



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:11 PM UTC

PDB ID : 2Q3O / pdb_00002q3o
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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

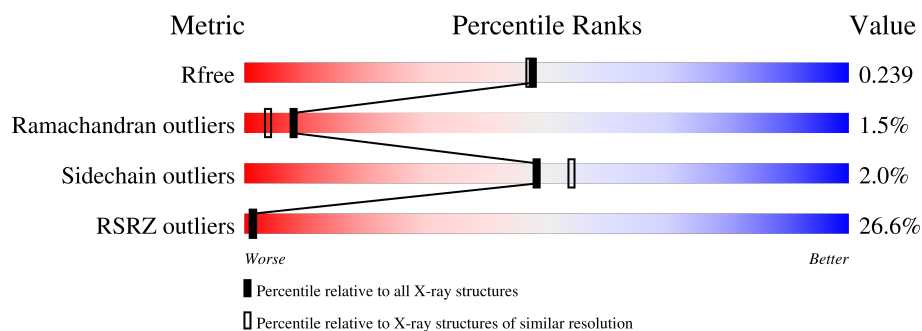
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	10052 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	1-A	391	26% 90% 7%
1	1-B	391	24% 91% 6%
1	10-A	391	87% 6% 7%
1	10-B	391	92% 6%
1	11-A	391	92% 7%
1	11-B	391	91% 6%

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Mol	Chain	Length	Quality of chain
1	12-A	391	 90% • 7%
1	12-B	391	 91% • 6%
1	13-A	391	 91% • 7%
1	13-B	391	 90% • 6%
1	14-A	391	 91% • 7%
1	14-B	391	 90% • 6%
1	15-A	391	 91% • 7%
1	15-B	391	 90% • 6%
1	16-A	391	 91% • 7%
1	16-B	391	 91% • 6%
1	2-A	391	 90% • 7%
1	2-B	391	 91% • 6%
1	3-A	391	 92% • 7%
1	3-B	391	 90% • 6%
1	4-A	391	 91% • 7%
1	4-B	391	 91% • 6%
1	5-A	391	 92% • 7%
1	5-B	391	 91% • 6%
1	6-A	391	 92% • 7%
1	6-B	391	 92% • 6%
1	7-A	391	 91% • 7%
1	7-B	391	 90% • 6%
1	8-A	391	 91% • 7%
1	8-B	391	 91% • 6%
1	9-A	391	 90% • 7%

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Mol	Chain	Length	Quality of chain
1	9-B	391	91% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 97936 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 12-oxophytodienoate reductase 3.

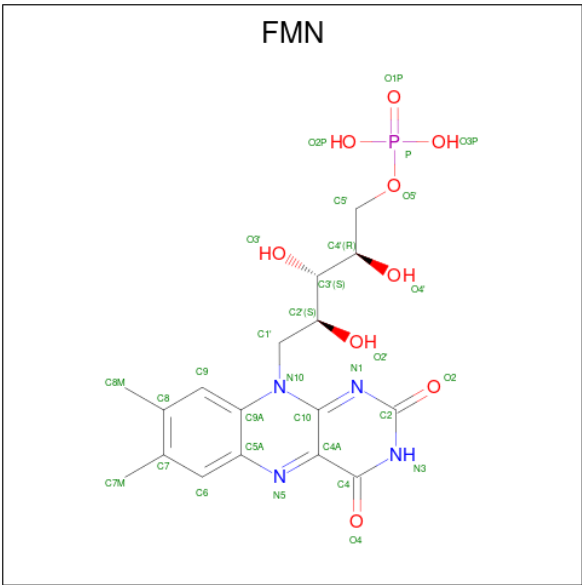
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	2-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	3-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	4-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	5-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	6-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	7-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	8-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	9-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	10-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	11-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	12-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	13-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	14-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	15-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	16-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	2-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	3-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	4-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	5-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	6-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	7-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	8-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	9-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	10-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	11-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	12-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	13-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	14-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	15-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	16-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	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	3-A	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	5-A	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	7-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	8-A	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	10-A	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	12-A	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	14-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	15-A	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	1-B	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-B	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-B	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-B	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-B	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-B	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-B	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-B	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	2-A	202	Total O 202 202	0	0
3	3-A	202	Total O 202 202	0	0
3	4-A	203	Total O 203 203	0	0
3	5-A	205	Total O 205 205	0	0
3	6-A	203	Total O 203 203	0	0
3	7-A	203	Total O 203 203	0	0
3	8-A	201	Total O 201 201	0	0
3	9-A	205	Total O 205 205	0	0
3	10-A	200	Total O 200 200	0	0
3	11-A	203	Total O 203 203	0	0
3	12-A	206	Total O 206 206	0	0
3	13-A	206	Total O 206 206	0	0
3	14-A	202	Total O 202 202	0	0
3	15-A	200	Total O 200 200	0	0
3	16-A	204	Total O 204 204	0	0
3	1-B	208	Total O 208 208	0	0
3	2-B	208	Total O 208 208	0	0
3	3-B	208	Total O 208 208	0	0
3	4-B	207	Total O 207 207	0	0
3	5-B	205	Total O 205 205	0	0
3	6-B	207	Total O 207 207	0	0

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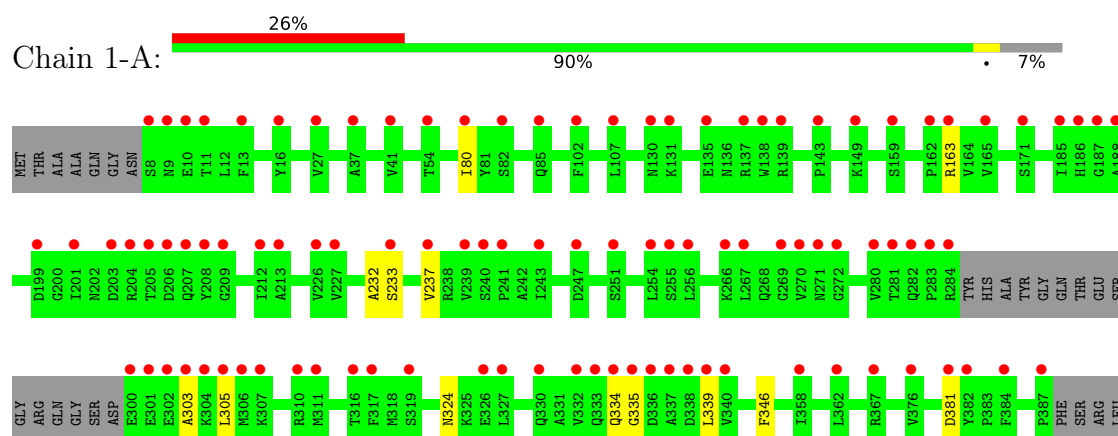
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	7-B	207	Total 207	O 207	0	0
3	8-B	209	Total 209	O 209	0	0
3	9-B	205	Total 205	O 205	0	0
3	10-B	210	Total 210	O 210	0	0
3	11-B	207	Total 207	O 207	0	0
3	12-B	204	Total 204	O 204	0	0
3	13-B	204	Total 204	O 204	0	0
3	14-B	208	Total 208	O 208	0	0
3	15-B	210	Total 210	O 210	0	0
3	16-B	206	Total 206	O 206	0	0

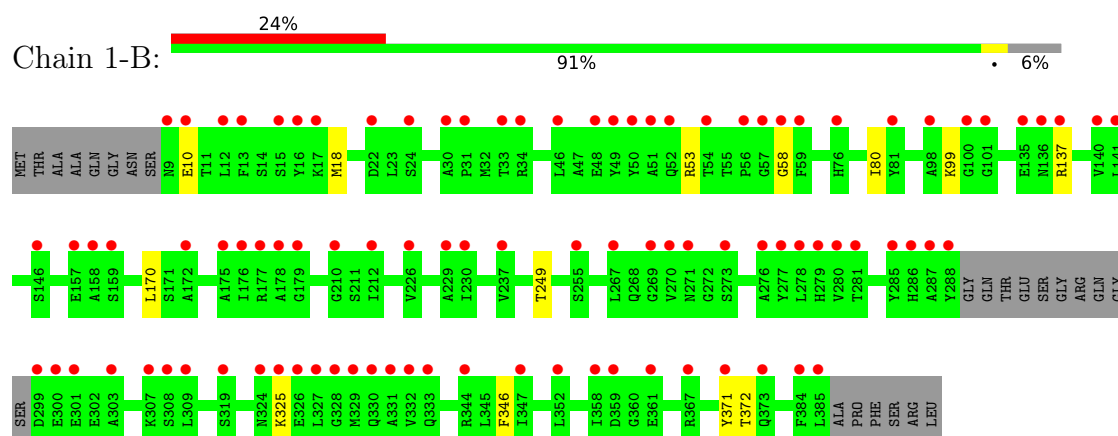
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

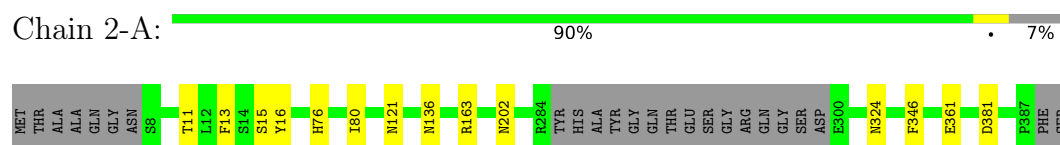
- Molecule 1: 12-oxophytodienoate reductase 3



- Molecule 1: 12-oxophytodienoate reductase 3

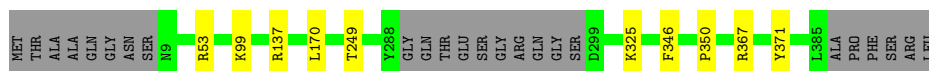


- Molecule 1: 12-oxophytodienoate reductase 3

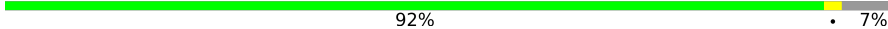


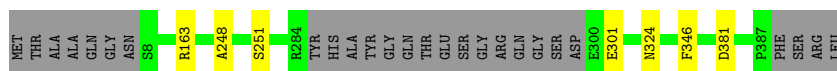
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 2-B:  91% • 6%



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 3-A:  92% • 7%



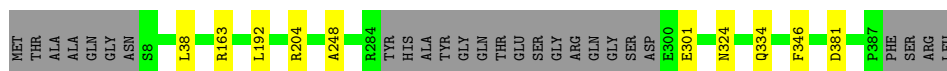
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 3-B:  90% • 6%



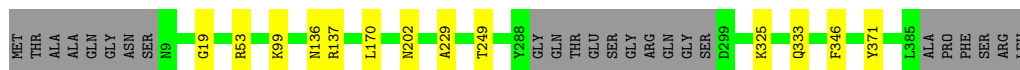
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 4-A:  91% • 7%



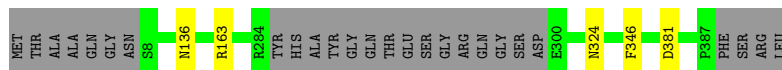
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 4-B:  91% • 6%



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 5-A:  92% • 7%



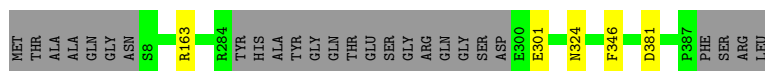
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 5-B:  91% • 6%



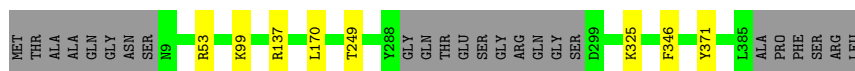
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 6-A:  92% • 7%



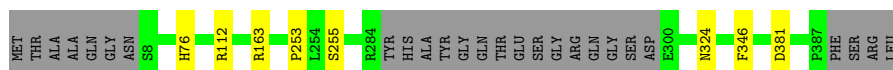
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 6-B:  92% • 6%



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 7-A:  91% • 7%



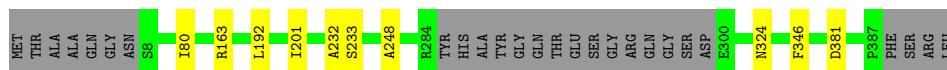
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 7-B:  90% • 6%



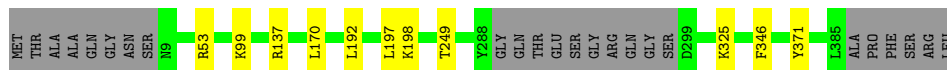
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 8-A:  91% • 7%



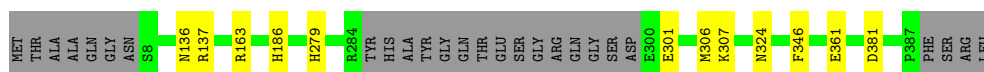
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 8-B:  91% • 6%



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 9-A:  90% • 7%



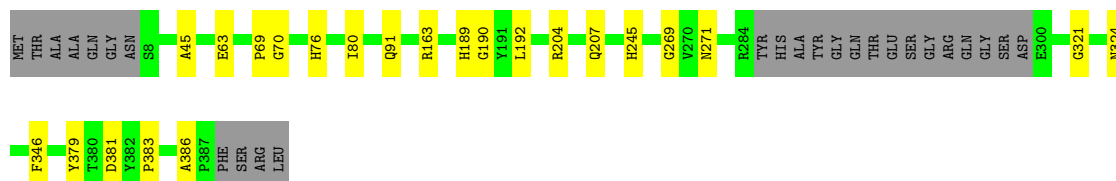
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 9-B:  91% • 6%



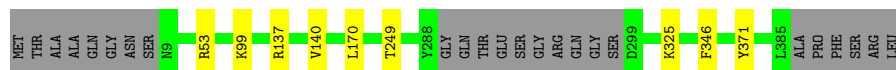
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 10-A:  87% 6% 7%



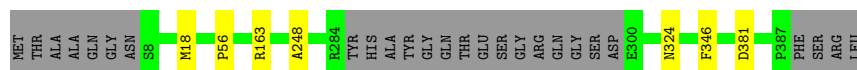
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 10-B:  92% • 6%



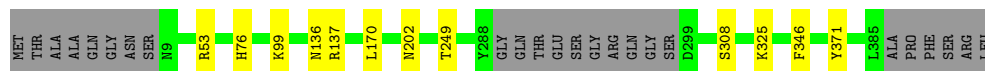
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 11-A:  92% • 7%



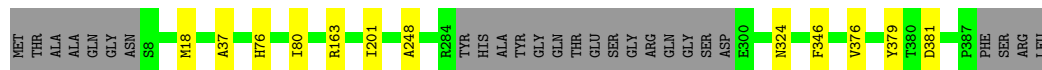
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 11-B:  91% • 6%



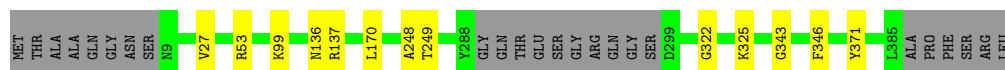
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 12-A:  90% • 7%

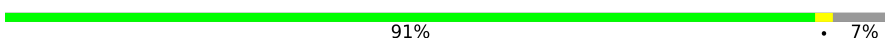
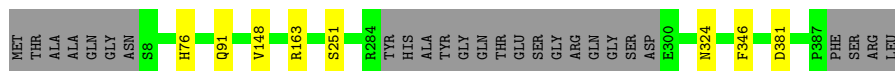


- Molecule 1: 12-oxophytodienoate reductase 3

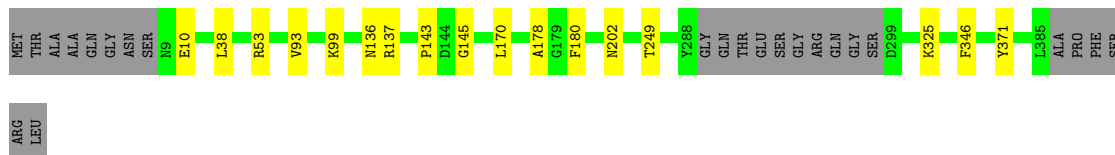
Chain 12-B:  91% • 6%



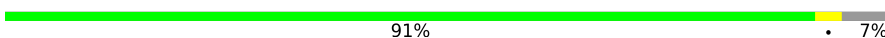
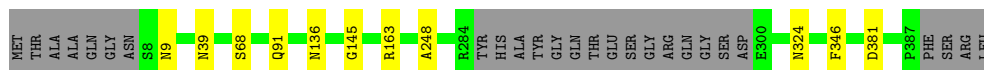
● Molecule 1: 12-oxophytodienoate reductase 3

Chain 13-A:  91% 7%

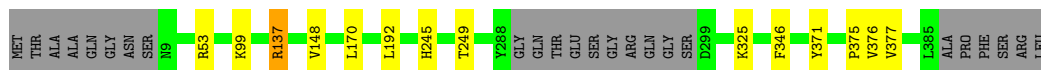
● Molecule 1: 12-oxophytodienoate reductase 3

Chain 13-B:  90% 6%

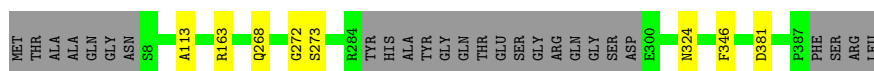
● Molecule 1: 12-oxophytodienoate reductase 3

Chain 14-A:  91% 7%

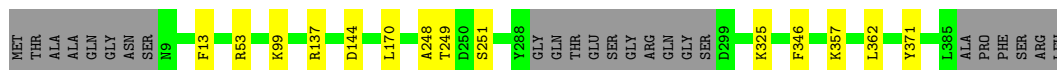
● Molecule 1: 12-oxophytodienoate reductase 3

Chain 14-B:  90% 6%

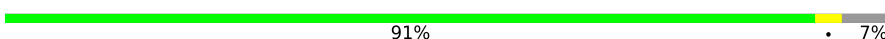
● Molecule 1: 12-oxophytodienoate reductase 3

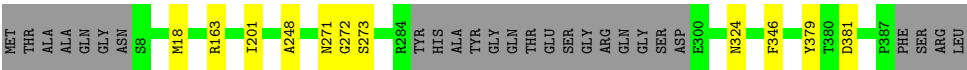
Chain 15-A:  91% 7%

● Molecule 1: 12-oxophytodienoate reductase 3

Chain 15-B:  90% 6%

● Molecule 1: 12-oxophytodienoate reductase 3

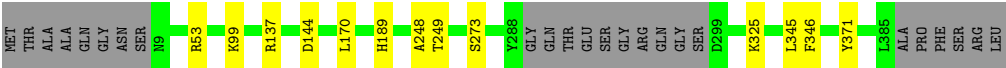
Chain 16-A:  91% 7%



● Molecule 1: 12-oxophytodienoate reductase 3

Chain 16-B:

91%6%



4 Data and refinement statistics

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 24.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (24.90-2.00) 91.2 (24.90-2.00)	Depositor EDS
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 0.186 , 0.239	Depositor DCC
R_{free} test set	2572 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
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.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.21	0/2875	0.42	0/3895
1	1-B	0.23	0/2906	0.44	0/3937
1	2-A	0.21	0/2875	0.42	0/3895
1	2-B	0.23	0/2906	0.44	0/3937
1	3-A	0.21	0/2875	0.42	0/3895
1	3-B	0.23	0/2906	0.44	0/3937
1	4-A	0.21	0/2875	0.42	0/3895
1	4-B	0.23	0/2906	0.44	0/3937
1	5-A	0.21	0/2875	0.42	0/3895
1	5-B	0.23	0/2906	0.44	0/3937
1	6-A	0.21	0/2875	0.42	0/3895
1	6-B	0.23	0/2906	0.44	0/3937
1	7-A	0.21	0/2875	0.42	0/3895
1	7-B	0.23	0/2906	0.44	0/3937
1	8-A	0.21	0/2875	0.42	0/3895
1	8-B	0.23	0/2906	0.44	0/3937
1	9-A	0.21	0/2875	0.42	0/3895
1	9-B	0.23	0/2906	0.44	0/3937
1	10-A	0.21	0/2875	0.42	0/3895
1	10-B	0.23	0/2906	0.44	0/3937
1	11-A	0.21	0/2875	0.42	0/3895
1	11-B	0.23	0/2906	0.44	0/3937
1	12-A	0.21	0/2875	0.42	0/3895
1	12-B	0.23	0/2906	0.44	0/3937
1	13-A	0.21	0/2875	0.42	0/3895
1	13-B	0.23	0/2906	0.44	0/3937
1	14-A	0.21	0/2875	0.42	0/3895
1	14-B	0.23	0/2906	0.44	0/3937
1	15-A	0.21	0/2875	0.42	0/3895
1	15-B	0.23	0/2906	0.44	0/3937
1	16-A	0.21	0/2875	0.42	0/3895
1	16-B	0.23	0/2906	0.44	0/3937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.22	0/92496	0.43	0/125312

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	0
3	1-B	208	0	0	0	0
3	2-A	202	0	0	0	0

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

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

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%)	4	1
1	1-B	363/391 (93%)	333 (92%)	25 (7%)	5 (1%)	9	4
1	2-A	361/391 (92%)	300 (83%)	51 (14%)	10 (3%)	4	1
1	2-B	363/391 (93%)	337 (93%)	24 (7%)	2 (1%)	21	17
1	3-A	361/391 (92%)	336 (93%)	22 (6%)	3 (1%)	16	11
1	3-B	363/391 (93%)	339 (93%)	18 (5%)	6 (2%)	7	3
1	4-A	361/391 (92%)	322 (89%)	33 (9%)	6 (2%)	7	3
1	4-B	363/391 (93%)	338 (93%)	20 (6%)	5 (1%)	9	4
1	5-A	361/391 (92%)	331 (92%)	29 (8%)	1 (0%)	36	35
1	5-B	363/391 (93%)	341 (94%)	20 (6%)	2 (1%)	21	17
1	6-A	361/391 (92%)	338 (94%)	22 (6%)	1 (0%)	36	35
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%)	11	7
1	7-B	363/391 (93%)	334 (92%)	23 (6%)	6 (2%)	7	3
1	8-A	361/391 (92%)	324 (90%)	31 (9%)	6 (2%)	7	3
1	8-B	363/391 (93%)	332 (92%)	28 (8%)	3 (1%)	16	11
1	9-A	361/391 (92%)	330 (91%)	23 (6%)	8 (2%)	5	2
1	9-B	363/391 (93%)	335 (92%)	26 (7%)	2 (1%)	21	17
1	10-A	361/391 (92%)	309 (86%)	33 (9%)	19 (5%)	1	0
1	10-B	363/391 (93%)	338 (93%)	24 (7%)	1 (0%)	36	35
1	11-A	361/391 (92%)	336 (93%)	22 (6%)	3 (1%)	16	11
1	11-B	363/391 (93%)	337 (93%)	22 (6%)	4 (1%)	11	7
1	12-A	361/391 (92%)	328 (91%)	25 (7%)	8 (2%)	5	2
1	12-B	363/391 (93%)	326 (90%)	32 (9%)	5 (1%)	9	4
1	13-A	361/391 (92%)	322 (89%)	35 (10%)	4 (1%)	11	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13-B	363/391 (93%)	327 (90%)	27 (7%)	9 (2%)	4	1
1	14-A	361/391 (92%)	312 (86%)	42 (12%)	7 (2%)	6	3
1	14-B	363/391 (93%)	311 (86%)	45 (12%)	7 (2%)	6	3
1	15-A	361/391 (92%)	324 (90%)	33 (9%)	4 (1%)	11	7
1	15-B	363/391 (93%)	326 (90%)	31 (8%)	6 (2%)	7	3
1	16-A	361/391 (92%)	324 (90%)	30 (8%)	7 (2%)	6	3
1	16-B	363/391 (93%)	332 (92%)	26 (7%)	5 (1%)	9	4
All	All	11584/12512 (93%)	10513 (91%)	903 (8%)	168 (2%)	8	4

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	294 (99%)	4 (1%)	61	68
1	1-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	2-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	2-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	3-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	3-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	4-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	4-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	5-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	5-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	6-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	6-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	7-A	298/317 (94%)	294 (99%)	4 (1%)	61	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	8-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	8-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	9-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	9-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	10-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	10-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	11-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	11-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	12-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	12-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	13-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	13-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	14-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	14-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	15-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	15-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
1	16-A	298/317 (94%)	294 (99%)	4 (1%)	61	68
1	16-B	300/317 (95%)	292 (97%)	8 (3%)	39	42
All	All	9568/10144 (94%)	9376 (98%)	192 (2%)	48	54

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	163	ARG
1	1-A	324	ASN
1	1-A	346	PHE
1	1-A	381	ASP
1	1-B	53	ARG
1	1-B	99	LYS
1	1-B	137	ARG
1	1-B	170	LEU
1	1-B	249	THR
1	1-B	325	LYS
1	1-B	346	PHE

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Mol	Chain	Res	Type
1	1-B	371	TYR
1	2-A	163	ARG
1	2-A	324	ASN
1	2-A	346	PHE
1	2-A	381	ASP
1	2-B	53	ARG
1	2-B	99	LYS
1	2-B	137	ARG
1	2-B	170	LEU
1	2-B	249	THR
1	2-B	325	LYS
1	2-B	346	PHE
1	2-B	371	TYR
1	3-A	163	ARG
1	3-A	324	ASN
1	3-A	346	PHE
1	3-A	381	ASP
1	3-B	53	ARG
1	3-B	99	LYS
1	3-B	137	ARG
1	3-B	170	LEU
1	3-B	249	THR
1	3-B	325	LYS
1	3-B	346	PHE
1	3-B	371	TYR
1	4-A	163	ARG
1	4-A	324	ASN
1	4-A	346	PHE
1	4-A	381	ASP
1	4-B	53	ARG
1	4-B	99	LYS
1	4-B	137	ARG
1	4-B	170	LEU
1	4-B	249	THR
1	4-B	325	LYS
1	4-B	346	PHE
1	4-B	371	TYR
1	5-A	163	ARG
1	5-A	324	ASN
1	5-A	346	PHE
1	5-A	381	ASP
1	5-B	53	ARG

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Mol	Chain	Res	Type
1	5-B	99	LYS
1	5-B	137	ARG
1	5-B	170	LEU
1	5-B	249	THR
1	5-B	325	LYS
1	5-B	346	PHE
1	5-B	371	TYR
1	6-A	163	ARG
1	6-A	324	ASN
1	6-A	346	PHE
1	6-A	381	ASP
1	6-B	53	ARG
1	6-B	99	LYS
1	6-B	137	ARG
1	6-B	170	LEU
1	6-B	249	THR
1	6-B	325	LYS
1	6-B	346	PHE
1	6-B	371	TYR
1	7-A	163	ARG
1	7-A	324	ASN
1	7-A	346	PHE
1	7-A	381	ASP
1	7-B	53	ARG
1	7-B	99	LYS
1	7-B	137	ARG
1	7-B	170	LEU
1	7-B	249	THR
1	7-B	325	LYS
1	7-B	346	PHE
1	7-B	371	TYR
1	8-A	163	ARG
1	8-A	324	ASN
1	8-A	346	PHE
1	8-A	381	ASP
1	8-B	53	ARG
1	8-B	99	LYS
1	8-B	137	ARG
1	8-B	170	LEU
1	8-B	249	THR
1	8-B	325	LYS
1	8-B	346	PHE

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Mol	Chain	Res	Type
1	8-B	371	TYR
1	9-A	163	ARG
1	9-A	324	ASN
1	9-A	346	PHE
1	9-A	381	ASP
1	9-B	53	ARG
1	9-B	99	LYS
1	9-B	137	ARG
1	9-B	170	LEU
1	9-B	249	THR
1	9-B	325	LYS
1	9-B	346	PHE
1	9-B	371	TYR
1	10-A	163	ARG
1	10-A	324	ASN
1	10-A	346	PHE
1	10-A	381	ASP
1	10-B	53	ARG
1	10-B	99	LYS
1	10-B	137	ARG
1	10-B	170	LEU
1	10-B	249	THR
1	10-B	325	LYS
1	10-B	346	PHE
1	10-B	371	TYR
1	11-A	163	ARG
1	11-A	324	ASN
1	11-A	346	PHE
1	11-A	381	ASP
1	11-B	53	ARG
1	11-B	99	LYS
1	11-B	137	ARG
1	11-B	170	LEU
1	11-B	249	THR
1	11-B	325	LYS
1	11-B	346	PHE
1	11-B	371	TYR
1	12-A	163	ARG
1	12-A	324	ASN
1	12-A	346	PHE
1	12-A	381	ASP
1	12-B	53	ARG

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Mol	Chain	Res	Type
1	12-B	99	LYS
1	12-B	137	ARG
1	12-B	170	LEU
1	12-B	249	THR
1	12-B	325	LYS
1	12-B	346	PHE
1	12-B	371	TYR
1	13-A	163	ARG
1	13-A	324	ASN
1	13-A	346	PHE
1	13-A	381	ASP
1	13-B	53	ARG
1	13-B	99	LYS
1	13-B	137	ARG
1	13-B	170	LEU
1	13-B	249	THR
1	13-B	325	LYS
1	13-B	346	PHE
1	13-B	371	TYR
1	14-A	163	ARG
1	14-A	324	ASN
1	14-A	346	PHE
1	14-A	381	ASP
1	14-B	53	ARG
1	14-B	99	LYS
1	14-B	137	ARG
1	14-B	170	LEU
1	14-B	249	THR
1	14-B	325	LYS
1	14-B	346	PHE
1	14-B	371	TYR
1	15-A	163	ARG
1	15-A	324	ASN
1	15-A	346	PHE
1	15-A	381	ASP
1	15-B	53	ARG
1	15-B	99	LYS
1	15-B	137	ARG
1	15-B	170	LEU
1	15-B	249	THR
1	15-B	325	LYS
1	15-B	346	PHE

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Mol	Chain	Res	Type
1	15-B	371	TYR
1	16-A	163	ARG
1	16-A	324	ASN
1	16-A	346	PHE
1	16-A	381	ASP
1	16-B	53	ARG
1	16-B	99	LYS
1	16-B	137	ARG
1	16-B	170	LEU
1	16-B	249	THR
1	16-B	325	LYS
1	16-B	346	PHE
1	16-B	371	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (356) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	39	ASN
1	1-A	52	GLN
1	1-A	97	HIS
1	1-A	119	GLN
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-A	366	ASN
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	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	186	HIS
1	2-A	195	GLN

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Mol	Chain	Res	Type
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-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	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	119	GLN
1	3-A	195	GLN
1	3-A	221	GLN
1	3-A	268	GLN
1	3-A	282	GLN
1	3-A	324	ASN
1	3-A	330	GLN
1	3-A	334	GLN
1	3-B	39	ASN
1	3-B	43	ASN
1	3-B	91	GLN
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	271	ASN
1	3-B	314	ASN
1	3-B	334	GLN
1	3-B	373	GLN
1	4-A	39	ASN
1	4-A	91	GLN
1	4-A	97	HIS
1	4-A	119	GLN
1	4-A	147	HIS

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Mol	Chain	Res	Type
1	4-A	195	GLN
1	4-A	202	ASN
1	4-A	268	GLN
1	4-A	282	GLN
1	4-A	314	ASN
1	4-A	324	ASN
1	4-A	334	GLN
1	4-A	373	GLN
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	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
1	5-A	271	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	119	GLN
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	373	GLN
1	6-A	39	ASN

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Mol	Chain	Res	Type
1	6-A	52	GLN
1	6-A	97	HIS
1	6-A	119	GLN
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-A	333	GLN
1	6-A	366	ASN
1	6-B	39	ASN
1	6-B	76	HIS
1	6-B	97	HIS
1	6-B	119	GLN
1	6-B	147	HIS
1	6-B	174	ASN
1	6-B	189	HIS
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	373	GLN
1	7-A	39	ASN
1	7-A	52	GLN
1	7-A	119	GLN
1	7-A	221	GLN
1	7-A	268	GLN
1	7-A	271	ASN
1	7-A	282	GLN
1	7-A	314	ASN
1	7-A	324	ASN
1	7-A	334	GLN
1	7-A	363	ASN
1	7-A	373	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

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Mol	Chain	Res	Type
1	7-B	207	GLN
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	7-B	373	GLN
1	8-A	52	GLN
1	8-A	97	HIS
1	8-A	119	GLN
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	119	GLN
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
1	9-A	97	HIS
1	9-A	195	GLN
1	9-A	268	GLN
1	9-A	271	ASN
1	9-A	314	ASN
1	9-A	324	ASN
1	9-A	330	GLN
1	9-A	333	GLN

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Mol	Chain	Res	Type
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	330	GLN
1	9-B	334	GLN
1	9-B	373	GLN
1	10-A	52	GLN
1	10-A	119	GLN
1	10-A	147	HIS
1	10-A	189	HIS
1	10-A	195	GLN
1	10-A	245	HIS
1	10-A	268	GLN
1	10-A	324	ASN
1	10-A	330	GLN
1	10-A	333	GLN
1	10-A	334	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	195	GLN
1	10-B	214	ASN
1	10-B	268	GLN
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
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-B	39	ASN
1	11-B	97	HIS
1	11-B	119	GLN

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Mol	Chain	Res	Type
1	11-B	174	ASN
1	11-B	195	GLN
1	11-B	214	ASN
1	11-B	268	GLN
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	221	GLN
1	12-A	268	GLN
1	12-A	271	ASN
1	12-A	314	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	174	ASN
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	373	GLN
1	13-A	39	ASN
1	13-A	97	HIS
1	13-A	119	GLN
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	97	HIS
1	13-B	119	GLN
1	13-B	174	ASN
1	13-B	186	HIS

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Mol	Chain	Res	Type
1	13-B	214	ASN
1	13-B	268	GLN
1	13-B	373	GLN
1	14-A	39	ASN
1	14-A	52	GLN
1	14-A	97	HIS
1	14-A	119	GLN
1	14-A	130	ASN
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	363	ASN
1	14-B	39	ASN
1	14-B	76	HIS
1	14-B	91	GLN
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	282	GLN
1	14-B	314	ASN
1	14-B	330	GLN
1	14-B	363	ASN
1	14-B	366	ASN
1	15-A	39	ASN
1	15-A	76	HIS
1	15-A	97	HIS
1	15-A	186	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

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Mol	Chain	Res	Type
1	15-B	119	GLN
1	15-B	174	ASN
1	15-B	189	HIS
1	15-B	195	GLN
1	15-B	207	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	147	HIS
1	16-A	195	GLN
1	16-A	214	ASN
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	349	ASN
1	16-A	373	GLN
1	16-B	39	ASN
1	16-B	136	ASN
1	16-B	147	HIS
1	16-B	174	ASN
1	16-B	195	GLN
1	16-B	207	GLN
1	16-B	214	ASN
1	16-B	245	HIS
1	16-B	268	GLN
1	16-B	330	GLN
1	16-B	373	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	16-A	7401	-	33,33,33	2.25	10 (30%)	48,50,50	3.35	19 (39%)
2	FMN	13-B	9401	-	33,33,33	2.63	13 (39%)	48,50,50	3.86	23 (47%)
2	FMN	9-B	9401	-	33,33,33	2.07	11 (33%)	48,50,50	3.53	13 (27%)
2	FMN	12-B	9401	-	33,33,33	2.01	12 (36%)	48,50,50	3.27	15 (31%)
2	FMN	10-B	9401	-	33,33,33	2.00	9 (27%)	48,50,50	3.46	14 (29%)
2	FMN	4-B	9401	-	33,33,33	1.59	7 (21%)	48,50,50	3.22	13 (27%)
2	FMN	12-A	7401	-	33,33,33	1.64	8 (24%)	48,50,50	2.69	16 (33%)
2	FMN	3-A	7401	-	33,33,33	2.05	9 (27%)	48,50,50	3.01	15 (31%)
2	FMN	8-A	7401	-	33,33,33	1.96	11 (33%)	48,50,50	2.78	16 (33%)
2	FMN	5-B	9401	-	33,33,33	1.93	7 (21%)	48,50,50	3.44	18 (37%)
2	FMN	14-A	7401	-	33,33,33	2.22	14 (42%)	48,50,50	3.11	20 (41%)
2	FMN	8-B	9401	-	33,33,33	1.69	7 (21%)	48,50,50	3.44	19 (39%)
2	FMN	16-B	9401	-	33,33,33	1.98	10 (30%)	48,50,50	3.68	21 (43%)
2	FMN	9-A	7401	-	33,33,33	1.82	10 (30%)	48,50,50	2.81	15 (31%)
2	FMN	14-B	9401	-	33,33,33	2.08	10 (30%)	48,50,50	3.50	16 (33%)
2	FMN	6-A	7401	-	33,33,33	2.15	6 (18%)	48,50,50	2.89	16 (33%)
2	FMN	1-B	9401	-	33,33,33	1.97	6 (18%)	48,50,50	3.39	13 (27%)
2	FMN	2-A	7401	-	33,33,33	1.65	8 (24%)	48,50,50	2.56	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	7-B	9401	-	33,33,33	2.38	9 (27%)	48,50,50	3.73	21 (43%)
2	FMN	2-B	9401	-	33,33,33	2.20	13 (39%)	48,50,50	3.88	20 (41%)
2	FMN	4-A	7401	-	33,33,33	1.88	5 (15%)	48,50,50	2.88	14 (29%)
2	FMN	3-B	9401	-	33,33,33	1.99	8 (24%)	48,50,50	3.70	19 (39%)
2	FMN	11-B	9401	-	33,33,33	2.09	5 (15%)	48,50,50	3.44	11 (22%)
2	FMN	15-B	9401	-	33,33,33	2.64	12 (36%)	48,50,50	3.88	24 (50%)
2	FMN	10-A	7401	-	33,33,33	1.53	7 (21%)	48,50,50	2.65	18 (37%)
2	FMN	7-A	7401	-	33,33,33	2.34	8 (24%)	48,50,50	3.34	23 (47%)
2	FMN	6-B	9401	-	33,33,33	2.14	13 (39%)	48,50,50	3.83	19 (39%)
2	FMN	5-A	7401	-	33,33,33	1.98	7 (21%)	48,50,50	2.88	15 (31%)
2	FMN	11-A	7401	-	33,33,33	1.96	5 (15%)	48,50,50	2.86	14 (29%)
2	FMN	13-A	7401	-	33,33,33	2.28	11 (33%)	48,50,50	3.37	20 (41%)
2	FMN	15-A	7401	-	33,33,33	1.94	9 (27%)	48,50,50	2.89	15 (31%)
2	FMN	1-A	7401	-	33,33,33	2.04	7 (21%)	48,50,50	2.85	13 (27%)

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	16-A	7401	-	-	4/18/18/18	0/3/3/3
2	FMN	13-B	9401	-	-	4/18/18/18	0/3/3/3
2	FMN	9-B	9401	-	-	2/18/18/18	0/3/3/3
2	FMN	12-B	9401	-	-	3/18/18/18	0/3/3/3
2	FMN	10-B	9401	-	-	4/18/18/18	0/3/3/3
2	FMN	4-B	9401	-	-	2/18/18/18	0/3/3/3
2	FMN	12-A	7401	-	-	1/18/18/18	0/3/3/3
2	FMN	3-A	7401	-	-	4/18/18/18	0/3/3/3
2	FMN	8-A	7401	-	-	3/18/18/18	0/3/3/3
2	FMN	5-B	9401	-	-	4/18/18/18	0/3/3/3
2	FMN	14-A	7401	-	-	1/18/18/18	0/3/3/3
2	FMN	8-B	9401	-	-	2/18/18/18	0/3/3/3
2	FMN	16-B	9401	-	-	4/18/18/18	0/3/3/3
2	FMN	9-A	7401	-	-	3/18/18/18	0/3/3/3
2	FMN	14-B	9401	-	-	4/18/18/18	0/3/3/3

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

All (287) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-A	7401	FMN	C1'-C2'	-9.03	1.40	1.52
2	11-B	9401	FMN	C5'-C4'	-8.35	1.40	1.51
2	1-B	9401	FMN	C5'-C4'	-7.97	1.41	1.51
2	7-B	9401	FMN	C1'-C2'	-7.56	1.42	1.52
2	6-A	7401	FMN	C5'-C4'	-7.54	1.41	1.51
2	13-B	9401	FMN	C1'-C2'	-7.31	1.42	1.52
2	15-B	9401	FMN	C1'-C2'	-7.16	1.42	1.52
2	15-B	9401	FMN	C9A-N10	7.13	1.53	1.41
2	13-B	9401	FMN	C9A-N10	6.91	1.53	1.41
2	2-B	9401	FMN	C1'-C2'	-6.77	1.43	1.52
2	13-A	7401	FMN	C1'-C2'	-6.72	1.43	1.52
2	16-A	7401	FMN	C1'-C2'	-6.65	1.43	1.52
2	6-B	9401	FMN	C1'-C2'	-6.42	1.43	1.52
2	1-A	7401	FMN	C1'-C2'	-6.36	1.43	1.52
2	3-A	7401	FMN	C1'-C2'	-6.36	1.43	1.52
2	7-B	9401	FMN	C9A-N10	6.07	1.51	1.41
2	3-B	9401	FMN	C1'-C2'	-5.91	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	11-A	7401	FMN	C1'-C2'	-5.89	1.44	1.52
2	14-A	7401	FMN	C4'-C3'	-5.84	1.43	1.53
2	5-A	7401	FMN	C1'-C2'	-5.68	1.44	1.52
2	5-B	9401	FMN	C9A-N10	5.54	1.50	1.41
2	15-A	7401	FMN	C1'-C2'	-5.38	1.45	1.52
2	5-A	7401	FMN	C9A-N10	5.36	1.50	1.41
2	4-A	7401	FMN	C1'-C2'	-5.33	1.45	1.52
2	16-B	9401	FMN	C5'-C4'	5.29	1.59	1.51
2	13-A	7401	FMN	C9A-N10	5.18	1.50	1.41
2	7-A	7401	FMN	C9A-N10	5.16	1.50	1.41
2	11-A	7401	FMN	C9A-N10	5.15	1.50	1.41
2	10-B	9401	FMN	C9A-N10	5.15	1.50	1.41
2	10-B	9401	FMN	C1'-C2'	-5.14	1.45	1.52
2	6-A	7401	FMN	C9A-N10	5.01	1.49	1.41
2	4-A	7401	FMN	C9A-N10	4.97	1.49	1.41
2	8-A	7401	FMN	C9A-N10	4.95	1.49	1.41
2	16-A	7401	FMN	C9A-N10	4.91	1.49	1.41
2	14-B	9401	FMN	C9A-N10	4.91	1.49	1.41
2	3-B	9401	FMN	C9A-N10	4.90	1.49	1.41
2	9-A	7401	FMN	C9A-N10	4.89	1.49	1.41
2	14-B	9401	FMN	C5'-C4'	4.87	1.58	1.51
2	1-A	7401	FMN	C9A-N10	4.82	1.49	1.41
2	9-B	9401	FMN	C1'-C2'	-4.67	1.46	1.52
2	16-B	9401	FMN	C9A-N10	4.62	1.49	1.41
2	12-B	9401	FMN	C9A-N10	4.54	1.49	1.41
2	12-B	9401	FMN	C1'-C2'	4.53	1.59	1.52
2	14-A	7401	FMN	C5'-C4'	-4.53	1.45	1.51
2	3-A	7401	FMN	C9A-N10	4.41	1.48	1.41
2	9-B	9401	FMN	C9A-N10	4.29	1.48	1.41
2	15-A	7401	FMN	C5'-C4'	-4.27	1.46	1.51
2	5-B	9401	FMN	C1'-C2'	-4.25	1.46	1.52
2	9-B	9401	FMN	C4'-C3'	-4.18	1.46	1.53
2	15-B	9401	FMN	C5'-C4'	4.18	1.57	1.51
2	7-B	9401	FMN	C5'-C4'	4.14	1.57	1.51
2	4-B	9401	FMN	C9A-N10	4.10	1.48	1.41
2	15-B	9401	FMN	C1'-N10	4.04	1.57	1.47
2	13-B	9401	FMN	C5'-C4'	4.00	1.57	1.51
2	8-A	7401	FMN	C5A-N5	-4.00	1.32	1.39
2	15-A	7401	FMN	C5A-N5	-3.99	1.32	1.39
2	2-A	7401	FMN	C2-N3	-3.97	1.30	1.39
2	9-A	7401	FMN	C5A-N5	-3.95	1.32	1.39
2	8-B	9401	FMN	C1'-C2'	3.95	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-B	9401	FMN	C6-C5A	3.95	1.46	1.40
2	14-A	7401	FMN	P-O5'	-3.91	1.48	1.60
2	14-A	7401	FMN	C6-C5A	3.90	1.45	1.40
2	13-B	9401	FMN	C1'-N10	3.89	1.57	1.47
2	2-B	9401	FMN	C9A-N10	3.87	1.47	1.41
2	15-B	9401	FMN	C6-C5A	3.87	1.45	1.40
2	12-A	7401	FMN	C9A-C5A	3.80	1.47	1.41
2	11-B	9401	FMN	C9-C9A	3.80	1.45	1.39
2	2-A	7401	FMN	C9A-C5A	3.79	1.47	1.41
2	10-B	9401	FMN	C9-C9A	3.76	1.45	1.39
2	10-A	7401	FMN	C2'-C3'	3.74	1.60	1.53
2	16-B	9401	FMN	C2'-C3'	3.72	1.59	1.53
2	1-B	9401	FMN	C9-C9A	3.69	1.45	1.39
2	6-A	7401	FMN	C5A-N5	-3.67	1.32	1.39
2	4-A	7401	FMN	C5A-N5	-3.64	1.32	1.39
2	15-A	7401	FMN	C9A-N10	3.64	1.47	1.41
2	6-B	9401	FMN	C9A-N10	3.63	1.47	1.41
2	11-A	7401	FMN	C5A-N5	-3.63	1.32	1.39
2	1-A	7401	FMN	C5A-N5	-3.60	1.32	1.39
2	5-A	7401	FMN	C5A-N5	-3.60	1.32	1.39
2	6-A	7401	FMN	C1'-C2'	-3.60	1.47	1.52
2	3-A	7401	FMN	C5A-N5	-3.58	1.32	1.39
2	13-A	7401	FMN	C5A-N5	-3.57	1.32	1.39
2	12-A	7401	FMN	C2-N3	-3.57	1.31	1.39
2	14-A	7401	FMN	C9-C9A	3.56	1.45	1.39
2	9-B	9401	FMN	C9-C9A	3.54	1.45	1.39
2	5-B	9401	FMN	C9-C9A	3.49	1.45	1.39
2	16-A	7401	FMN	C5A-N5	-3.46	1.33	1.39
2	3-A	7401	FMN	C4'-C3'	-3.43	1.47	1.53
2	2-B	9401	FMN	C2'-C3'	3.43	1.59	1.53
2	12-B	9401	FMN	C5A-N5	-3.42	1.33	1.39
2	8-A	7401	FMN	C1'-C2'	3.41	1.57	1.52
2	11-B	9401	FMN	C9A-N10	3.35	1.47	1.41
2	7-B	9401	FMN	C9-C9A	3.32	1.45	1.39
2	8-A	7401	FMN	C9A-C5A	3.30	1.46	1.41
2	14-B	9401	FMN	C6-C5A	3.29	1.45	1.40
2	9-B	9401	FMN	C6-C5A	3.29	1.45	1.40
2	9-A	7401	FMN	C9A-C5A	3.28	1.46	1.41
2	15-B	9401	FMN	C2-N1	-3.27	1.29	1.36
2	12-A	7401	FMN	C4A-C10	3.26	1.53	1.44
2	8-B	9401	FMN	C6-C5A	3.25	1.44	1.40
2	6-B	9401	FMN	C9-C9A	3.24	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-B	9401	FMN	C9-C9A	3.24	1.44	1.39
2	3-A	7401	FMN	P-O5'	-3.20	1.50	1.60
2	16-A	7401	FMN	C9-C9A	3.18	1.44	1.39
2	2-B	9401	FMN	C9-C9A	3.14	1.44	1.39
2	7-B	9401	FMN	C9A-C5A	3.14	1.46	1.41
2	3-B	9401	FMN	C9-C9A	3.13	1.44	1.39
2	7-A	7401	FMN	C2'-C3'	-3.12	1.48	1.53
2	13-A	7401	FMN	C9-C9A	3.11	1.44	1.39
2	13-B	9401	FMN	C2-N1	-3.11	1.29	1.36
2	4-B	9401	FMN	C9-C9A	3.10	1.44	1.39
2	14-B	9401	FMN	C2'-C3'	3.10	1.58	1.53
2	5-B	9401	FMN	C6-C5A	3.10	1.44	1.40
2	14-B	9401	FMN	C9A-C5A	3.09	1.46	1.41
2	10-B	9401	FMN	C6-C5A	3.09	1.44	1.40
2	7-B	9401	FMN	C6-C5A	3.08	1.44	1.40
2	14-A	7401	FMN	O2'-C2'	3.07	1.49	1.43
2	14-B	9401	FMN	C1'-N10	3.05	1.55	1.47
2	11-B	9401	FMN	C5A-N5	-3.04	1.33	1.39
2	6-B	9401	FMN	P-O5'	-3.03	1.50	1.60
2	6-A	7401	FMN	C9-C9A	3.01	1.44	1.39
2	15-B	9401	FMN	C9-C9A	3.01	1.44	1.39
2	16-B	9401	FMN	C9A-C5A	3.00	1.46	1.41
2	9-B	9401	FMN	O2'-C2'	2.99	1.49	1.43
2	1-B	9401	FMN	C5A-N5	-2.98	1.34	1.39
2	13-B	9401	FMN	C9-C9A	2.98	1.44	1.39
2	4-B	9401	FMN	C6-C5A	2.98	1.44	1.40
2	14-B	9401	FMN	O3'-C3'	-2.96	1.35	1.43
2	13-B	9401	FMN	P-O5'	-2.96	1.51	1.60
2	6-B	9401	FMN	C4'-C3'	-2.95	1.48	1.53
2	2-A	7401	FMN	C4A-C10	2.95	1.52	1.44
2	6-B	9401	FMN	C6-C5A	2.95	1.44	1.40
2	7-A	7401	FMN	C6-C5A	2.94	1.44	1.40
2	1-A	7401	FMN	P-O5'	-2.94	1.51	1.60
2	16-B	9401	FMN	C9-C9A	2.92	1.44	1.39
2	3-B	9401	FMN	C9A-C5A	2.91	1.45	1.41
2	8-B	9401	FMN	C4A-C10	2.89	1.52	1.44
2	16-A	7401	FMN	O3'-C3'	-2.89	1.35	1.43
2	3-B	9401	FMN	C6-C5A	2.88	1.44	1.40
2	13-A	7401	FMN	O3'-C3'	-2.87	1.35	1.43
2	9-B	9401	FMN	P-O5'	-2.87	1.51	1.60
2	2-B	9401	FMN	C6-C5A	2.86	1.44	1.40
2	13-A	7401	FMN	C6-C5A	2.86	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-B	9401	FMN	O2'-C2'	2.85	1.49	1.43
2	10-B	9401	FMN	P-O5'	-2.85	1.51	1.60
2	16-A	7401	FMN	C6-C5A	2.84	1.44	1.40
2	13-B	9401	FMN	C9A-C5A	2.83	1.45	1.41
2	7-A	7401	FMN	C2-N1	-2.83	1.30	1.36
2	1-A	7401	FMN	C9-C9A	2.83	1.44	1.39
2	8-B	9401	FMN	C9A-N10	2.83	1.46	1.41
2	12-B	9401	FMN	C2'-C3'	2.83	1.58	1.53
2	15-B	9401	FMN	C9A-C5A	2.82	1.45	1.41
2	5-A	7401	FMN	C9-C9A	2.80	1.44	1.39
2	15-B	9401	FMN	P-O5'	-2.80	1.51	1.60
2	8-A	7401	FMN	C10-N10	2.78	1.43	1.37
2	11-A	7401	FMN	C9-C9A	2.74	1.44	1.39
2	7-A	7401	FMN	C5A-N5	-2.73	1.34	1.39
2	10-A	7401	FMN	C6-C5A	2.72	1.44	1.40
2	3-A	7401	FMN	C9-C9A	2.71	1.44	1.39
2	12-B	9401	FMN	C4'-C3'	2.71	1.58	1.53
2	6-B	9401	FMN	O2'-C2'	2.69	1.49	1.43
2	8-A	7401	FMN	C2'-C3'	2.69	1.58	1.53
2	4-B	9401	FMN	C5A-N5	-2.69	1.34	1.39
2	6-B	9401	FMN	C2'-C3'	2.69	1.58	1.53
2	4-A	7401	FMN	C9-C9A	2.69	1.44	1.39
2	8-A	7401	FMN	C1'-N10	2.68	1.54	1.47
2	2-B	9401	FMN	P-O5'	-2.67	1.51	1.60
2	10-A	7401	FMN	C9A-C5A	2.67	1.45	1.41
2	16-A	7401	FMN	C9A-C5A	2.67	1.45	1.41
2	9-A	7401	FMN	C1'-C2'	2.66	1.56	1.52
2	15-A	7401	FMN	C9-C9A	2.66	1.43	1.39
2	8-B	9401	FMN	C5A-N5	-2.65	1.34	1.39
2	12-B	9401	FMN	C4A-C10	2.63	1.51	1.44
2	4-B	9401	FMN	C4A-C10	2.62	1.51	1.44
2	13-A	7401	FMN	C9A-C5A	2.61	1.45	1.41
2	5-B	9401	FMN	C5A-N5	-2.61	1.34	1.39
2	8-B	9401	FMN	C9-C9A	2.61	1.43	1.39
2	12-B	9401	FMN	C9A-C5A	2.61	1.45	1.41
2	12-B	9401	FMN	C1'-N10	2.54	1.54	1.47
2	8-A	7401	FMN	C4A-C10	2.53	1.51	1.44
2	16-B	9401	FMN	C1'-C2'	-2.53	1.49	1.52
2	9-A	7401	FMN	C10-N10	2.53	1.42	1.37
2	16-B	9401	FMN	C6-C5A	2.53	1.43	1.40
2	2-B	9401	FMN	C4'-C3'	-2.53	1.49	1.53
2	7-B	9401	FMN	C5A-N5	-2.50	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	14-A	7401	FMN	C2-N1	-2.49	1.31	1.36
2	7-A	7401	FMN	C9A-C5A	2.49	1.45	1.41
2	9-A	7401	FMN	C9-C9A	2.48	1.43	1.39
2	6-B	9401	FMN	P-O3P	2.48	1.64	1.54
2	12-B	9401	FMN	C2-N3	-2.48	1.33	1.39
2	15-B	9401	FMN	C4'-C3'	2.47	1.57	1.53
2	8-A	7401	FMN	C9-C9A	2.47	1.43	1.39
2	2-A	7401	FMN	C1'-N10	2.45	1.53	1.47
2	2-B	9401	FMN	C9A-C5A	2.45	1.45	1.41
2	12-A	7401	FMN	C9A-N10	2.44	1.45	1.41
2	10-A	7401	FMN	C1'-N10	2.44	1.53	1.47
2	9-A	7401	FMN	C4A-C10	2.43	1.51	1.44
2	12-A	7401	FMN	P-O2P	2.43	1.63	1.54
2	4-A	7401	FMN	C6-C5A	2.42	1.43	1.40
2	5-B	9401	FMN	C9A-C5A	2.41	1.45	1.41
2	16-A	7401	FMN	C5'-C4'	2.40	1.55	1.51
2	10-B	9401	FMN	C5A-N5	-2.40	1.35	1.39
2	16-B	9401	FMN	O2'-C2'	2.38	1.48	1.43
2	13-B	9401	FMN	C4'-C3'	2.37	1.57	1.53
2	3-B	9401	FMN	C5A-N5	-2.37	1.35	1.39
2	3-B	9401	FMN	C2-N1	-2.36	1.31	1.36
2	1-A	7401	FMN	C6-C5A	2.36	1.43	1.40
2	7-B	9401	FMN	C2-N1	-2.36	1.31	1.36
2	10-A	7401	FMN	C4A-C10	2.35	1.51	1.44
2	14-B	9401	FMN	C5A-N5	-2.34	1.35	1.39
2	16-A	7401	FMN	C2-N1	-2.33	1.31	1.36
2	2-B	9401	FMN	C2-N1	-2.33	1.31	1.36
2	9-A	7401	FMN	C1'-N10	2.33	1.53	1.47
2	13-A	7401	FMN	C2-N1	-2.32	1.31	1.36
2	12-B	9401	FMN	C9-C9A	2.31	1.43	1.39
2	14-A	7401	FMN	P-O1P	-2.31	1.43	1.50
2	2-B	9401	FMN	P-O3P	2.30	1.63	1.54
2	9-B	9401	FMN	P-O3P	2.30	1.63	1.54
2	5-A	7401	FMN	C6-C5A	2.29	1.43	1.40
2	13-A	7401	FMN	C5'-C4'	2.29	1.54	1.51
2	2-B	9401	FMN	C5A-N5	-2.28	1.35	1.39
2	9-B	9401	FMN	C5A-N5	-2.28	1.35	1.39
2	2-B	9401	FMN	O3'-C3'	2.27	1.48	1.43
2	3-A	7401	FMN	C6-C5A	2.27	1.43	1.40
2	16-A	7401	FMN	C4'-C3'	-2.27	1.49	1.53
2	14-A	7401	FMN	P-O2P	2.26	1.63	1.54
2	14-A	7401	FMN	C10-N10	-2.25	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-B	9401	FMN	O2-C2	-2.25	1.19	1.24
2	12-A	7401	FMN	C1'-N10	2.24	1.53	1.47
2	9-A	7401	FMN	C6-C5A	2.24	1.43	1.40
2	13-B	9401	FMN	C2'-C3'	-2.24	1.49	1.53
2	7-A	7401	FMN	C9-C9A	2.24	1.43	1.39
2	1-A	7401	FMN	C4'-C3'	-2.23	1.49	1.53
2	8-A	7401	FMN	C6-C5A	2.22	1.43	1.40
2	14-A	7401	FMN	C1'-N10	-2.22	1.42	1.47
2	15-B	9401	FMN	P-O3P	2.22	1.63	1.54
2	15-A	7401	FMN	C10-N10	-2.21	1.32	1.37
2	11-A	7401	FMN	C6-C5A	2.21	1.43	1.40
2	5-B	9401	FMN	C4A-C10	2.21	1.50	1.44
2	4-B	9401	FMN	C9A-C5A	2.21	1.44	1.41
2	10-B	9401	FMN	C9A-C5A	2.20	1.44	1.41
2	7-B	9401	FMN	O3'-C3'	2.20	1.48	1.43
2	14-B	9401	FMN	C4A-C10	2.20	1.50	1.44
2	12-B	9401	FMN	C6-C5A	2.19	1.43	1.40
2	9-A	7401	FMN	P-O2P	2.19	1.63	1.54
2	6-B	9401	FMN	C5A-N5	-2.19	1.35	1.39
2	15-A	7401	FMN	C6-C5A	2.18	1.43	1.40
2	14-A	7401	FMN	C9-C8	-2.17	1.36	1.39
2	6-B	9401	FMN	C9A-C5A	2.17	1.44	1.41
2	15-A	7401	FMN	P-O5'	-2.16	1.53	1.60
2	3-A	7401	FMN	C9A-C5A	2.16	1.44	1.41
2	3-A	7401	FMN	C2-N1	-2.16	1.31	1.36
2	15-B	9401	FMN	C2'-C3'	-2.16	1.49	1.53
2	6-A	7401	FMN	C6-C5A	2.16	1.43	1.40
2	10-B	9401	FMN	O2'-C2'	2.15	1.47	1.43
2	8-B	9401	FMN	C2-N3	-2.15	1.34	1.39
2	13-A	7401	FMN	C4'-C3'	-2.14	1.49	1.53
2	2-A	7401	FMN	P-O2P	2.14	1.62	1.54
2	2-A	7401	FMN	C6-C7	-2.14	1.36	1.39
2	6-B	9401	FMN	O3'-C3'	2.14	1.48	1.43
2	3-B	9401	FMN	O2'-C2'	2.14	1.47	1.43
2	6-B	9401	FMN	C2-N1	-2.13	1.31	1.36
2	13-B	9401	FMN	P-O3P	2.13	1.62	1.54
2	12-B	9401	FMN	C4-N3	-2.12	1.34	1.38
2	2-A	7401	FMN	C5A-N5	-2.11	1.35	1.39
2	10-A	7401	FMN	O2-C2	-2.11	1.20	1.24
2	9-B	9401	FMN	C2-N1	-2.11	1.31	1.36
2	12-A	7401	FMN	C5A-N5	-2.10	1.35	1.39
2	15-A	7401	FMN	C2-N1	-2.10	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-A	7401	FMN	C5'-C4'	-2.09	1.49	1.51
2	8-A	7401	FMN	P-O2P	2.09	1.62	1.54
2	12-A	7401	FMN	O2'-C2'	-2.09	1.39	1.43
2	16-B	9401	FMN	C4A-C10	2.08	1.50	1.44
2	1-B	9401	FMN	C9A-N10	2.08	1.44	1.41
2	16-B	9401	FMN	C2-N1	-2.08	1.31	1.36
2	13-B	9401	FMN	C5A-N5	-2.07	1.35	1.39
2	2-A	7401	FMN	O2'-C2'	-2.07	1.39	1.43
2	14-A	7401	FMN	C2'-C3'	-2.05	1.49	1.53
2	10-B	9401	FMN	C4A-C10	2.05	1.50	1.44
2	14-A	7401	FMN	O5'-C5'	-2.05	1.36	1.44
2	4-B	9401	FMN	C1'-C2'	2.04	1.55	1.52
2	10-A	7401	FMN	C9-C9A	2.04	1.42	1.39
2	1-B	9401	FMN	C6-C5A	2.04	1.43	1.40
2	5-A	7401	FMN	P-O3P	2.02	1.62	1.54
2	11-B	9401	FMN	C6-C5A	2.01	1.43	1.40
2	13-A	7401	FMN	O2-C2	-2.01	1.20	1.24
2	9-B	9401	FMN	C9A-C5A	2.00	1.44	1.41

All (541) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-B	9401	FMN	C4'-C3'-C2'	-11.95	93.68	113.57
2	11-B	9401	FMN	O3P-P-O5'	-11.73	76.08	106.67
2	4-A	7401	FMN	O3P-P-O5'	-11.55	76.56	106.67
2	6-B	9401	FMN	C4'-C3'-C2'	-11.42	94.56	113.57
2	1-B	9401	FMN	O3P-P-O5'	-11.28	77.27	106.67
2	15-B	9401	FMN	O5'-P-O1P	-11.17	76.25	106.44
2	5-A	7401	FMN	O3P-P-O5'	-11.15	77.60	106.67
2	11-A	7401	FMN	O3P-P-O5'	-11.12	77.67	106.67
2	13-B	9401	FMN	O5'-P-O1P	-11.12	76.40	106.44
2	8-B	9401	FMN	O5'-P-O1P	-11.05	76.59	106.44
2	7-A	7401	FMN	O3P-P-O5'	-11.02	77.94	106.67
2	14-A	7401	FMN	O3P-P-O5'	-11.02	77.95	106.67
2	14-B	9401	FMN	O3P-P-O2P	-10.88	67.00	107.80
2	14-B	9401	FMN	O3P-P-O5'	-10.80	78.50	106.67
2	10-B	9401	FMN	O5'-P-O1P	-10.79	77.27	106.44
2	7-B	9401	FMN	O5'-P-O1P	-10.79	77.27	106.44
2	1-B	9401	FMN	O2P-P-O5'	10.62	134.36	106.67
2	3-B	9401	FMN	O2P-P-O5'	10.56	134.21	106.67
2	16-B	9401	FMN	O3P-P-O2P	-10.56	68.22	107.80
2	9-A	7401	FMN	O3P-P-O5'	-10.49	79.33	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	11-B	9401	FMN	O2P-P-O5'	10.48	133.98	106.67
2	9-B	9401	FMN	O5'-P-O1P	-10.44	78.23	106.44
2	5-B	9401	FMN	O5'-P-O1P	-10.40	78.34	106.44
2	10-B	9401	FMN	O2P-P-O5'	10.31	133.55	106.67
2	6-B	9401	FMN	O5'-P-O1P	-10.30	78.60	106.44
2	1-B	9401	FMN	O5'-P-O1P	-10.30	78.61	106.44
2	9-B	9401	FMN	O2P-P-O5'	10.28	133.46	106.67
2	11-B	9401	FMN	O5'-P-O1P	-10.27	78.68	106.44
2	13-B	9401	FMN	O2P-P-O5'	10.20	133.28	106.67
2	9-B	9401	FMN	O3P-P-O5'	-10.15	80.20	106.67
2	10-B	9401	FMN	O3P-P-O5'	-10.12	80.28	106.67
2	5-B	9401	FMN	O2P-P-O5'	10.07	132.93	106.67
2	3-B	9401	FMN	O3P-P-O5'	-10.07	80.41	106.67
2	14-B	9401	FMN	O2P-P-O5'	10.07	132.92	106.67
2	15-B	9401	FMN	O2P-P-O5'	10.06	132.90	106.67
2	8-A	7401	FMN	O3P-P-O5'	-10.04	80.48	106.67
2	12-A	7401	FMN	O3P-P-O5'	-9.95	80.72	106.67
2	4-B	9401	FMN	O2P-P-O5'	9.92	132.54	106.67
2	16-B	9401	FMN	O3P-P-O5'	-9.85	81.00	106.67
2	7-B	9401	FMN	O3P-P-O5'	-9.77	81.19	106.67
2	13-B	9401	FMN	O3P-P-O5'	-9.73	81.29	106.67
2	2-B	9401	FMN	O5'-P-O1P	-9.73	80.15	106.44
2	15-B	9401	FMN	O3P-P-O5'	-9.70	81.39	106.67
2	12-B	9401	FMN	O2P-P-O1P	-9.69	73.07	110.83
2	1-A	7401	FMN	O3P-P-O5'	-9.65	81.52	106.67
2	12-B	9401	FMN	O2P-P-O5'	9.64	131.79	106.67
2	8-B	9401	FMN	O2P-P-O1P	-9.61	73.41	110.83
2	3-B	9401	FMN	O5'-P-O1P	-9.60	80.50	106.44
2	7-B	9401	FMN	O2P-P-O5'	9.57	131.62	106.67
2	3-B	9401	FMN	C4'-C3'-C2'	-9.56	97.67	113.57
2	2-A	7401	FMN	O3P-P-O5'	-9.53	81.82	106.67
2	8-B	9401	FMN	O2P-P-O5'	9.50	131.43	106.67
2	7-A	7401	FMN	C4'-C3'-C2'	-9.46	97.83	113.57
2	2-B	9401	FMN	O2P-P-O1P	-9.43	74.08	110.83
2	12-B	9401	FMN	O5'-P-O1P	-9.42	80.98	106.44
2	6-B	9401	FMN	O2P-P-O1P	-9.23	74.87	110.83
2	6-A	7401	FMN	O3P-P-O5'	-9.17	82.75	106.67
2	3-B	9401	FMN	O2P-P-O1P	-9.14	75.24	110.83
2	13-A	7401	FMN	O3P-P-O1P	-9.12	75.30	110.83
2	4-B	9401	FMN	O2P-P-O1P	-9.08	75.45	110.83
2	9-B	9401	FMN	O2P-P-O1P	-9.04	75.60	110.83
2	16-A	7401	FMN	O3P-P-O1P	-9.00	75.76	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	4-B	9401	FMN	O3P-P-O5'	-8.98	83.24	106.67
2	5-B	9401	FMN	O3P-P-O5'	-8.93	83.39	106.67
2	16-B	9401	FMN	C4'-C3'-C2'	-8.91	98.74	113.57
2	16-B	9401	FMN	O2P-P-O5'	8.84	129.72	106.67
2	4-B	9401	FMN	O5'-P-O1P	-8.81	82.62	106.44
2	15-A	7401	FMN	C4'-C3'-C2'	-8.80	98.92	113.57
2	13-A	7401	FMN	C4'-C3'-C2'	-8.68	99.13	113.57
2	7-B	9401	FMN	C4'-C3'-C2'	-8.60	99.26	113.57
2	2-B	9401	FMN	O2P-P-O5'	8.53	128.91	106.67
2	3-A	7401	FMN	O3P-P-O5'	-8.51	84.47	106.67
2	16-A	7401	FMN	C4'-C3'-C2'	-8.49	99.44	113.57
2	6-B	9401	FMN	O2P-P-O5'	8.44	128.69	106.67
2	3-A	7401	FMN	C4'-C3'-C2'	-8.35	99.68	113.57
2	12-B	9401	FMN	O3P-P-O5'	-8.34	84.92	106.67
2	10-A	7401	FMN	O3P-P-O5'	-8.31	85.00	106.67
2	13-A	7401	FMN	O5'-C5'-C4'	-8.27	87.30	109.36
2	16-A	7401	FMN	O5'-C5'-C4'	-8.24	87.36	109.36
2	2-B	9401	FMN	O3P-P-O2P	-8.16	77.20	107.80
2	15-A	7401	FMN	O3P-P-O1P	-8.13	79.14	110.83
2	16-A	7401	FMN	O5'-P-O1P	8.10	128.35	106.44
2	10-B	9401	FMN	O2P-P-O1P	-8.05	79.45	110.83
2	1-B	9401	FMN	O2P-P-O1P	-8.02	79.60	110.83
2	6-B	9401	FMN	O3P-P-O2P	-7.97	77.91	107.80
2	8-B	9401	FMN	O3P-P-O5'	-7.92	86.01	106.67
2	5-B	9401	FMN	O2P-P-O1P	-7.87	80.16	110.83
2	13-A	7401	FMN	O5'-P-O1P	7.87	127.70	106.44
2	7-B	9401	FMN	O2P-P-O1P	-7.65	81.01	110.83
2	15-B	9401	FMN	O3P-P-O2P	-7.62	79.22	107.80
2	13-B	9401	FMN	O3P-P-O2P	-7.59	79.32	107.80
2	11-B	9401	FMN	O2P-P-O1P	-7.57	81.35	110.83
2	7-A	7401	FMN	O5'-P-O1P	7.53	126.79	106.44
2	1-A	7401	FMN	C4'-C3'-C2'	-7.53	101.04	113.57
2	15-B	9401	FMN	C4'-C3'-C2'	-7.53	101.05	113.57
2	6-B	9401	FMN	O3P-P-O5'	-7.47	87.20	106.67
2	13-B	9401	FMN	C4'-C3'-C2'	-7.45	101.17	113.57
2	2-B	9401	FMN	O3P-P-O5'	-7.41	87.34	106.67
2	13-B	9401	FMN	O2P-P-O1P	-7.41	81.97	110.83
2	15-B	9401	FMN	O2P-P-O1P	-7.38	82.08	110.83
2	5-B	9401	FMN	O3P-P-O2P	-7.37	80.15	107.80
2	4-B	9401	FMN	O3P-P-O2P	-7.31	80.38	107.80
2	9-B	9401	FMN	C4'-C3'-C2'	-7.30	101.43	113.57
2	15-A	7401	FMN	O3P-P-O5'	-7.29	87.65	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	16-B	9401	FMN	O2P-P-O1P	-7.27	82.51	110.83
2	14-A	7401	FMN	C4'-C3'-C2'	-7.25	101.51	113.57
2	7-A	7401	FMN	O3P-P-O1P	-7.19	82.83	110.83
2	15-A	7401	FMN	O5'-P-O1P	7.18	125.84	106.44
2	12-A	7401	FMN	O3P-P-O1P	-7.15	82.97	110.83
2	7-B	9401	FMN	O3P-P-O2P	-7.11	81.14	107.80
2	3-A	7401	FMN	O5'-P-O1P	7.04	125.48	106.44
2	14-A	7401	FMN	O3P-P-O1P	-6.96	83.71	110.83
2	3-A	7401	FMN	O3P-P-O1P	-6.94	83.79	110.83
2	6-B	9401	FMN	O5'-C5'-C4'	-6.91	90.91	109.36
2	12-B	9401	FMN	O3P-P-O2P	-6.89	81.97	107.80
2	10-A	7401	FMN	O3P-P-O1P	-6.85	84.16	110.83
2	2-A	7401	FMN	O3P-P-O1P	-6.85	84.16	110.83
2	2-B	9401	FMN	O5'-C5'-C4'	-6.81	91.18	109.36
2	9-A	7401	FMN	O3P-P-O1P	-6.76	84.50	110.83
2	3-A	7401	FMN	O5'-C5'-C4'	-6.72	91.41	109.36
2	8-A	7401	FMN	O3P-P-O1P	-6.71	84.69	110.83
2	14-A	7401	FMN	O5'-P-O1P	6.67	124.47	106.44
2	3-A	7401	FMN	O3P-P-O2P	-6.65	82.86	107.80
2	6-A	7401	FMN	O3P-P-O2P	-6.63	82.93	107.80
2	8-A	7401	FMN	O5'-P-O1P	6.61	124.30	106.44
2	10-A	7401	FMN	O3P-P-O2P	-6.58	83.12	107.80
2	8-A	7401	FMN	O3P-P-O2P	-6.57	83.17	107.80
2	14-B	9401	FMN	O2P-P-O1P	-6.54	85.35	110.83
2	6-A	7401	FMN	O3P-P-O1P	-6.54	85.36	110.83
2	16-B	9401	FMN	O5'-P-O1P	-6.48	88.93	106.44
2	2-A	7401	FMN	O5'-P-O1P	6.48	123.95	106.44
2	1-A	7401	FMN	O3P-P-O1P	-6.46	85.66	110.83
2	4-A	7401	FMN	C4'-C3'-C2'	-6.45	102.84	113.57
2	10-B	9401	FMN	O3P-P-O2P	-6.43	83.69	107.80
2	5-A	7401	FMN	O3P-P-O1P	-6.42	85.82	110.83
2	1-A	7401	FMN	O5'-P-O1P	6.40	123.75	106.44
2	9-A	7401	FMN	O3P-P-O2P	-6.40	83.82	107.80
2	12-A	7401	FMN	O3P-P-O2P	-6.37	83.90	107.80
2	5-A	7401	FMN	O5'-P-O1P	6.37	123.66	106.44
2	9-A	7401	FMN	O5'-P-O1P	6.35	123.61	106.44
2	13-A	7401	FMN	O3P-P-O2P	-6.34	84.03	107.80
2	14-A	7401	FMN	O5'-C5'-C4'	-6.33	92.45	109.36
2	5-A	7401	FMN	C4'-C3'-C2'	-6.33	103.04	113.57
2	16-A	7401	FMN	O3P-P-O5'	-6.32	90.20	106.67
2	11-A	7401	FMN	O3P-P-O1P	-6.31	86.26	110.83
2	1-A	7401	FMN	O3P-P-O2P	-6.29	84.21	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	11-A	7401	FMN	C4'-C3'-C2'	-6.27	103.14	113.57
2	12-A	7401	FMN	O5'-P-O1P	6.26	123.37	106.44
2	2-A	7401	FMN	O3P-P-O2P	-6.22	84.48	107.80
2	3-B	9401	FMN	O3P-P-O2P	-6.22	84.48	107.80
2	16-A	7401	FMN	O3P-P-O2P	-6.19	84.58	107.80
2	5-B	9401	FMN	C4'-C3'-C2'	-6.19	103.28	113.57
2	9-B	9401	FMN	O3P-P-O2P	-6.17	84.67	107.80
2	10-B	9401	FMN	C4'-C3'-C2'	-6.15	103.34	113.57
2	11-A	7401	FMN	O5'-P-O1P	6.11	122.95	106.44
2	10-A	7401	FMN	O5'-P-O1P	6.10	122.93	106.44
2	4-A	7401	FMN	O5'-P-O1P	6.04	122.77	106.44
2	13-A	7401	FMN	O3P-P-O5'	-6.04	90.92	106.67
2	14-A	7401	FMN	O3P-P-O2P	-6.02	85.22	107.80
2	8-B	9401	FMN	O3P-P-O2P	-6.02	85.24	107.80
2	4-A	7401	FMN	O3P-P-O1P	-5.96	87.59	110.83
2	14-B	9401	FMN	C4'-C3'-C2'	-5.93	103.70	113.57
2	14-B	9401	FMN	O5'-P-O1P	-5.88	90.55	106.44
2	16-A	7401	FMN	C5'-C4'-C3'	5.77	123.10	112.22
2	6-A	7401	FMN	O2P-P-O5'	5.73	121.61	106.67
2	15-A	7401	FMN	O3P-P-O2P	-5.72	86.37	107.80
2	4-A	7401	FMN	O3P-P-O2P	-5.70	86.43	107.80
2	13-A	7401	FMN	C5'-C4'-C3'	5.69	122.94	112.22
2	1-B	9401	FMN	O3P-P-O2P	-5.68	86.49	107.80
2	11-B	9401	FMN	O3P-P-O2P	-5.68	86.50	107.80
2	11-A	7401	FMN	O3P-P-O2P	-5.45	87.36	107.80
2	6-A	7401	FMN	C4'-C3'-C2'	-5.44	104.51	113.57
2	7-A	7401	FMN	C1'-N10-C9A	5.38	131.09	120.63
2	16-B	9401	FMN	O5'-C5'-C4'	-5.37	95.04	109.36
2	2-B	9401	FMN	C5'-C4'-C3'	5.36	122.34	112.22
2	15-B	9401	FMN	C1'-N10-C9A	5.34	131.01	120.63
2	15-B	9401	FMN	C1'-C2'-C3'	5.32	124.08	109.66
2	16-B	9401	FMN	C5'-C4'-C3'	5.27	122.16	112.22
2	5-A	7401	FMN	O3P-P-O2P	-5.24	88.15	107.80
2	5-B	9401	FMN	O3P-P-O1P	5.22	131.16	110.83
2	7-A	7401	FMN	O3P-P-O2P	-5.20	88.30	107.80
2	13-B	9401	FMN	C1'-N10-C9A	5.19	130.73	120.63
2	4-A	7401	FMN	O2P-P-O5'	5.17	120.16	106.67
2	13-B	9401	FMN	C1'-C2'-C3'	5.17	123.67	109.66
2	4-B	9401	FMN	O3P-P-O1P	5.12	130.79	110.83
2	7-B	9401	FMN	O3P-P-O1P	5.07	130.59	110.83
2	6-A	7401	FMN	O5'-C5'-C4'	5.07	122.89	109.36
2	11-B	9401	FMN	O3P-P-O1P	5.03	130.42	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	11-A	7401	FMN	O2P-P-O5'	5.02	119.76	106.67
2	8-B	9401	FMN	O3P-P-O1P	4.99	130.27	110.83
2	16-B	9401	FMN	O3P-P-O1P	4.97	130.18	110.83
2	6-B	9401	FMN	O3P-P-O1P	4.95	130.12	110.83
2	12-B	9401	FMN	O3P-P-O1P	4.94	130.10	110.83
2	2-B	9401	FMN	O3P-P-O1P	4.90	129.93	110.83
2	13-A	7401	FMN	C1'-N10-C9A	4.85	130.06	120.63
2	6-A	7401	FMN	O5'-P-O1P	4.80	119.42	106.44
2	11-B	9401	FMN	C4'-C3'-C2'	-4.79	105.60	113.57
2	5-A	7401	FMN	O2P-P-O5'	4.76	119.09	106.67
2	7-B	9401	FMN	C1'-N10-C9A	4.75	129.87	120.63
2	9-A	7401	FMN	O2P-P-O5'	4.73	119.00	106.67
2	1-B	9401	FMN	O3P-P-O1P	4.72	129.22	110.83
2	6-A	7401	FMN	C5'-C4'-C3'	-4.70	103.35	112.22
2	8-A	7401	FMN	O2P-P-O5'	4.70	118.92	106.67
2	6-B	9401	FMN	C5'-C4'-C3'	4.61	120.92	112.22
2	7-B	9401	FMN	C1'-C2'-C3'	4.61	122.15	109.66
2	16-A	7401	FMN	C1'-N10-C9A	4.60	129.58	120.63
2	10-B	9401	FMN	O3P-P-O1P	4.52	128.44	110.83
2	15-B	9401	FMN	O2'-C2'-C3'	-4.37	99.02	109.25
2	9-B	9401	FMN	O5'-C5'-C4'	-4.36	97.73	109.36
2	13-B	9401	FMN	O5'-C5'-C4'	-4.32	97.83	109.36
2	8-B	9401	FMN	C5'-C4'-C3'	-4.32	104.07	112.22
2	3-B	9401	FMN	O3P-P-O1P	4.31	127.61	110.83
2	15-B	9401	FMN	O5'-C5'-C4'	-4.30	97.88	109.36
2	7-A	7401	FMN	O5'-C5'-C4'	-4.29	97.92	109.36
2	13-B	9401	FMN	O2'-C2'-C3'	-4.27	99.25	109.25
2	10-A	7401	FMN	C4'-C3'-C2'	-4.17	106.63	113.57
2	15-B	9401	FMN	O3P-P-O1P	4.15	127.01	110.83
2	1-A	7401	FMN	O2P-P-O5'	4.08	117.31	106.67
2	14-A	7401	FMN	C4-C4A-N5	4.06	123.81	118.21
2	13-B	9401	FMN	O3P-P-O1P	4.05	126.63	110.83
2	8-B	9401	FMN	C1'-N10-C9A	-4.01	112.85	120.63
2	14-B	9401	FMN	O3P-P-O1P	3.95	126.24	110.83
2	10-A	7401	FMN	O2P-P-O5'	3.89	116.82	106.67
2	15-B	9401	FMN	C4-C4A-N5	3.89	123.58	118.21
2	2-A	7401	FMN	O2P-P-O5'	3.82	116.62	106.67
2	6-A	7401	FMN	C1'-C2'-C3'	3.81	120.00	109.66
2	9-B	9401	FMN	O3P-P-O1P	3.79	125.59	110.83
2	13-B	9401	FMN	C4-C4A-N5	3.77	123.42	118.21
2	12-A	7401	FMN	O2P-P-O5'	3.71	116.35	106.67
2	3-B	9401	FMN	O5'-C5'-C4'	-3.64	99.65	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	8-A	7401	FMN	C9A-N10-C10	-3.63	115.22	120.75
2	13-A	7401	FMN	C1'-C2'-C3'	3.62	119.48	109.66
2	9-A	7401	FMN	C9A-N10-C10	-3.57	115.31	120.75
2	5-A	7401	FMN	C1'-C2'-C3'	3.57	119.33	109.66
2	16-A	7401	FMN	O4'-C4'-C5'	-3.55	102.16	109.99
2	13-A	7401	FMN	O4'-C4'-C5'	-3.54	102.19	109.99
2	12-A	7401	FMN	C4-C4A-N5	3.49	123.03	118.21
2	14-B	9401	FMN	C1'-C2'-C3'	3.48	119.09	109.66
2	5-B	9401	FMN	C1'-C2'-C3'	3.46	119.04	109.66
2	11-A	7401	FMN	C1'-C2'-C3'	3.46	119.03	109.66
2	8-B	9401	FMN	C5A-C9A-N10	3.42	121.06	117.97
2	6-B	9401	FMN	C4-C4A-N5	3.42	122.93	118.21
2	2-A	7401	FMN	C4-C4A-N5	3.41	122.92	118.21
2	14-B	9401	FMN	C5'-C4'-C3'	3.40	118.64	112.22
2	7-A	7401	FMN	O2P-P-O5'	3.40	115.53	106.67
2	7-A	7401	FMN	C4-C4A-N5	3.39	122.89	118.21
2	14-B	9401	FMN	O5'-C5'-C4'	-3.37	100.37	109.36
2	16-A	7401	FMN	C1'-C2'-C3'	3.36	118.77	109.66
2	7-A	7401	FMN	C1'-C2'-C3'	3.35	118.74	109.66
2	2-B	9401	FMN	C4-C4A-N5	3.33	122.81	118.21
2	9-A	7401	FMN	C4'-C3'-C2'	-3.33	108.03	113.57
2	10-A	7401	FMN	C4-C4A-N5	3.31	122.78	118.21
2	3-B	9401	FMN	C1'-N10-C9A	3.30	127.04	120.63
2	8-B	9401	FMN	O3'-C3'-C2'	-3.29	101.44	108.93
2	3-B	9401	FMN	C4-C4A-N5	3.29	122.75	118.21
2	8-A	7401	FMN	C1'-C2'-C3'	3.29	118.57	109.66
2	10-A	7401	FMN	O5'-C5'-C4'	-3.28	100.62	109.36
2	2-B	9401	FMN	O4'-C4'-C3'	-3.27	101.59	109.25
2	15-A	7401	FMN	O5'-C5'-C4'	-3.26	100.66	109.36
2	13-A	7401	FMN	C9-C9A-N10	3.23	126.20	121.85
2	8-B	9401	FMN	C4'-C3'-C2'	3.21	118.92	113.57
2	6-B	9401	FMN	O4'-C4'-C3'	-3.21	101.73	109.25
2	13-A	7401	FMN	C5A-N5-C4A	3.20	123.26	118.09
2	9-B	9401	FMN	C4-C4A-N5	3.18	122.61	118.21
2	7-B	9401	FMN	C4-C4A-N5	3.16	122.58	118.21
2	1-A	7401	FMN	O5'-C5'-C4'	-3.15	100.94	109.36
2	1-B	9401	FMN	C4'-C3'-C2'	-3.13	108.36	113.57
2	12-A	7401	FMN	C4'-C3'-C2'	-3.12	108.38	113.57
2	16-A	7401	FMN	C4-C4A-N5	3.12	122.51	118.21
2	14-B	9401	FMN	C4-C4A-N5	3.11	122.51	118.21
2	12-B	9401	FMN	C4A-C10-N1	-3.11	116.96	124.59
2	16-B	9401	FMN	C4-C4A-N5	3.10	122.49	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	16-A	7401	FMN	C5A-N5-C4A	3.10	123.09	118.09
2	9-A	7401	FMN	C1'-C2'-C3'	3.09	118.03	109.66
2	8-A	7401	FMN	C4'-C3'-C2'	-3.08	108.45	113.57
2	14-A	7401	FMN	C9A-C5A-N5	-3.05	119.22	122.45
2	8-A	7401	FMN	C4A-C10-N1	-3.05	117.11	124.59
2	16-A	7401	FMN	C9-C9A-N10	3.05	125.95	121.85
2	10-A	7401	FMN	O2-C2-N1	-3.02	116.78	121.80
2	14-A	7401	FMN	O2-C2-N1	-3.02	116.78	121.80
2	3-B	9401	FMN	C5'-C4'-C3'	3.01	117.91	112.22
2	12-B	9401	FMN	C9A-N10-C10	-3.00	116.18	120.75
2	10-B	9401	FMN	C4-C4A-N5	2.99	122.34	118.21
2	15-A	7401	FMN	C9A-C5A-N5	-2.99	119.28	122.45
2	3-A	7401	FMN	C5'-C4'-C3'	2.98	117.84	112.22
2	8-A	7401	FMN	C5A-N5-C4A	2.98	122.90	118.09
2	13-A	7401	FMN	C4-C4A-N5	2.97	122.31	118.21
2	9-A	7401	FMN	C4A-C10-N1	-2.96	117.32	124.59
2	15-A	7401	FMN	O4-C4-C4A	-2.96	118.72	126.53
2	9-A	7401	FMN	C5A-N5-C4A	2.94	122.85	118.09
2	6-A	7401	FMN	C5A-N5-C4A	2.93	122.83	118.09
2	7-A	7401	FMN	O2-C2-N1	-2.93	116.93	121.80
2	15-B	9401	FMN	C4A-C10-N10	2.92	120.66	116.48
2	13-A	7401	FMN	O2P-P-O1P	2.92	122.19	110.83
2	5-A	7401	FMN	C5A-N5-C4A	2.90	122.77	118.09
2	15-B	9401	FMN	C10-N1-C2	2.89	123.11	116.85
2	13-B	9401	FMN	C10-N1-C2	2.89	123.11	116.85
2	16-B	9401	FMN	C1'-C2'-C3'	2.87	117.45	109.66
2	15-B	9401	FMN	C9A-N10-C10	-2.85	116.40	120.75
2	11-B	9401	FMN	C5A-N5-C4A	2.85	122.69	118.09
2	11-A	7401	FMN	C5A-N5-C4A	2.85	122.69	118.09
2	14-A	7401	FMN	O2P-P-O5'	2.84	114.08	106.67
2	12-B	9401	FMN	C5A-N5-C4A	2.84	122.68	118.09
2	4-A	7401	FMN	C1'-C2'-C3'	2.84	117.35	109.66
2	1-B	9401	FMN	C4-C4A-N5	2.83	122.12	118.21
2	14-B	9401	FMN	C5A-N5-C4A	2.81	122.64	118.09
2	7-B	9401	FMN	O5'-C5'-C4'	-2.81	101.87	109.36
2	13-B	9401	FMN	C9A-N10-C10	-2.80	116.48	120.75
2	13-B	9401	FMN	C4A-C10-N10	2.79	120.48	116.48
2	4-A	7401	FMN	C5A-N5-C4A	2.79	122.60	118.09
2	5-B	9401	FMN	C4-C4A-N5	2.78	122.05	118.21
2	1-B	9401	FMN	C5A-N5-C4A	2.78	122.58	118.09
2	8-B	9401	FMN	C1'-C2'-C3'	-2.76	102.17	109.66
2	15-B	9401	FMN	O2-C2-N1	-2.76	117.22	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-A	7401	FMN	O2-C2-N1	-2.76	117.22	121.80
2	14-A	7401	FMN	O4'-C4'-C5'	-2.75	103.91	109.99
2	16-A	7401	FMN	O2P-P-O1P	2.74	121.51	110.83
2	5-B	9401	FMN	C1'-N10-C9A	2.74	125.95	120.63
2	3-B	9401	FMN	C1'-C2'-C3'	2.73	117.05	109.66
2	16-B	9401	FMN	O2-C2-N1	-2.72	117.28	121.80
2	1-A	7401	FMN	C1'-C2'-C3'	2.72	117.03	109.66
2	1-A	7401	FMN	C5A-N5-C4A	2.70	122.46	118.09
2	2-B	9401	FMN	O3'-C3'-C4'	2.69	115.04	108.93
2	6-A	7401	FMN	O4-C4-C4A	-2.69	119.44	126.53
2	7-B	9401	FMN	C9-C9A-N10	2.68	125.46	121.85
2	15-A	7401	FMN	C5A-N5-C4A	2.68	122.42	118.09
2	15-B	9401	FMN	C9-C9A-N10	2.68	125.45	121.85
2	16-B	9401	FMN	C1'-N10-C9A	2.68	125.83	120.63
2	11-A	7401	FMN	O4-C4-C4A	-2.68	119.47	126.53
2	7-A	7401	FMN	C9-C9A-N10	2.67	125.45	121.85
2	9-B	9401	FMN	C9A-C5A-N5	-2.67	119.62	122.45
2	3-A	7401	FMN	C5A-N5-C4A	2.67	122.41	118.09
2	1-A	7401	FMN	O2-C2-N1	-2.67	117.37	121.80
2	16-B	9401	FMN	C10-N1-C2	2.67	122.62	116.85
2	8-B	9401	FMN	C9A-C5A-N5	-2.66	119.63	122.45
2	13-B	9401	FMN	O2-C2-N1	-2.66	117.38	121.80
2	3-B	9401	FMN	O2-C2-N1	-2.65	117.39	121.80
2	7-B	9401	FMN	O2-C2-N1	-2.65	117.40	121.80
2	7-A	7401	FMN	C10-N1-C2	2.64	122.58	116.85
2	8-A	7401	FMN	O4-C4-C4A	-2.64	119.55	126.53
2	11-B	9401	FMN	C4-C4A-N5	2.64	121.85	118.21
2	5-A	7401	FMN	O4-C4-C4A	-2.64	119.57	126.53
2	1-A	7401	FMN	O4-C4-C4A	-2.64	119.58	126.53
2	9-A	7401	FMN	O4-C4-C4A	-2.64	119.58	126.53
2	14-B	9401	FMN	C4A-C10-N1	-2.62	118.16	124.59
2	5-B	9401	FMN	C5A-N5-C4A	2.62	122.32	118.09
2	7-A	7401	FMN	C5A-N5-C4A	2.61	122.32	118.09
2	3-A	7401	FMN	O2P-P-O5'	2.61	113.48	106.67
2	15-A	7401	FMN	C2'-C1'-N10	-2.61	97.87	110.20
2	13-B	9401	FMN	C9-C9A-N10	2.61	125.36	121.85
2	12-A	7401	FMN	C5A-C9A-N10	2.61	120.33	117.97
2	9-A	7401	FMN	C10-N1-C2	2.60	122.48	116.85
2	4-A	7401	FMN	O4-C4-C4A	-2.60	119.67	126.53
2	2-A	7401	FMN	C4A-C10-N1	-2.60	118.22	124.59
2	3-A	7401	FMN	O4-C4-C4A	-2.59	119.68	126.53
2	10-B	9401	FMN	C1'-C2'-C3'	2.59	116.69	109.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-B	9401	FMN	O2-C2-N1	-2.59	117.50	121.80
2	16-A	7401	FMN	O2-C2-N1	-2.59	117.50	121.80
2	6-B	9401	FMN	O2-C2-N1	-2.59	117.50	121.80
2	15-A	7401	FMN	C1'-C2'-C3'	2.58	116.65	109.66
2	4-A	7401	FMN	O2-C2-N1	-2.57	117.52	121.80
2	10-A	7401	FMN	C5'-C4'-C3'	2.57	117.07	112.22
2	13-B	9401	FMN	C5A-N5-C4A	2.56	122.23	118.09
2	10-B	9401	FMN	C5A-N5-C4A	2.56	122.22	118.09
2	14-B	9401	FMN	C10-N1-C2	2.55	122.37	116.85
2	12-A	7401	FMN	C4A-C10-N1	-2.55	118.33	124.59
2	6-B	9401	FMN	O3'-C3'-C4'	2.55	114.71	108.93
2	15-B	9401	FMN	C5A-N5-C4A	2.54	122.20	118.09
2	16-B	9401	FMN	C4A-C10-N10	2.54	120.12	116.48
2	7-B	9401	FMN	O3'-C3'-C2'	2.53	114.68	108.93
2	6-A	7401	FMN	C2'-C1'-N10	-2.53	98.25	110.20
2	4-B	9401	FMN	C5A-N5-C4A	2.52	122.16	118.09
2	15-A	7401	FMN	O2P-P-O5'	2.52	113.23	106.67
2	8-A	7401	FMN	C10-N1-C2	2.51	122.29	116.85
2	16-B	9401	FMN	C5A-N5-C4A	2.51	122.15	118.09
2	15-B	9401	FMN	C9-C9A-C5A	-2.51	115.60	120.03
2	11-A	7401	FMN	O2-C2-N1	-2.50	117.64	121.80
2	8-B	9401	FMN	C4A-C10-N1	-2.49	118.48	124.59
2	13-A	7401	FMN	O2-C2-N1	-2.49	117.66	121.80
2	7-A	7401	FMN	C5'-C4'-C3'	2.48	116.91	112.22
2	14-A	7401	FMN	O4-C4-C4A	-2.48	119.98	126.53
2	7-B	9401	FMN	C5A-N5-C4A	2.48	122.10	118.09
2	14-A	7401	FMN	O4'-C4'-C3'	-2.47	103.47	109.25
2	15-A	7401	FMN	O2-C2-N1	-2.47	117.70	121.80
2	10-A	7401	FMN	O4'-C4'-C5'	-2.47	104.54	109.99
2	13-B	9401	FMN	C9-C9A-C5A	-2.46	115.67	120.03
2	16-B	9401	FMN	C4-N3-C2	-2.46	121.28	125.64
2	7-A	7401	FMN	O2'-C2'-C3'	-2.45	103.51	109.25
2	7-A	7401	FMN	O3'-C3'-C4'	2.45	114.49	108.93
2	6-B	9401	FMN	C5A-N5-C4A	2.45	122.05	118.09
2	5-A	7401	FMN	O2-C2-N1	-2.44	117.75	121.80
2	2-B	9401	FMN	C5A-N5-C4A	2.44	122.03	118.09
2	7-B	9401	FMN	C10-N1-C2	2.43	122.12	116.85
2	7-B	9401	FMN	C4A-C10-N10	2.43	119.96	116.48
2	5-A	7401	FMN	C1'-N10-C9A	2.43	125.35	120.63
2	7-A	7401	FMN	C4A-C10-N10	2.43	119.95	116.48
2	9-B	9401	FMN	O2-C2-N1	-2.42	117.79	121.80
2	6-B	9401	FMN	C9A-C5A-N5	-2.41	119.90	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	12-B	9401	FMN	C10-N1-C2	2.41	122.06	116.85
2	9-A	7401	FMN	O2-C2-N1	-2.40	117.82	121.80
2	2-B	9401	FMN	O4-C4-C4A	-2.39	120.22	126.53
2	4-B	9401	FMN	O3'-C3'-C2'	-2.39	103.50	108.93
2	12-A	7401	FMN	O2-C2-N1	-2.39	117.83	121.80
2	3-B	9401	FMN	C5A-N5-C4A	2.39	121.95	118.09
2	9-B	9401	FMN	C5A-N5-C4A	2.39	121.95	118.09
2	16-A	7401	FMN	C10-N1-C2	2.39	122.02	116.85
2	9-B	9401	FMN	O4-C4-C4A	-2.38	120.24	126.53
2	15-A	7401	FMN	C5'-C4'-C3'	2.38	116.71	112.22
2	12-B	9401	FMN	C4'-C3'-C2'	-2.38	109.61	113.57
2	4-B	9401	FMN	C9A-C5A-N5	-2.38	119.93	122.45
2	10-B	9401	FMN	C9A-C5A-N5	-2.38	119.93	122.45
2	6-B	9401	FMN	O4-C4-C4A	-2.37	120.29	126.53
2	4-B	9401	FMN	C4-C4A-N5	2.36	121.47	118.21
2	12-A	7401	FMN	N3-C2-N1	2.36	124.52	119.50
2	8-B	9401	FMN	C5A-N5-C4A	2.36	121.91	118.09
2	16-B	9401	FMN	O4'-C4'-C5'	-2.36	104.79	109.99
2	1-B	9401	FMN	O4-C4-C4A	-2.36	120.31	126.53
2	11-B	9401	FMN	O4-C4-C4A	-2.35	120.32	126.53
2	2-B	9401	FMN	C9A-C5A-N5	-2.35	119.96	122.45
2	4-B	9401	FMN	C4A-C10-N1	-2.35	118.84	124.59
2	10-B	9401	FMN	O4-C4-C4A	-2.34	120.34	126.53
2	14-B	9401	FMN	C9A-N10-C10	-2.33	117.19	120.75
2	2-A	7401	FMN	C5A-C9A-N10	2.33	120.08	117.97
2	13-A	7401	FMN	C10-N1-C2	2.33	121.90	116.85
2	2-B	9401	FMN	O4'-C4'-C5'	-2.33	104.86	109.99
2	12-A	7401	FMN	O4'-C4'-C5'	-2.32	104.86	109.99
2	14-A	7401	FMN	O3'-C3'-C2'	-2.32	103.65	108.93
2	1-B	9401	FMN	O4'-C4'-C5'	-2.32	104.87	109.99
2	2-A	7401	FMN	C4A-C10-N10	2.32	119.80	116.48
2	14-A	7401	FMN	C5'-C4'-C3'	2.31	116.58	112.22
2	16-B	9401	FMN	C4A-C10-N1	-2.31	118.92	124.59
2	15-B	9401	FMN	C9A-C9-C8	2.31	123.87	119.22
2	3-B	9401	FMN	C10-N1-C2	2.30	121.84	116.85
2	14-A	7401	FMN	C10-N1-C2	2.30	121.83	116.85
2	13-B	9401	FMN	C9A-C9-C8	2.29	123.82	119.22
2	14-B	9401	FMN	C4-N3-C2	-2.29	121.58	125.64
2	7-A	7401	FMN	O4-C4-C4A	-2.28	120.50	126.53
2	14-A	7401	FMN	C5A-N5-C4A	2.28	121.78	118.09
2	5-B	9401	FMN	O4-C4-C4A	-2.28	120.52	126.53
2	9-A	7401	FMN	C4-N3-C2	-2.27	121.60	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2-A	7401	FMN	N3-C2-N1	2.27	124.32	119.50
2	10-A	7401	FMN	C4-N3-C2	-2.26	121.62	125.64
2	4-B	9401	FMN	C5A-C9A-N10	2.26	120.01	117.97
2	16-B	9401	FMN	C9A-N10-C10	-2.25	117.31	120.75
2	8-B	9401	FMN	C4-C4A-N5	2.25	121.32	118.21
2	6-A	7401	FMN	O2-C2-N1	-2.25	118.06	121.80
2	8-A	7401	FMN	C9-C9A-C5A	-2.25	116.05	120.03
2	9-A	7401	FMN	C9-C9A-C5A	-2.25	116.05	120.03
2	3-B	9401	FMN	O4-C4-C4A	-2.25	120.59	126.53
2	7-A	7401	FMN	O3'-C3'-C2'	2.25	114.03	108.93
2	6-A	7401	FMN	C9A-C5A-N5	-2.24	120.08	122.45
2	11-B	9401	FMN	C4A-C10-N1	-2.24	119.11	124.59
2	12-A	7401	FMN	C10-N1-C2	2.23	121.68	116.85
2	2-B	9401	FMN	C1'-N10-C9A	2.23	124.97	120.63
2	7-A	7401	FMN	C9A-C5A-N5	-2.23	120.09	122.45
2	12-B	9401	FMN	C5A-C9A-N10	2.23	119.98	117.97
2	3-A	7401	FMN	O4'-C4'-C5'	-2.22	105.08	109.99
2	14-A	7401	FMN	C6-C5A-N5	2.22	122.14	118.44
2	12-A	7401	FMN	C9A-N10-C10	-2.22	117.36	120.75
2	4-B	9401	FMN	O4-C4-C4A	-2.22	120.68	126.53
2	13-A	7401	FMN	C4A-C10-N10	2.21	119.65	116.48
2	7-B	9401	FMN	O4-C4-C4A	-2.20	120.71	126.53
2	5-A	7401	FMN	C9A-N10-C10	-2.20	117.39	120.75
2	4-A	7401	FMN	C9A-N10-C10	-2.20	117.39	120.75
2	14-A	7401	FMN	C10-C4A-N5	-2.20	120.31	124.81
2	15-B	9401	FMN	O3'-C3'-C2'	2.20	113.93	108.93
2	10-A	7401	FMN	C4A-C10-N10	2.20	119.63	116.48
2	10-A	7401	FMN	C10-N1-C2	2.20	121.61	116.85
2	1-A	7401	FMN	C9A-C5A-N5	-2.19	120.13	122.45
2	12-A	7401	FMN	C4A-C10-N10	2.19	119.62	116.48
2	8-A	7401	FMN	C4-N3-C2	-2.19	121.75	125.64
2	13-A	7401	FMN	C4-N3-C2	-2.19	121.76	125.64
2	8-B	9401	FMN	N10-C10-N1	2.18	124.94	118.51
2	11-A	7401	FMN	C1'-N10-C9A	2.18	124.87	120.63
2	13-A	7401	FMN	C9-C9A-C5A	-2.18	116.18	120.03
2	2-B	9401	FMN	C10-N1-C2	2.18	121.56	116.85
2	15-A	7401	FMN	O4-C4-N3	2.17	124.19	120.11
2	5-A	7401	FMN	C10-N1-C2	2.17	121.54	116.85
2	5-A	7401	FMN	C9A-C5A-N5	-2.17	120.16	122.45
2	3-A	7401	FMN	C9A-C5A-N5	-2.16	120.16	122.45
2	16-A	7401	FMN	C4A-C10-N10	2.16	119.58	116.48
2	8-A	7401	FMN	O2-C2-N1	-2.16	118.22	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-B	9401	FMN	C9-C9A-C5A	-2.16	116.22	120.03
2	7-B	9401	FMN	C9A-N10-C10	-2.15	117.47	120.75
2	1-B	9401	FMN	C4A-C10-N1	-2.15	119.32	124.59
2	16-A	7401	FMN	C4-N3-C2	-2.15	121.83	125.64
2	2-A	7401	FMN	C10-N1-C2	2.14	121.49	116.85
2	3-A	7401	FMN	C10-N1-C2	2.14	121.49	116.85
2	12-A	7401	FMN	C1'-C2'-C3'	2.14	115.47	109.66
2	10-A	7401	FMN	C5A-N5-C4A	2.14	121.55	118.09
2	3-B	9401	FMN	C4A-C10-N10	2.14	119.55	116.48
2	5-B	9401	FMN	C9A-C5A-N5	-2.14	120.19	122.45
2	14-A	7401	FMN	C4-N3-C2	-2.13	121.86	125.64
2	11-A	7401	FMN	C9A-C5A-N5	-2.13	120.19	122.45
2	4-A	7401	FMN	C10-N1-C2	2.13	121.45	116.85
2	2-A	7401	FMN	C9A-N10-C10	-2.13	117.51	120.75
2	1-A	7401	FMN	C10-N1-C2	2.12	121.44	116.85
2	13-B	9401	FMN	O3'-C3'-C2'	2.12	113.75	108.93
2	12-B	9401	FMN	N10-C10-N1	2.12	124.75	118.51
2	10-A	7401	FMN	C10-C4A-N5	-2.12	120.49	124.81
2	16-B	9401	FMN	C9-C9A-N10	2.11	124.70	121.85
2	6-B	9401	FMN	C10-N1-C2	2.11	121.42	116.85
2	7-A	7401	FMN	C9A-C9-C8	2.11	123.47	119.22
2	6-A	7401	FMN	C10-N1-C2	2.11	121.42	116.85
2	10-A	7401	FMN	C4A-C10-N1	-2.10	119.44	124.59
2	11-A	7401	FMN	C9A-N10-C10	-2.10	117.55	120.75
2	7-A	7401	FMN	C9-C9A-C5A	-2.10	116.32	120.03
2	11-A	7401	FMN	C10-N1-C2	2.10	121.39	116.85
2	10-B	9401	FMN	O2-C2-N1	-2.10	118.32	121.80
2	4-A	7401	FMN	C9A-C5A-N5	-2.10	120.23	122.45
2	10-A	7401	FMN	C9A-C5A-N5	-2.08	120.25	122.45
2	13-B	9401	FMN	C4-N3-C2	-2.08	121.95	125.64
2	16-A	7401	FMN	C9-C9A-C5A	-2.08	116.36	120.03
2	8-B	9401	FMN	O4-C4-C4A	-2.08	121.06	126.53
2	1-B	9401	FMN	C9A-C5A-N5	-2.07	120.26	122.45
2	8-B	9401	FMN	O3'-C3'-C4'	-2.07	104.23	108.93
2	13-A	7401	FMN	C9A-N10-C10	-2.07	117.60	120.75
2	3-A	7401	FMN	C4-C4A-N5	2.07	121.06	118.21
2	3-B	9401	FMN	C9-C9A-N10	2.06	124.63	121.85
2	6-B	9401	FMN	O2'-C2'-C3'	2.06	114.07	109.25
2	13-B	9401	FMN	O4'-C4'-C5'	-2.06	105.45	109.99
2	12-B	9401	FMN	O4-C4-C4A	-2.06	121.10	126.53
2	6-B	9401	FMN	O4'-C4'-C5'	-2.06	105.45	109.99
2	15-B	9401	FMN	O2'-C2'-C1'	-2.05	101.75	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-B	9401	FMN	C4A-C10-N1	-2.05	119.56	124.59
2	5-B	9401	FMN	C9-C9A-C5A	-2.05	116.40	120.03
2	3-B	9401	FMN	O4'-C4'-C5'	-2.05	105.47	109.99
2	15-B	9401	FMN	O4'-C4'-C5'	-2.05	105.47	109.99
2	2-A	7401	FMN	O2-C2-N1	-2.05	118.40	121.80
2	4-A	7401	FMN	C4A-C10-N1	-2.04	119.59	124.59
2	6-A	7401	FMN	C4A-C10-N1	-2.03	119.62	124.59
2	2-B	9401	FMN	C4-N3-C2	-2.03	122.05	125.64
2	5-B	9401	FMN	C10-N1-C2	2.02	121.23	116.85
2	5-B	9401	FMN	O2-C2-N1	-2.02	118.44	121.80
2	15-B	9401	FMN	C4-N3-C2	-2.02	122.05	125.64
2	7-B	9401	FMN	O4'-C4'-C3'	2.02	113.98	109.25
2	5-B	9401	FMN	C9-C9A-N10	2.02	124.57	121.85
2	5-A	7401	FMN	C4A-C10-N1	-2.02	119.65	124.59
2	12-B	9401	FMN	C9-C9A-C5A	-2.02	116.47	120.03
2	8-A	7401	FMN	C5A-C9A-N10	2.01	119.79	117.97
2	10-B	9401	FMN	C10-N1-C2	2.01	121.20	116.85

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-A	7401	FMN	C2'-C1'-N10-C10
2	1-A	7401	FMN	C5'-O5'-P-O3P
2	2-A	7401	FMN	C2'-C1'-N10-C10
2	2-A	7401	FMN	C5'-O5'-P-O3P
2	3-A	7401	FMN	C2'-C1'-N10-C10
2	3-A	7401	FMN	C5'-O5'-P-O3P
2	4-A	7401	FMN	C2'-C1'-N10-C9A
2	4-A	7401	FMN	C2'-C1'-N10-C10
2	4-A	7401	FMN	C5'-O5'-P-O3P
2	5-A	7401	FMN	C2'-C1'-N10-C9A
2	5-A	7401	FMN	C2'-C1'-N10-C10
2	5-A	7401	FMN	C5'-O5'-P-O3P
2	6-A	7401	FMN	C2'-C1'-N10-C10
2	6-A	7401	FMN	C5'-O5'-P-O3P
2	7-A	7401	FMN	C2'-C1'-N10-C9A
2	7-A	7401	FMN	C2'-C1'-N10-C10
2	7-A	7401	FMN	C5'-O5'-P-O3P
2	8-A	7401	FMN	C2'-C1'-N10-C10
2	8-A	7401	FMN	C5'-O5'-P-O3P
2	9-A	7401	FMN	C2'-C1'-N10-C9A

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Mol	Chain	Res	Type	Atoms
2	9-A	7401	FMN	C2'-C1'-N10-C10
2	9-A	7401	FMN	C5'-O5'-P-O3P
2	10-A	7401	FMN	C2'-C1'-N10-C10
2	10-A	7401	FMN	C5'-O5'-P-O3P
2	11-A	7401	FMN	C2'-C1'-N10-C9A
2	11-A	7401	FMN	C2'-C1'-N10-C10
2	11-A	7401	FMN	C5'-O5'-P-O3P
2	12-A	7401	FMN	C5'-O5'-P-O3P
2	13-A	7401	FMN	C2'-C1'-N10-C9A
2	13-A	7401	FMN	C2'-C1'-N10-C10
2	13-A	7401	FMN	C5'-O5'-P-O3P
2	14-A	7401	FMN	C5'-O5'-P-O3P
2	15-A	7401	FMN	C5'-O5'-P-O1P
2	15-A	7401	FMN	C5'-O5'-P-O3P
2	16-A	7401	FMN	C2'-C1'-N10-C9A
2	16-A	7401	FMN	C2'-C1'-N10-C10
2	16-A	7401	FMN	C5'-O5'-P-O3P
2	1-B	9401	FMN	C5'-O5'-P-O1P
2	1-B	9401	FMN	C5'-O5'-P-O3P
2	2-B	9401	FMN	C2'-C1'-N10-C10
2	2-B	9401	FMN	C5'-O5'-P-O1P
2	2-B	9401	FMN	C5'-O5'-P-O3P
2	3-B	9401	FMN	C2'-C1'-N10-C10
2	3-B	9401	FMN	C5'-O5'-P-O1P
2	3-B	9401	FMN	C5'-O5'-P-O3P
2	4-B	9401	FMN	C5'-O5'-P-O1P
2	4-B	9401	FMN	C5'-O5'-P-O3P
2	5-B	9401	FMN	C2'-C1'-N10-C9A
2	5-B	9401	FMN	C2'-C1'-N10-C10
2	5-B	9401	FMN	C5'-O5'-P-O1P
2	5-B	9401	FMN	C5'-O5'-P-O3P
2	6-B	9401	FMN	C5'-O5'-P-O1P
2	6-B	9401	FMN	C5'-O5'-P-O3P
2	7-B	9401	FMN	C2'-C1'-N10-C9A
2	7-B	9401	FMN	C2'-C1'-N10-C10
2	7-B	9401	FMN	C5'-O5'-P-O1P
2	7-B	9401	FMN	C5'-O5'-P-O3P
2	8-B	9401	FMN	C5'-O5'-P-O1P
2	8-B	9401	FMN	C5'-O5'-P-O3P
2	9-B	9401	FMN	C5'-O5'-P-O1P
2	9-B	9401	FMN	C5'-O5'-P-O3P
2	10-B	9401	FMN	C2'-C1'-N10-C10

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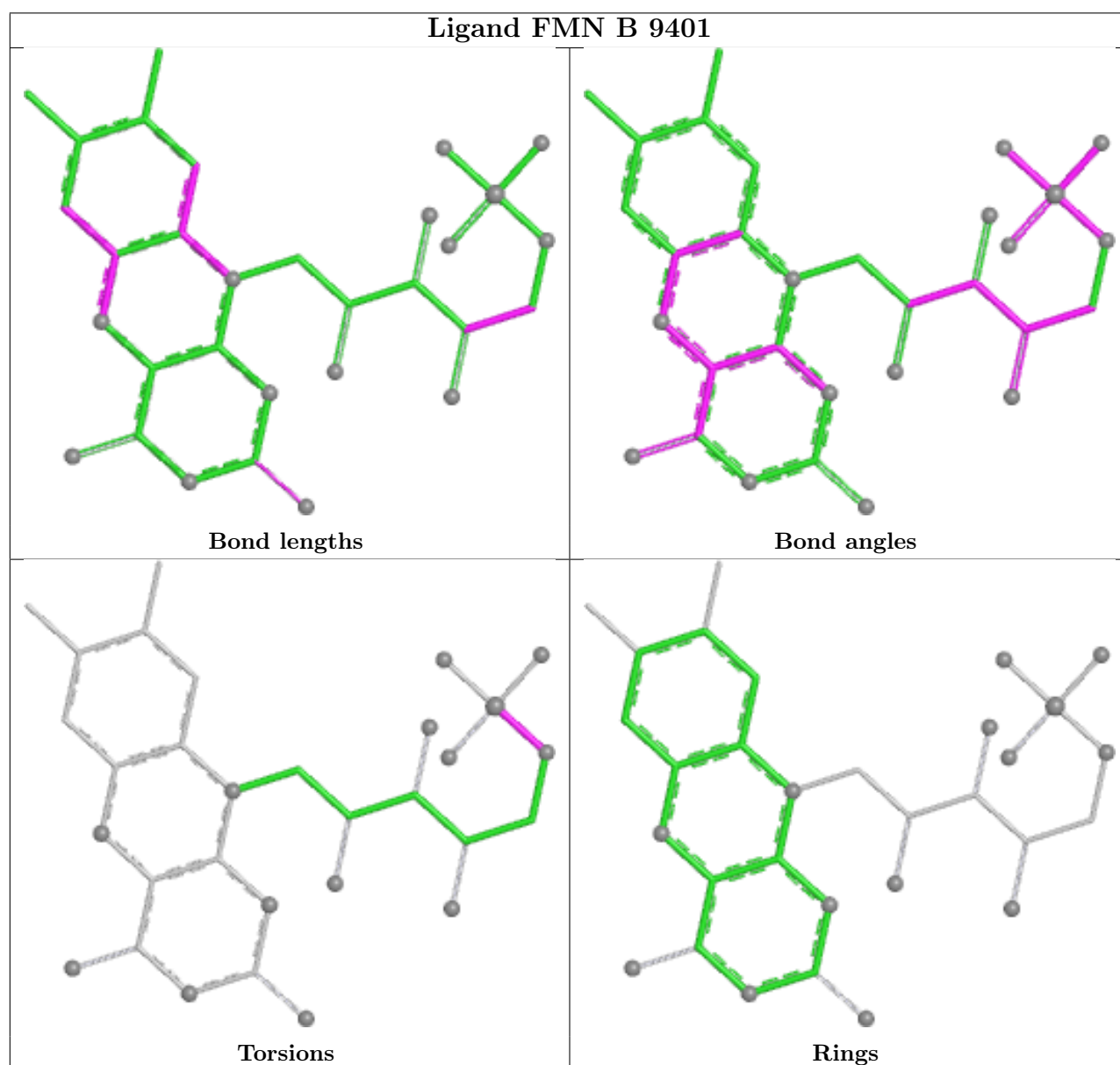
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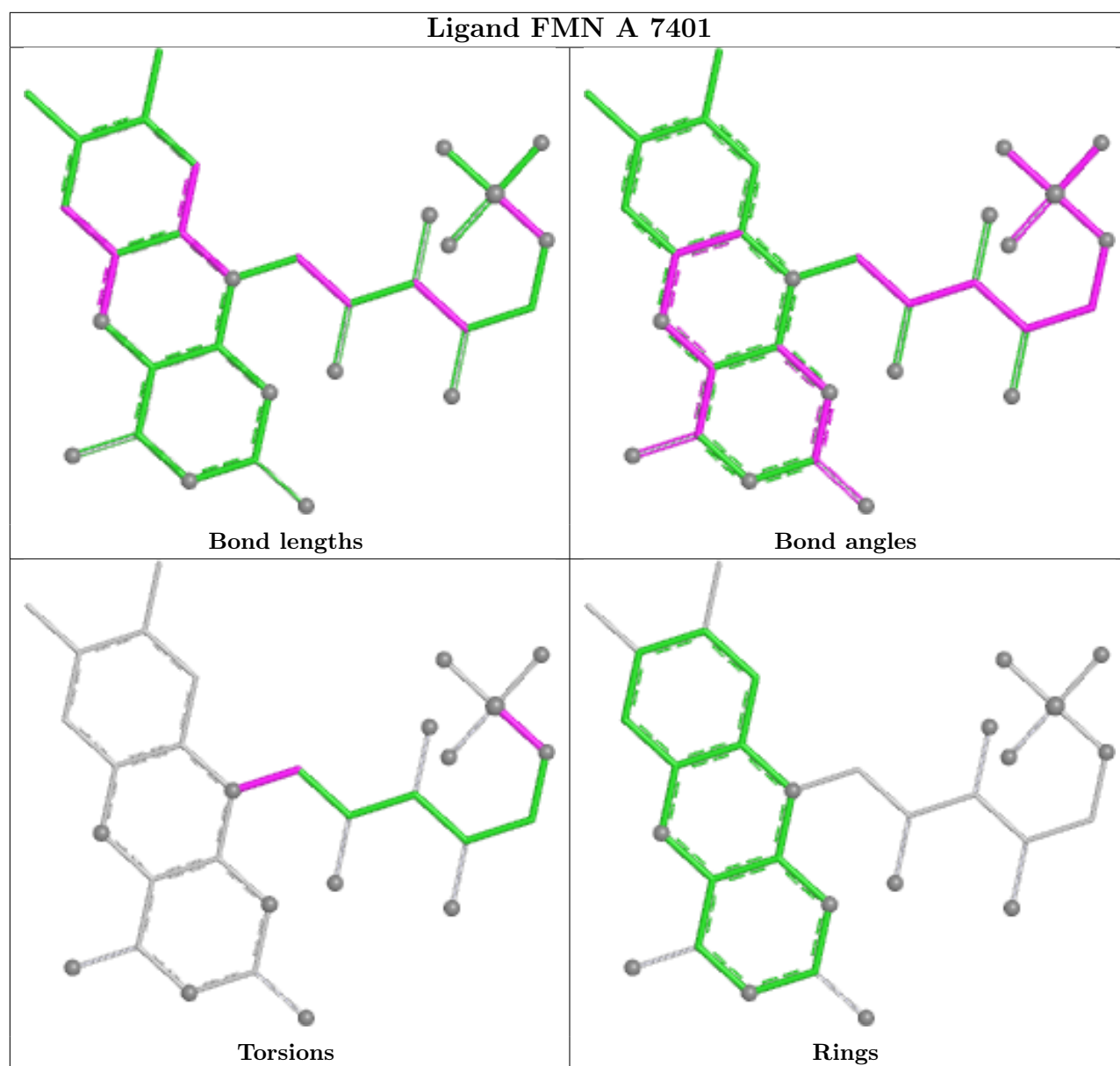
Mol	Chain	Res	Type	Atoms
2	10-B	9401	FMN	C5'-O5'-P-O1P
2	10-B	9401	FMN	C5'-O5'-P-O3P
2	11-B	9401	FMN	C5'-O5'-P-O1P
2	11-B	9401	FMN	C5'-O5'-P-O3P
2	12-B	9401	FMN	C2'-C1'-N10-C10
2	12-B	9401	FMN	C5'-O5'-P-O1P
2	12-B	9401	FMN	C5'-O5'-P-O3P
2	13-B	9401	FMN	C2'-C1'-N10-C9A
2	13-B	9401	FMN	C2'-C1'-N10-C10
2	13-B	9401	FMN	C5'-O5'-P-O1P
2	13-B	9401	FMN	C5'-O5'-P-O3P
2	14-B	9401	FMN	C2'-C1'-N10-C9A
2	14-B	9401	FMN	C2'-C1'-N10-C10
2	14-B	9401	FMN	C5'-O5'-P-O3P
2	15-B	9401	FMN	C2'-C1'-N10-C9A
2	15-B	9401	FMN	C2'-C1'-N10-C10
2	15-B	9401	FMN	C5'-O5'-P-O1P
2	15-B	9401	FMN	C5'-O5'-P-O3P
2	16-B	9401	FMN	C2'-C1'-N10-C9A
2	16-B	9401	FMN	C2'-C1'-N10-C10
2	16-B	9401	FMN	C5'-O5'-P-O3P
2	1-A	7401	FMN	C2'-C1'-N10-C9A
2	3-A	7401	FMN	C2'-C1'-N10-C9A
2	6-A	7401	FMN	C2'-C1'-N10-C9A
2	8-A	7401	FMN	C2'-C1'-N10-C9A
2	3-B	9401	FMN	C2'-C1'-N10-C9A
2	10-B	9401	FMN	C2'-C1'-N10-C9A
2	14-B	9401	FMN	C5'-O5'-P-O1P
2	16-B	9401	FMN	C5'-O5'-P-O1P
2	1-A	7401	FMN	C5'-O5'-P-O1P
2	2-A	7401	FMN	C5'-O5'-P-O1P
2	3-A	7401	FMN	C5'-O5'-P-O1P
2	4-A	7401	FMN	C5'-O5'-P-O1P
2	5-A	7401	FMN	C5'-O5'-P-O1P
2	6-A	7401	FMN	C5'-O5'-P-O1P
2	7-A	7401	FMN	C5'-O5'-P-O1P
2	10-A	7401	FMN	C5'-O5'-P-O1P
2	11-A	7401	FMN	C5'-O5'-P-O1P
2	13-A	7401	FMN	C5'-O5'-P-O1P
2	16-A	7401	FMN	C5'-O5'-P-O1P

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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 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	365/391 (93%)	1.69	100 (27%) ⓘ ⓘ	1, 1, 2, 3	365 (100%)
1	1-B	367/391 (93%)	1.47	95 (25%) ⓘ ⓘ	1, 1, 2, 3	367 (100%)
1	2-A	0/391	-	-	-	-
1	2-B	0/391	-	-	-	-
1	3-A	0/391	-	-	-	-
1	3-B	0/391	-	-	-	-
1	4-A	0/391	-	-	-	-
1	4-B	0/391	-	-	-	-
1	5-A	0/391	-	-	-	-
1	5-B	0/391	-	-	-	-
1	6-A	0/391	-	-	-	-
1	6-B	0/391	-	-	-	-
1	7-A	0/391	-	-	-	-
1	7-B	0/391	-	-	-	-
1	8-A	0/391	-	-	-	-
1	8-B	0/391	-	-	-	-
1	9-A	0/391	-	-	-	-
1	9-B	0/391	-	-	-	-
1	10-A	0/391	-	-	-	-
1	10-B	0/391	-	-	-	-
1	11-A	0/391	-	-	-	-
1	11-B	0/391	-	-	-	-
1	12-A	0/391	-	-	-	-
1	12-B	0/391	-	-	-	-
1	13-A	0/391	-	-	-	-
1	13-B	0/391	-	-	-	-
1	14-A	0/391	-	-	-	-
1	14-B	0/391	-	-	-	-
1	15-A	0/391	-	-	-	-
1	15-B	0/391	-	-	-	-
1	16-A	0/391	-	-	-	-
1	16-B	0/391	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	732/12512 (5%)	1.58	195 (26%) 1 1	1, 1, 2, 3	732 (100%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	303	ALA	11.2
1	1-B	371	TYR	10.6
1	1-B	9	ASN	9.8
1	1-A	107	LEU	9.3
1	1-B	57	GLY	7.7
1	1-A	272	GLY	7.5
1	1-A	305	LEU	7.2
1	1-A	237	VAL	7.2
1	1-A	270	VAL	7.2
1	1-A	271	ASN	7.0
1	1-B	100	GLY	6.8
1	1-A	336	ASP	6.8
1	1-B	299	ASP	6.2
1	1-A	381	ASP	6.0
1	1-A	240	SER	5.9
1	1-A	239	VAL	5.9
1	1-A	337	ALA	5.8
1	1-B	270	VAL	5.7
1	1-A	302	GLU	5.7
1	1-B	269	GLY	5.4
1	1-A	310	ARG	5.4
1	1-A	334	GLN	5.3
1	1-B	278	LEU	5.2
1	1-B	17	LYS	5.2
1	1-B	286	HIS	5.1
1	1-A	188	ALA	5.1
1	1-B	285	TYR	5.0
1	1-A	319	SER	4.9
1	1-A	300	GLU	4.9
1	1-A	138	TRP	4.8
1	1-A	338	ASP	4.7
1	1-A	185	ILE	4.7
1	1-A	137	ARG	4.6
1	1-A	8	SER	4.6
1	1-B	276	ALA	4.5
1	1-B	326	GLU	4.4
1	1-A	283	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	1-B	271	ASN	4.3
1	1-A	333	GLN	4.2
1	1-B	333	GLN	4.1
1	1-A	327	LEU	4.1
1	1-A	162	PRO	4.1
1	1-A	9	ASN	4.1
1	1-B	324	ASN	4.1
1	1-A	207	GLN	4.1
1	1-B	10	GLU	4.0
1	1-B	229	ALA	3.9
1	1-A	301	GLU	3.9
1	1-A	269	GLY	3.9
1	1-A	335	GLY	3.9
1	1-A	159	SER	3.9
1	1-A	311	MET	3.9
1	1-A	139	ARG	3.8
1	1-A	306	MET	3.8
1	1-A	387	PRO	3.8
1	1-A	326	GLU	3.8
1	1-B	327	LEU	3.8
1	1-A	266	LYS	3.8
1	1-A	382	TYR	3.7
1	1-A	243	ILE	3.7
1	1-B	281	THR	3.6
1	1-B	16	TYR	3.6
1	1-B	51	ALA	3.6
1	1-B	325	LYS	3.5
1	1-B	288	TYR	3.5
1	1-A	41	VAL	3.5
1	1-B	279	HIS	3.5
1	1-B	179	GLY	3.4
1	1-A	281	THR	3.4
1	1-B	280	VAL	3.4
1	1-A	206	ASP	3.4
1	1-A	205	THR	3.3
1	1-B	178	ALA	3.3
1	1-A	304	LYS	3.3
1	1-B	54	THR	3.3
1	1-A	187	GLY	3.3
1	1-A	16	TYR	3.3
1	1-B	140	VAL	3.3
1	1-A	282	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	1-A	163	ARG	3.2
1	1-A	332	VAL	3.2
1	1-A	254	LEU	3.2
1	1-A	339	LEU	3.2
1	1-B	385	LEU	3.2
1	1-A	233	SER	3.2
1	1-B	226	VAL	3.2
1	1-A	208	TYR	3.2
1	1-A	203	ASP	3.2
1	1-A	54	THR	3.2
1	1-A	149	LYS	3.2
1	1-B	237	VAL	3.1
1	1-B	347	ILE	3.1
1	1-B	34	ARG	3.1
1	1-B	81	TYR	3.1
1	1-A	316	THR	3.1
1	1-B	52	GLN	3.0
1	1-A	209	GLY	3.0
1	1-B	158	ALA	3.0
1	1-B	287	ALA	3.0
1	1-B	331	ALA	2.9
1	1-B	359	ASP	2.9
1	1-B	344	ARG	2.9
1	1-A	143	PRO	2.9
1	1-A	284	ARG	2.9
1	1-A	307	LYS	2.9
1	1-A	376	VAL	2.8
1	1-B	332	VAL	2.8
1	1-A	201	ILE	2.8
1	1-A	241	PRO	2.8
1	1-A	280	VAL	2.8
1	1-A	204	ARG	2.7
1	1-A	267	LEU	2.7
1	1-A	102	PHE	2.7
1	1-B	49	TYR	2.7
1	1-A	227	VAL	2.7
1	1-B	137	ARG	2.7
1	1-B	30	ALA	2.7
1	1-B	328	GLY	2.7
1	1-B	361	GLU	2.6
1	1-B	373	GLN	2.6
1	1-B	172	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	1-B	15	SER	2.6
1	1-B	301	GLU	2.6
1	1-B	136	ASN	2.6
1	1-B	384	PHE	2.6
1	1-A	165	VAL	2.6
1	1-B	98	ALA	2.6
1	1-B	24	SER	2.5
1	1-B	176	ILE	2.5
1	1-A	199	ASP	2.5
1	1-B	59	PHE	2.5
1	1-B	22	ASP	2.5
1	1-A	330	GLN	2.5
1	1-B	330	GLN	2.5
1	1-B	141	LEU	2.5
1	1-A	247	ASP	2.4
1	1-A	82	SER	2.4
1	1-B	273	SER	2.4
1	1-B	303	ALA	2.4
1	1-A	358	ILE	2.4
1	1-B	367	ARG	2.4
1	1-B	277	TYR	2.4
1	1-B	101	GLY	2.4
1	1-A	384	PHE	2.4
1	1-A	212	ILE	2.4
1	1-B	212	ILE	2.4
1	1-A	255	SER	2.4
1	1-B	307	LYS	2.4
1	1-B	58	GLY	2.3
1	1-A	186	HIS	2.3
1	1-B	33	THR	2.3
1	1-B	135	GLU	2.3
1	1-B	175	ALA	2.3
1	1-B	309	LEU	2.3
1	1-A	317	PHE	2.3
1	1-B	255	SER	2.3
1	1-B	300	GLU	2.3
1	1-A	171	SER	2.3
1	1-B	177	ARG	2.3
1	1-A	37	ALA	2.3
1	1-A	131	LYS	2.2
1	1-A	130	ASN	2.2
1	1-B	358	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	1-A	340	VAL	2.2
1	1-B	329	MET	2.2
1	1-A	213	ALA	2.2
1	1-B	48	GLU	2.2
1	1-B	267	LEU	2.2
1	1-B	13	PHE	2.2
1	1-B	230	ILE	2.2
1	1-A	362	LEU	2.2
1	1-B	319	SER	2.2
1	1-A	13	PHE	2.1
1	1-B	157	GLU	2.1
1	1-B	76	HIS	2.1
1	1-B	46	LEU	2.1
1	1-A	135	GLU	2.1
1	1-B	31	PRO	2.1
1	1-A	226	VAL	2.1
1	1-A	256	LEU	2.1
1	1-A	85	GLN	2.1
1	1-A	367	ARG	2.1
1	1-B	210	GLY	2.1
1	1-B	146	SER	2.1
1	1-B	308	SER	2.1
1	1-A	10	GLU	2.1
1	1-A	11	THR	2.1
1	1-A	27	VAL	2.1
1	1-B	12	LEU	2.0
1	1-B	352	LEU	2.0
1	1-B	56	PRO	2.0
1	1-B	50	TYR	2.0
1	1-A	80	ILE	2.0
1	1-A	251	SER	2.0
1	1-B	159	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

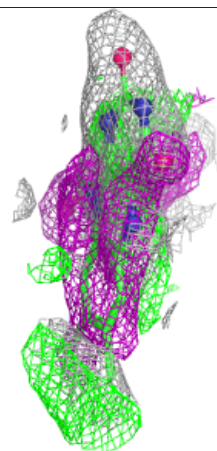
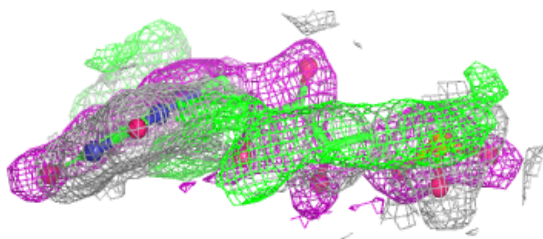
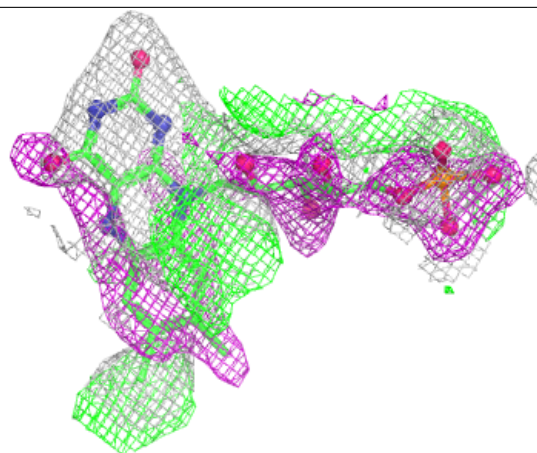
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	1-B	9401	31/31	0.70	0.20	1,12,18,23	31
2	FMN	2-A	7401	31/31	-	-	1,8,20,22	31
2	FMN	3-A	7401	31/31	-	-	1,6,18,24	31
2	FMN	4-A	7401	31/31	-	-	1,8,19,24	31
2	FMN	5-A	7401	31/31	-	-	1,8,18,24	31
2	FMN	6-A	7401	31/31	-	-	1,7,17,19	31
2	FMN	7-A	7401	31/31	-	-	1,5,14,20	31
2	FMN	8-A	7401	31/31	-	-	1,5,21,25	31
2	FMN	9-A	7401	31/31	-	-	1,4,21,25	31
2	FMN	10-A	7401	31/31	-	-	1,4,8,15	31
2	FMN	11-A	7401	31/31	-	-	1,8,18,23	31
2	FMN	12-A	7401	31/31	-	-	1,9,17,18	31
2	FMN	13-A	7401	31/31	-	-	1,2,14,16	31
2	FMN	14-A	7401	31/31	-	-	1,7,10,14	31
2	FMN	15-A	7401	31/31	-	-	1,6,14,18	31
2	FMN	16-A	7401	31/31	-	-	1,2,12,16	31
2	FMN	1-A	7401	31/31	0.77	0.15	1,8,19,24	31
2	FMN	2-B	9401	31/31	-	-	1,8,14,19	31
2	FMN	3-B	9401	31/31	-	-	1,8,18,19	31
2	FMN	4-B	9401	31/31	-	-	1,8,14,15	31
2	FMN	5-B	9401	31/31	-	-	1,8,15,16	31
2	FMN	6-B	9401	31/31	-	-	1,8,15,19	31
2	FMN	7-B	9401	31/31	-	-	1,7,12,14	31
2	FMN	8-B	9401	31/31	-	-	1,6,17,20	31
2	FMN	9-B	9401	31/31	-	-	1,9,16,18	31
2	FMN	10-B	9401	31/31	-	-	4,10,14,16	31
2	FMN	11-B	9401	31/31	-	-	1,11,18,21	31
2	FMN	12-B	9401	31/31	-	-	1,8,16,17	31
2	FMN	13-B	9401	31/31	-	-	1,8,16,20	31
2	FMN	14-B	9401	31/31	-	-	1,8,14,15	31
2	FMN	15-B	9401	31/31	-	-	1,8,15,20	31
2	FMN	16-B	9401	31/31	-	-	1,9,15,18	31

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.

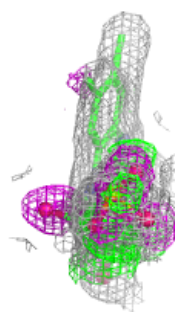
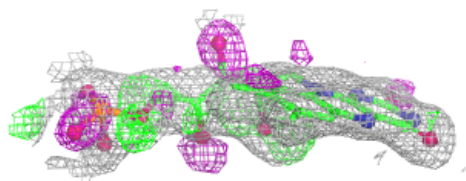
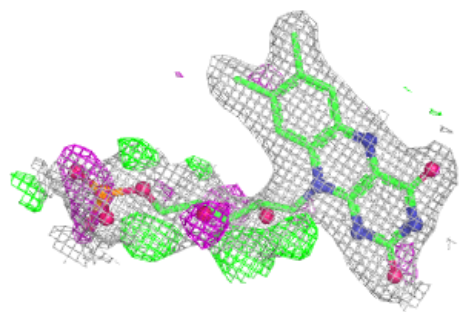
Electron density around FMN B 9401:

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



Electron density around FMN A 7401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.