



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 05:30 AM GMT

PDB ID : 2Q3O
Title : Ensemble refinement of the protein crystal structure of 12-oxo-phytodienoate reductase isoform 3
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-30
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

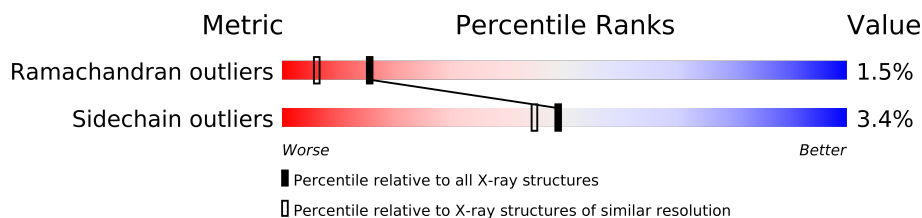
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)







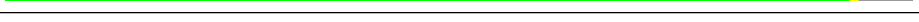

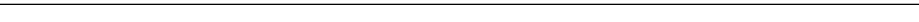

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	391	
1	1-B	391	
1	10-A	391	
1	10-B	391	
1	11-A	391	
1	11-B	391	
1	12-A	391	
1	12-B	391	
1	13-A	391	
1	13-B	391	
1	14-A	391	
1	14-B	391	
1	15-A	391	
1	15-B	391	
1	16-A	391	
1	16-B	391	
1	2-A	391	
1	2-B	391	
1	3-A	391	

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Mol	Chain	Length	Quality of chain
1	3-B	391	
1	4-A	391	
1	4-B	391	
1	5-A	391	
1	5-B	391	
1	6-A	391	
1	6-B	391	
1	7-A	391	
1	7-B	391	
1	8-A	391	
1	8-B	391	
1	9-A	391	
1	9-B	391	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 97936 atoms, of which 0 are hydrogen and 0 are deuterium.

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 12-oxophytodienoate reductase 3.

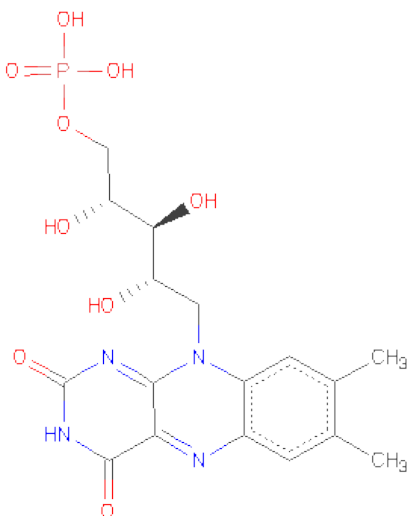
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	1-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	2-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	2-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	3-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	3-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	4-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	4-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	5-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	5-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	6-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	6-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	7-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	7-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	8-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	8-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	9-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	9-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	10-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	10-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	11-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	11-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	12-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	12-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	13-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	13-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	14-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	14-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	15-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	15-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	16-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	16-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	1-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	2-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	2-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	3-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	3-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	4-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	4-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	5-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	5-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	6-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	6-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	7-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	7-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	8-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	8-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	9-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	9-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	10-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	10-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	11-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	11-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	12-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	12-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	13-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	13-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	14-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	14-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	15-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	15-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	16-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	16-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	202	Total	O	0	0
			202	202		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-B	208	Total 208	O 208	0	0
3	2-A	202	Total 202	O 202	0	0
3	2-B	208	Total 208	O 208	0	0
3	3-A	202	Total 202	O 202	0	0
3	3-B	208	Total 208	O 208	0	0
3	4-A	203	Total 203	O 203	0	0
3	4-B	207	Total 207	O 207	0	0
3	5-A	205	Total 205	O 205	0	0
3	5-B	205	Total 205	O 205	0	0
3	6-A	203	Total 203	O 203	0	0
3	6-B	207	Total 207	O 207	0	0
3	7-A	203	Total 203	O 203	0	0
3	7-B	207	Total 207	O 207	0	0
3	8-A	201	Total 201	O 201	0	0
3	8-B	209	Total 209	O 209	0	0
3	9-A	205	Total 205	O 205	0	0
3	9-B	205	Total 205	O 205	0	0
3	10-A	200	Total 200	O 200	0	0
3	10-B	210	Total 210	O 210	0	0
3	11-A	203	Total 203	O 203	0	0
3	11-B	207	Total 207	O 207	0	0

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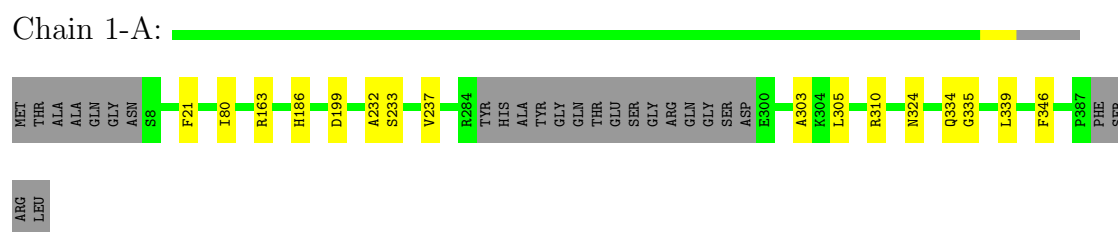
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	12-A	206	Total 206	O 206	0	0
3	12-B	204	Total 204	O 204	0	0
3	13-A	206	Total 206	O 206	0	0
3	13-B	204	Total 204	O 204	0	0
3	14-A	202	Total 202	O 202	0	0
3	14-B	208	Total 208	O 208	0	0
3	15-A	200	Total 200	O 200	0	0
3	15-B	210	Total 210	O 210	0	0
3	16-A	204	Total 204	O 204	0	0
3	16-B	206	Total 206	O 206	0	0

3 Residue-property plots

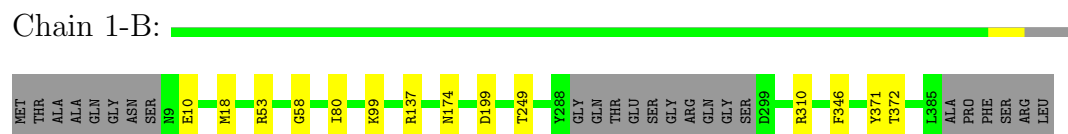
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

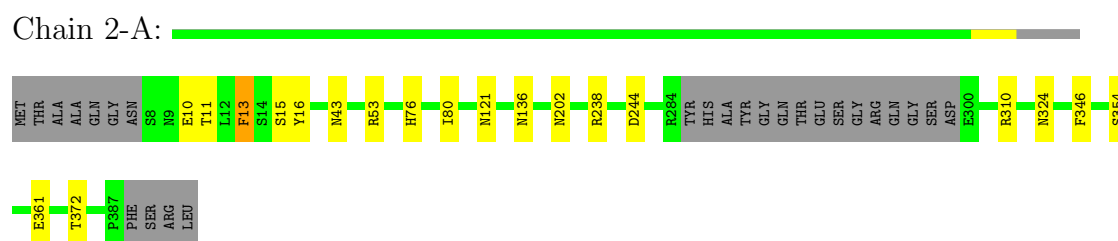
- Molecule 1: 12-oxophytodienoate reductase 3



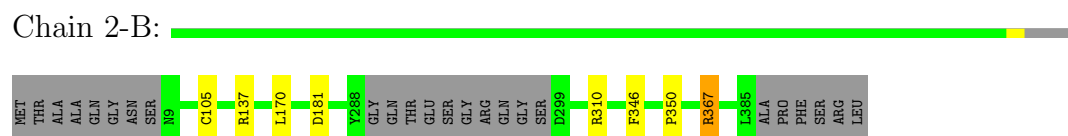
- Molecule 1: 12-oxophytodienoate reductase 3



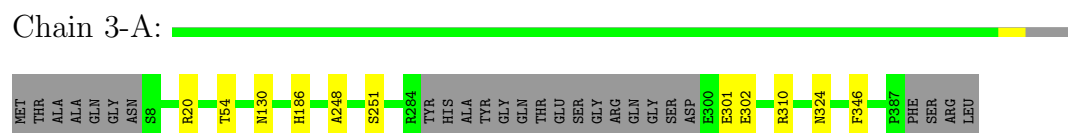
- Molecule 1: 12-oxophytodienoate reductase 3



- Molecule 1: 12-oxophytodienoate reductase 3



- Molecule 1: 12-oxophytodienoate reductase 3



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 3-B:

- Molecule 1: 12-oxophytodienoate reductase 3

Chain 4-A:

LEU

- Molecule 1: 12-oxophytodienoate reductase 3

Chain 4-B:

- Molecule 1: 12-oxophytodienoate reductase 3

Chain 5-A:

- Molecule 1: 12-oxophytodienoate reductase 3

Chain 5-B:

- Molecule 1: 12-oxophytodienoate reductase 3

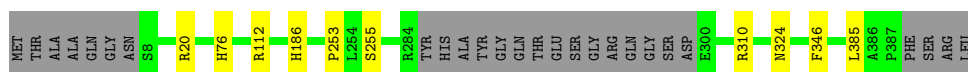
Chain 6-A:

- Molecule 1: 12-oxophytodienoate reductase 3

Chain 6-B:

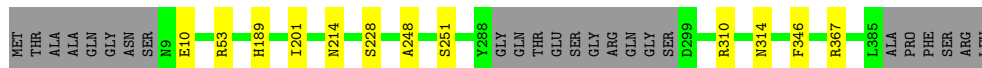
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 7-A:



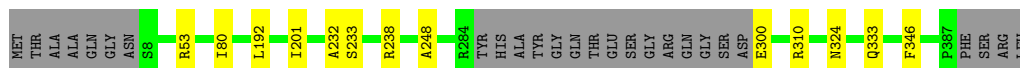
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 7-B:



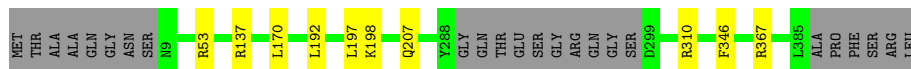
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 8-B:



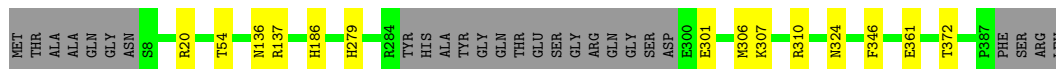
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 9-B:



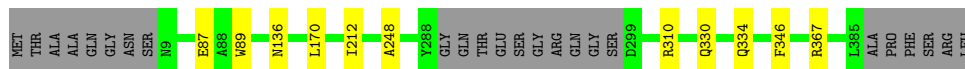
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 10-B:



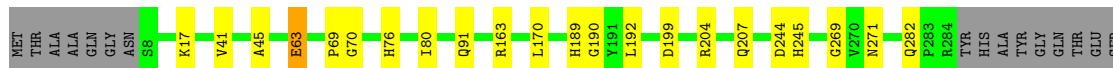
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 11-B:



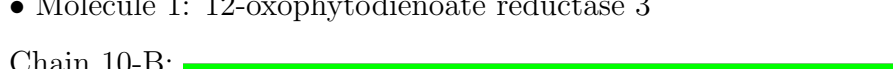
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 12-B:



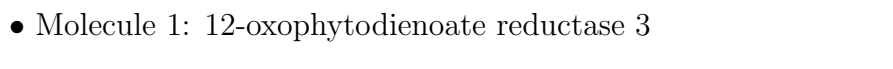
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 13-B:



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 14-B:



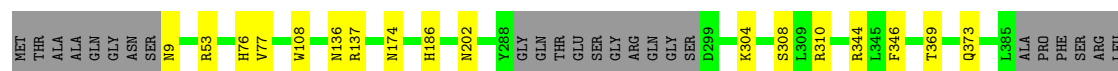
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 11-A: 



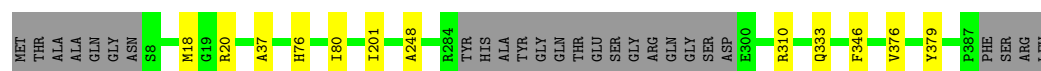
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 11-B: 



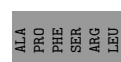
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 12-A: 



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 12-B: 



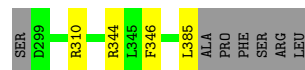
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 13-A: 



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 13-B: 



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 14-A: 





- Molecule 1: 12-oxophytodienoate reductase 3

Chain 14-B:



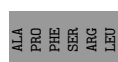
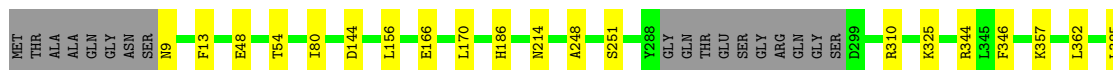
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 15-A:



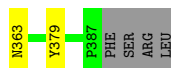
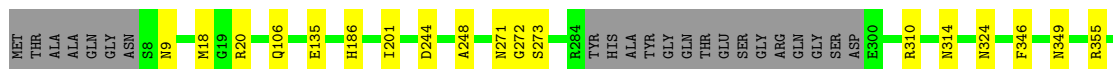
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 15-B:



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 16-A:



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 16-B:



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.11Å 85.07Å 121.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.90 – 2.00	Depositor
% Data completeness (in resolution range)	91.1 (24.90-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.235	Depositor
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.057	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 50628 reflections (0.004%)	Xtriage
Total number of atoms	97936	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1-A	0.41	0/2875	0.64	0/3895
1	1-B	0.40	0/2906	0.64	0/3937
1	2-A	0.43	0/2875	0.65	0/3895
1	2-B	0.41	0/2906	0.63	0/3937
1	3-A	0.41	0/2875	0.64	0/3895
1	3-B	0.42	0/2906	0.65	0/3937
1	4-A	0.42	0/2875	0.64	0/3895
1	4-B	0.41	0/2906	0.64	0/3937
1	5-A	0.41	0/2875	0.64	0/3895
1	5-B	0.41	0/2906	0.64	0/3937
1	6-A	0.41	0/2875	0.64	0/3895
1	6-B	0.41	0/2906	0.64	0/3937
1	7-A	0.41	0/2875	0.64	0/3895
1	7-B	0.41	0/2906	0.65	0/3937
1	8-A	0.41	0/2875	0.65	0/3895
1	8-B	0.42	0/2906	0.64	0/3937
1	9-A	0.41	0/2875	0.63	0/3895
1	9-B	0.41	0/2906	0.63	0/3937
1	10-A	0.41	0/2875	0.66	0/3895
1	10-B	0.41	0/2906	0.64	0/3937
1	11-A	0.41	0/2875	0.65	0/3895
1	11-B	0.41	0/2906	0.64	0/3937
1	12-A	0.41	0/2875	0.64	0/3895
1	12-B	0.41	0/2906	0.64	0/3937
1	13-A	0.46	0/2875	0.70	0/3895
1	13-B	0.47	0/2906	0.72	1/3937 (0.0%)
1	14-A	0.46	0/2875	0.70	0/3895
1	14-B	0.48	0/2906	0.71	0/3937
1	15-A	0.46	0/2875	0.72	0/3895
1	15-B	0.46	0/2906	0.71	1/3937 (0.0%)
1	16-A	0.45	0/2875	0.71	0/3895
1	16-B	0.46	0/2906	0.71	1/3937 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.43	0/92496	0.66	3/125312 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	13-B	170	LEU	CA-CB-CG	5.53	128.01	115.30
1	16-B	108	TRP	N-CA-C	5.14	124.88	111.00
1	15-B	170	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	2810	0	2766	0	0
1	1-B	2839	0	2783	0	0
1	2-A	2810	0	2766	0	0
1	2-B	2839	0	2783	0	0
1	3-A	2810	0	2766	0	0
1	3-B	2839	0	2783	0	0
1	4-A	2810	0	2766	0	0
1	4-B	2839	0	2783	0	0
1	5-A	2810	0	2766	0	0
1	5-B	2839	0	2783	0	0
1	6-A	2810	0	2766	0	0
1	6-B	2839	0	2783	0	0
1	7-A	2810	0	2766	0	0
1	7-B	2839	0	2783	0	0
1	8-A	2810	0	2766	0	0
1	8-B	2839	0	2783	0	0
1	9-A	2810	0	2766	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	9-B	2839	0	2783	0	0
1	10-A	2810	0	2766	0	0
1	10-B	2839	0	2783	0	0
1	11-A	2810	0	2766	0	0
1	11-B	2839	0	2783	0	0
1	12-A	2810	0	2766	0	0
1	12-B	2839	0	2783	0	0
1	13-A	2810	0	2766	0	0
1	13-B	2839	0	2783	0	0
1	14-A	2810	0	2766	0	0
1	14-B	2839	0	2783	0	0
1	15-A	2810	0	2766	0	0
1	15-B	2839	0	2783	0	0
1	16-A	2810	0	2766	0	0
1	16-B	2839	0	2783	0	0
2	1-A	31	0	19	0	0
2	1-B	31	0	19	0	0
2	2-A	31	0	19	0	0
2	2-B	31	0	19	0	0
2	3-A	31	0	19	0	0
2	3-B	31	0	19	0	0
2	4-A	31	0	19	0	0
2	4-B	31	0	19	0	0
2	5-A	31	0	19	0	0
2	5-B	31	0	19	0	0
2	6-A	31	0	19	0	0
2	6-B	31	0	19	0	0
2	7-A	31	0	19	0	0
2	7-B	31	0	19	0	0
2	8-A	31	0	19	0	0
2	8-B	31	0	19	0	0
2	9-A	31	0	19	0	0
2	9-B	31	0	19	0	0
2	10-A	31	0	19	0	0
2	10-B	31	0	19	0	0
2	11-A	31	0	19	0	0
2	11-B	31	0	19	0	0
2	12-A	31	0	19	0	0
2	12-B	31	0	19	0	0
2	13-A	31	0	18	0	0
2	13-B	31	0	19	0	0
2	14-A	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	14-B	31	0	18	0	0
2	15-A	31	0	19	0	0
2	15-B	31	0	19	0	0
2	16-A	31	0	18	0	0
2	16-B	31	0	19	0	0
3	1-A	202	0	0	0	1
3	1-B	208	0	0	0	1
3	2-A	202	0	0	0	1
3	2-B	208	0	0	0	1
3	3-A	202	0	0	0	1
3	3-B	208	0	0	0	1
3	4-A	203	0	0	0	1
3	4-B	207	0	0	0	1
3	5-A	205	0	0	0	1
3	5-B	205	0	0	0	1
3	6-A	203	0	0	0	1
3	6-B	207	0	0	0	1
3	7-A	203	0	0	0	1
3	7-B	207	0	0	0	1
3	8-A	201	0	0	0	1
3	8-B	209	0	0	0	1
3	9-A	205	0	0	0	1
3	9-B	205	0	0	0	1
3	10-A	200	0	0	0	1
3	10-B	210	0	0	0	1
3	11-A	203	0	0	0	1
3	11-B	207	0	0	0	1
3	12-A	206	0	0	0	1
3	12-B	204	0	0	0	1
3	13-A	206	0	0	0	1
3	13-B	204	0	0	0	1
3	14-A	202	0	0	0	1
3	14-B	208	0	0	0	1
3	15-A	200	0	0	0	1
3	15-B	210	0	0	0	1
3	16-A	204	0	0	0	1
3	16-B	206	0	0	0	1
All	All	97936	0	89389	0	16

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

All (16) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:7506:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7506:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7506:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7507:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7509:HOH:O	3:B:9428:HOH:O[3_655]	2.11	0.09
3:A:7507:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7508:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7506:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7508:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7504:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7507:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7509:HOH:O	3:B:9428:HOH:O[3_655]	2.11	0.09
3:A:7508:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7505:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09
3:A:7504:HOH:O	3:B:9430:HOH:O[3_655]	2.11	0.09
3:A:7508:HOH:O	3:B:9429:HOH:O[3_655]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	361/391 (92%)	317 (88%)	35 (10%)	9 (2%)	9	2
1	1-B	363/391 (93%)	333 (92%)	25 (7%)	5 (1%)	16	7
1	2-A	361/391 (92%)	300 (83%)	51 (14%)	10 (3%)	8	2
1	2-B	363/391 (93%)	337 (93%)	24 (7%)	2 (1%)	33	24
1	3-A	361/391 (92%)	336 (93%)	22 (6%)	3 (1%)	27	17
1	3-B	363/391 (93%)	339 (93%)	18 (5%)	6 (2%)	14	5
1	4-A	361/391 (92%)	322 (89%)	33 (9%)	6 (2%)	14	5
1	4-B	363/391 (93%)	338 (93%)	20 (6%)	5 (1%)	16	7
1	5-A	361/391 (92%)	331 (92%)	29 (8%)	1 (0%)	50	44
1	5-B	363/391 (93%)	341 (94%)	20 (6%)	2 (1%)	33	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6-A	361/391 (92%)	338 (94%)	22 (6%)	1 (0%)	50	44
1	6-B	363/391 (93%)	341 (94%)	22 (6%)	0	100	100
1	7-A	361/391 (92%)	333 (92%)	24 (7%)	4 (1%)	21	10
1	7-B	363/391 (93%)	334 (92%)	23 (6%)	6 (2%)	14	5
1	8-A	361/391 (92%)	324 (90%)	31 (9%)	6 (2%)	14	5
1	8-B	363/391 (93%)	332 (92%)	28 (8%)	3 (1%)	27	17
1	9-A	361/391 (92%)	330 (91%)	23 (6%)	8 (2%)	10	3
1	9-B	363/391 (93%)	335 (92%)	26 (7%)	2 (1%)	33	24
1	10-A	361/391 (92%)	309 (86%)	33 (9%)	19 (5%)	3	0
1	10-B	363/391 (93%)	338 (93%)	24 (7%)	1 (0%)	50	44
1	11-A	361/391 (92%)	336 (93%)	22 (6%)	3 (1%)	27	17
1	11-B	363/391 (93%)	337 (93%)	22 (6%)	4 (1%)	21	10
1	12-A	361/391 (92%)	328 (91%)	25 (7%)	8 (2%)	10	3
1	12-B	363/391 (93%)	326 (90%)	32 (9%)	5 (1%)	16	7
1	13-A	361/391 (92%)	322 (89%)	35 (10%)	4 (1%)	21	10
1	13-B	363/391 (93%)	327 (90%)	27 (7%)	9 (2%)	9	2
1	14-A	361/391 (92%)	312 (86%)	42 (12%)	7 (2%)	12	4
1	14-B	363/391 (93%)	311 (86%)	45 (12%)	7 (2%)	12	4
1	15-A	361/391 (92%)	324 (90%)	33 (9%)	4 (1%)	21	10
1	15-B	363/391 (93%)	326 (90%)	31 (8%)	6 (2%)	14	5
1	16-A	361/391 (92%)	324 (90%)	30 (8%)	7 (2%)	12	4
1	16-B	363/391 (93%)	332 (92%)	26 (7%)	5 (1%)	16	7
All	All	11584/12512 (93%)	10513 (91%)	903 (8%)	168 (2%)	15	6

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	233	SER
1	1-A	303	ALA
1	2-A	13	PHE
1	2-A	15	SER
1	2-A	76	HIS
1	2-A	80	ILE
1	2-A	121	ASN

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Mol	Chain	Res	Type
1	4-B	136	ASN
1	7-B	251	SER
1	8-A	248	ALA
1	9-B	136	ASN
1	10-A	76	HIS
1	10-A	189	HIS
1	10-A	190	GLY
1	10-A	204	ARG
1	10-A	245	HIS
1	11-A	18	MET
1	11-A	248	ALA
1	11-B	136	ASN
1	11-B	202	ASN
1	12-A	37	ALA
1	12-B	136	ASN
1	13-A	251	SER
1	13-B	136	ASN
1	13-B	180	PHE
1	14-A	39	ASN
1	1-A	305	LEU
1	1-A	335	GLY
1	1-A	339	LEU
1	1-B	18	MET
1	1-B	58	GLY
1	1-B	372	THR
1	2-A	16	TYR
1	2-A	202	ASN
1	3-A	248	ALA
1	4-A	192	LEU
1	4-B	202	ASN
1	6-A	301	GLU
1	7-A	76	HIS
1	7-B	189	HIS
1	7-B	201	ILE
1	8-A	80	ILE
1	8-A	232	ALA
1	8-B	197	LEU
1	9-A	279	HIS
1	9-A	306	MET
1	10-A	269	GLY
1	10-A	271	ASN
1	11-B	76	HIS

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Mol	Chain	Res	Type
1	12-A	18	MET
1	12-A	379	TYR
1	13-A	76	HIS
1	13-B	145	GLY
1	13-B	202	ASN
1	14-A	145	GLY
1	14-B	192	LEU
1	15-A	273	SER
1	15-B	13	PHE
1	16-A	18	MET
1	16-A	248	ALA
1	16-A	379	TYR
1	16-B	248	ALA
1	16-B	273	SER
1	1-A	80	ILE
1	2-A	361	GLU
1	3-B	20	ARG
1	3-B	248	ALA
1	3-B	272	GLY
1	4-A	38	LEU
1	4-A	204	ARG
1	4-A	248	ALA
1	4-A	334	GLN
1	5-B	229	ALA
1	7-B	10	GLU
1	7-B	228	SER
1	8-A	233	SER
1	8-B	192	LEU
1	8-B	198	LYS
1	9-A	307	LYS
1	9-B	248	ALA
1	10-A	45	ALA
1	10-A	70	GLY
1	10-A	379	TYR
1	10-A	383	PRO
1	12-A	201	ILE
1	12-A	248	ALA
1	13-A	91	GLN
1	14-A	91	GLN
1	14-B	148	VAL
1	14-B	377	VAL
1	15-A	268	GLN

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Mol	Chain	Res	Type
1	15-A	272	GLY
1	15-B	251	SER
1	16-A	273	SER
1	2-A	11	THR
1	2-A	136	ASN
1	3-A	251	SER
1	3-A	301	GLU
1	3-B	377	VAL
1	5-A	136	ASN
1	9-A	186	HIS
1	9-A	301	GLU
1	10-A	91	GLN
1	11-B	308	SER
1	12-A	76	HIS
1	12-B	27	VAL
1	14-A	9	ASN
1	14-A	136	ASN
1	15-B	248	ALA
1	15-B	362	LEU
1	16-B	144	ASP
1	16-B	345	LEU
1	1-A	232	ALA
1	1-A	334	GLN
1	2-B	367	ARG
1	4-B	229	ALA
1	4-B	333	GLN
1	5-B	248	ALA
1	7-A	112	ARG
1	7-A	255	SER
1	7-B	248	ALA
1	9-A	136	ASN
1	9-A	361	GLU
1	10-A	192	LEU
1	10-A	207	GLN
1	10-A	386	ALA
1	13-A	148	VAL
1	13-B	10	GLU
1	13-B	38	LEU
1	13-B	178	ALA
1	14-A	248	ALA
1	14-B	245	HIS
1	14-B	375	PRO

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Mol	Chain	Res	Type
1	15-A	113	ALA
1	15-B	144	ASP
1	15-B	357	LYS
1	16-A	201	ILE
1	16-A	271	ASN
1	16-A	272	GLY
1	16-B	189	HIS
1	1-B	10	GLU
1	3-B	376	VAL
1	4-A	301	GLU
1	4-B	19	GLY
1	8-A	192	LEU
1	9-A	137	ARG
1	10-A	63	GLU
1	12-B	248	ALA
1	14-B	137	ARG
1	14-B	376	VAL
1	3-B	375	PRO
1	8-A	201	ILE
1	10-A	321	GLY
1	12-B	343	GLY
1	13-B	93	VAL
1	1-B	80	ILE
1	7-A	253	PRO
1	10-A	69	PRO
1	10-B	140	VAL
1	12-A	80	ILE
1	10-A	80	ILE
1	11-A	56	PRO
1	1-A	237	VAL
1	2-B	350	PRO
1	12-A	376	VAL
1	12-B	322	GLY
1	13-B	143	PRO
1	14-A	68	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	298/317 (94%)	291 (98%)	7 (2%)	63	63
1	1-B	300/317 (95%)	291 (97%)	9 (3%)	53	50
1	2-A	298/317 (94%)	287 (96%)	11 (4%)	45	40
1	2-B	300/317 (95%)	293 (98%)	7 (2%)	63	63
1	3-A	298/317 (94%)	290 (97%)	8 (3%)	57	56
1	3-B	300/317 (95%)	291 (97%)	9 (3%)	53	50
1	4-A	298/317 (94%)	288 (97%)	10 (3%)	49	45
1	4-B	300/317 (95%)	291 (97%)	9 (3%)	53	50
1	5-A	298/317 (94%)	292 (98%)	6 (2%)	68	69
1	5-B	300/317 (95%)	292 (97%)	8 (3%)	57	56
1	6-A	298/317 (94%)	291 (98%)	7 (2%)	63	63
1	6-B	300/317 (95%)	295 (98%)	5 (2%)	73	75
1	7-A	298/317 (94%)	292 (98%)	6 (2%)	68	69
1	7-B	300/317 (95%)	294 (98%)	6 (2%)	68	69
1	8-A	298/317 (94%)	291 (98%)	7 (2%)	63	63
1	8-B	300/317 (95%)	293 (98%)	7 (2%)	63	63
1	9-A	298/317 (94%)	292 (98%)	6 (2%)	68	69
1	9-B	300/317 (95%)	291 (97%)	9 (3%)	53	50
1	10-A	298/317 (94%)	284 (95%)	14 (5%)	36	29
1	10-B	300/317 (95%)	292 (97%)	8 (3%)	57	56
1	11-A	298/317 (94%)	289 (97%)	9 (3%)	53	50
1	11-B	300/317 (95%)	287 (96%)	13 (4%)	40	33
1	12-A	298/317 (94%)	294 (99%)	4 (1%)	80	82
1	12-B	300/317 (95%)	287 (96%)	13 (4%)	40	33
1	13-A	298/317 (94%)	285 (96%)	13 (4%)	39	32
1	13-B	300/317 (95%)	284 (95%)	16 (5%)	32	24
1	14-A	298/317 (94%)	276 (93%)	22 (7%)	20	12
1	14-B	300/317 (95%)	277 (92%)	23 (8%)	18	11
1	15-A	298/317 (94%)	282 (95%)	16 (5%)	31	24
1	15-B	300/317 (95%)	287 (96%)	13 (4%)	40	33
1	16-A	298/317 (94%)	285 (96%)	13 (4%)	39	32
1	16-B	300/317 (95%)	290 (97%)	10 (3%)	50	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9568/10144 (94%)	9244 (97%)	324 (3%)	49 45

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	21	PHE
1	1-A	163	ARG
1	1-A	186	HIS
1	1-A	199	ASP
1	1-A	310	ARG
1	1-A	324	ASN
1	1-A	346	PHE
1	1-B	53	ARG
1	1-B	99	LYS
1	1-B	137	ARG
1	1-B	174	ASN
1	1-B	199	ASP
1	1-B	249	THR
1	1-B	310	ARG
1	1-B	346	PHE
1	1-B	371	TYR
1	2-A	10	GLU
1	2-A	13	PHE
1	2-A	43	ASN
1	2-A	53	ARG
1	2-A	238	ARG
1	2-A	244	ASP
1	2-A	310	ARG
1	2-A	324	ASN
1	2-A	346	PHE
1	2-A	354	SER
1	2-A	372	THR
1	2-B	105	CYS
1	2-B	137	ARG
1	2-B	170	LEU
1	2-B	181	ASP
1	2-B	310	ARG
1	2-B	346	PHE
1	2-B	367	ARG
1	3-A	20	ARG
1	3-A	54	THR
1	3-A	130	ASN

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Mol	Chain	Res	Type
1	3-A	186	HIS
1	3-A	302	GLU
1	3-A	310	ARG
1	3-A	324	ASN
1	3-A	346	PHE
1	3-B	54	THR
1	3-B	77	VAL
1	3-B	109	HIS
1	3-B	181	ASP
1	3-B	186	HIS
1	3-B	310	ARG
1	3-B	326	GLU
1	3-B	346	PHE
1	3-B	367	ARG
1	4-A	38	LEU
1	4-A	54	THR
1	4-A	94	GLU
1	4-A	144	ASP
1	4-A	186	HIS
1	4-A	310	ARG
1	4-A	324	ASN
1	4-A	346	PHE
1	4-A	349	ASN
1	4-A	354	SER
1	4-B	22	ASP
1	4-B	53	ARG
1	4-B	60	LEU
1	4-B	137	ARG
1	4-B	174	ASN
1	4-B	207	GLN
1	4-B	244	ASP
1	4-B	310	ARG
1	4-B	346	PHE
1	5-A	21	PHE
1	5-A	54	THR
1	5-A	302	GLU
1	5-A	310	ARG
1	5-A	324	ASN
1	5-A	346	PHE
1	5-B	54	THR
1	5-B	136	ASN
1	5-B	146	SER

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Mol	Chain	Res	Type
1	5-B	186	HIS
1	5-B	199	ASP
1	5-B	212	ILE
1	5-B	310	ARG
1	5-B	346	PHE
1	6-A	54	THR
1	6-A	174	ASN
1	6-A	244	ASP
1	6-A	310	ARG
1	6-A	324	ASN
1	6-A	336	ASP
1	6-A	346	PHE
1	6-B	137	ARG
1	6-B	170	LEU
1	6-B	199	ASP
1	6-B	310	ARG
1	6-B	346	PHE
1	7-A	20	ARG
1	7-A	186	HIS
1	7-A	310	ARG
1	7-A	324	ASN
1	7-A	346	PHE
1	7-A	385	LEU
1	7-B	53	ARG
1	7-B	214	ASN
1	7-B	310	ARG
1	7-B	314	ASN
1	7-B	346	PHE
1	7-B	367	ARG
1	8-A	53	ARG
1	8-A	238	ARG
1	8-A	300	GLU
1	8-A	310	ARG
1	8-A	324	ASN
1	8-A	333	GLN
1	8-A	346	PHE
1	8-B	53	ARG
1	8-B	137	ARG
1	8-B	170	LEU
1	8-B	207	GLN
1	8-B	310	ARG
1	8-B	346	PHE

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Mol	Chain	Res	Type
1	8-B	367	ARG
1	9-A	20	ARG
1	9-A	54	THR
1	9-A	310	ARG
1	9-A	324	ASN
1	9-A	346	PHE
1	9-A	372	THR
1	9-B	87	GLU
1	9-B	89	TRP
1	9-B	170	LEU
1	9-B	212	ILE
1	9-B	310	ARG
1	9-B	330	GLN
1	9-B	334	GLN
1	9-B	346	PHE
1	9-B	367	ARG
1	10-A	17	LYS
1	10-A	41	VAL
1	10-A	63	GLU
1	10-A	163	ARG
1	10-A	170	LEU
1	10-A	199	ASP
1	10-A	244	ASP
1	10-A	282	GLN
1	10-A	310	ARG
1	10-A	311	MET
1	10-A	324	ASN
1	10-A	326	GLU
1	10-A	330	GLN
1	10-A	346	PHE
1	10-B	54	THR
1	10-B	170	LEU
1	10-B	214	ASN
1	10-B	285	TYR
1	10-B	310	ARG
1	10-B	333	GLN
1	10-B	346	PHE
1	10-B	367	ARG
1	11-A	21	PHE
1	11-A	60	LEU
1	11-A	134	SER
1	11-A	186	HIS

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Mol	Chain	Res	Type
1	11-A	251	SER
1	11-A	252	ASP
1	11-A	310	ARG
1	11-A	324	ASN
1	11-A	346	PHE
1	11-B	9	ASN
1	11-B	53	ARG
1	11-B	77	VAL
1	11-B	108	TRP
1	11-B	137	ARG
1	11-B	174	ASN
1	11-B	186	HIS
1	11-B	304	LYS
1	11-B	310	ARG
1	11-B	344	ARG
1	11-B	346	PHE
1	11-B	369	THR
1	11-B	373	GLN
1	12-A	20	ARG
1	12-A	310	ARG
1	12-A	333	GLN
1	12-A	346	PHE
1	12-B	54	THR
1	12-B	87	GLU
1	12-B	131	LYS
1	12-B	163	ARG
1	12-B	166	GLU
1	12-B	170	LEU
1	12-B	184	GLU
1	12-B	310	ARG
1	12-B	314	ASN
1	12-B	324	ASN
1	12-B	341	SER
1	12-B	346	PHE
1	12-B	367	ARG
1	13-A	20	ARG
1	13-A	54	THR
1	13-A	80	ILE
1	13-A	105	CYS
1	13-A	130	ASN
1	13-A	184	GLU
1	13-A	186	HIS

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Mol	Chain	Res	Type
1	13-A	284	ARG
1	13-A	310	ARG
1	13-A	324	ASN
1	13-A	346	PHE
1	13-A	354	SER
1	13-A	372	THR
1	13-B	54	THR
1	13-B	80	ILE
1	13-B	87	GLU
1	13-B	97	HIS
1	13-B	99	LYS
1	13-B	137	ARG
1	13-B	151	PRO
1	13-B	170	LEU
1	13-B	174	ASN
1	13-B	184	GLU
1	13-B	194	ASP
1	13-B	247	ASP
1	13-B	310	ARG
1	13-B	344	ARG
1	13-B	346	PHE
1	13-B	385	LEU
1	14-A	14	SER
1	14-A	20	ARG
1	14-A	54	THR
1	14-A	63	GLU
1	14-A	71	SER
1	14-A	104	PHE
1	14-A	105	CYS
1	14-A	106	GLN
1	14-A	130	ASN
1	14-A	147	HIS
1	14-A	149	LYS
1	14-A	184	GLU
1	14-A	186	HIS
1	14-A	199	ASP
1	14-A	310	ARG
1	14-A	314	ASN
1	14-A	324	ASN
1	14-A	336	ASP
1	14-A	341	SER
1	14-A	346	PHE

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Mol	Chain	Res	Type
1	14-A	365	TYR
1	14-A	385	LEU
1	14-B	46	LEU
1	14-B	52	GLN
1	14-B	54	THR
1	14-B	60	LEU
1	14-B	80	ILE
1	14-B	84	GLU
1	14-B	106	GLN
1	14-B	135	GLU
1	14-B	137	ARG
1	14-B	151	PRO
1	14-B	157	GLU
1	14-B	186	HIS
1	14-B	203	ASP
1	14-B	214	ASN
1	14-B	216	CYS
1	14-B	278	LEU
1	14-B	285	TYR
1	14-B	304	LYS
1	14-B	310	ARG
1	14-B	314	ASN
1	14-B	346	PHE
1	14-B	367	ARG
1	14-B	385	LEU
1	15-A	21	PHE
1	15-A	54	THR
1	15-A	105	CYS
1	15-A	114	SER
1	15-A	147	HIS
1	15-A	174	ASN
1	15-A	184	GLU
1	15-A	186	HIS
1	15-A	195	GLN
1	15-A	228	SER
1	15-A	244	ASP
1	15-A	300	GLU
1	15-A	310	ARG
1	15-A	324	ASN
1	15-A	346	PHE
1	15-A	372	THR
1	15-B	9	ASN

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Mol	Chain	Res	Type
1	15-B	48	GLU
1	15-B	54	THR
1	15-B	80	ILE
1	15-B	156	LEU
1	15-B	166	GLU
1	15-B	186	HIS
1	15-B	214	ASN
1	15-B	310	ARG
1	15-B	325	LYS
1	15-B	344	ARG
1	15-B	346	PHE
1	15-B	385	LEU
1	16-A	9	ASN
1	16-A	20	ARG
1	16-A	106	GLN
1	16-A	135	GLU
1	16-A	186	HIS
1	16-A	244	ASP
1	16-A	310	ARG
1	16-A	314	ASN
1	16-A	324	ASN
1	16-A	346	PHE
1	16-A	349	ASN
1	16-A	355	ARG
1	16-A	363	ASN
1	16-B	46	LEU
1	16-B	53	ARG
1	16-B	137	ARG
1	16-B	138	TRP
1	16-B	186	HIS
1	16-B	214	ASN
1	16-B	240	SER
1	16-B	310	ARG
1	16-B	346	PHE
1	16-B	385	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (348) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	39	ASN
1	1-A	52	GLN
1	1-A	97	HIS

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Mol	Chain	Res	Type
1	1-A	195	GLN
1	1-A	268	GLN
1	1-A	271	ASN
1	1-A	324	ASN
1	1-A	333	GLN
1	1-B	39	ASN
1	1-B	97	HIS
1	1-B	174	ASN
1	1-B	195	GLN
1	1-B	214	ASN
1	1-B	268	GLN
1	1-B	314	ASN
1	1-B	330	GLN
1	1-B	334	GLN
1	1-B	366	ASN
1	2-A	39	ASN
1	2-A	43	ASN
1	2-A	52	GLN
1	2-A	97	HIS
1	2-A	195	GLN
1	2-A	214	ASN
1	2-A	221	GLN
1	2-A	268	GLN
1	2-A	271	ASN
1	2-A	324	ASN
1	2-A	334	GLN
1	2-B	39	ASN
1	2-B	76	HIS
1	2-B	119	GLN
1	2-B	174	ASN
1	2-B	195	GLN
1	2-B	214	ASN
1	2-B	268	GLN
1	2-B	271	ASN
1	2-B	282	GLN
1	2-B	314	ASN
1	2-B	334	GLN
1	3-A	39	ASN
1	3-A	52	GLN
1	3-A	97	HIS
1	3-A	195	GLN
1	3-A	221	GLN

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Mol	Chain	Res	Type
1	3-A	268	GLN
1	3-A	271	ASN
1	3-A	282	GLN
1	3-A	324	ASN
1	3-A	334	GLN
1	3-B	39	ASN
1	3-B	91	GLN
1	3-B	109	HIS
1	3-B	119	GLN
1	3-B	174	ASN
1	3-B	195	GLN
1	3-B	214	ASN
1	3-B	268	GLN
1	3-B	314	ASN
1	3-B	334	GLN
1	3-B	373	GLN
1	4-A	39	ASN
1	4-A	97	HIS
1	4-A	119	GLN
1	4-A	147	HIS
1	4-A	195	GLN
1	4-A	268	GLN
1	4-A	282	GLN
1	4-A	314	ASN
1	4-A	324	ASN
1	4-B	39	ASN
1	4-B	76	HIS
1	4-B	97	HIS
1	4-B	174	ASN
1	4-B	195	GLN
1	4-B	207	GLN
1	4-B	214	ASN
1	4-B	268	GLN
1	4-B	271	ASN
1	4-B	314	ASN
1	4-B	334	GLN
1	5-A	39	ASN
1	5-A	52	GLN
1	5-A	97	HIS
1	5-A	195	GLN
1	5-A	221	GLN
1	5-A	268	GLN

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Mol	Chain	Res	Type
1	5-A	314	ASN
1	5-A	324	ASN
1	5-A	334	GLN
1	5-B	9	ASN
1	5-B	39	ASN
1	5-B	76	HIS
1	5-B	97	HIS
1	5-B	174	ASN
1	5-B	189	HIS
1	5-B	195	GLN
1	5-B	214	ASN
1	5-B	268	GLN
1	5-B	271	ASN
1	5-B	282	GLN
1	5-B	314	ASN
1	5-B	334	GLN
1	5-B	373	GLN
1	6-A	39	ASN
1	6-A	52	GLN
1	6-A	97	HIS
1	6-A	195	GLN
1	6-A	221	GLN
1	6-A	268	GLN
1	6-A	282	GLN
1	6-A	324	ASN
1	6-B	39	ASN
1	6-B	76	HIS
1	6-B	97	HIS
1	6-B	174	ASN
1	6-B	195	GLN
1	6-B	214	ASN
1	6-B	268	GLN
1	6-B	271	ASN
1	6-B	282	GLN
1	6-B	314	ASN
1	6-B	334	GLN
1	7-A	39	ASN
1	7-A	52	GLN
1	7-A	97	HIS
1	7-A	119	GLN
1	7-A	195	GLN
1	7-A	221	GLN

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Mol	Chain	Res	Type
1	7-A	268	GLN
1	7-A	282	GLN
1	7-A	314	ASN
1	7-A	324	ASN
1	7-A	334	GLN
1	7-B	39	ASN
1	7-B	76	HIS
1	7-B	97	HIS
1	7-B	174	ASN
1	7-B	189	HIS
1	7-B	195	GLN
1	7-B	214	ASN
1	7-B	265	ASN
1	7-B	286	HIS
1	7-B	314	ASN
1	7-B	333	GLN
1	7-B	334	GLN
1	8-A	52	GLN
1	8-A	97	HIS
1	8-A	195	GLN
1	8-A	221	GLN
1	8-A	268	GLN
1	8-A	271	ASN
1	8-A	282	GLN
1	8-A	314	ASN
1	8-A	324	ASN
1	8-A	333	GLN
1	8-A	334	GLN
1	8-A	366	ASN
1	8-B	39	ASN
1	8-B	76	HIS
1	8-B	97	HIS
1	8-B	174	ASN
1	8-B	195	GLN
1	8-B	207	GLN
1	8-B	214	ASN
1	8-B	268	GLN
1	8-B	282	GLN
1	8-B	314	ASN
1	8-B	373	GLN
1	9-A	39	ASN
1	9-A	52	GLN

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Mol	Chain	Res	Type
1	9-A	97	HIS
1	9-A	195	GLN
1	9-A	221	GLN
1	9-A	268	GLN
1	9-A	271	ASN
1	9-A	314	ASN
1	9-A	324	ASN
1	9-A	334	GLN
1	9-B	9	ASN
1	9-B	39	ASN
1	9-B	76	HIS
1	9-B	174	ASN
1	9-B	195	GLN
1	9-B	214	ASN
1	9-B	268	GLN
1	9-B	282	GLN
1	9-B	330	GLN
1	10-A	52	GLN
1	10-A	147	HIS
1	10-A	189	HIS
1	10-A	195	GLN
1	10-A	268	GLN
1	10-A	271	ASN
1	10-A	324	ASN
1	10-A	330	GLN
1	10-A	334	GLN
1	10-A	373	GLN
1	10-B	39	ASN
1	10-B	76	HIS
1	10-B	97	HIS
1	10-B	147	HIS
1	10-B	174	ASN
1	10-B	189	HIS
1	10-B	195	GLN
1	10-B	214	ASN
1	10-B	268	GLN
1	10-B	271	ASN
1	10-B	282	GLN
1	10-B	314	ASN
1	10-B	333	GLN
1	11-A	39	ASN
1	11-A	195	GLN

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Mol	Chain	Res	Type
1	11-A	221	GLN
1	11-A	268	GLN
1	11-A	271	ASN
1	11-A	314	ASN
1	11-A	324	ASN
1	11-A	333	GLN
1	11-A	334	GLN
1	11-B	39	ASN
1	11-B	97	HIS
1	11-B	106	GLN
1	11-B	174	ASN
1	11-B	195	GLN
1	11-B	214	ASN
1	11-B	268	GLN
1	11-B	271	ASN
1	11-B	314	ASN
1	11-B	330	GLN
1	11-B	366	ASN
1	11-B	373	GLN
1	12-A	39	ASN
1	12-A	52	GLN
1	12-A	97	HIS
1	12-A	195	GLN
1	12-A	221	GLN
1	12-A	268	GLN
1	12-A	271	ASN
1	12-A	334	GLN
1	12-B	39	ASN
1	12-B	76	HIS
1	12-B	91	GLN
1	12-B	97	HIS
1	12-B	119	GLN
1	12-B	147	HIS
1	12-B	195	GLN
1	12-B	214	ASN
1	12-B	268	GLN
1	12-B	314	ASN
1	12-B	333	GLN
1	12-B	334	GLN
1	12-B	373	GLN
1	13-A	39	ASN
1	13-A	91	GLN

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Mol	Chain	Res	Type
1	13-A	97	HIS
1	13-A	186	HIS
1	13-A	195	GLN
1	13-A	268	GLN
1	13-A	324	ASN
1	13-A	334	GLN
1	13-A	373	GLN
1	13-B	76	HIS
1	13-B	97	HIS
1	13-B	174	ASN
1	13-B	186	HIS
1	13-B	214	ASN
1	13-B	268	GLN
1	13-B	334	GLN
1	14-A	39	ASN
1	14-A	52	GLN
1	14-A	91	GLN
1	14-A	97	HIS
1	14-A	130	ASN
1	14-A	147	HIS
1	14-A	195	GLN
1	14-A	221	GLN
1	14-A	245	HIS
1	14-A	268	GLN
1	14-A	324	ASN
1	14-A	330	GLN
1	14-A	333	GLN
1	14-A	334	GLN
1	14-B	9	ASN
1	14-B	39	ASN
1	14-B	76	HIS
1	14-B	121	ASN
1	14-B	174	ASN
1	14-B	195	GLN
1	14-B	202	ASN
1	14-B	214	ASN
1	14-B	268	GLN
1	14-B	314	ASN
1	14-B	330	GLN
1	14-B	366	ASN
1	15-A	39	ASN
1	15-A	52	GLN

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Mol	Chain	Res	Type
1	15-A	76	HIS
1	15-A	97	HIS
1	15-A	195	GLN
1	15-A	214	ASN
1	15-A	268	GLN
1	15-A	324	ASN
1	15-A	334	GLN
1	15-B	9	ASN
1	15-B	39	ASN
1	15-B	76	HIS
1	15-B	97	HIS
1	15-B	119	GLN
1	15-B	174	ASN
1	15-B	189	HIS
1	15-B	195	GLN
1	15-B	214	ASN
1	15-B	268	GLN
1	15-B	314	ASN
1	15-B	333	GLN
1	15-B	334	GLN
1	15-B	363	ASN
1	16-A	9	ASN
1	16-A	39	ASN
1	16-A	52	GLN
1	16-A	97	HIS
1	16-A	189	HIS
1	16-A	195	GLN
1	16-A	214	ASN
1	16-A	221	GLN
1	16-A	268	GLN
1	16-A	271	ASN
1	16-A	282	GLN
1	16-A	324	ASN
1	16-A	330	GLN
1	16-A	333	GLN
1	16-A	334	GLN
1	16-A	349	ASN
1	16-A	373	GLN
1	16-B	39	ASN
1	16-B	136	ASN
1	16-B	174	ASN
1	16-B	195	GLN

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Mol	Chain	Res	Type
1	16-B	207	GLN
1	16-B	214	ASN
1	16-B	221	GLN
1	16-B	245	HIS
1	16-B	268	GLN
1	16-B	286	HIS
1	16-B	330	GLN
1	16-B	363	ASN
1	16-B	373	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

32 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	FMN	1-A	7401	-	33,33,33	2.49	6 (18%)	46,50,50	3.27	17 (36%)
2	FMN	1-B	9401	-	33,33,33	2.06	6 (18%)	46,50,50	4.04	17 (36%)
2	FMN	10-A	7401	-	33,33,33	2.16	6 (18%)	46,50,50	2.93	16 (34%)
2	FMN	10-B	9401	-	33,33,33	2.39	7 (21%)	46,50,50	4.00	18 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	11-A	7401	-	33,33,33	2.41	7 (21%)	46,50,50	3.45	17 (36%)
2	FMN	11-B	9401	-	33,33,33	2.14	5 (15%)	46,50,50	4.12	17 (36%)
2	FMN	12-A	7401	-	33,33,33	2.26	9 (27%)	46,50,50	3.03	15 (32%)
2	FMN	12-B	9401	-	33,33,33	2.74	9 (27%)	46,50,50	3.83	17 (36%)
2	FMN	13-A	7401	-	33,33,33	2.81	9 (27%)	46,50,50	3.81	19 (41%)
2	FMN	13-B	9401	-	33,33,33	3.33	11 (33%)	46,50,50	4.33	20 (43%)
2	FMN	14-A	7401	-	33,33,33	2.43	14 (42%)	46,50,50	3.30	18 (39%)
2	FMN	14-B	9401	-	33,33,33	2.68	10 (30%)	46,50,50	3.84	18 (39%)
2	FMN	15-A	7401	-	33,33,33	2.23	8 (24%)	46,50,50	3.52	20 (43%)
2	FMN	15-B	9401	-	33,33,33	3.37	12 (36%)	46,50,50	4.36	22 (47%)
2	FMN	16-A	7401	-	33,33,33	2.75	10 (30%)	46,50,50	3.76	19 (41%)
2	FMN	16-B	9401	-	33,33,33	2.37	9 (27%)	46,50,50	3.91	17 (36%)
2	FMN	2-A	7401	-	33,33,33	2.18	8 (24%)	46,50,50	2.96	13 (28%)
2	FMN	2-B	9401	-	33,33,33	2.57	12 (36%)	46,50,50	3.94	19 (41%)
2	FMN	3-A	7401	-	33,33,33	2.45	7 (21%)	46,50,50	3.17	17 (36%)
2	FMN	3-B	9401	-	33,33,33	2.43	5 (15%)	46,50,50	4.02	18 (39%)
2	FMN	4-A	7401	-	33,33,33	2.32	7 (21%)	46,50,50	3.32	17 (36%)
2	FMN	4-B	9401	-	33,33,33	2.08	6 (18%)	46,50,50	3.69	17 (36%)
2	FMN	5-A	7401	-	33,33,33	2.42	7 (21%)	46,50,50	3.47	17 (36%)
2	FMN	5-B	9401	-	33,33,33	2.38	8 (24%)	46,50,50	4.01	19 (41%)
2	FMN	6-A	7401	-	33,33,33	2.35	7 (21%)	46,50,50	3.83	19 (41%)
2	FMN	6-B	9401	-	33,33,33	2.52	14 (42%)	46,50,50	3.87	19 (41%)
2	FMN	7-A	7401	-	33,33,33	2.98	11 (33%)	46,50,50	3.81	18 (39%)
2	FMN	7-B	9401	-	33,33,33	2.95	9 (27%)	46,50,50	4.18	18 (39%)
2	FMN	8-A	7401	-	33,33,33	2.59	10 (30%)	46,50,50	3.35	18 (39%)
2	FMN	8-B	9401	-	33,33,33	2.29	6 (18%)	46,50,50	4.12	21 (45%)
2	FMN	9-A	7401	-	33,33,33	2.41	7 (21%)	46,50,50	3.36	18 (39%)
2	FMN	9-B	9401	-	33,33,33	2.38	12 (36%)	46,50,50	3.78	17 (36%)

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	FMN	1-A	7401	-	-	0/18/18/18	0/0/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	1-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	10-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	10-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	11-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	11-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	12-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	12-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	13-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	13-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	14-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	14-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	15-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	15-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	16-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	16-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	2-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	2-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	3-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	3-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	4-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	4-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	5-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	5-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	6-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	6-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	7-A	7401	-	-	2/18/18/18	0/0/3/3
2	FMN	7-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	8-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	8-B	9401	-	-	0/18/18/18	0/0/3/3
2	FMN	9-A	7401	-	-	0/18/18/18	0/0/3/3
2	FMN	9-B	9401	-	-	0/18/18/18	0/0/3/3

All (274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-A	7401	FMN	C1'-C2'	-12.07	1.40	1.51
2	7-B	9401	FMN	C1'-C2'	-9.93	1.42	1.51
2	15-B	9401	FMN	C9A-N10	9.91	1.53	1.38
2	13-B	9401	FMN	C9A-N10	9.66	1.53	1.38
2	13-B	9401	FMN	C1'-C2'	-9.56	1.42	1.51
2	15-B	9401	FMN	C1'-C2'	-9.34	1.42	1.51
2	2-B	9401	FMN	C1'-C2'	-8.77	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-A	7401	FMN	C1'-C2'	-8.70	1.43	1.51
2	7-B	9401	FMN	C9A-N10	8.67	1.51	1.38
2	16-A	7401	FMN	C1'-C2'	-8.61	1.43	1.51
2	15-B	9401	FMN	C1'-N10	8.37	1.57	1.48
2	6-B	9401	FMN	C1'-C2'	-8.26	1.43	1.51
2	1-A	7401	FMN	C1'-C2'	-8.17	1.43	1.51
2	3-A	7401	FMN	C1'-C2'	-8.17	1.43	1.51
2	5-B	9401	FMN	C9A-N10	8.06	1.50	1.38
2	13-B	9401	FMN	C1'-N10	8.03	1.57	1.48
2	5-A	7401	FMN	C9A-N10	7.84	1.50	1.38
2	12-B	9401	FMN	C1'-C2'	7.74	1.59	1.51
2	13-A	7401	FMN	C9A-N10	7.63	1.50	1.38
2	7-A	7401	FMN	C9A-N10	7.61	1.50	1.38
2	11-A	7401	FMN	C9A-N10	7.60	1.50	1.38
2	10-B	9401	FMN	C9A-N10	7.60	1.50	1.38
2	3-B	9401	FMN	C1'-C2'	-7.52	1.44	1.51
2	11-A	7401	FMN	C1'-C2'	-7.49	1.44	1.51
2	6-A	7401	FMN	C9A-N10	7.43	1.49	1.38
2	12-A	7401	FMN	C4A-C10	7.41	1.53	1.40
2	4-A	7401	FMN	C9A-N10	7.38	1.49	1.38
2	8-A	7401	FMN	C9A-N10	7.37	1.49	1.38
2	16-A	7401	FMN	C9A-N10	7.32	1.49	1.38
2	14-B	9401	FMN	C9A-N10	7.31	1.49	1.38
2	3-B	9401	FMN	C9A-N10	7.31	1.49	1.38
2	9-A	7401	FMN	C9A-N10	7.29	1.49	1.38
2	1-A	7401	FMN	C9A-N10	7.21	1.49	1.38
2	5-A	7401	FMN	C1'-C2'	-7.18	1.44	1.51
2	11-B	9401	FMN	C5'-C4'	-7.06	1.40	1.51
2	16-B	9401	FMN	C9A-N10	6.97	1.49	1.38
2	8-B	9401	FMN	C1'-C2'	6.88	1.58	1.51
2	12-B	9401	FMN	C9A-N10	6.88	1.49	1.38
2	2-A	7401	FMN	C4A-C10	6.88	1.52	1.40
2	8-B	9401	FMN	C4A-C10	6.78	1.52	1.40
2	15-A	7401	FMN	C1'-C2'	-6.74	1.45	1.51
2	1-B	9401	FMN	C5'-C4'	-6.74	1.41	1.51
2	3-A	7401	FMN	C9A-N10	6.73	1.48	1.38
2	4-A	7401	FMN	C1'-C2'	-6.68	1.45	1.51
2	9-B	9401	FMN	C9A-N10	6.59	1.48	1.38
2	14-B	9401	FMN	C4-C4A	6.39	1.51	1.41
2	10-B	9401	FMN	C1'-C2'	-6.39	1.45	1.51
2	6-A	7401	FMN	C5'-C4'	-6.37	1.41	1.51
2	4-B	9401	FMN	C9A-N10	6.36	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	12-B	9401	FMN	C4A-C10	6.33	1.51	1.40
2	4-B	9401	FMN	C4A-C10	6.31	1.51	1.40
2	14-B	9401	FMN	C1'-N10	6.25	1.55	1.48
2	8-A	7401	FMN	C4A-C10	6.17	1.51	1.40
2	2-B	9401	FMN	C9A-N10	6.10	1.47	1.38
2	8-A	7401	FMN	C1'-C2'	6.10	1.57	1.51
2	9-A	7401	FMN	C4A-C10	6.00	1.51	1.40
2	10-A	7401	FMN	C4A-C10	5.86	1.51	1.40
2	15-A	7401	FMN	C9A-N10	5.83	1.47	1.38
2	6-B	9401	FMN	C9A-N10	5.82	1.47	1.38
2	10-A	7401	FMN	C4-C4A	5.73	1.50	1.41
2	9-B	9401	FMN	C1'-C2'	-5.70	1.46	1.51
2	5-B	9401	FMN	C4A-C10	5.62	1.50	1.40
2	14-B	9401	FMN	C4A-C10	5.60	1.50	1.40
2	11-B	9401	FMN	C9A-N10	5.49	1.47	1.38
2	8-A	7401	FMN	C1'-N10	5.46	1.54	1.48
2	16-B	9401	FMN	C4A-C10	5.41	1.50	1.40
2	10-B	9401	FMN	C4A-C10	5.36	1.50	1.40
2	7-B	9401	FMN	C4A-C10	5.24	1.50	1.40
2	9-B	9401	FMN	C4A-C10	5.20	1.49	1.40
2	3-B	9401	FMN	C4A-C10	5.17	1.49	1.40
2	12-B	9401	FMN	C1'-N10	5.15	1.54	1.48
2	4-A	7401	FMN	C4A-C10	5.10	1.49	1.40
2	5-B	9401	FMN	C1'-C2'	-5.08	1.46	1.51
2	14-A	7401	FMN	C1'-N10	-5.03	1.42	1.48
2	12-B	9401	FMN	C4-C4A	5.02	1.49	1.41
2	9-A	7401	FMN	C1'-C2'	5.01	1.56	1.51
2	1-A	7401	FMN	C4A-C10	5.01	1.49	1.40
2	2-A	7401	FMN	C1'-N10	4.96	1.53	1.48
2	15-B	9401	FMN	C4A-C10	4.95	1.49	1.40
2	14-A	7401	FMN	C4'-C3'	-4.94	1.43	1.53
2	10-A	7401	FMN	C1'-N10	4.94	1.53	1.48
2	3-A	7401	FMN	C4A-C10	4.92	1.49	1.40
2	16-B	9401	FMN	C4-C4A	4.90	1.49	1.41
2	8-B	9401	FMN	C9A-N10	4.88	1.46	1.38
2	13-B	9401	FMN	C4A-C10	4.88	1.49	1.40
2	11-B	9401	FMN	C4A-C10	4.87	1.49	1.40
2	11-A	7401	FMN	C4A-C10	4.83	1.49	1.40
2	6-A	7401	FMN	C4A-C10	4.82	1.49	1.40
2	5-A	7401	FMN	C4A-C10	4.79	1.49	1.40
2	16-A	7401	FMN	C4A-C10	4.75	1.49	1.40
2	1-B	9401	FMN	C4A-C10	4.73	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-B	9401	FMN	C4A-C10	4.73	1.49	1.40
2	2-B	9401	FMN	C4A-C10	4.71	1.49	1.40
2	9-A	7401	FMN	C1'-N10	4.70	1.53	1.48
2	12-A	7401	FMN	C4-C4A	4.67	1.48	1.41
2	15-A	7401	FMN	C4A-C10	4.62	1.48	1.40
2	16-B	9401	FMN	C5'-C4'	4.61	1.59	1.51
2	13-A	7401	FMN	C4A-C10	4.59	1.48	1.40
2	15-B	9401	FMN	C4-C4A	4.59	1.48	1.41
2	12-A	7401	FMN	C1'-N10	4.52	1.53	1.48
2	13-B	9401	FMN	C4-C4A	4.49	1.48	1.41
2	12-A	7401	FMN	C9A-N10	4.43	1.45	1.38
2	13-A	7401	FMN	C4-C4A	4.34	1.48	1.41
2	2-A	7401	FMN	C4-C4A	4.31	1.48	1.41
2	14-B	9401	FMN	C5'-C4'	4.25	1.58	1.51
2	16-A	7401	FMN	C4-C4A	4.17	1.48	1.41
2	7-A	7401	FMN	C4A-C10	4.16	1.48	1.40
2	6-A	7401	FMN	C1'-C2'	-4.14	1.47	1.51
2	4-B	9401	FMN	C1'-C2'	4.11	1.55	1.51
2	8-B	9401	FMN	C4-C4A	4.08	1.47	1.41
2	1-B	9401	FMN	C9A-N10	4.01	1.44	1.38
2	14-A	7401	FMN	C4A-C10	3.99	1.47	1.40
2	5-B	9401	FMN	C4-C4A	3.99	1.47	1.41
2	7-B	9401	FMN	C4-C4A	3.92	1.47	1.41
2	1-B	9401	FMN	C4-C4A	3.90	1.47	1.41
2	10-A	7401	FMN	C9A-N10	3.89	1.44	1.38
2	4-B	9401	FMN	C4-C4A	3.86	1.47	1.41
2	7-B	9401	FMN	C1'-N10	3.81	1.52	1.48
2	13-A	7401	FMN	C1'-N10	3.80	1.52	1.48
2	14-A	7401	FMN	C5'-C4'	-3.79	1.45	1.51
2	10-B	9401	FMN	C4-C4A	3.76	1.47	1.41
2	3-B	9401	FMN	C4-C4A	3.73	1.47	1.41
2	8-A	7401	FMN	C4-C4A	3.71	1.47	1.41
2	11-B	9401	FMN	C4-C4A	3.68	1.47	1.41
2	15-B	9401	FMN	C5'-C4'	3.66	1.57	1.51
2	2-A	7401	FMN	C2-N3	-3.66	1.30	1.37
2	9-A	7401	FMN	C4-C4A	3.65	1.47	1.41
2	7-B	9401	FMN	C5'-C4'	3.63	1.57	1.51
2	14-A	7401	FMN	C1'-C2'	3.63	1.55	1.51
2	6-B	9401	FMN	C4-C4A	3.62	1.47	1.41
2	15-A	7401	FMN	C5'-C4'	-3.57	1.46	1.51
2	9-B	9401	FMN	C4'-C3'	-3.55	1.46	1.53
2	7-A	7401	FMN	C4-C4A	3.54	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-B	9401	FMN	C6-C5A	3.54	1.46	1.41
2	2-A	7401	FMN	C9A-N10	3.51	1.44	1.38
2	14-A	7401	FMN	P-O5'	-3.51	1.48	1.60
2	13-B	9401	FMN	C5'-C4'	3.51	1.57	1.51
2	16-A	7401	FMN	C1'-N10	3.51	1.52	1.48
2	14-A	7401	FMN	C6-C5A	3.48	1.45	1.41
2	15-B	9401	FMN	C6-C5A	3.45	1.45	1.41
2	2-B	9401	FMN	C4-C4A	3.42	1.46	1.41
2	14-B	9401	FMN	C1'-C2'	3.41	1.54	1.51
2	16-B	9401	FMN	C1'-N10	3.34	1.52	1.48
2	9-B	9401	FMN	C4-C4A	3.30	1.46	1.41
2	12-A	7401	FMN	C2-N3	-3.20	1.31	1.37
2	13-A	7401	FMN	C4A-N5	-3.19	1.29	1.36
2	10-A	7401	FMN	C2'-C3'	3.10	1.60	1.53
2	16-B	9401	FMN	C2'-C3'	3.09	1.59	1.53
2	14-B	9401	FMN	O3'-C3'	-3.04	1.35	1.43
2	12-A	7401	FMN	C1'-C2'	3.04	1.54	1.51
2	16-A	7401	FMN	C4A-N5	-2.99	1.29	1.36
2	16-A	7401	FMN	O3'-C3'	-2.96	1.35	1.43
2	13-A	7401	FMN	O3'-C3'	-2.95	1.35	1.43
2	14-A	7401	FMN	C10-N10	-2.92	1.32	1.38
2	3-A	7401	FMN	C4'-C3'	-2.92	1.47	1.53
2	14-A	7401	FMN	C4-C4A	2.90	1.46	1.41
2	15-A	7401	FMN	C10-N10	-2.89	1.32	1.38
2	2-A	7401	FMN	C1'-C2'	2.86	1.54	1.51
2	5-B	9401	FMN	C1'-N10	2.86	1.51	1.48
2	3-A	7401	FMN	P-O5'	-2.86	1.50	1.60
2	9-A	7401	FMN	C4A-N5	-2.84	1.30	1.36
2	2-B	9401	FMN	C2'-C3'	2.84	1.59	1.53
2	10-A	7401	FMN	C1'-C2'	2.83	1.54	1.51
2	14-A	7401	FMN	O2'-C2'	2.77	1.49	1.43
2	8-A	7401	FMN	C4A-N5	-2.73	1.30	1.36
2	6-B	9401	FMN	P-O5'	-2.70	1.50	1.60
2	14-B	9401	FMN	C6-C5A	2.70	1.45	1.41
2	9-B	9401	FMN	C6-C5A	2.70	1.45	1.41
2	9-B	9401	FMN	O2'-C2'	2.70	1.49	1.43
2	1-B	9401	FMN	C1'-N10	-2.67	1.45	1.48
2	7-A	7401	FMN	C2'-C3'	-2.66	1.48	1.53
2	8-B	9401	FMN	C6-C5A	2.65	1.44	1.41
2	13-B	9401	FMN	P-O5'	-2.64	1.51	1.60
2	15-B	9401	FMN	C2-N1	-2.63	1.29	1.35
2	1-A	7401	FMN	P-O5'	-2.62	1.51	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-A	7401	FMN	C1'-N10	2.60	1.51	1.48
2	16-B	9401	FMN	C1'-C2'	-2.58	1.49	1.51
2	2-B	9401	FMN	O2'-C2'	2.57	1.49	1.43
2	14-B	9401	FMN	C2'-C3'	2.57	1.58	1.53
2	9-B	9401	FMN	P-O5'	-2.56	1.51	1.60
2	6-B	9401	FMN	P-O3P	2.55	1.64	1.54
2	5-A	7401	FMN	C1'-N10	2.54	1.51	1.48
2	11-B	9401	FMN	C9-C9A	2.54	1.45	1.40
2	10-B	9401	FMN	P-O5'	-2.54	1.51	1.60
2	3-A	7401	FMN	C4A-N5	-2.53	1.30	1.36
2	6-B	9401	FMN	C4'-C3'	-2.52	1.48	1.53
2	9-B	9401	FMN	C1'-N10	-2.51	1.45	1.48
2	10-B	9401	FMN	C9-C9A	2.51	1.45	1.40
2	15-A	7401	FMN	C4A-N5	-2.49	1.30	1.36
2	15-B	9401	FMN	P-O5'	-2.49	1.51	1.60
2	12-A	7401	FMN	P-O2P	2.49	1.63	1.54
2	13-B	9401	FMN	C2-N1	-2.48	1.29	1.35
2	5-B	9401	FMN	C6-C5A	2.46	1.44	1.41
2	1-B	9401	FMN	C9-C9A	2.45	1.45	1.40
2	10-B	9401	FMN	C6-C5A	2.45	1.44	1.41
2	7-B	9401	FMN	C6-C5A	2.44	1.44	1.41
2	6-B	9401	FMN	O2'-C2'	2.43	1.49	1.43
2	1-A	7401	FMN	C4A-N5	-2.43	1.31	1.36
2	5-A	7401	FMN	C4-C4A	2.42	1.45	1.41
2	4-A	7401	FMN	C4-C4A	2.41	1.45	1.41
2	12-A	7401	FMN	C10-N1	-2.40	1.31	1.35
2	6-A	7401	FMN	C4-C4A	2.39	1.45	1.41
2	11-A	7401	FMN	C4A-N5	-2.38	1.31	1.36
2	2-B	9401	FMN	P-O5'	-2.37	1.51	1.60
2	2-B	9401	FMN	P-O3P	2.37	1.63	1.54
2	14-A	7401	FMN	P-O1P	-2.36	1.43	1.51
2	9-B	9401	FMN	P-O3P	2.36	1.63	1.54
2	11-A	7401	FMN	C1'-N10	2.35	1.50	1.48
2	14-A	7401	FMN	C9-C9A	2.34	1.45	1.40
2	5-A	7401	FMN	C4A-N5	-2.34	1.31	1.36
2	11-A	7401	FMN	C4-C4A	2.34	1.45	1.41
2	4-A	7401	FMN	C4A-N5	-2.33	1.31	1.36
2	12-B	9401	FMN	C2'-C3'	2.33	1.58	1.53
2	9-B	9401	FMN	C10-N10	-2.33	1.33	1.38
2	6-A	7401	FMN	C4A-N5	-2.33	1.31	1.36
2	14-A	7401	FMN	P-O2P	2.33	1.63	1.54
2	2-B	9401	FMN	O3'-C3'	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9-B	9401	FMN	C9-C9A	2.32	1.45	1.40
2	12-A	7401	FMN	C9A-C5A	2.31	1.47	1.42
2	4-B	9401	FMN	C6-C5A	2.31	1.44	1.41
2	2-A	7401	FMN	C9A-C5A	2.30	1.47	1.42
2	12-B	9401	FMN	O4-C4	-2.30	1.20	1.24
2	7-A	7401	FMN	C4-N3	2.29	1.41	1.37
2	1-A	7401	FMN	C4-C4A	2.29	1.45	1.41
2	5-B	9401	FMN	C9-C9A	2.28	1.45	1.40
2	3-A	7401	FMN	C4-C4A	2.28	1.44	1.41
2	15-B	9401	FMN	P-O3P	2.28	1.63	1.54
2	6-B	9401	FMN	C6-C5A	2.27	1.44	1.41
2	7-A	7401	FMN	C6-C5A	2.25	1.44	1.41
2	7-A	7401	FMN	C10-N10	-2.25	1.33	1.38
2	9-A	7401	FMN	P-O2P	2.25	1.63	1.54
2	7-B	9401	FMN	O3'-C3'	2.25	1.48	1.43
2	7-A	7401	FMN	C2-N1	-2.24	1.30	1.35
2	12-B	9401	FMN	C4'-C3'	2.24	1.58	1.53
2	8-A	7401	FMN	C2'-C3'	2.22	1.58	1.53
2	6-B	9401	FMN	C2'-C3'	2.22	1.58	1.53
2	12-B	9401	FMN	C4A-N5	-2.21	1.31	1.36
2	2-A	7401	FMN	P-O2P	2.20	1.62	1.54
2	15-A	7401	FMN	O4-C4	-2.19	1.20	1.24
2	6-B	9401	FMN	O3'-C3'	2.19	1.48	1.43
2	13-B	9401	FMN	P-O3P	2.19	1.62	1.54
2	3-B	9401	FMN	C6-C5A	2.18	1.44	1.41
2	7-A	7401	FMN	C4A-N5	-2.16	1.31	1.36
2	2-B	9401	FMN	C6-C5A	2.16	1.44	1.41
2	2-B	9401	FMN	C4'-C3'	-2.16	1.49	1.53
2	13-A	7401	FMN	C6-C5A	2.15	1.44	1.41
2	7-B	9401	FMN	C9-C9A	2.15	1.45	1.40
2	8-A	7401	FMN	P-O2P	2.14	1.62	1.54
2	16-B	9401	FMN	O2'-C2'	2.14	1.48	1.43
2	16-A	7401	FMN	C5'-C4'	2.14	1.55	1.51
2	2-B	9401	FMN	C10-N10	-2.14	1.34	1.38
2	6-B	9401	FMN	C1'-N10	-2.13	1.45	1.48
2	16-A	7401	FMN	C6-C5A	2.13	1.44	1.41
2	8-B	9401	FMN	O4-C4	-2.13	1.20	1.24
2	8-A	7401	FMN	C10-N10	2.11	1.43	1.38
2	4-B	9401	FMN	O4-C4	-2.10	1.20	1.24
2	5-A	7401	FMN	P-O3P	2.08	1.62	1.54
2	6-B	9401	FMN	C9-C9A	2.08	1.44	1.40
2	14-B	9401	FMN	C9-C9A	2.08	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	4-A	7401	FMN	C1'-N10	2.06	1.50	1.48
2	14-A	7401	FMN	C9A-N10	2.05	1.41	1.38
2	13-A	7401	FMN	C5'-C4'	2.04	1.54	1.51
2	15-B	9401	FMN	P-O2P	2.04	1.62	1.54
2	5-B	9401	FMN	P-O3P	2.04	1.62	1.54
2	15-B	9401	FMN	C4'-C3'	2.03	1.57	1.53
2	6-B	9401	FMN	C10-N10	-2.03	1.34	1.38
2	16-A	7401	FMN	C9-C9A	2.03	1.44	1.40
2	6-A	7401	FMN	C1'-N10	2.03	1.50	1.48
2	11-A	7401	FMN	P-O3P	2.03	1.62	1.54
2	4-A	7401	FMN	P-O3P	2.02	1.62	1.54
2	13-B	9401	FMN	P-O2P	2.02	1.62	1.54
2	16-B	9401	FMN	C4A-N5	-2.02	1.31	1.36
2	8-A	7401	FMN	C5A-N5	-2.01	1.32	1.35
2	15-A	7401	FMN	C5A-N5	-2.00	1.32	1.35

All (572) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	7401	FMN	C1'-N10-C9A	12.56	131.09	118.87
2	15-B	9401	FMN	C1'-N10-C9A	12.47	131.01	118.87
2	13-B	9401	FMN	C1'-N10-C9A	12.19	130.73	118.87
2	13-A	7401	FMN	C1'-N10-C9A	11.51	130.06	118.87
2	12-B	9401	FMN	O2P-P-O1P	-11.43	73.07	110.44
2	8-B	9401	FMN	O2P-P-O1P	-11.33	73.41	110.44
2	7-B	9401	FMN	C1'-N10-C9A	11.30	129.87	118.87
2	2-B	9401	FMN	O2P-P-O1P	-11.12	74.08	110.44
2	11-B	9401	FMN	O3P-P-O5'	-11.08	76.08	106.65
2	16-A	7401	FMN	C1'-N10-C9A	11.01	129.58	118.87
2	15-A	7401	FMN	C2'-C1'-N10	-10.99	97.87	112.45
2	4-A	7401	FMN	O3P-P-O5'	-10.90	76.56	106.65
2	6-B	9401	FMN	O2P-P-O1P	-10.88	74.87	110.44
2	3-B	9401	FMN	O2P-P-O1P	-10.77	75.24	110.44
2	13-A	7401	FMN	O3P-P-O1P	-10.75	75.30	110.44
2	4-B	9401	FMN	O2P-P-O1P	-10.71	75.45	110.44
2	6-A	7401	FMN	C2'-C1'-N10	-10.70	98.25	112.45
2	9-B	9401	FMN	O2P-P-O1P	-10.66	75.60	110.44
2	1-B	9401	FMN	O3P-P-O5'	-10.65	77.27	106.65
2	16-A	7401	FMN	O3P-P-O1P	-10.61	75.76	110.44
2	5-A	7401	FMN	O3P-P-O5'	-10.52	77.60	106.65
2	11-A	7401	FMN	O3P-P-O5'	-10.50	77.67	106.65
2	6-A	7401	FMN	P-O5'-C5'	-10.46	87.95	118.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	14-B	9401	FMN	O3P-P-O2P	-10.43	67.00	107.61
2	7-A	7401	FMN	O3P-P-O5'	-10.40	77.94	106.65
2	14-A	7401	FMN	O3P-P-O5'	-10.40	77.95	106.65
2	15-B	9401	FMN	O5'-P-O1P	-10.39	76.25	106.71
2	13-B	9401	FMN	O5'-P-O1P	-10.34	76.40	106.71
2	8-B	9401	FMN	O5'-P-O1P	-10.27	76.59	106.71
2	14-B	9401	FMN	O3P-P-O5'	-10.20	78.50	106.65
2	16-B	9401	FMN	O3P-P-O2P	-10.11	68.22	107.61
2	10-B	9401	FMN	O5'-P-O1P	-10.04	77.27	106.71
2	1-B	9401	FMN	O2P-P-O5'	10.04	134.36	106.65
2	7-B	9401	FMN	O5'-P-O1P	-10.04	77.27	106.71
2	3-B	9401	FMN	O2P-P-O5'	9.99	134.21	106.65
2	11-B	9401	FMN	O2P-P-O5'	9.90	133.98	106.65
2	9-A	7401	FMN	O3P-P-O5'	-9.90	79.33	106.65
2	10-B	9401	FMN	O2P-P-O5'	9.75	133.55	106.65
2	9-B	9401	FMN	O2P-P-O5'	9.72	133.46	106.65
2	9-B	9401	FMN	O5'-P-O1P	-9.71	78.23	106.71
2	5-B	9401	FMN	O5'-P-O1P	-9.68	78.34	106.71
2	13-B	9401	FMN	O2P-P-O5'	9.65	133.28	106.65
2	6-B	9401	FMN	O5'-P-O1P	-9.59	78.60	106.71
2	1-B	9401	FMN	O5'-P-O1P	-9.58	78.61	106.71
2	9-B	9401	FMN	O3P-P-O5'	-9.58	80.20	106.65
2	15-A	7401	FMN	O3P-P-O1P	-9.57	79.14	110.44
2	11-B	9401	FMN	O5'-P-O1P	-9.56	78.68	106.71
2	10-B	9401	FMN	O3P-P-O5'	-9.55	80.28	106.65
2	5-B	9401	FMN	O2P-P-O5'	9.52	132.93	106.65
2	14-B	9401	FMN	O2P-P-O5'	9.52	132.92	106.65
2	15-B	9401	FMN	O2P-P-O5'	9.51	132.90	106.65
2	3-B	9401	FMN	O3P-P-O5'	-9.51	80.41	106.65
2	10-B	9401	FMN	O2P-P-O1P	-9.48	79.45	110.44
2	8-A	7401	FMN	O3P-P-O5'	-9.48	80.48	106.65
2	1-B	9401	FMN	O2P-P-O1P	-9.44	79.60	110.44
2	12-A	7401	FMN	O3P-P-O5'	-9.39	80.72	106.65
2	4-B	9401	FMN	O2P-P-O5'	9.38	132.54	106.65
2	16-B	9401	FMN	O3P-P-O5'	-9.29	81.00	106.65
2	11-B	9401	FMN	P-O5'-C5'	-9.26	91.40	118.19
2	5-B	9401	FMN	O2P-P-O1P	-9.26	80.16	110.44
2	7-B	9401	FMN	O3P-P-O5'	-9.22	81.19	106.65
2	13-B	9401	FMN	O3P-P-O5'	-9.19	81.29	106.65
2	15-B	9401	FMN	O3P-P-O5'	-9.15	81.39	106.65
2	12-B	9401	FMN	O2P-P-O5'	9.11	131.79	106.65
2	1-A	7401	FMN	O3P-P-O5'	-9.11	81.52	106.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-B	9401	FMN	O5'-P-O1P	-9.06	80.15	106.71
2	7-B	9401	FMN	O2P-P-O5'	9.05	131.62	106.65
2	7-B	9401	FMN	O2P-P-O1P	-9.00	81.01	110.44
2	2-A	7401	FMN	O3P-P-O5'	-9.00	81.82	106.65
2	8-B	9401	FMN	O2P-P-O5'	8.98	131.43	106.65
2	3-B	9401	FMN	O5'-P-O1P	-8.94	80.50	106.71
2	11-B	9401	FMN	O2P-P-O1P	-8.90	81.35	110.44
2	12-B	9401	FMN	O5'-P-O1P	-8.78	80.98	106.71
2	13-B	9401	FMN	O2P-P-O1P	-8.71	81.97	110.44
2	15-B	9401	FMN	O2P-P-O1P	-8.68	82.08	110.44
2	6-A	7401	FMN	O3P-P-O5'	-8.66	82.75	106.65
2	2-B	9401	FMN	C4'-C3'-C2'	-8.66	93.68	113.25
2	16-B	9401	FMN	O2P-P-O1P	-8.55	82.51	110.44
2	1-B	9401	FMN	P-O5'-C5'	-8.53	93.52	118.19
2	4-B	9401	FMN	O3P-P-O5'	-8.48	83.24	106.65
2	7-A	7401	FMN	O3P-P-O1P	-8.45	82.83	110.44
2	5-B	9401	FMN	O3P-P-O5'	-8.43	83.39	106.65
2	12-A	7401	FMN	O3P-P-O1P	-8.40	82.97	110.44
2	3-B	9401	FMN	C1'-N10-C9A	8.40	127.04	118.87
2	16-B	9401	FMN	O2P-P-O5'	8.36	129.72	106.65
2	6-B	9401	FMN	C4'-C3'-C2'	-8.27	94.56	113.25
2	4-B	9401	FMN	O5'-P-O1P	-8.22	82.62	106.71
2	14-A	7401	FMN	O3P-P-O1P	-8.18	83.71	110.44
2	3-A	7401	FMN	O3P-P-O1P	-8.15	83.79	110.44
2	1-B	9401	FMN	C2'-C1'-N10	-8.09	101.71	112.45
2	15-B	9401	FMN	C2-N1-C10	8.07	123.11	114.98
2	2-B	9401	FMN	O2P-P-O5'	8.07	128.91	106.65
2	13-B	9401	FMN	C2-N1-C10	8.06	123.11	114.98
2	10-A	7401	FMN	O3P-P-O1P	-8.04	84.16	110.44
2	2-A	7401	FMN	O3P-P-O1P	-8.04	84.16	110.44
2	3-A	7401	FMN	O3P-P-O5'	-8.03	84.47	106.65
2	6-B	9401	FMN	O2P-P-O5'	7.98	128.69	106.65
2	9-A	7401	FMN	O3P-P-O1P	-7.94	84.50	110.44
2	8-A	7401	FMN	O3P-P-O1P	-7.88	84.69	110.44
2	12-B	9401	FMN	O3P-P-O5'	-7.87	84.92	106.65
2	8-B	9401	FMN	C4A-C10-N10	-7.86	116.59	120.51
2	10-A	7401	FMN	O3P-P-O5'	-7.85	85.00	106.65
2	10-B	9401	FMN	C2'-C1'-N10	-7.81	102.09	112.45
2	2-B	9401	FMN	O3P-P-O2P	-7.81	77.20	107.61
2	14-A	7401	FMN	C2'-C1'-N10	-7.71	102.22	112.45
2	14-B	9401	FMN	O2P-P-O1P	-7.68	85.35	110.44
2	6-A	7401	FMN	O3P-P-O1P	-7.67	85.36	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6-B	9401	FMN	O3P-P-O2P	-7.63	77.91	107.61
2	16-B	9401	FMN	C2-N1-C10	7.58	122.62	114.98
2	1-A	7401	FMN	O3P-P-O1P	-7.58	85.66	110.44
2	11-B	9401	FMN	C2'-C1'-N10	-7.56	102.42	112.45
2	7-A	7401	FMN	C2-N1-C10	7.54	122.58	114.98
2	5-A	7401	FMN	O3P-P-O1P	-7.53	85.82	110.44
2	8-B	9401	FMN	O3P-P-O5'	-7.48	86.01	106.65
2	9-A	7401	FMN	C2-N1-C10	7.44	122.48	114.98
2	11-A	7401	FMN	O3P-P-O1P	-7.40	86.26	110.44
2	16-A	7401	FMN	O5'-P-O1P	7.38	128.35	106.71
2	14-B	9401	FMN	C2-N1-C10	7.34	122.37	114.98
2	15-B	9401	FMN	O3P-P-O2P	-7.29	79.22	107.61
2	5-B	9401	FMN	C1'-N10-C9A	7.27	125.95	118.87
2	13-B	9401	FMN	O3P-P-O2P	-7.26	79.32	107.61
2	8-A	7401	FMN	C2-N1-C10	7.25	122.29	114.98
2	13-A	7401	FMN	O5'-P-O1P	7.16	127.70	106.71
2	16-B	9401	FMN	C1'-N10-C9A	7.16	125.83	118.87
2	7-B	9401	FMN	C2-N1-C10	7.08	122.12	114.98
2	5-B	9401	FMN	O3P-P-O2P	-7.05	80.15	107.61
2	6-B	9401	FMN	O3P-P-O5'	-7.05	87.20	106.65
2	12-B	9401	FMN	C2-N1-C10	7.03	122.06	114.98
2	2-B	9401	FMN	O3P-P-O5'	-6.99	87.34	106.65
2	4-B	9401	FMN	O3P-P-O2P	-6.99	80.38	107.61
2	4-A	7401	FMN	O3P-P-O1P	-6.99	87.59	110.44
2	16-A	7401	FMN	C2-N1-C10	6.98	122.02	114.98
2	3-B	9401	FMN	C4'-C3'-C2'	-6.89	97.67	113.25
2	15-A	7401	FMN	O3P-P-O5'	-6.88	87.65	106.65
2	11-A	7401	FMN	C2'-C1'-N10	-6.87	103.34	112.45
2	13-A	7401	FMN	C2-N1-C10	6.86	121.90	114.98
2	7-A	7401	FMN	O5'-P-O1P	6.85	126.79	106.71
2	7-A	7401	FMN	C4'-C3'-C2'	-6.82	97.83	113.25
2	3-B	9401	FMN	C2-N1-C10	6.80	121.84	114.98
2	14-A	7401	FMN	C2-N1-C10	6.80	121.83	114.98
2	7-B	9401	FMN	O3P-P-O2P	-6.80	81.14	107.61
2	1-A	7401	FMN	C2'-C1'-N10	-6.72	103.53	112.45
2	8-A	7401	FMN	C9A-N10-C10	-6.67	115.22	121.77
2	5-A	7401	FMN	C1'-N10-C9A	6.66	125.35	118.87
2	12-A	7401	FMN	C2-N1-C10	6.65	121.68	114.98
2	12-B	9401	FMN	O3P-P-O2P	-6.58	81.97	107.61
2	9-A	7401	FMN	C9A-N10-C10	-6.58	115.31	121.77
2	10-A	7401	FMN	C2-N1-C10	6.58	121.61	114.98
2	5-B	9401	FMN	C2'-C1'-N10	-6.58	103.72	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-B	9401	FMN	C1'-N10-C10	6.57	128.49	119.17
2	2-B	9401	FMN	C2-N1-C10	6.53	121.56	114.98
2	15-A	7401	FMN	O5'-P-O1P	6.53	125.84	106.71
2	5-A	7401	FMN	C2-N1-C10	6.51	121.54	114.98
2	2-A	7401	FMN	C2-N1-C10	6.46	121.49	114.98
2	3-A	7401	FMN	C2-N1-C10	6.46	121.49	114.98
2	5-A	7401	FMN	C2'-C1'-N10	-6.45	103.90	112.45
2	10-B	9401	FMN	P-O5'-C5'	-6.44	99.57	118.19
2	4-A	7401	FMN	C2-N1-C10	6.43	121.45	114.98
2	16-B	9401	FMN	C4'-C3'-C2'	-6.42	98.74	113.25
2	1-A	7401	FMN	C2-N1-C10	6.41	121.44	114.98
2	15-A	7401	FMN	C4A-C10-N10	-6.41	117.31	120.51
2	3-A	7401	FMN	O5'-P-O1P	6.40	125.48	106.71
2	6-B	9401	FMN	C2-N1-C10	6.39	121.42	114.98
2	6-A	7401	FMN	C2-N1-C10	6.39	121.42	114.98
2	11-A	7401	FMN	C2-N1-C10	6.36	121.39	114.98
2	3-A	7401	FMN	O3P-P-O2P	-6.36	82.86	107.61
2	15-A	7401	FMN	C4'-C3'-C2'	-6.34	98.92	113.25
2	5-B	9401	FMN	O3P-P-O1P	6.34	131.16	110.44
2	6-A	7401	FMN	O3P-P-O2P	-6.34	82.93	107.61
2	10-A	7401	FMN	O3P-P-O2P	-6.29	83.12	107.61
2	8-A	7401	FMN	O3P-P-O2P	-6.28	83.17	107.61
2	2-B	9401	FMN	C1'-N10-C9A	6.27	124.97	118.87
2	13-A	7401	FMN	C4'-C3'-C2'	-6.25	99.13	113.25
2	5-B	9401	FMN	P-O5'-C5'	-6.23	100.17	118.19
2	4-B	9401	FMN	O3P-P-O1P	6.23	130.79	110.44
2	9-B	9401	FMN	C2'-C1'-N10	-6.22	104.20	112.45
2	5-B	9401	FMN	C2-N1-C10	6.21	121.23	114.98
2	8-B	9401	FMN	C1'-N10-C9A	-6.20	112.85	118.87
2	7-B	9401	FMN	C4'-C3'-C2'	-6.19	99.26	113.25
2	10-B	9401	FMN	C2-N1-C10	6.17	121.20	114.98
2	11-A	7401	FMN	C1'-N10-C9A	6.17	124.87	118.87
2	7-B	9401	FMN	O3P-P-O1P	6.16	130.59	110.44
2	4-B	9401	FMN	C4A-C10-N10	-6.14	117.44	120.51
2	10-B	9401	FMN	O3P-P-O2P	-6.14	83.69	107.61
2	11-A	7401	FMN	P-O5'-C5'	-6.14	100.43	118.19
2	11-B	9401	FMN	O3P-P-O1P	6.11	130.42	110.44
2	16-A	7401	FMN	C4'-C3'-C2'	-6.11	99.44	113.25
2	9-A	7401	FMN	O3P-P-O2P	-6.11	83.82	107.61
2	12-A	7401	FMN	O3P-P-O2P	-6.09	83.90	107.61
2	8-B	9401	FMN	O3P-P-O1P	6.07	130.27	110.44
2	16-B	9401	FMN	O5'-P-O1P	-6.06	88.93	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	14-A	7401	FMN	O5'-P-O1P	6.06	124.47	106.71
2	13-A	7401	FMN	O3P-P-O2P	-6.05	84.03	107.61
2	16-B	9401	FMN	O3P-P-O1P	6.04	130.18	110.44
2	5-A	7401	FMN	P-O5'-C5'	-6.02	100.77	118.19
2	6-B	9401	FMN	O3P-P-O1P	6.02	130.12	110.44
2	12-B	9401	FMN	O3P-P-O1P	6.01	130.10	110.44
2	1-A	7401	FMN	O3P-P-O2P	-6.01	84.21	107.61
2	9-B	9401	FMN	C2-N1-C10	6.00	121.03	114.98
2	3-A	7401	FMN	C4'-C3'-C2'	-6.00	99.68	113.25
2	8-A	7401	FMN	O5'-P-O1P	6.00	124.30	106.71
2	2-B	9401	FMN	O3P-P-O1P	5.96	129.93	110.44
2	16-A	7401	FMN	O3P-P-O5'	-5.96	90.20	106.65
2	1-B	9401	FMN	C4A-C10-N10	-5.96	117.54	120.51
2	2-A	7401	FMN	O3P-P-O2P	-5.94	84.48	107.61
2	3-B	9401	FMN	O3P-P-O2P	-5.94	84.48	107.61
2	15-A	7401	FMN	C2-N1-C10	5.93	120.96	114.98
2	16-A	7401	FMN	O3P-P-O2P	-5.91	84.58	107.61
2	4-B	9401	FMN	C2-N1-C10	5.89	120.92	114.98
2	9-B	9401	FMN	O3P-P-O2P	-5.89	84.67	107.61
2	2-A	7401	FMN	O5'-P-O1P	5.88	123.95	106.71
2	16-A	7401	FMN	C5'-C4'-C3'	5.85	123.10	112.06
2	13-A	7401	FMN	C4A-N5-C5A	5.85	123.26	116.69
2	8-B	9401	FMN	C2-N1-C10	5.85	120.87	114.98
2	1-A	7401	FMN	O5'-P-O1P	5.81	123.75	106.71
2	5-A	7401	FMN	O5'-P-O1P	5.78	123.66	106.71
2	12-B	9401	FMN	C4A-C10-N1	-5.78	116.96	122.73
2	13-A	7401	FMN	C5'-C4'-C3'	5.77	122.94	112.06
2	9-A	7401	FMN	O5'-P-O1P	5.77	123.61	106.71
2	11-B	9401	FMN	C2-N1-C10	5.76	120.78	114.98
2	14-A	7401	FMN	O3P-P-O2P	-5.75	85.22	107.61
2	1-B	9401	FMN	O3P-P-O1P	5.74	129.22	110.44
2	8-B	9401	FMN	O3P-P-O2P	-5.74	85.24	107.61
2	2-A	7401	FMN	C1'-N10-C9A	5.73	124.44	118.87
2	13-A	7401	FMN	O3P-P-O5'	-5.70	90.92	106.65
2	16-A	7401	FMN	C4A-N5-C5A	5.70	123.09	116.69
2	12-B	9401	FMN	C9A-N10-C10	-5.70	116.18	121.77
2	12-A	7401	FMN	O5'-P-O1P	5.68	123.37	106.71
2	7-A	7401	FMN	C1'-N10-C10	-5.68	111.11	119.17
2	3-A	7401	FMN	C1'-N10-C9A	5.66	124.38	118.87
2	10-A	7401	FMN	C1'-N10-C9A	5.66	124.38	118.87
2	1-B	9401	FMN	C2-N1-C10	5.66	120.69	114.98
2	8-A	7401	FMN	C4A-C10-N1	-5.62	117.11	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-B	9401	FMN	C1'-N10-C9A	5.58	124.31	118.87
2	11-A	7401	FMN	O5'-P-O1P	5.54	122.95	106.71
2	10-A	7401	FMN	O5'-P-O1P	5.53	122.93	106.71
2	8-A	7401	FMN	C4A-N5-C5A	5.53	122.90	116.69
2	14-B	9401	FMN	O5'-P-O1P	-5.51	90.55	106.71
2	10-B	9401	FMN	O3P-P-O1P	5.51	128.44	110.44
2	14-B	9401	FMN	C1'-N10-C9A	5.49	124.22	118.87
2	9-A	7401	FMN	C4A-N5-C5A	5.48	122.85	116.69
2	4-A	7401	FMN	O5'-P-O1P	5.48	122.77	106.71
2	6-A	7401	FMN	C4A-N5-C5A	5.47	122.83	116.69
2	15-B	9401	FMN	C9A-N10-C10	-5.47	116.40	121.77
2	15-A	7401	FMN	O3P-P-O2P	-5.45	86.37	107.61
2	2-B	9401	FMN	C5'-C4'-C3'	5.45	122.34	112.06
2	6-A	7401	FMN	C4A-C10-N10	-5.44	117.80	120.51
2	4-A	7401	FMN	O3P-P-O2P	-5.44	86.43	107.61
2	1-B	9401	FMN	O3P-P-O2P	-5.42	86.49	107.61
2	11-B	9401	FMN	O3P-P-O2P	-5.42	86.50	107.61
2	6-A	7401	FMN	O2P-P-O5'	5.42	121.61	106.65
2	5-A	7401	FMN	C4A-N5-C5A	5.41	122.77	116.69
2	9-A	7401	FMN	C4A-C10-N1	-5.41	117.32	122.73
2	1-A	7401	FMN	C4'-C3'-C2'	-5.40	101.04	113.25
2	15-B	9401	FMN	C4'-C3'-C2'	-5.40	101.05	113.25
2	13-B	9401	FMN	C9A-N10-C10	-5.38	116.48	121.77
2	16-B	9401	FMN	C5'-C4'-C3'	5.35	122.16	112.06
2	11-B	9401	FMN	C4A-N5-C5A	5.34	122.69	116.69
2	13-B	9401	FMN	C4'-C3'-C2'	-5.34	101.17	113.25
2	11-A	7401	FMN	C4A-N5-C5A	5.34	122.69	116.69
2	12-B	9401	FMN	C4A-N5-C5A	5.33	122.68	116.69
2	4-A	7401	FMN	C1'-N10-C9A	5.32	124.05	118.87
2	14-B	9401	FMN	C4A-N5-C5A	5.29	122.64	116.69
2	4-A	7401	FMN	C2'-C1'-N10	-5.27	105.46	112.45
2	4-A	7401	FMN	C4A-N5-C5A	5.26	122.60	116.69
2	3-B	9401	FMN	O3P-P-O1P	5.25	127.61	110.44
2	1-B	9401	FMN	C4A-N5-C5A	5.24	122.58	116.69
2	9-B	9401	FMN	C4'-C3'-C2'	-5.23	101.43	113.25
2	11-B	9401	FMN	C4A-C10-N10	-5.23	117.90	120.51
2	14-A	7401	FMN	C4A-C10-N10	-5.22	117.90	120.51
2	11-A	7401	FMN	O3P-P-O2P	-5.20	87.36	107.61
2	14-A	7401	FMN	C4'-C3'-C2'	-5.19	101.51	113.25
2	1-A	7401	FMN	C4A-N5-C5A	5.14	122.46	116.69
2	15-A	7401	FMN	C4A-N5-C5A	5.10	122.42	116.69
2	3-A	7401	FMN	C4A-N5-C5A	5.09	122.41	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6-B	9401	FMN	C1'-N10-C9A	5.07	123.81	118.87
2	15-B	9401	FMN	O3P-P-O1P	5.07	127.01	110.44
2	5-B	9401	FMN	C4A-N5-C5A	5.01	122.32	116.69
2	7-A	7401	FMN	C4A-N5-C5A	5.01	122.32	116.69
2	5-A	7401	FMN	O3P-P-O2P	-5.00	88.15	107.61
2	15-B	9401	FMN	C1'-C2'-C3'	4.99	124.08	109.82
2	7-A	7401	FMN	O3P-P-O2P	-4.96	88.30	107.61
2	13-B	9401	FMN	O3P-P-O1P	4.95	126.63	110.44
2	13-B	9401	FMN	C4A-N5-C5A	4.93	122.23	116.69
2	14-B	9401	FMN	C2'-C1'-N10	-4.93	105.91	112.45
2	10-B	9401	FMN	C4A-N5-C5A	4.93	122.22	116.69
2	9-B	9401	FMN	C4A-C10-N10	-4.93	118.05	120.51
2	15-B	9401	FMN	C4A-N5-C5A	4.91	122.20	116.69
2	4-A	7401	FMN	O2P-P-O5'	4.90	120.16	106.65
2	4-B	9401	FMN	C4A-N5-C5A	4.87	122.16	116.69
2	16-B	9401	FMN	C4A-N5-C5A	4.86	122.15	116.69
2	13-B	9401	FMN	C1'-C2'-C3'	4.84	123.67	109.82
2	14-B	9401	FMN	O3P-P-O1P	4.83	126.24	110.44
2	13-A	7401	FMN	C1'-N10-C10	-4.82	112.33	119.17
2	7-B	9401	FMN	C4A-N5-C5A	4.82	122.10	116.69
2	11-B	9401	FMN	C1'-N10-C9A	4.80	123.55	118.87
2	4-A	7401	FMN	P-O5'-C5'	-4.79	104.33	118.19
2	6-B	9401	FMN	C4A-N5-C5A	4.77	122.05	116.69
2	11-A	7401	FMN	O2P-P-O5'	4.75	119.76	106.65
2	2-B	9401	FMN	C4A-N5-C5A	4.75	122.03	116.69
2	6-B	9401	FMN	C5'-C4'-C3'	4.70	120.92	112.06
2	1-A	7401	FMN	C1'-N10-C9A	4.69	123.44	118.87
2	9-B	9401	FMN	C4A-N5-C5A	4.68	121.95	116.69
2	3-B	9401	FMN	C4A-N5-C5A	4.68	121.95	116.69
2	14-B	9401	FMN	C9A-N10-C10	-4.66	117.19	121.77
2	3-B	9401	FMN	C2'-C1'-N10	-4.65	106.28	112.45
2	8-B	9401	FMN	C4A-N5-C5A	4.64	121.91	116.69
2	15-B	9401	FMN	C1'-N10-C10	-4.64	112.59	119.17
2	9-B	9401	FMN	O3P-P-O1P	4.63	125.59	110.44
2	6-A	7401	FMN	C5'-C4'-C3'	-4.61	103.35	112.06
2	4-A	7401	FMN	C4'-C3'-C2'	-4.60	102.84	113.25
2	7-B	9401	FMN	C1'-N10-C10	-4.60	112.64	119.17
2	16-A	7401	FMN	C1'-N10-C10	-4.59	112.65	119.17
2	14-B	9401	FMN	C4A-C10-N1	-4.57	118.16	122.73
2	16-B	9401	FMN	C9A-N10-C10	-4.54	117.31	121.77
2	14-A	7401	FMN	C4A-N5-C5A	4.53	121.78	116.69
2	2-A	7401	FMN	C4A-C10-N1	-4.52	118.22	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-A	7401	FMN	C4'-C3'-C2'	-4.52	103.04	113.25
2	12-A	7401	FMN	C1'-N10-C9A	4.52	123.27	118.87
2	5-A	7401	FMN	O2P-P-O5'	4.51	119.09	106.65
2	13-B	9401	FMN	C1'-N10-C10	-4.50	112.78	119.17
2	12-A	7401	FMN	C9A-N10-C10	-4.49	117.36	121.77
2	9-A	7401	FMN	O2P-P-O5'	4.48	119.00	106.65
2	11-A	7401	FMN	C4'-C3'-C2'	-4.47	103.14	113.25
2	5-A	7401	FMN	C9A-N10-C10	-4.46	117.39	121.77
2	4-A	7401	FMN	C9A-N10-C10	-4.46	117.39	121.77
2	8-A	7401	FMN	O2P-P-O5'	4.44	118.92	106.65
2	12-B	9401	FMN	C4A-C10-N10	-4.44	118.30	120.51
2	9-A	7401	FMN	C1'-N10-C9A	4.43	123.18	118.87
2	5-B	9401	FMN	C4'-C3'-C2'	-4.41	103.28	113.25
2	12-A	7401	FMN	C4A-C10-N1	-4.40	118.33	122.73
2	10-B	9401	FMN	C4'-C3'-C2'	-4.38	103.34	113.25
2	7-B	9401	FMN	C9A-N10-C10	-4.38	117.47	121.77
2	3-A	7401	FMN	C2'-C1'-N10	-4.35	106.68	112.45
2	10-B	9401	FMN	C4A-C10-N10	-4.34	118.34	120.51
2	2-A	7401	FMN	C9A-N10-C10	-4.34	117.51	121.77
2	6-A	7401	FMN	O5'-P-O1P	4.34	119.42	106.71
2	10-A	7401	FMN	C4A-N5-C5A	4.33	121.55	116.69
2	8-B	9401	FMN	C5A-C9A-N10	4.32	121.06	116.80
2	7-B	9401	FMN	C1'-C2'-C3'	4.31	122.15	109.82
2	11-A	7401	FMN	C9A-N10-C10	-4.30	117.55	121.77
2	8-B	9401	FMN	C4A-C10-N1	-4.26	118.48	122.73
2	13-A	7401	FMN	C9A-N10-C10	-4.24	117.60	121.77
2	8-B	9401	FMN	C5'-C4'-C3'	-4.23	104.07	112.06
2	14-B	9401	FMN	C4'-C3'-C2'	-4.22	103.70	113.25
2	11-A	7401	FMN	C4A-C10-N10	-4.18	118.42	120.51
2	1-A	7401	FMN	P-O5'-C5'	-4.15	106.19	118.19
2	1-A	7401	FMN	C9A-N10-C10	-4.13	117.71	121.77
2	8-A	7401	FMN	C1'-N10-C9A	4.13	122.89	118.87
2	1-A	7401	FMN	C4A-C10-N10	-4.09	118.47	120.51
2	4-A	7401	FMN	C4A-C10-N10	-4.08	118.47	120.51
2	16-A	7401	FMN	C9A-N10-C10	-4.08	117.77	121.77
2	8-A	7401	FMN	C4A-C10-N10	-4.07	118.48	120.51
2	7-A	7401	FMN	C9A-N10-C10	-4.06	117.78	121.77
2	15-B	9401	FMN	O2'-C2'-C3'	-4.03	99.02	109.05
2	6-A	7401	FMN	C9A-N10-C10	-4.02	117.82	121.77
2	5-B	9401	FMN	C4A-C10-N10	-4.01	118.51	120.51
2	16-A	7401	FMN	P-O5'-C5'	4.00	129.75	118.19
2	3-A	7401	FMN	C9A-N10-C10	-3.98	117.86	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6-A	7401	FMN	C1'-N10-C9A	3.94	122.71	118.87
2	13-B	9401	FMN	O2'-C2'-C3'	-3.93	99.25	109.05
2	15-A	7401	FMN	P-O5'-C5'	-3.93	106.82	118.19
2	5-A	7401	FMN	C4A-C10-N10	-3.91	118.56	120.51
2	13-A	7401	FMN	P-O5'-C5'	3.91	129.49	118.19
2	4-B	9401	FMN	C4A-C10-N1	-3.89	118.84	122.73
2	6-B	9401	FMN	C4A-C10-N10	-3.89	118.57	120.51
2	16-A	7401	FMN	O4'-C4'-C5'	-3.88	102.16	110.12
2	6-A	7401	FMN	C4'-C3'-C2'	-3.87	104.51	113.25
2	1-A	7401	FMN	O2P-P-O5'	3.86	117.31	106.65
2	13-A	7401	FMN	O4'-C4'-C5'	-3.86	102.19	110.12
2	6-B	9401	FMN	C2'-C1'-N10	-3.84	107.36	112.45
2	12-B	9401	FMN	P-O5'-C5'	-3.83	107.12	118.19
2	9-A	7401	FMN	C4A-C10-N10	-3.82	118.60	120.51
2	16-B	9401	FMN	C4A-C10-N1	-3.82	118.92	122.73
2	9-B	9401	FMN	P-O5'-C5'	-3.78	107.25	118.19
2	5-B	9401	FMN	C9A-N10-C10	-3.72	118.11	121.77
2	8-B	9401	FMN	P-O5'-C5'	-3.72	107.44	118.19
2	16-B	9401	FMN	C2'-C1'-N10	-3.71	107.53	112.45
2	10-A	7401	FMN	O2P-P-O5'	3.69	116.82	106.65
2	7-B	9401	FMN	C2'-C1'-N10	-3.65	107.61	112.45
2	11-B	9401	FMN	C4A-C10-N1	-3.63	119.11	122.73
2	4-B	9401	FMN	P-O5'-C5'	-3.61	107.74	118.19
2	2-A	7401	FMN	O2P-P-O5'	3.61	116.62	106.65
2	13-A	7401	FMN	O2P-P-O1P	3.60	122.19	110.44
2	12-A	7401	FMN	C4A-N5-C5A	3.58	120.72	116.69
2	12-A	7401	FMN	C5A-C9A-N10	3.58	120.33	116.80
2	6-A	7401	FMN	C1'-C2'-C3'	3.56	120.00	109.82
2	12-A	7401	FMN	O2P-P-O5'	3.52	116.35	106.65
2	14-B	9401	FMN	C5'-C4'-C3'	3.49	118.64	112.06
2	2-B	9401	FMN	C4A-C10-N10	-3.45	118.79	120.51
2	3-A	7401	FMN	C4A-C10-N10	-3.44	118.79	120.51
2	3-B	9401	FMN	C9A-N10-C10	-3.44	118.39	121.77
2	4-B	9401	FMN	C9A-N10-C10	-3.43	118.40	121.77
2	1-B	9401	FMN	C4A-C10-N1	-3.41	119.32	122.73
2	8-B	9401	FMN	N1-C10-N10	3.41	124.94	115.97
2	16-A	7401	FMN	O2P-P-O1P	3.39	121.51	110.44
2	11-B	9401	FMN	C4'-C3'-C2'	-3.38	105.60	113.25
2	13-A	7401	FMN	C1'-C2'-C3'	3.38	119.48	109.82
2	2-A	7401	FMN	C4A-N5-C5A	3.34	120.45	116.69
2	12-B	9401	FMN	N1-C10-N10	3.34	124.75	115.97
2	2-A	7401	FMN	C5A-C9A-N10	3.33	120.08	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-A	7401	FMN	C1'-C2'-C3'	3.32	119.33	109.82
2	10-A	7401	FMN	C4A-C10-N1	-3.29	119.44	122.73
2	2-B	9401	FMN	C2'-C1'-N10	-3.29	108.08	112.45
2	2-A	7401	FMN	P-O5'-C5'	-3.28	108.72	118.19
2	10-A	7401	FMN	C9A-N10-C10	-3.26	118.56	121.77
2	8-B	9401	FMN	C2'-C1'-N10	3.26	116.78	112.45
2	4-B	9401	FMN	C5A-C9A-N10	3.26	120.01	116.80
2	3-B	9401	FMN	C1'-N10-C10	-3.25	114.55	119.17
2	14-B	9401	FMN	C1'-C2'-C3'	3.24	119.09	109.82
2	12-B	9401	FMN	C5A-C9A-N10	3.23	119.98	116.80
2	5-B	9401	FMN	C1'-C2'-C3'	3.23	119.04	109.82
2	11-A	7401	FMN	C1'-C2'-C3'	3.22	119.03	109.82
2	7-A	7401	FMN	O2P-P-O5'	3.22	115.53	106.65
2	8-A	7401	FMN	N1-C10-N10	3.21	124.40	115.97
2	15-B	9401	FMN	O2'-C2'-C1'	-3.20	101.75	109.71
2	5-B	9401	FMN	C4A-C10-N1	-3.17	119.56	122.73
2	8-B	9401	FMN	C9A-N10-C10	-3.17	118.65	121.77
2	4-A	7401	FMN	C4A-C10-N1	-3.14	119.59	122.73
2	16-A	7401	FMN	C1'-C2'-C3'	3.13	118.77	109.82
2	7-A	7401	FMN	C1'-C2'-C3'	3.12	118.74	109.82
2	6-A	7401	FMN	C4A-C10-N1	-3.11	119.62	122.73
2	3-B	9401	FMN	C5'-C4'-C3'	3.10	117.91	112.06
2	5-A	7401	FMN	C4A-C10-N1	-3.09	119.65	122.73
2	9-A	7401	FMN	N1-C10-N10	3.08	124.07	115.97
2	9-A	7401	FMN	P-O5'-C5'	-3.07	109.32	118.19
2	3-A	7401	FMN	C5'-C4'-C3'	3.07	117.84	112.06
2	13-B	9401	FMN	O2'-C2'-C1'	-3.06	102.10	109.71
2	8-A	7401	FMN	C1'-C2'-C3'	3.06	118.57	109.82
2	15-B	9401	FMN	C2'-C1'-N10	-3.05	108.40	112.45
2	8-A	7401	FMN	C5A-C9A-N10	3.03	119.79	116.80
2	11-A	7401	FMN	C4A-C10-N1	-3.03	119.70	122.73
2	13-A	7401	FMN	C4A-C10-N1	-3.03	119.70	122.73
2	14-A	7401	FMN	O4'-C4'-C5'	-3.02	103.91	110.12
2	14-B	9401	FMN	C4A-C10-N10	-3.02	119.00	120.51
2	7-B	9401	FMN	C4A-C10-N1	-3.00	119.73	122.73
2	2-B	9401	FMN	O4'-C4'-C3'	-2.99	101.59	109.05
2	15-A	7401	FMN	C9A-N10-C10	-2.98	118.85	121.77
2	10-B	9401	FMN	C9A-N10-C10	-2.96	118.86	121.77
2	4-B	9401	FMN	N1-C10-N10	2.95	123.72	115.97
2	15-A	7401	FMN	C5A-C9A-N10	2.94	119.70	116.80
2	6-B	9401	FMN	O4'-C4'-C3'	-2.94	101.73	109.05
2	10-A	7401	FMN	C4'-C3'-C2'	-2.93	106.63	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-A	7401	FMN	C5A-C9A-N10	2.91	119.67	116.80
2	8-B	9401	FMN	O3'-C3'-C2'	-2.88	101.44	108.74
2	9-A	7401	FMN	C1'-C2'-C3'	2.87	118.03	109.82
2	1-A	7401	FMN	C4A-C10-N1	-2.86	119.88	122.73
2	3-B	9401	FMN	P-O5'-C5'	-2.85	109.96	118.19
2	13-B	9401	FMN	C4A-C10-N1	-2.83	119.90	122.73
2	15-B	9401	FMN	C4A-C10-N1	-2.82	119.91	122.73
2	11-B	9401	FMN	C9A-N10-C10	-2.78	119.03	121.77
2	16-A	7401	FMN	C4A-C10-N1	-2.78	119.95	122.73
2	12-A	7401	FMN	P-O5'-C5'	-2.77	110.17	118.19
2	10-A	7401	FMN	C5A-C9A-N10	2.75	119.51	116.80
2	1-B	9401	FMN	N1-C10-N10	2.73	123.14	115.97
2	10-B	9401	FMN	C4A-C10-N1	-2.72	120.01	122.73
2	3-A	7401	FMN	C4A-C10-N1	-2.72	120.02	122.73
2	10-A	7401	FMN	O4'-C4'-C5'	-2.72	104.54	110.12
2	14-A	7401	FMN	C6-C5A-N5	2.71	122.14	118.97
2	16-A	7401	FMN	O2'-C2'-C1'	-2.70	103.00	109.71
2	3-B	9401	FMN	C4A-C10-N1	-2.70	120.03	122.73
2	14-A	7401	FMN	O2P-P-O5'	2.69	114.08	106.65
2	4-B	9401	FMN	C2'-C1'-N10	-2.68	108.90	112.45
2	8-B	9401	FMN	C1'-C2'-C3'	-2.67	102.17	109.82
2	11-B	9401	FMN	N1-C10-N10	2.67	122.99	115.97
2	16-B	9401	FMN	C1'-C2'-C3'	2.67	117.45	109.82
2	4-B	9401	FMN	C1'-N10-C10	2.66	122.94	119.17
2	12-B	9401	FMN	C1'-N10-C10	2.66	122.94	119.17
2	10-A	7401	FMN	C5'-C4'-C3'	2.65	117.07	112.06
2	4-A	7401	FMN	C1'-C2'-C3'	2.63	117.35	109.82
2	8-A	7401	FMN	P-O5'-C5'	-2.63	110.58	118.19
2	2-B	9401	FMN	C1'-N10-C10	-2.62	115.45	119.17
2	14-B	9401	FMN	N1-C10-N10	2.61	122.82	115.97
2	13-A	7401	FMN	O2'-C2'-C1'	-2.60	103.25	109.71
2	16-B	9401	FMN	O4'-C4'-C5'	-2.60	104.79	110.12
2	7-A	7401	FMN	C5'-C4'-C3'	2.57	116.91	112.06
2	2-B	9401	FMN	O4'-C4'-C5'	-2.56	104.86	110.12
2	12-A	7401	FMN	O4'-C4'-C5'	-2.56	104.86	110.12
2	13-B	9401	FMN	C2'-C1'-N10	-2.56	109.06	112.45
2	1-B	9401	FMN	O4'-C4'-C5'	-2.56	104.87	110.12
2	3-B	9401	FMN	C1'-C2'-C3'	2.53	117.05	109.82
2	6-A	7401	FMN	C5A-C9A-N10	2.53	119.29	116.80
2	1-A	7401	FMN	C1'-C2'-C3'	2.52	117.03	109.82
2	6-A	7401	FMN	N1-C10-N10	2.51	122.58	115.97
2	8-B	9401	FMN	C4'-C3'-C2'	2.51	118.92	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-B	9401	FMN	O3'-C3'-C4'	2.49	115.04	108.74
2	9-B	9401	FMN	C1'-N10-C9A	2.48	121.29	118.87
2	3-A	7401	FMN	O2P-P-O5'	2.48	113.48	106.65
2	15-A	7401	FMN	C5'-C4'-C3'	2.47	116.71	112.06
2	3-A	7401	FMN	O4'-C4'-C5'	-2.45	105.08	110.12
2	14-A	7401	FMN	C5A-C9A-N10	2.45	119.21	116.80
2	4-A	7401	FMN	C5A-C9A-N10	2.43	119.19	116.80
2	10-A	7401	FMN	P-O5'-C5'	-2.40	111.24	118.19
2	10-B	9401	FMN	C1'-C2'-C3'	2.40	116.69	109.82
2	14-A	7401	FMN	C5'-C4'-C3'	2.40	116.58	112.06
2	14-B	9401	FMN	C5A-C9A-N10	2.39	119.16	116.80
2	15-A	7401	FMN	C1'-C2'-C3'	2.39	116.65	109.82
2	15-A	7401	FMN	O2P-P-O5'	2.38	113.23	106.65
2	6-B	9401	FMN	O3'-C3'-C4'	2.36	114.71	108.74
2	7-B	9401	FMN	O3'-C3'-C2'	2.35	114.68	108.74
2	1-A	7401	FMN	C5A-C9A-N10	2.31	119.08	116.80
2	12-A	7401	FMN	N1-C10-N10	2.31	122.05	115.97
2	5-A	7401	FMN	C5A-C9A-N10	2.31	119.08	116.80
2	2-B	9401	FMN	C4A-C10-N1	-2.31	120.42	122.73
2	9-A	7401	FMN	C4'-C3'-C2'	-2.31	108.03	113.25
2	15-A	7401	FMN	N1-C10-N10	2.29	122.00	115.97
2	15-A	7401	FMN	O2P-P-O1P	2.29	117.93	110.44
2	2-A	7401	FMN	N1-C10-N10	2.29	121.98	115.97
2	5-B	9401	FMN	C1'-N10-C10	-2.28	115.93	119.17
2	11-A	7401	FMN	C5A-C9A-N10	2.28	119.05	116.80
2	7-A	7401	FMN	O3'-C3'-C4'	2.28	114.49	108.74
2	6-B	9401	FMN	C4A-C10-N1	-2.28	120.45	122.73
2	13-B	9401	FMN	O4'-C4'-C5'	-2.28	105.45	110.12
2	6-B	9401	FMN	O4'-C4'-C5'	-2.27	105.45	110.12
2	4-A	7401	FMN	N1-C10-N10	2.27	121.93	115.97
2	15-B	9401	FMN	C9-C9A-C5A	-2.27	115.60	119.38
2	3-B	9401	FMN	O4'-C4'-C5'	-2.27	105.47	110.12
2	15-B	9401	FMN	O4'-C4'-C5'	-2.26	105.47	110.12
2	5-B	9401	FMN	N1-C10-N10	2.27	121.92	115.97
2	13-A	7401	FMN	O5'-C5'-C4'	-2.26	87.30	105.77
2	16-A	7401	FMN	O5'-C5'-C4'	-2.26	87.36	105.77
2	5-B	9401	FMN	C5A-C9A-N10	2.25	119.02	116.80
2	11-A	7401	FMN	N1-C10-N10	2.24	121.87	115.97
2	14-A	7401	FMN	O4'-C4'-C3'	-2.24	103.47	109.05
2	7-A	7401	FMN	O2'-C2'-C3'	-2.22	103.51	109.05
2	2-B	9401	FMN	C9A-N10-C10	-2.22	119.58	121.77
2	13-B	9401	FMN	C9-C9A-C5A	-2.22	115.67	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-A	7401	FMN	N1-C10-N10	2.21	121.79	115.97
2	9-B	9401	FMN	C5A-C9A-N10	2.19	118.96	116.80
2	13-B	9401	FMN	C5A-C9A-N10	2.19	118.96	116.80
2	15-B	9401	FMN	C5A-C9A-N10	2.17	118.94	116.80
2	1-B	9401	FMN	C4'-C3'-C2'	-2.16	108.36	113.25
2	1-A	7401	FMN	N1-C10-N10	2.16	121.66	115.97
2	10-B	9401	FMN	N1-C10-N10	2.16	121.64	115.97
2	9-A	7401	FMN	O2'-C2'-C1'	-2.16	104.35	109.71
2	12-A	7401	FMN	C4'-C3'-C2'	-2.16	108.38	113.25
2	1-B	9401	FMN	C9A-N10-C10	-2.16	119.65	121.77
2	3-A	7401	FMN	O2P-P-O1P	2.15	117.48	110.44
2	8-A	7401	FMN	O2'-C2'-C1'	-2.15	104.37	109.71
2	15-A	7401	FMN	O4'-C4'-C5'	-2.14	105.72	110.12
2	13-A	7401	FMN	C9-C9A-N10	2.14	126.20	121.59
2	10-B	9401	FMN	C5A-C9A-N10	2.13	118.90	116.80
2	8-A	7401	FMN	C4'-C3'-C2'	-2.12	108.45	113.25
2	12-B	9401	FMN	C2'-C1'-N10	2.11	115.25	112.45
2	7-A	7401	FMN	O4'-C4'-C5'	-2.11	105.80	110.12
2	1-B	9401	FMN	C5A-C9A-N10	2.10	118.87	116.80
2	7-B	9401	FMN	O2'-C2'-C1'	-2.10	104.50	109.71
2	6-A	7401	FMN	O5'-C5'-C4'	2.10	122.89	105.77
2	7-A	7401	FMN	O3'-C3'-C2'	2.10	114.03	108.74
2	11-B	9401	FMN	O4'-C4'-C5'	-2.10	105.82	110.12
2	9-B	9401	FMN	C4A-C10-N1	-2.10	120.64	122.73
2	7-A	7401	FMN	C4A-C10-N1	-2.09	120.64	122.73
2	15-A	7401	FMN	C4A-C10-N1	-2.08	120.65	122.73
2	8-A	7401	FMN	C2'-C1'-N10	-2.07	109.70	112.45
2	14-A	7401	FMN	P-O5'-C5'	-2.07	112.20	118.19
2	4-B	9401	FMN	O3'-C3'-C2'	-2.07	103.50	108.74
2	12-B	9401	FMN	C1'-N10-C9A	2.07	120.88	118.87
2	14-A	7401	FMN	C9A-C5A-N5	-2.06	119.22	122.37
2	9-A	7401	FMN	C2'-C1'-N10	-2.06	109.72	112.45
2	15-B	9401	FMN	O3'-C3'-C2'	2.06	113.93	108.74
2	10-A	7401	FMN	O2P-P-O1P	2.04	117.12	110.44
2	9-B	9401	FMN	C9A-N10-C10	-2.04	119.77	121.77
2	3-A	7401	FMN	C5A-C9A-N10	2.03	118.80	116.80
2	9-B	9401	FMN	N1-C10-N10	2.03	121.31	115.97
2	16-A	7401	FMN	C9-C9A-N10	2.02	125.95	121.59
2	6-B	9401	FMN	C9A-N10-C10	-2.02	119.78	121.77
2	6-B	9401	FMN	O2'-C2'-C3'	2.02	114.07	109.05
2	7-B	9401	FMN	C5'-C4'-C3'	2.02	115.86	112.06
2	15-B	9401	FMN	C8-C9-C9A	2.01	123.87	119.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	14-A	7401	FMN	O3'-C3'-C2'	-2.01	103.65	108.74
2	15-A	7401	FMN	C9A-C5A-N5	-2.01	119.28	122.37
2	16-B	9401	FMN	C4-N3-C2	-2.00	121.28	125.39

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	7-A	7401	FMN	C2'-C1'-N10-C10
2	7-A	7401	FMN	C2'-C1'-N10-C9A

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.