB-CG-CD
2	72-A	201	FOL	CA-CB-CG-CD
2	53-A	201	FOL	C11-C-N-CA

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Mol	Chain	Res	Type	Atoms
2	48-A	201	FOL	N-CA-CB-CG
2	54-A	201	FOL	C11-C-N-CA
2	38-A	201	FOL	CB-CA-CT-O1
2	53-A	201	FOL	O-C-N-CA
2	57-A	201	FOL	N-CA-CB-CG
2	68-A	201	FOL	O-C-C11-C16
2	71-A	201	FOL	CB-CA-CT-O2
2	75-A	201	FOL	CB-CA-CT-O1
3	2-A	202	NAP	C2B-O2B-P2B-O3X
3	5-A	202	NAP	C2B-O2B-P2B-O3X
3	8-A	202	NAP	C2B-O2B-P2B-O3X
3	12-A	202	NAP	C2B-O2B-P2B-O3X
3	14-A	202	NAP	C2B-O2B-P2B-O3X
3	15-A	202	NAP	C2B-O2B-P2B-O3X
3	18-A	202	NAP	C2B-O2B-P2B-O3X
3	20-A	202	NAP	C2B-O2B-P2B-O3X
3	22-A	202	NAP	C2B-O2B-P2B-O3X
3	25-A	202	NAP	C2B-O2B-P2B-O3X
3	28-A	202	NAP	C2B-O2B-P2B-O3X
3	31-A	202	NAP	C2B-O2B-P2B-O3X
3	33-A	202	NAP	C2B-O2B-P2B-O3X
3	37-A	202	NAP	C2B-O2B-P2B-O3X
3	46-A	202	NAP	C2B-O2B-P2B-O3X
3	50-A	202	NAP	C2B-O2B-P2B-O3X
3	53-A	202	NAP	C2B-O2B-P2B-O3X
3	57-A	202	NAP	C2B-O2B-P2B-O3X
3	59-A	202	NAP	C2B-O2B-P2B-O3X
3	60-A	202	NAP	C2B-O2B-P2B-O3X
3	61-A	202	NAP	C2B-O2B-P2B-O3X
3	63-A	202	NAP	C2B-O2B-P2B-O3X
3	73-A	202	NAP	C2B-O2B-P2B-O3X
3	74-A	202	NAP	C2B-O2B-P2B-O3X
3	78-A	202	NAP	C2B-O2B-P2B-O3X
2	24-A	201	FOL	OE2-CD-CG-CB
2	71-A	201	FOL	N-CA-CB-CG
2	31-A	201	FOL	C11-C-N-CA
2	45-A	201	FOL	OE2-CD-CG-CB
3	3-A	202	NAP	C2D-C1D-N1N-C2N
3	4-A	202	NAP	C2D-C1D-N1N-C2N
3	6-A	202	NAP	C2D-C1D-N1N-C2N
3	13-A	202	NAP	C2D-C1D-N1N-C2N
3	16-A	202	NAP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	18-A	202	NAP	C2D-C1D-N1N-C2N
3	19-A	202	NAP	C2D-C1D-N1N-C2N
3	20-A	202	NAP	C2D-C1D-N1N-C2N
3	26-A	202	NAP	C2D-C1D-N1N-C2N
3	27-A	202	NAP	C2D-C1D-N1N-C2N
3	29-A	202	NAP	C2D-C1D-N1N-C2N
3	32-A	202	NAP	C2D-C1D-N1N-C2N
3	44-A	202	NAP	C2D-C1D-N1N-C2N
3	45-A	202	NAP	C2D-C1D-N1N-C2N
3	46-A	202	NAP	C2D-C1D-N1N-C2N
3	48-A	202	NAP	C2D-C1D-N1N-C2N
3	53-A	202	NAP	C2D-C1D-N1N-C2N
3	54-A	202	NAP	C2D-C1D-N1N-C2N
3	60-A	202	NAP	C2D-C1D-N1N-C2N
3	68-A	202	NAP	C2D-C1D-N1N-C2N
3	69-A	202	NAP	C2D-C1D-N1N-C2N
3	70-A	202	NAP	C2D-C1D-N1N-C2N
3	73-A	202	NAP	C2D-C1D-N1N-C6N
3	76-A	202	NAP	C2D-C1D-N1N-C2N
2	36-A	201	FOL	CT-CA-CB-CG
2	41-A	201	FOL	CT-CA-CB-CG
2	78-A	201	FOL	OE2-CD-CG-CB
2	61-A	201	FOL	N-CA-CT-O1
2	3-A	201	FOL	O-C-N-CA
2	45-A	201	FOL	OE1-CD-CG-CB
2	71-A	201	FOL	OE2-CD-CG-CB
2	77-A	201	FOL	OE1-CD-CG-CB
2	40-A	201	FOL	CA-CB-CG-CD
2	71-A	201	FOL	OE1-CD-CG-CB
2	70-A	201	FOL	C6-C9-N10-C14
2	46-A	201	FOL	C11-C-N-CA
2	68-A	201	FOL	N-C-C11-C16
2	36-A	201	FOL	N-CA-CB-CG
2	27-A	201	FOL	OE1-CD-CG-CB
2	29-A	201	FOL	OE2-CD-CG-CB
2	34-A	201	FOL	OE1-CD-CG-CB
2	78-A	201	FOL	OE1-CD-CG-CB
2	8-A	201	FOL	OE1-CD-CG-CB
2	24-A	201	FOL	OE1-CD-CG-CB
2	16-A	201	FOL	OE1-CD-CG-CB
2	59-A	201	FOL	OE1-CD-CG-CB
2	4-A	201	FOL	OE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
2	6-A	201	FOL	OE1-CD-CG-CB
2	44-A	201	FOL	OE1-CD-CG-CB
2	59-A	201	FOL	OE2-CD-CG-CB
2	69-A	201	FOL	OE1-CD-CG-CB
2	7-A	201	FOL	OE1-CD-CG-CB
2	20-A	201	FOL	OE1-CD-CG-CB
2	27-A	201	FOL	OE2-CD-CG-CB
2	29-A	201	FOL	OE1-CD-CG-CB
2	38-A	201	FOL	OE1-CD-CG-CB
2	71-A	201	FOL	CA-CB-CG-CD
2	7-A	201	FOL	OE2-CD-CG-CB
2	41-A	201	FOL	OE2-CD-CG-CB
2	67-A	201	FOL	OE1-CD-CG-CB
2	66-A	201	FOL	N-CA-CB-CG
2	18-A	201	FOL	O-C-N-CA
2	11-A	201	FOL	OE2-CD-CG-CB
2	28-A	201	FOL	OE1-CD-CG-CB
3	1-A	202	NAP	O4D-C1D-N1N-C2N
3	2-A	202	NAP	O4D-C1D-N1N-C2N
3	2-A	202	NAP	O4D-C1D-N1N-C6N
3	3-A	202	NAP	O4D-C1D-N1N-C2N
3	4-A	202	NAP	O4D-C1D-N1N-C2N
3	5-A	202	NAP	O4D-C1D-N1N-C2N
3	6-A	202	NAP	O4D-C1D-N1N-C2N
3	7-A	202	NAP	O4D-C1D-N1N-C2N
3	8-A	202	NAP	O4D-C1D-N1N-C2N
3	9-A	202	NAP	O4D-C1D-N1N-C2N
3	9-A	202	NAP	O4D-C1D-N1N-C6N
3	10-A	202	NAP	O4D-C1D-N1N-C2N
3	11-A	202	NAP	O4D-C1D-N1N-C2N
3	12-A	202	NAP	O4D-C1D-N1N-C2N
3	13-A	202	NAP	O4D-C1D-N1N-C2N
3	14-A	202	NAP	O4D-C1D-N1N-C2N
3	14-A	202	NAP	O4D-C1D-N1N-C6N
3	16-A	202	NAP	O4D-C1D-N1N-C2N
3	17-A	202	NAP	O4D-C1D-N1N-C2N
3	18-A	202	NAP	O4D-C1D-N1N-C2N
3	19-A	202	NAP	O4D-C1D-N1N-C2N
3	20-A	202	NAP	O4D-C1D-N1N-C2N
3	21-A	202	NAP	O4D-C1D-N1N-C2N
3	22-A	202	NAP	O4D-C1D-N1N-C2N
3	23-A	202	NAP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	24-A	202	NAP	O4D-C1D-N1N-C2N
3	25-A	202	NAP	O4D-C1D-N1N-C2N
3	26-A	202	NAP	O4D-C1D-N1N-C2N
3	27-A	202	NAP	O4D-C1D-N1N-C2N
3	28-A	202	NAP	O4D-C1D-N1N-C2N
3	29-A	202	NAP	O4D-C1D-N1N-C2N
3	30-A	202	NAP	O4D-C1D-N1N-C2N
3	31-A	202	NAP	O4D-C1D-N1N-C2N
3	33-A	202	NAP	O4D-C1D-N1N-C2N
3	34-A	202	NAP	O4D-C1D-N1N-C2N
3	36-A	202	NAP	O4D-C1D-N1N-C2N
3	37-A	202	NAP	O4D-C1D-N1N-C2N
3	38-A	202	NAP	O4D-C1D-N1N-C2N
3	38-A	202	NAP	O4D-C1D-N1N-C6N
3	39-A	202	NAP	O4D-C1D-N1N-C2N
3	40-A	202	NAP	O4D-C1D-N1N-C2N
3	41-A	202	NAP	O4D-C1D-N1N-C2N
3	42-A	202	NAP	O4D-C1D-N1N-C2N
3	43-A	202	NAP	O4D-C1D-N1N-C2N
3	43-A	202	NAP	O4D-C1D-N1N-C6N
3	44-A	202	NAP	O4D-C1D-N1N-C2N
3	45-A	202	NAP	O4D-C1D-N1N-C2N
3	46-A	202	NAP	O4D-C1D-N1N-C2N
3	47-A	202	NAP	O4D-C1D-N1N-C2N
3	48-A	202	NAP	O4D-C1D-N1N-C2N
3	49-A	202	NAP	O4D-C1D-N1N-C2N
3	50-A	202	NAP	O4D-C1D-N1N-C2N
3	51-A	202	NAP	O4D-C1D-N1N-C2N
3	52-A	202	NAP	O4D-C1D-N1N-C2N
3	53-A	202	NAP	O4D-C1D-N1N-C2N
3	54-A	202	NAP	O4D-C1D-N1N-C2N
3	56-A	202	NAP	O4D-C1D-N1N-C2N
3	57-A	202	NAP	O4D-C1D-N1N-C2N
3	58-A	202	NAP	O4D-C1D-N1N-C2N
3	59-A	202	NAP	O4D-C1D-N1N-C2N
3	60-A	202	NAP	O4D-C1D-N1N-C2N
3	61-A	202	NAP	O4D-C1D-N1N-C2N
3	62-A	202	NAP	O4D-C1D-N1N-C2N
3	63-A	202	NAP	O4D-C1D-N1N-C2N
3	63-A	202	NAP	O4D-C1D-N1N-C6N
3	64-A	202	NAP	O4D-C1D-N1N-C2N
3	65-A	202	NAP	O4D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
3	66-A	202	NAP	O4D-C1D-N1N-C2N
3	67-A	202	NAP	O4D-C1D-N1N-C2N
3	67-A	202	NAP	O4D-C1D-N1N-C6N
3	68-A	202	NAP	O4D-C1D-N1N-C2N
3	69-A	202	NAP	O4D-C1D-N1N-C2N
3	70-A	202	NAP	O4D-C1D-N1N-C2N
3	71-A	202	NAP	O4D-C1D-N1N-C2N
3	72-A	202	NAP	O4D-C1D-N1N-C2N
3	74-A	202	NAP	O4D-C1D-N1N-C2N
3	75-A	202	NAP	O4D-C1D-N1N-C2N
3	76-A	202	NAP	O4D-C1D-N1N-C2N
3	77-A	202	NAP	O4D-C1D-N1N-C2N
3	77-A	202	NAP	O4D-C1D-N1N-C6N
3	78-A	202	NAP	O4D-C1D-N1N-C2N
3	79-A	202	NAP	O4D-C1D-N1N-C2N
3	80-A	202	NAP	O4D-C1D-N1N-C2N
2	62-A	201	FOL	OE2-CD-CG-CB
2	63-A	201	FOL	OE1-CD-CG-CB
2	72-A	201	FOL	OE1-CD-CG-CB
2	77-A	201	FOL	OE2-CD-CG-CB
2	20-A	201	FOL	C11-C-N-CA
2	15-A	201	FOL	OE2-CD-CG-CB
2	72-A	201	FOL	OE2-CD-CG-CB
3	5-A	202	NAP	C2B-O2B-P2B-O1X
3	8-A	202	NAP	C2B-O2B-P2B-O1X
3	10-A	202	NAP	C2B-O2B-P2B-O1X
3	12-A	202	NAP	C2B-O2B-P2B-O1X
3	13-A	202	NAP	C2B-O2B-P2B-O1X
3	15-A	202	NAP	C2B-O2B-P2B-O1X
3	16-A	202	NAP	C2B-O2B-P2B-O1X
3	20-A	202	NAP	C2B-O2B-P2B-O1X
3	46-A	202	NAP	C2B-O2B-P2B-O1X
3	47-A	202	NAP	C2B-O2B-P2B-O1X
3	53-A	202	NAP	C2B-O2B-P2B-O1X
3	55-A	202	NAP	C2B-O2B-P2B-O1X
3	63-A	202	NAP	C2B-O2B-P2B-O1X
3	68-A	202	NAP	C2B-O2B-P2B-O1X
3	74-A	202	NAP	C2B-O2B-P2B-O1X
3	80-A	202	NAP	C2B-O2B-P2B-O1X
2	79-A	201	FOL	CB-CA-CT-O1
2	4-A	201	FOL	OE1-CD-CG-CB
2	17-A	201	FOL	OE2-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
2	39-A	201	FOL	OE2-CD-CG-CB
2	41-A	201	FOL	OE1-CD-CG-CB
2	11-A	201	FOL	OE1-CD-CG-CB
2	31-A	201	FOL	OE1-CD-CG-CB
3	22-A	202	NAP	PA-O3-PN-O5D
3	44-A	202	NAP	PA-O3-PN-O5D
2	3-A	201	FOL	OE1-CD-CG-CB
2	6-A	201	FOL	OE2-CD-CG-CB
2	16-A	201	FOL	OE2-CD-CG-CB
2	44-A	201	FOL	OE2-CD-CG-CB
2	15-A	201	FOL	OE1-CD-CG-CB
2	34-A	201	FOL	OE2-CD-CG-CB
2	73-A	201	FOL	OE2-CD-CG-CB
2	20-A	201	FOL	OE2-CD-CG-CB
2	39-A	201	FOL	OE1-CD-CG-CB
2	67-A	201	FOL	OE2-CD-CG-CB
2	8-A	201	FOL	OE2-CD-CG-CB
2	28-A	201	FOL	OE2-CD-CG-CB
2	69-A	201	FOL	OE2-CD-CG-CB
2	38-A	201	FOL	OE2-CD-CG-CB
2	48-A	201	FOL	OE2-CD-CG-CB
2	62-A	201	FOL	OE1-CD-CG-CB
2	3-A	201	FOL	C11-C-N-CA
2	5-A	201	FOL	OE1-CD-CG-CB
2	33-A	201	FOL	N-CA-CB-CG
2	5-A	201	FOL	OE2-CD-CG-CB
2	17-A	201	FOL	OE1-CD-CG-CB
2	33-A	201	FOL	OE2-CD-CG-CB
2	35-A	201	FOL	OE1-CD-CG-CB
2	35-A	201	FOL	OE2-CD-CG-CB
2	63-A	201	FOL	OE2-CD-CG-CB
2	76-A	201	FOL	OE2-CD-CG-CB
2	24-A	201	FOL	CA-CB-CG-CD
2	56-A	201	FOL	OE1-CD-CG-CB
2	57-A	201	FOL	OE2-CD-CG-CB
2	50-A	201	FOL	CT-CA-CB-CG
2	66-A	201	FOL	OE2-CD-CG-CB
2	33-A	201	FOL	OE1-CD-CG-CB
2	57-A	201	FOL	OE1-CD-CG-CB
2	58-A	201	FOL	OE2-CD-CG-CB
2	8-A	201	FOL	C6-C9-N10-C14
2	19-A	201	FOL	C6-C9-N10-C14

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Mol	Chain	Res	Type	Atoms
2	47-A	201	FOL	C6-C9-N10-C14
3	54-A	202	NAP	C1B-C2B-O2B-P2B
2	56-A	201	FOL	OE2-CD-CG-CB
2	12-A	201	FOL	OE2-CD-CG-CB
2	73-A	201	FOL	OE1-CD-CG-CB
2	76-A	201	FOL	OE1-CD-CG-CB
2	52-A	201	FOL	OE2-CD-CG-CB
2	53-A	201	FOL	OE2-CD-CG-CB
2	70-A	201	FOL	OE1-CD-CG-CB
2	3-A	201	FOL	OE2-CD-CG-CB
2	12-A	201	FOL	OE1-CD-CG-CB
2	48-A	201	FOL	OE1-CD-CG-CB
2	58-A	201	FOL	OE1-CD-CG-CB
2	68-A	201	FOL	OE1-CD-CG-CB
2	69-A	201	FOL	N-CA-CB-CG
2	19-A	201	FOL	OE1-CD-CG-CB
2	31-A	201	FOL	OE2-CD-CG-CB
2	20-A	201	FOL	O-C-N-CA
2	66-A	201	FOL	OE1-CD-CG-CB
2	75-A	201	FOL	CA-CB-CG-CD
2	19-A	201	FOL	OE2-CD-CG-CB
2	53-A	201	FOL	OE1-CD-CG-CB
2	70-A	201	FOL	OE2-CD-CG-CB
2	18-A	201	FOL	C11-C-N-CA
3	75-A	202	NAP	C3B-C4B-C5B-O5B
3	30-A	202	NAP	C3B-C2B-O2B-P2B
2	7-A	201	FOL	CB-CA-CT-O2
2	48-A	201	FOL	CB-CA-CT-O2
2	80-A	201	FOL	CB-CA-CT-O2
2	3-A	201	FOL	N-CA-CB-CG
2	58-A	201	FOL	CT-CA-N-C
2	65-A	201	FOL	OE2-CD-CG-CB
3	80-A	202	NAP	O4B-C4B-C5B-O5B
3	5-A	202	NAP	C2B-O2B-P2B-O2X
3	7-A	202	NAP	C2B-O2B-P2B-O3X
3	10-A	202	NAP	C2B-O2B-P2B-O2X
3	19-A	202	NAP	C2B-O2B-P2B-O3X
3	20-A	202	NAP	C2B-O2B-P2B-O2X
3	22-A	202	NAP	C2B-O2B-P2B-O2X
3	23-A	202	NAP	C2B-O2B-P2B-O2X
3	29-A	202	NAP	C2B-O2B-P2B-O3X
3	32-A	202	NAP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
3	41-A	202	NAP	C2B-O2B-P2B-O3X
3	43-A	202	NAP	C2B-O2B-P2B-O3X
3	44-A	202	NAP	C2B-O2B-P2B-O3X
3	49-A	202	NAP	C2B-O2B-P2B-O3X
3	52-A	202	NAP	C2B-O2B-P2B-O3X
3	53-A	202	NAP	C2B-O2B-P2B-O2X
3	56-A	202	NAP	C2B-O2B-P2B-O3X
3	63-A	202	NAP	C2B-O2B-P2B-O2X
3	67-A	202	NAP	C2B-O2B-P2B-O3X
3	70-A	202	NAP	C2B-O2B-P2B-O3X
3	72-A	202	NAP	C2B-O2B-P2B-O3X
3	75-A	202	NAP	C2B-O2B-P2B-O3X
2	31-A	201	FOL	CA-CB-CG-CD
2	30-A	201	FOL	OE1-CD-CG-CB
2	42-A	201	FOL	OE1-CD-CG-CB
2	80-A	201	FOL	CB-CA-CT-O1
2	30-A	201	FOL	OE2-CD-CG-CB
2	42-A	201	FOL	OE2-CD-CG-CB
2	5-A	201	FOL	C6-C9-N10-C14
2	11-A	201	FOL	C6-C9-N10-C14
2	26-A	201	FOL	C6-C9-N10-C14
2	55-A	201	FOL	C6-C9-N10-C14
2	52-A	201	FOL	OE1-CD-CG-CB
2	51-A	201	FOL	OE2-CD-CG-CB
3	22-A	202	NAP	C2B-O2B-P2B-O1X
3	23-A	202	NAP	C2B-O2B-P2B-O1X
3	25-A	202	NAP	C2B-O2B-P2B-O1X
3	26-A	202	NAP	C2B-O2B-P2B-O1X
3	28-A	202	NAP	C2B-O2B-P2B-O1X
3	34-A	202	NAP	C2B-O2B-P2B-O1X
3	40-A	202	NAP	C2B-O2B-P2B-O1X
3	58-A	202	NAP	C2B-O2B-P2B-O1X
3	71-A	202	NAP	C2B-O2B-P2B-O1X
2	7-A	201	FOL	CB-CA-CT-O1
2	78-A	201	FOL	CB-CA-CT-O1
2	65-A	201	FOL	OE1-CD-CG-CB
2	68-A	201	FOL	OE2-CD-CG-CB
3	54-A	202	NAP	C3B-C2B-O2B-P2B
2	15-A	201	FOL	CA-CB-CG-CD
2	43-A	201	FOL	CA-CB-CG-CD
2	26-A	201	FOL	OE2-CD-CG-CB
2	64-A	201	FOL	CA-CB-CG-CD

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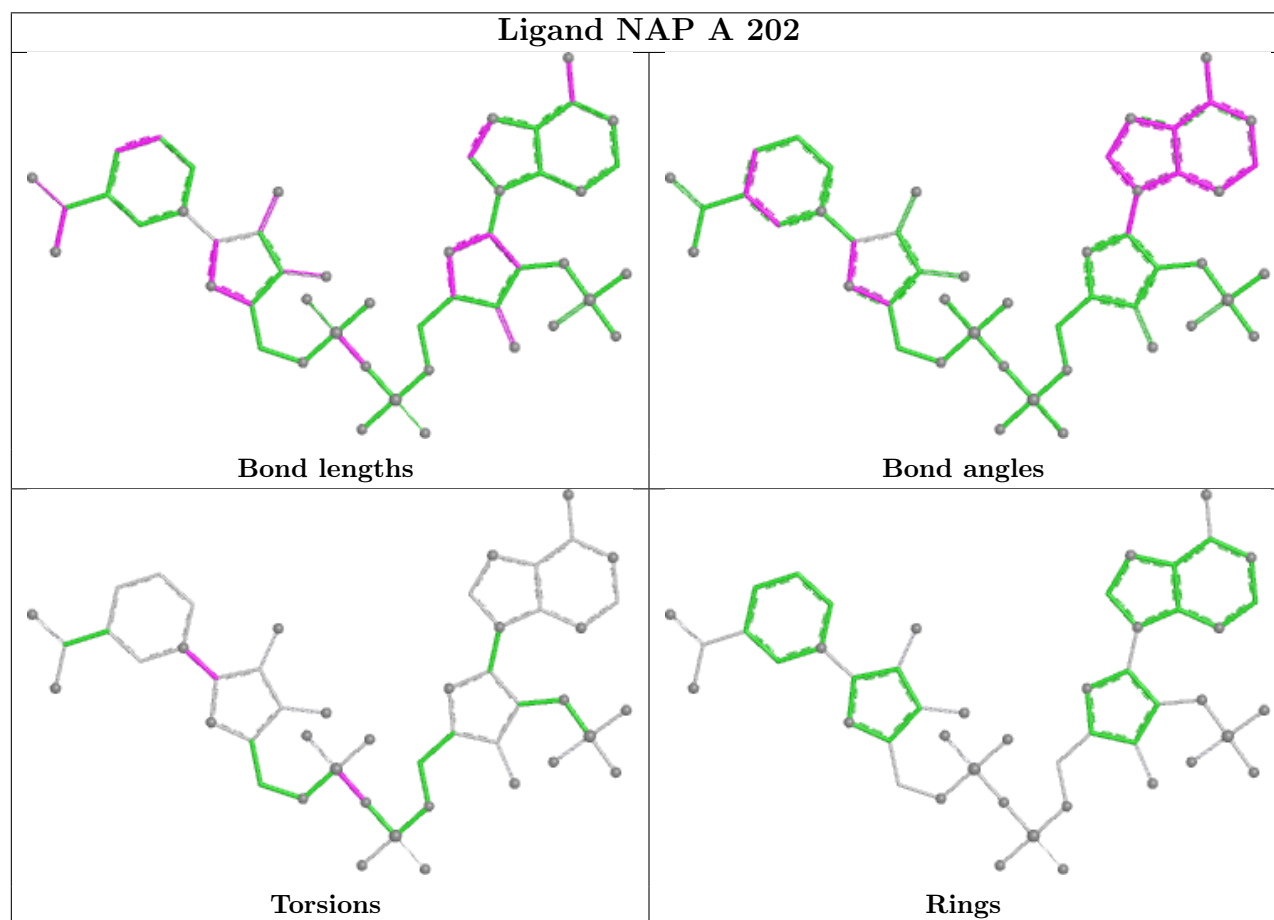
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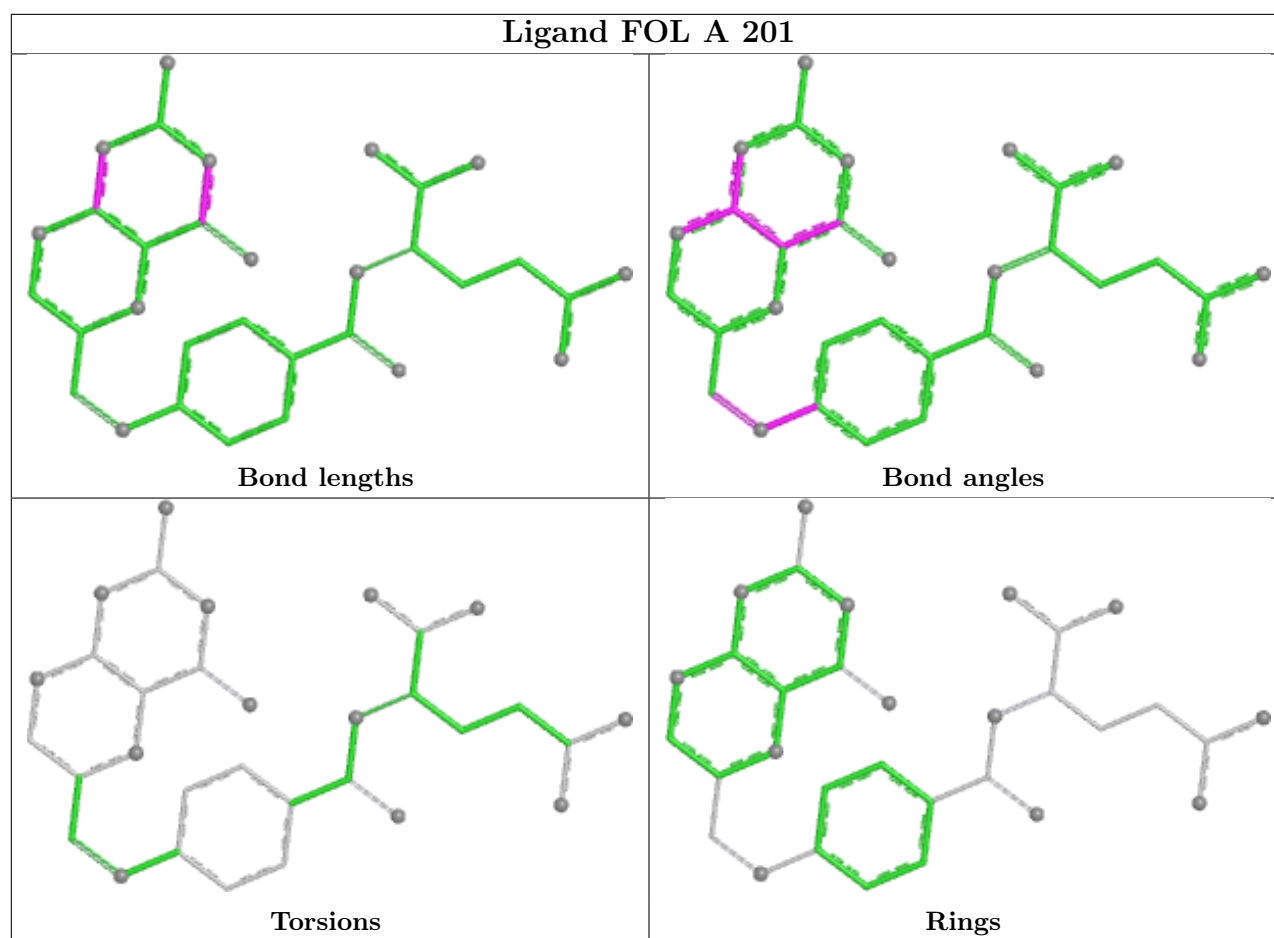
Mol	Chain	Res	Type	Atoms
2	59-A	201	FOL	C11-C-N-CA
3	74-A	202	NAP	C3B-C4B-C5B-O5B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	159/159 (100%)	2.32	72 (45%) 0 0	0, 0, 0, 0	159 (100%)
1	2-A	0/159	-	-	-	-
1	3-A	0/159	-	-	-	-
1	4-A	0/159	-	-	-	-
1	5-A	0/159	-	-	-	-
1	6-A	0/159	-	-	-	-
1	7-A	0/159	-	-	-	-
1	8-A	0/159	-	-	-	-
1	9-A	0/159	-	-	-	-
1	10-A	0/159	-	-	-	-
1	11-A	0/159	-	-	-	-
1	12-A	0/159	-	-	-	-
1	13-A	0/159	-	-	-	-
1	14-A	0/159	-	-	-	-
1	15-A	0/159	-	-	-	-
1	16-A	0/159	-	-	-	-
1	17-A	0/159	-	-	-	-
1	18-A	0/159	-	-	-	-
1	19-A	0/159	-	-	-	-
1	20-A	0/159	-	-	-	-
1	21-A	0/159	-	-	-	-
1	22-A	0/159	-	-	-	-
1	23-A	0/159	-	-	-	-
1	24-A	0/159	-	-	-	-
1	25-A	0/159	-	-	-	-
1	26-A	0/159	-	-	-	-
1	27-A	0/159	-	-	-	-
1	28-A	0/159	-	-	-	-
1	29-A	0/159	-	-	-	-
1	30-A	0/159	-	-	-	-
1	31-A	0/159	-	-	-	-
1	32-A	0/159	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	33-A	0/159	-	-	-	-
1	34-A	0/159	-	-	-	-
1	35-A	0/159	-	-	-	-
1	36-A	0/159	-	-	-	-
1	37-A	0/159	-	-	-	-
1	38-A	0/159	-	-	-	-
1	39-A	0/159	-	-	-	-
1	40-A	0/159	-	-	-	-
1	41-A	0/159	-	-	-	-
1	42-A	0/159	-	-	-	-
1	43-A	0/159	-	-	-	-
1	44-A	0/159	-	-	-	-
1	45-A	0/159	-	-	-	-
1	46-A	0/159	-	-	-	-
1	47-A	0/159	-	-	-	-
1	48-A	0/159	-	-	-	-
1	49-A	0/159	-	-	-	-
1	50-A	0/159	-	-	-	-
1	51-A	0/159	-	-	-	-
1	52-A	0/159	-	-	-	-
1	53-A	0/159	-	-	-	-
1	54-A	0/159	-	-	-	-
1	55-A	0/159	-	-	-	-
1	56-A	0/159	-	-	-	-
1	57-A	0/159	-	-	-	-
1	58-A	0/159	-	-	-	-
1	59-A	0/159	-	-	-	-
1	60-A	0/159	-	-	-	-
1	61-A	0/159	-	-	-	-
1	62-A	0/159	-	-	-	-
1	63-A	0/159	-	-	-	-
1	64-A	0/159	-	-	-	-
1	65-A	0/159	-	-	-	-
1	66-A	0/159	-	-	-	-
1	67-A	0/159	-	-	-	-
1	68-A	0/159	-	-	-	-
1	69-A	0/159	-	-	-	-
1	70-A	0/159	-	-	-	-
1	71-A	0/159	-	-	-	-
1	72-A	0/159	-	-	-	-
1	73-A	0/159	-	-	-	-
1	74-A	0/159	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	75-A	0/159	-	-	-	-
1	76-A	0/159	-	-	-	-
1	77-A	0/159	-	-	-	-
1	78-A	0/159	-	-	-	-
1	79-A	0/159	-	-	-	-
1	80-A	0/159	-	-	-	-
All	All	159/12720 (1%)	2.32	72 (45%) 0 0	0, 0, 0, 0	159 (100%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	130	PRO	15.6
1	1-A	20	MET	7.9
1	1-A	114	HIS	7.1
1	1-A	127	ASP	6.6
1	1-A	87	ASP	6.4
1	1-A	128	TYR	6.3
1	1-A	122	ASP	6.1
1	1-A	129	GLU	5.8
1	1-A	120	GLU	5.5
1	1-A	145	ALA	5.5
1	1-A	141	HIS	5.4
1	1-A	134	GLU	5.3
1	1-A	17	GLU	5.1
1	1-A	132	ASP	5.0
1	1-A	52	ARG	5.0
1	1-A	21	PRO	4.3
1	1-A	1	MET	4.2
1	1-A	65	GLN	4.0
1	1-A	10	VAL	4.0
1	1-A	137	PHE	4.0
1	1-A	48	GLU	3.9
1	1-A	55	PRO	3.9
1	1-A	119	VAL	3.8
1	1-A	106	LYS	3.8
1	1-A	16	MET	3.7
1	1-A	22	TRP	3.7
1	1-A	88	VAL	3.6
1	1-A	152	CYS	3.6
1	1-A	79	ASP	3.6
1	1-A	66	PRO	3.6
1	1-A	37	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	1-A	36	LEU	3.5
1	1-A	23	ASN	3.5
1	1-A	121	GLY	3.5
1	1-A	123	THR	3.3
1	1-A	148	SER	3.3
1	1-A	67	GLY	3.2
1	1-A	154	GLU	3.2
1	1-A	108	GLN	3.2
1	1-A	33	ARG	3.0
1	1-A	138	SER	2.9
1	1-A	47	TRP	2.9
1	1-A	157	GLU	2.9
1	1-A	101	GLU	2.8
1	1-A	118	GLU	2.8
1	1-A	45	HIS	2.8
1	1-A	135	SER	2.7
1	1-A	53	PRO	2.7
1	1-A	24	LEU	2.7
1	1-A	54	LEU	2.7
1	1-A	11	ASP	2.6
1	1-A	50	ILE	2.6
1	1-A	76	LYS	2.6
1	1-A	136	VAL	2.5
1	1-A	139	GLU	2.5
1	1-A	159	ARG	2.5
1	1-A	140	PHE	2.4
1	1-A	26	ALA	2.4
1	1-A	74	TRP	2.4
1	1-A	60	ILE	2.4
1	1-A	30	TRP	2.3
1	1-A	143	ALA	2.3
1	1-A	83	ALA	2.2
1	1-A	51	GLY	2.2
1	1-A	104	LEU	2.1
1	1-A	18	ASN	2.1
1	1-A	150	SER	2.1
1	1-A	82	ILE	2.1
1	1-A	49	SER	2.1
1	1-A	89	PRO	2.1
1	1-A	144	ASP	2.1
1	1-A	146	GLN	2.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	1-A	201	32/32	0.82	0.13	9,11,17,19	32
2	FOL	2-A	201	32/32	-	-	9,11,17,19	32
2	FOL	3-A	201	32/32	-	-	9,11,16,17	32
2	FOL	4-A	201	32/32	-	-	9,11,16,17	32
2	FOL	5-A	201	32/32	-	-	9,11,16,17	32
2	FOL	6-A	201	32/32	-	-	9,11,17,19	32
2	FOL	7-A	201	32/32	-	-	9,11,17,18	32
2	FOL	8-A	201	32/32	-	-	9,11,16,17	32
2	FOL	9-A	201	32/32	-	-	9,11,16,17	32
2	FOL	10-A	201	32/32	-	-	9,11,17,18	32
2	FOL	11-A	201	32/32	-	-	9,11,16,17	32
2	FOL	12-A	201	32/32	-	-	9,11,17,18	32
2	FOL	13-A	201	32/32	-	-	9,11,17,18	32
2	FOL	14-A	201	32/32	-	-	9,11,17,19	32
2	FOL	15-A	201	32/32	-	-	9,11,17,19	32
2	FOL	16-A	201	32/32	-	-	9,11,16,18	32
2	FOL	17-A	201	32/32	-	-	9,11,17,18	32
2	FOL	18-A	201	32/32	-	-	9,11,16,17	32
2	FOL	19-A	201	32/32	-	-	9,11,16,17	32
2	FOL	20-A	201	32/32	-	-	9,11,17,18	32
2	FOL	21-A	201	32/32	-	-	9,11,16,18	32
2	FOL	22-A	201	32/32	-	-	9,11,17,19	32
2	FOL	23-A	201	32/32	-	-	9,11,17,19	32
2	FOL	24-A	201	32/32	-	-	9,11,16,18	32
2	FOL	25-A	201	32/32	-	-	9,11,16,16	32
2	FOL	26-A	201	32/32	-	-	9,11,16,17	32
2	FOL	27-A	201	32/32	-	-	9,11,17,18	32

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	28-A	201	32/32	-	-	9,11,17,18	32
2	FOL	29-A	201	32/32	-	-	9,11,17,17	32
2	FOL	30-A	201	32/32	-	-	9,11,17,18	32
2	FOL	31-A	201	32/32	-	-	9,11,16,17	32
2	FOL	32-A	201	32/32	-	-	9,11,16,17	32
2	FOL	33-A	201	32/32	-	-	9,11,16,16	32
2	FOL	34-A	201	32/32	-	-	9,11,16,17	32
2	FOL	35-A	201	32/32	-	-	9,11,17,18	32
2	FOL	36-A	201	32/32	-	-	9,11,17,19	32
2	FOL	37-A	201	32/32	-	-	9,11,17,19	32
2	FOL	38-A	201	32/32	-	-	9,11,18,19	32
2	FOL	39-A	201	32/32	-	-	9,11,18,19	32
2	FOL	40-A	201	32/32	-	-	9,11,19,20	32
2	FOL	41-A	201	32/32	-	-	9,11,17,18	32
2	FOL	42-A	201	32/32	-	-	9,11,17,19	32
2	FOL	43-A	201	32/32	-	-	9,11,17,17	32
2	FOL	44-A	201	32/32	-	-	9,11,17,18	32
2	FOL	45-A	201	32/32	-	-	9,11,17,18	32
2	FOL	46-A	201	32/32	-	-	9,11,16,17	32
2	FOL	47-A	201	32/32	-	-	9,11,16,17	32
2	FOL	48-A	201	32/32	-	-	9,11,16,17	32
2	FOL	49-A	201	32/32	-	-	9,11,15,16	32
2	FOL	50-A	201	32/32	-	-	9,11,17,18	32
2	FOL	51-A	201	32/32	-	-	9,11,17,17	32
2	FOL	52-A	201	32/32	-	-	9,11,16,17	32
2	FOL	53-A	201	32/32	-	-	9,11,16,17	32
2	FOL	54-A	201	32/32	-	-	9,11,16,17	32
2	FOL	55-A	201	32/32	-	-	9,11,16,17	32
2	FOL	56-A	201	32/32	-	-	9,11,16,16	32
2	FOL	57-A	201	32/32	-	-	9,11,16,18	32
2	FOL	58-A	201	32/32	-	-	9,11,16,17	32
2	FOL	59-A	201	32/32	-	-	9,11,15,16	32
2	FOL	60-A	201	32/32	-	-	9,11,15,16	32
2	FOL	61-A	201	32/32	-	-	9,11,14,15	32
2	FOL	62-A	201	32/32	-	-	9,11,14,15	32
2	FOL	63-A	201	32/32	-	-	9,11,14,15	32
2	FOL	64-A	201	32/32	-	-	9,12,16,17	32
2	FOL	65-A	201	32/32	-	-	9,11,16,16	32
2	FOL	66-A	201	32/32	-	-	9,11,16,17	32
2	FOL	67-A	201	32/32	-	-	9,12,16,17	32
2	FOL	68-A	201	32/32	-	-	9,11,16,16	32
2	FOL	69-A	201	32/32	-	-	9,11,15,16	32

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	70-A	201	32/32	-	-	9,11,15,16	32
2	FOL	71-A	201	32/32	-	-	9,11,16,18	32
2	FOL	72-A	201	32/32	-	-	9,11,17,18	32
2	FOL	73-A	201	32/32	-	-	9,12,18,19	32
2	FOL	74-A	201	32/32	-	-	9,11,16,17	32
2	FOL	75-A	201	32/32	-	-	9,11,16,17	32
2	FOL	76-A	201	32/32	-	-	9,11,15,16	32
2	FOL	77-A	201	32/32	-	-	9,11,15,16	32
2	FOL	78-A	201	32/32	-	-	9,11,15,17	32
2	FOL	79-A	201	32/32	-	-	9,11,16,17	32
2	FOL	80-A	201	32/32	-	-	9,11,16,17	32
3	NAP	1-A	202	48/48	0.91	0.10	9,12,16,17	48
3	NAP	2-A	202	48/48	-	-	9,12,16,17	48
3	NAP	3-A	202	48/48	-	-	9,12,16,17	48
3	NAP	4-A	202	48/48	-	-	9,12,16,17	48
3	NAP	5-A	202	48/48	-	-	9,12,16,17	48
3	NAP	6-A	202	48/48	-	-	9,12,16,17	48
3	NAP	7-A	202	48/48	-	-	9,12,16,17	48
3	NAP	8-A	202	48/48	-	-	9,12,16,17	48
3	NAP	9-A	202	48/48	-	-	9,12,16,17	48
3	NAP	10-A	202	48/48	-	-	9,12,16,17	48
3	NAP	11-A	202	48/48	-	-	9,12,16,17	48
3	NAP	12-A	202	48/48	-	-	9,12,16,17	48
3	NAP	13-A	202	48/48	-	-	9,12,16,17	48
3	NAP	14-A	202	48/48	-	-	9,12,16,17	48
3	NAP	15-A	202	48/48	-	-	9,12,16,17	48
3	NAP	16-A	202	48/48	-	-	9,12,16,17	48
3	NAP	17-A	202	48/48	-	-	9,12,16,17	48
3	NAP	18-A	202	48/48	-	-	9,12,16,17	48
3	NAP	19-A	202	48/48	-	-	9,12,16,18	48
3	NAP	20-A	202	48/48	-	-	9,12,16,17	48
3	NAP	21-A	202	48/48	-	-	9,12,16,17	48
3	NAP	22-A	202	48/48	-	-	9,12,16,17	48
3	NAP	23-A	202	48/48	-	-	9,12,16,17	48
3	NAP	24-A	202	48/48	-	-	9,12,16,17	48
3	NAP	25-A	202	48/48	-	-	9,12,16,17	48
3	NAP	26-A	202	48/48	-	-	9,12,16,17	48
3	NAP	27-A	202	48/48	-	-	9,12,16,17	48
3	NAP	28-A	202	48/48	-	-	9,12,16,17	48
3	NAP	29-A	202	48/48	-	-	9,12,16,17	48
3	NAP	30-A	202	48/48	-	-	9,12,16,18	48
3	NAP	31-A	202	48/48	-	-	9,12,16,17	48

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	32-A	202	48/48	-	-	9,12,16,17	48
3	NAP	33-A	202	48/48	-	-	9,12,16,17	48
3	NAP	34-A	202	48/48	-	-	9,12,16,17	48
3	NAP	35-A	202	48/48	-	-	9,12,16,17	48
3	NAP	36-A	202	48/48	-	-	9,12,16,17	48
3	NAP	37-A	202	48/48	-	-	9,12,16,17	48
3	NAP	38-A	202	48/48	-	-	9,12,16,17	48
3	NAP	39-A	202	48/48	-	-	9,12,16,17	48
3	NAP	40-A	202	48/48	-	-	9,12,16,17	48
3	NAP	41-A	202	48/48	-	-	9,12,16,17	48
3	NAP	42-A	202	48/48	-	-	9,12,16,17	48
3	NAP	43-A	202	48/48	-	-	9,12,16,17	48
3	NAP	44-A	202	48/48	-	-	9,12,16,17	48
3	NAP	45-A	202	48/48	-	-	9,12,16,17	48
3	NAP	46-A	202	48/48	-	-	9,12,16,17	48
3	NAP	47-A	202	48/48	-	-	9,12,16,17	48
3	NAP	48-A	202	48/48	-	-	9,12,16,17	48
3	NAP	49-A	202	48/48	-	-	9,12,17,17	48
3	NAP	50-A	202	48/48	-	-	9,12,16,17	48
3	NAP	51-A	202	48/48	-	-	9,12,16,17	48
3	NAP	52-A	202	48/48	-	-	9,12,16,17	48
3	NAP	53-A	202	48/48	-	-	9,12,16,17	48
3	NAP	54-A	202	48/48	-	-	9,12,16,17	48
3	NAP	55-A	202	48/48	-	-	9,12,16,17	48
3	NAP	56-A	202	48/48	-	-	9,12,16,17	48
3	NAP	57-A	202	48/48	-	-	9,12,16,17	48
3	NAP	58-A	202	48/48	-	-	9,12,16,17	48
3	NAP	59-A	202	48/48	-	-	9,12,16,17	48
3	NAP	60-A	202	48/48	-	-	9,12,16,17	48
3	NAP	61-A	202	48/48	-	-	9,12,16,17	48
3	NAP	62-A	202	48/48	-	-	9,12,16,17	48
3	NAP	63-A	202	48/48	-	-	9,12,16,17	48
3	NAP	64-A	202	48/48	-	-	9,12,16,17	48
3	NAP	65-A	202	48/48	-	-	9,12,16,17	48
3	NAP	66-A	202	48/48	-	-	9,12,16,17	48
3	NAP	67-A	202	48/48	-	-	9,12,16,17	48
3	NAP	68-A	202	48/48	-	-	9,12,16,17	48
3	NAP	69-A	202	48/48	-	-	9,12,16,17	48
3	NAP	70-A	202	48/48	-	-	9,12,16,17	48
3	NAP	71-A	202	48/48	-	-	9,12,16,17	48
3	NAP	72-A	202	48/48	-	-	9,12,16,17	48
3	NAP	73-A	202	48/48	-	-	9,12,16,17	48

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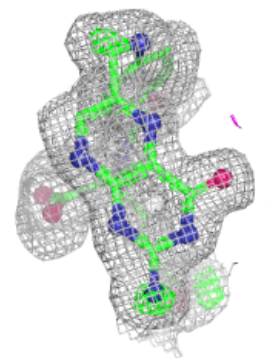
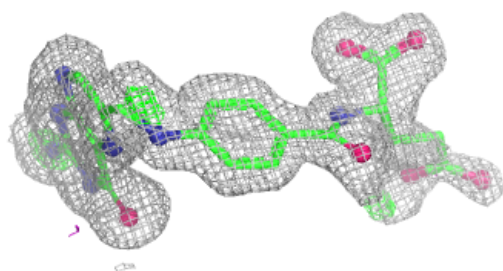
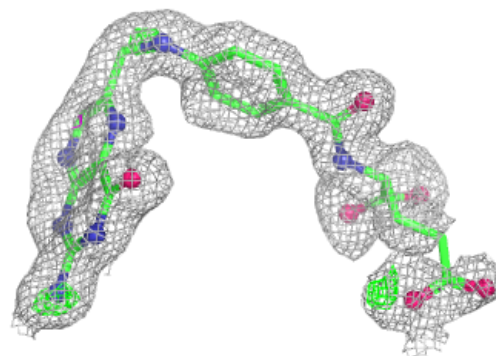
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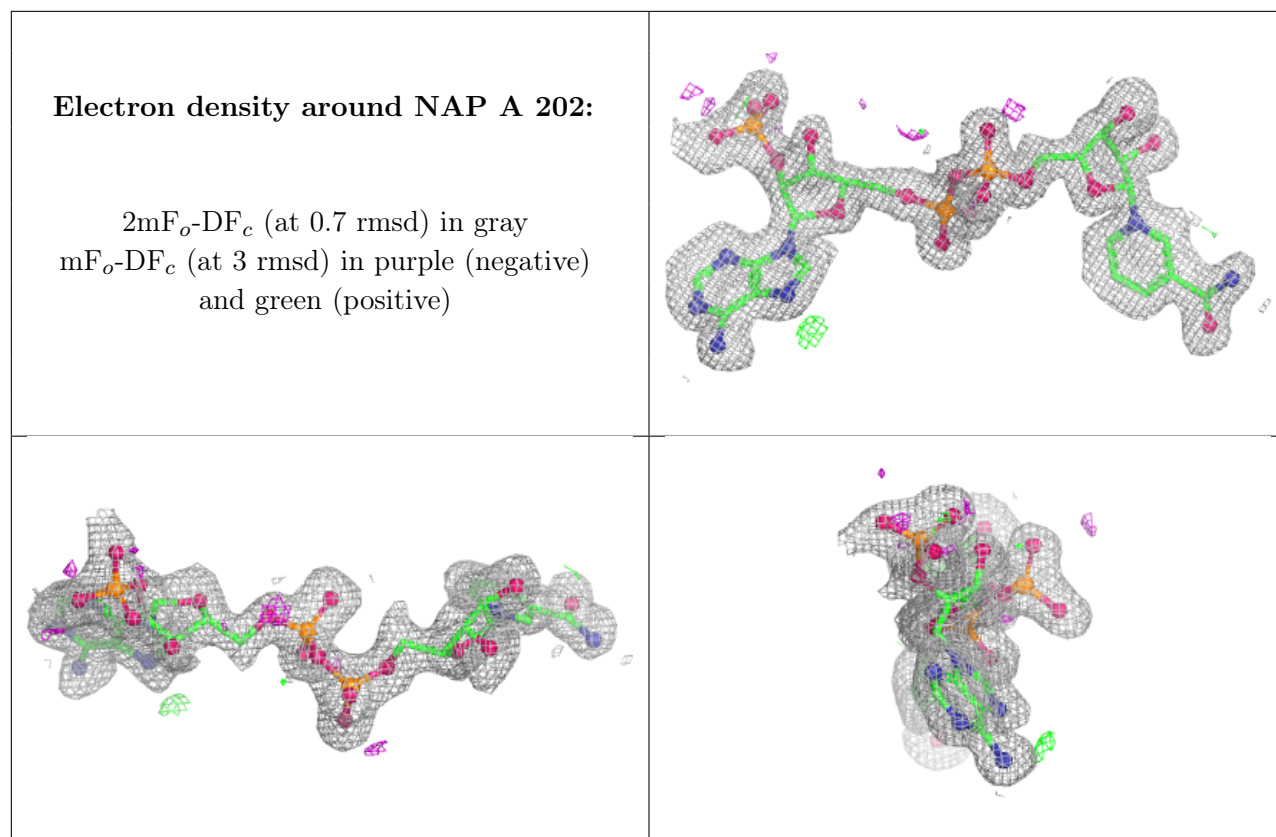
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	74-A	202	48/48	-	-	9,12,16,17	48
3	NAP	75-A	202	48/48	-	-	9,12,16,17	48
3	NAP	76-A	202	48/48	-	-	9,12,16,17	48
3	NAP	77-A	202	48/48	-	-	9,12,16,17	48
3	NAP	78-A	202	48/48	-	-	9,12,16,17	48
3	NAP	79-A	202	48/48	-	-	9,12,16,17	48
3	NAP	80-A	202	48/48	-	-	9,12,16,17	48

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FOL A 201:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





5.5 Other polymers [i](#)

There are no such residues in this entry.