Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 02:12 AM EDT

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

This is a Full wwPDB 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:

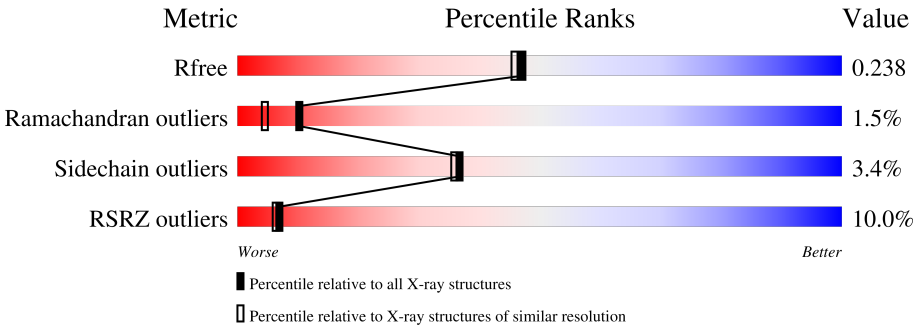
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	12% 89% • 7%
1	1-B	391	8% 90% • 6%
1	10-A	391	12% 85% 8% 7%
1	10-B	391	8% 92% • 6%
1	11-A	391	12% 90% • 7%
1	11-B	391	8% 90% • 6%

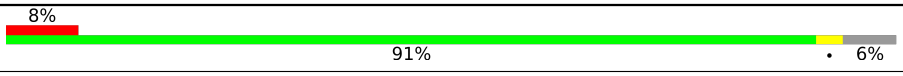
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	12-A	391	12% 90% 7%
1	12-B	391	8% 89% 5% 6%
1	13-A	391	12% 89% 7%
1	13-B	391	8% 87% 6% 6%
1	14-A	391	12% 86% 7% 7%
1	14-B	391	8% 86% 7% 6%
1	15-A	391	12% 88% 5% 7%
1	15-B	391	8% 89% 5% 6%
1	16-A	391	12% 88% 5% 7%
1	16-B	391	8% 90% 6%
1	2-A	391	12% 88% 5% 7%
1	2-B	391	8% 92% 6%
1	3-A	391	12% 91% 7%
1	3-B	391	8% 90% 6%
1	4-A	391	12% 90% 7%
1	4-B	391	8% 90% 6%
1	5-A	391	12% 92% 7%
1	5-B	391	8% 91% 6%
1	6-A	391	12% 91% 7%
1	6-B	391	8% 93% 6%
1	7-A	391	12% 91% 7%
1	7-B	391	8% 91% 6%
1	8-A	391	12% 90% 7%
1	8-B	391	8% 91% 6%
1	9-A	391	12% 90% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	9-B	391	

2 Entry composition (i)

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.

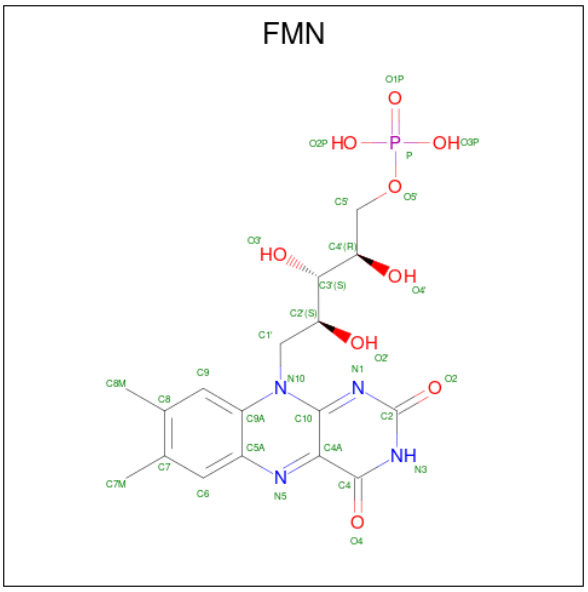
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	2-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	3-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	4-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	5-A	365	Total	C	N	O	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			

Continued on next page...

Continued from previous page...

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 (three-letter code: 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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

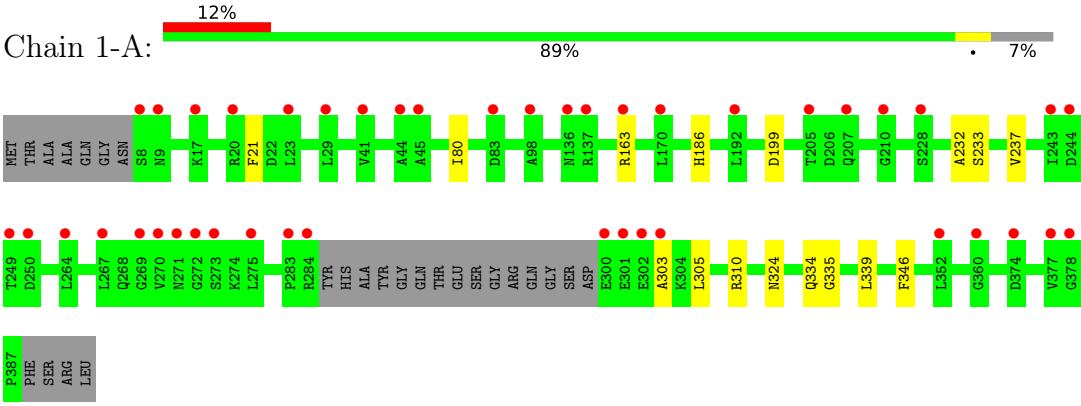
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	7-B	207	Total O 207 207	0	0
3	8-B	209	Total O 209 209	0	0
3	9-B	205	Total O 205 205	0	0
3	10-B	210	Total O 210 210	0	0
3	11-B	207	Total O 207 207	0	0
3	12-B	204	Total O 204 204	0	0
3	13-B	204	Total O 204 204	0	0
3	14-B	208	Total O 208 208	0	0
3	15-B	210	Total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

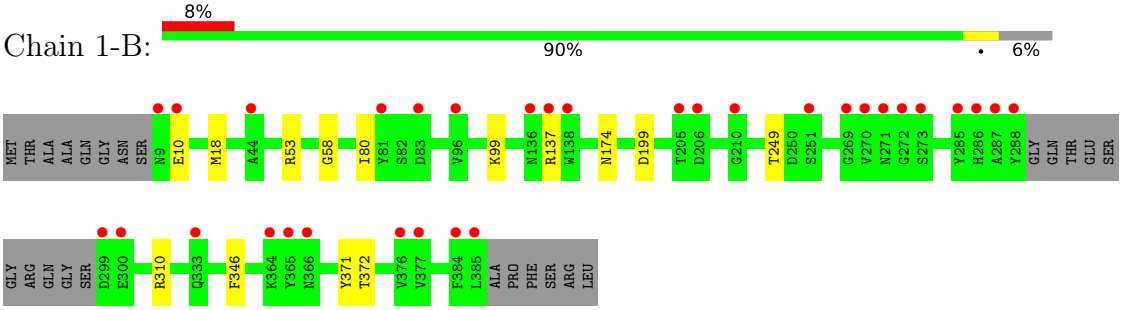
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 1-A:



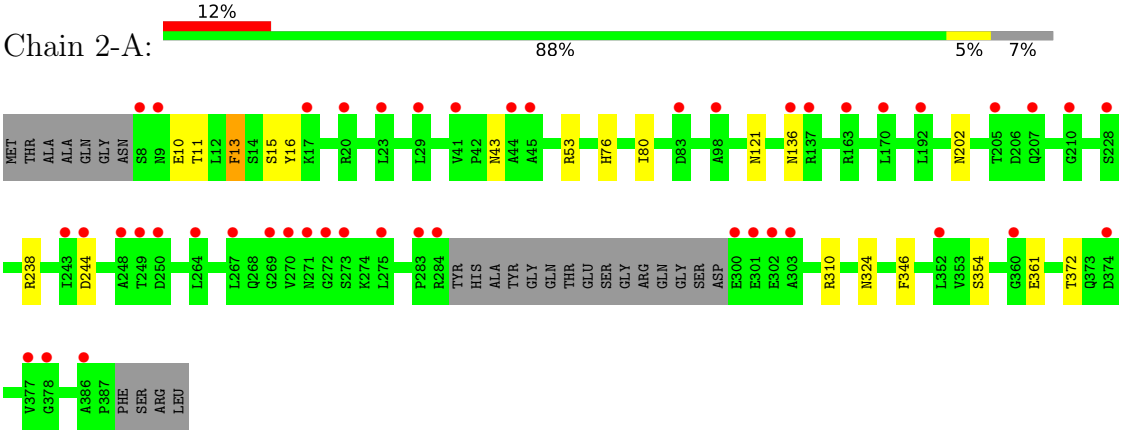
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 1-B:



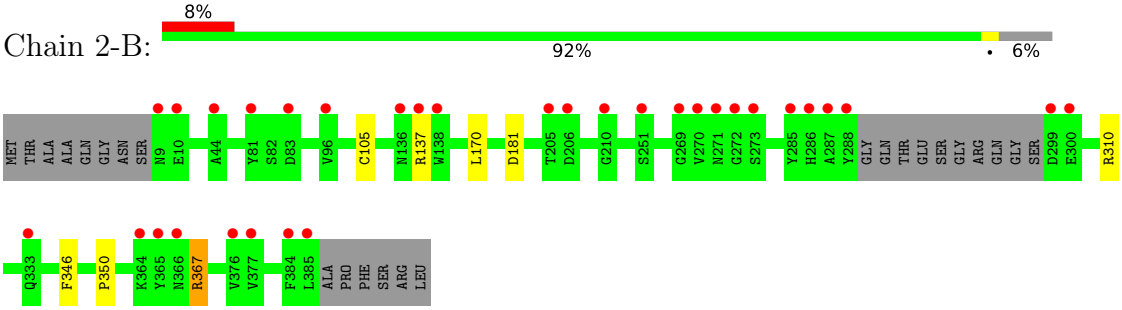
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 2-A:



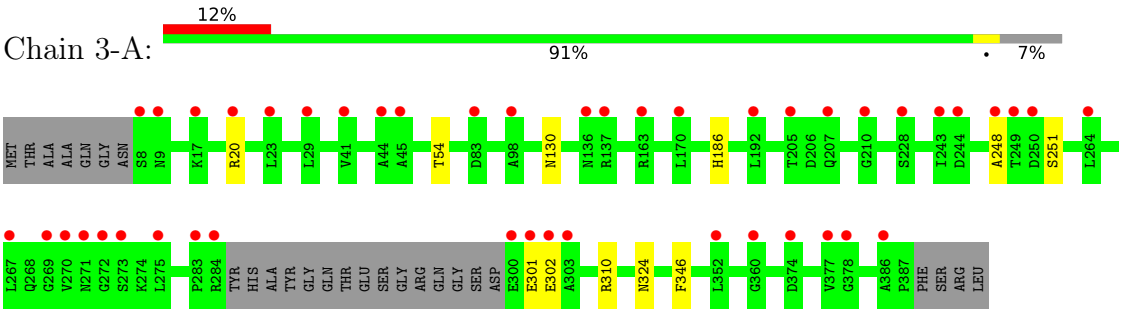
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 2-B:



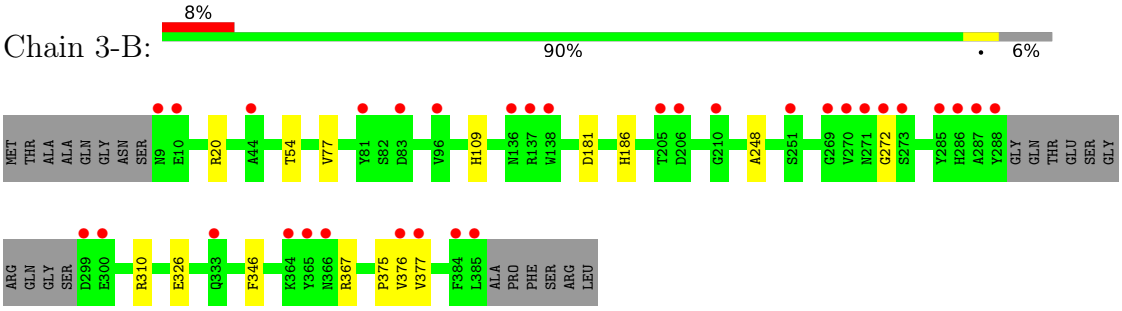
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 3-A:



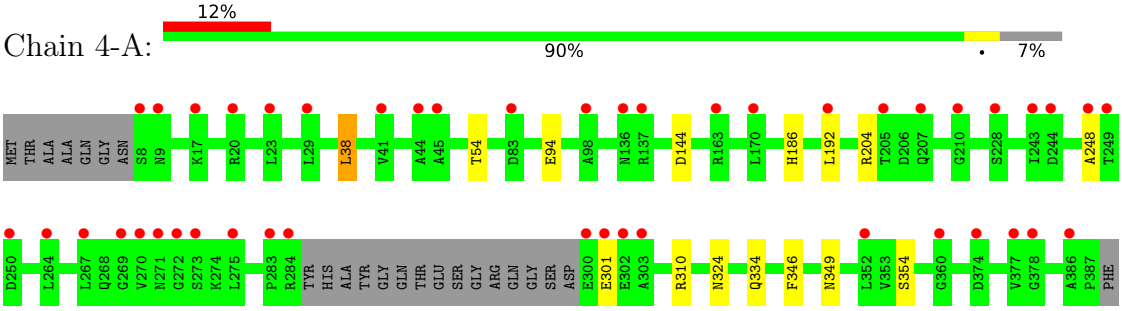
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 3-B:



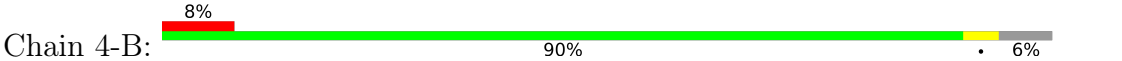
• Molecule 1: 12-oxophytodienoate reductase 3

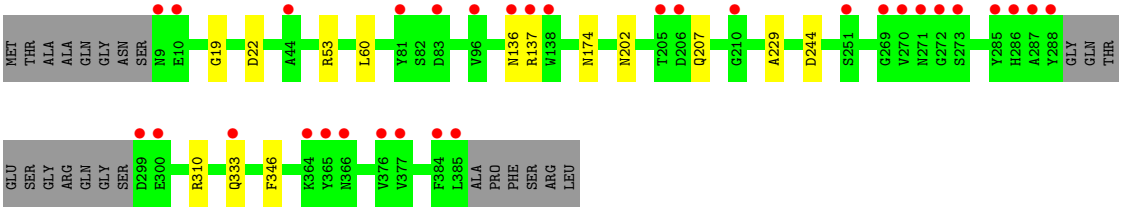
Chain 4-A:



• Molecule 1: 12-oxophytodienoate reductase 3

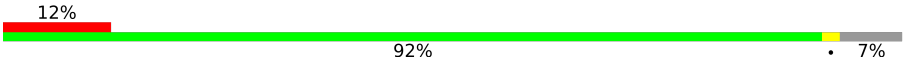
Chain 4-B:

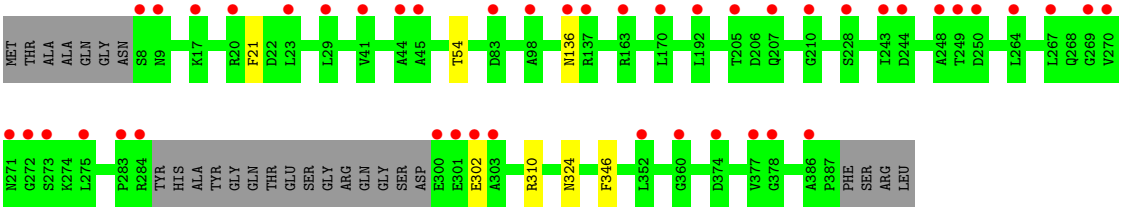




• Molecule 1: 12-oxophytodienoate reductase 3

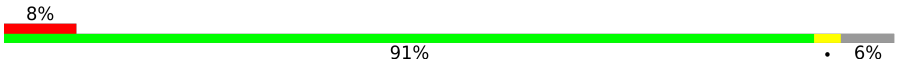
Chain 5-A:

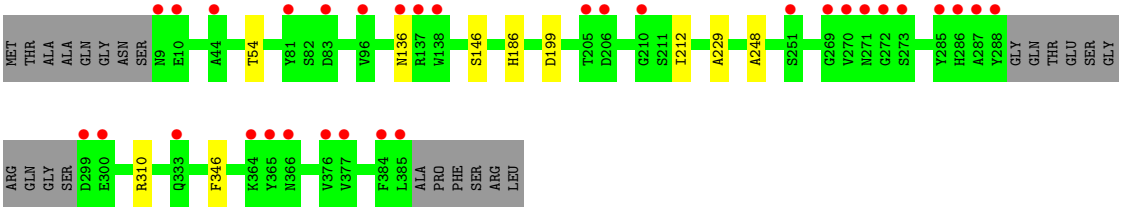




• Molecule 1: 12-oxophytodienoate reductase 3

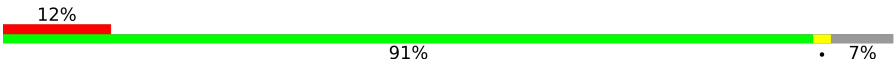
Chain 5-B:

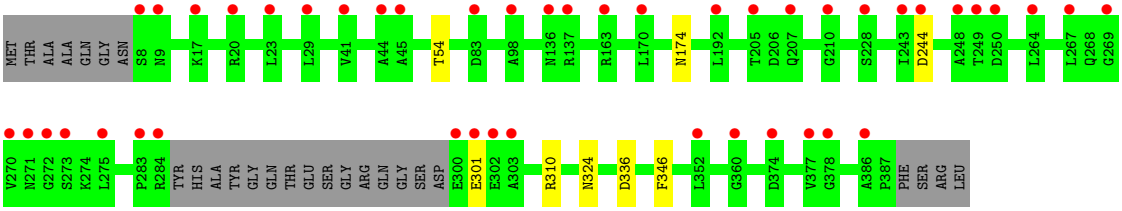




• Molecule 1: 12-oxophytodienoate reductase 3

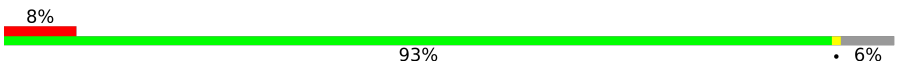
Chain 6-A:

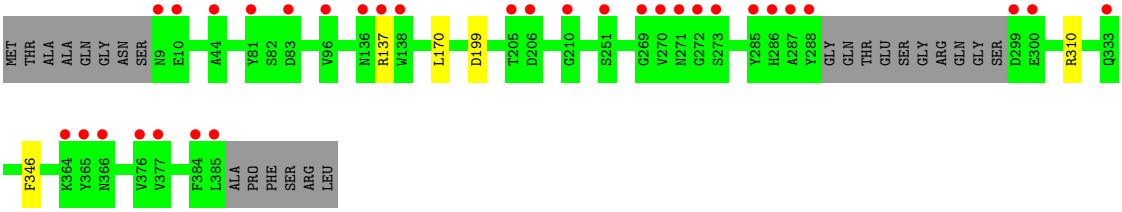




• Molecule 1: 12-oxophytodienoate reductase 3

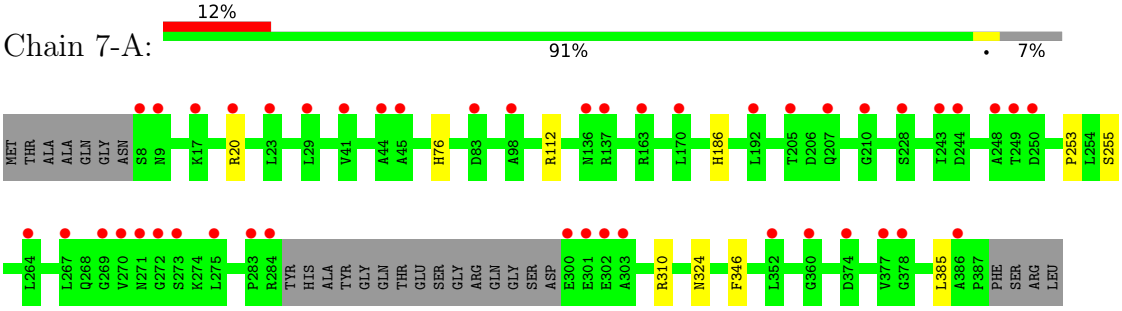
Chain 6-B:





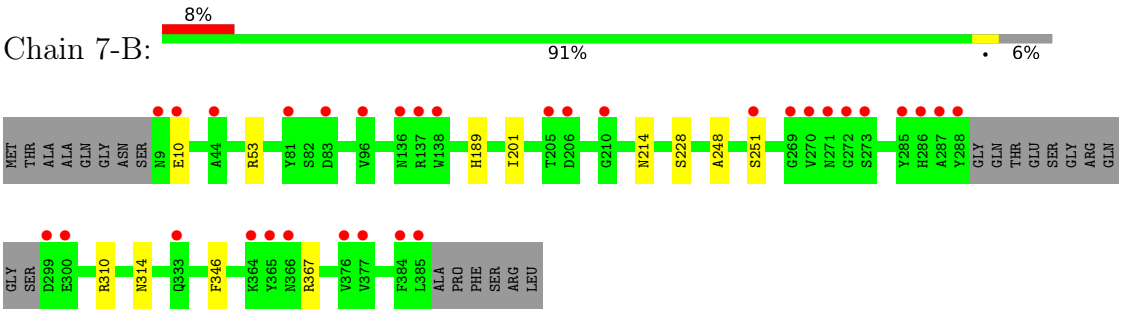
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 7-A:



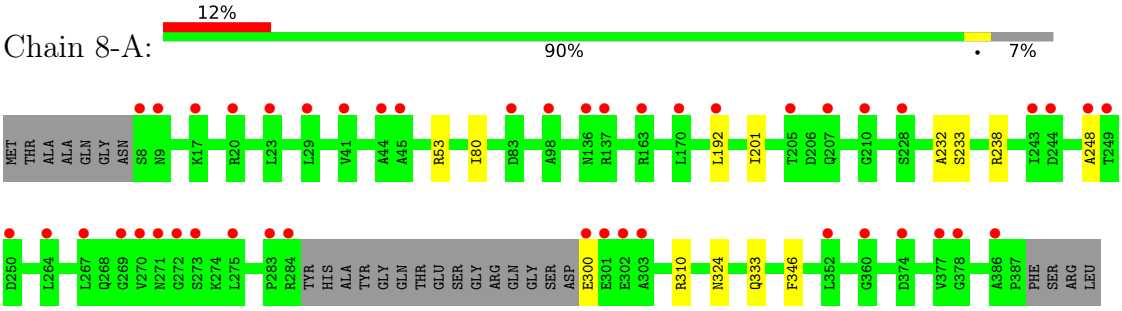
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 7-B:



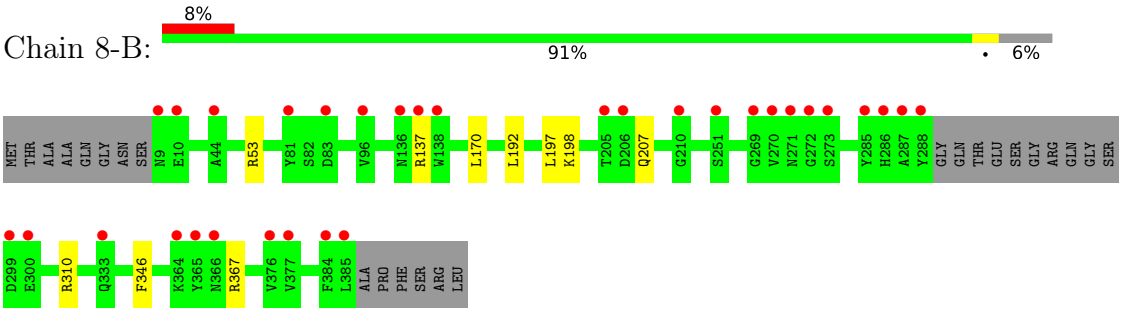
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 8-A:



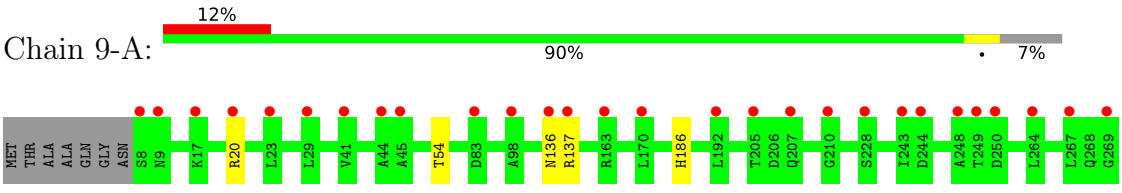
• Molecule 1: 12-oxophytodienoate reductase 3

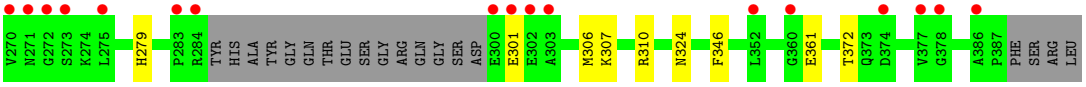
Chain 8-B:



• Molecule 1: 12-oxophytodienoate reductase 3

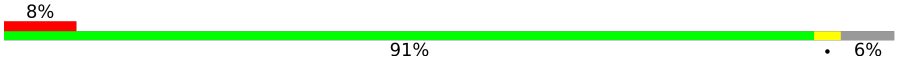
Chain 9-A:

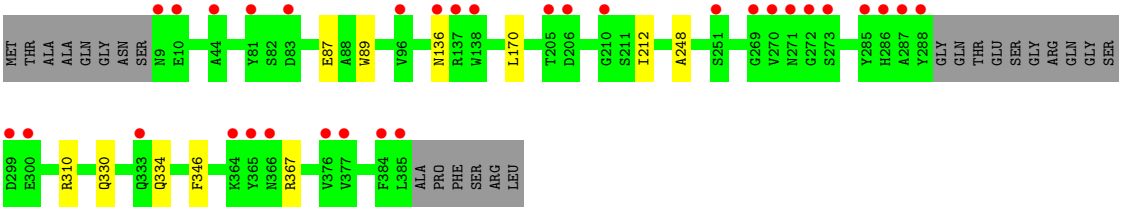




• Molecule 1: 12-oxophytodienoate reductase 3

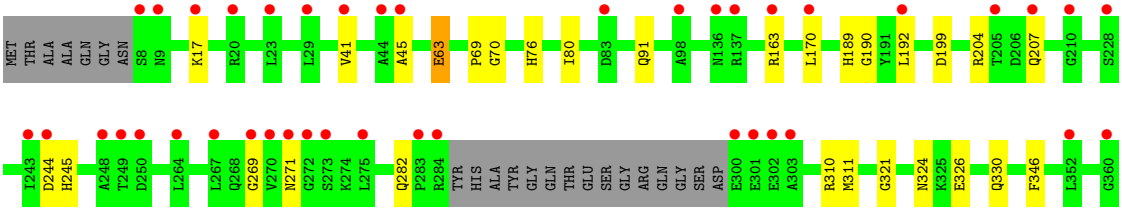
Chain 9-B:





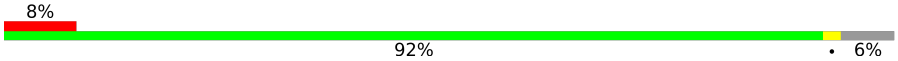
• Molecule 1: 12-oxophytodienoate reductase 3

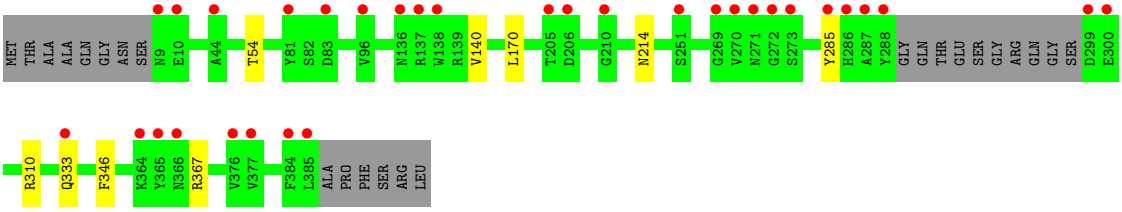
Chain 10-A:



• Molecule 1: 12-oxophytodienoate reductase 3

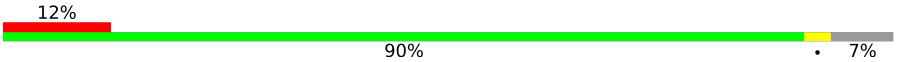
Chain 10-B:

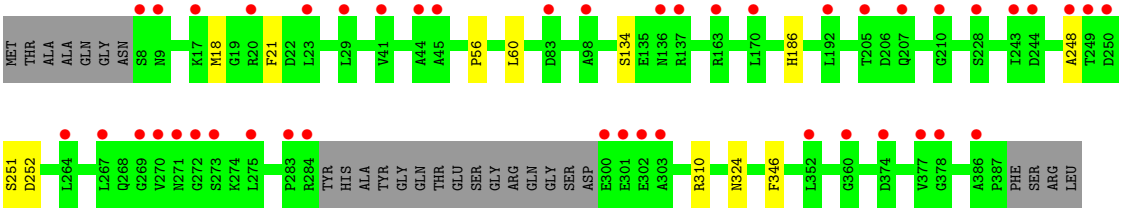




• Molecule 1: 12-oxophytodienoate reductase 3

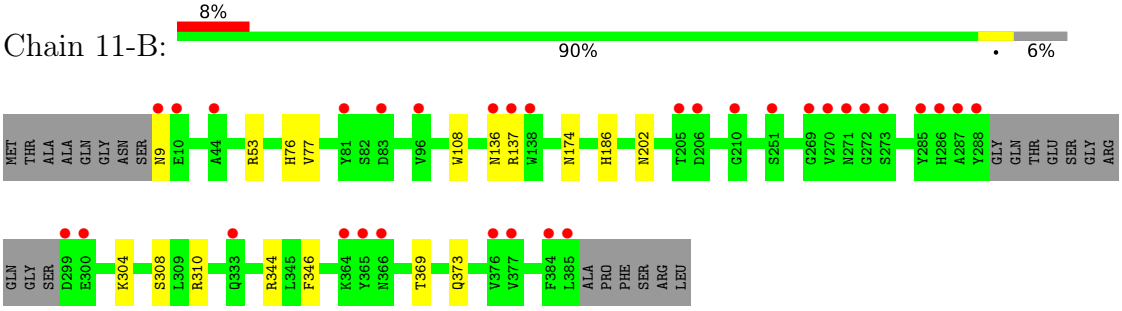
Chain 11-A:





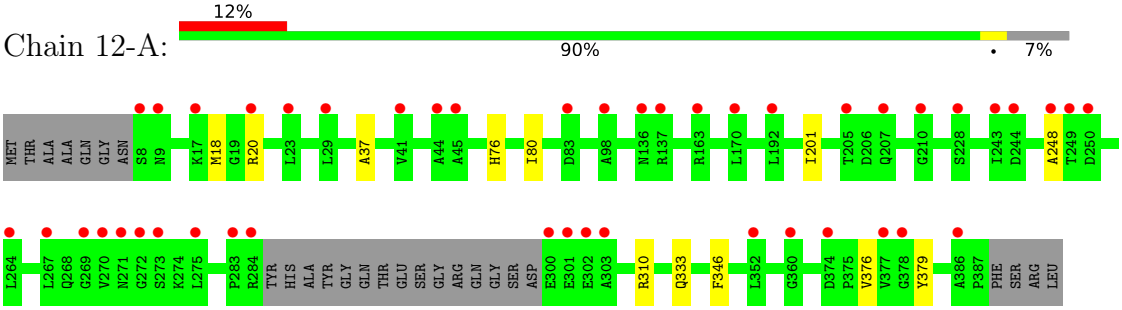
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 11-B:



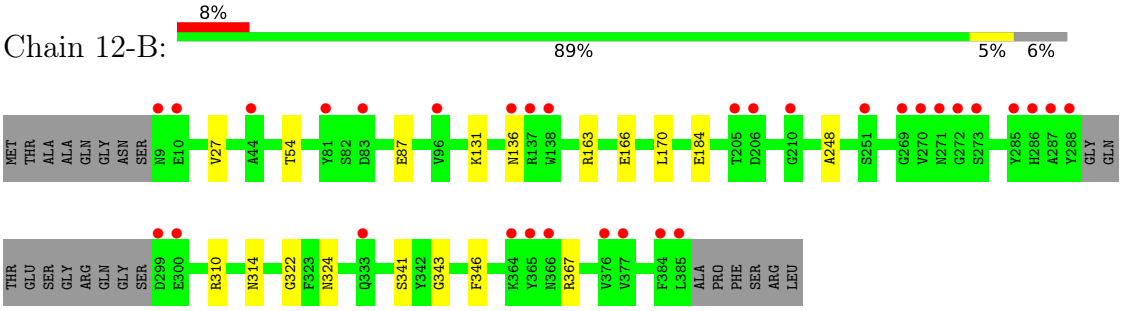
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 12-A:



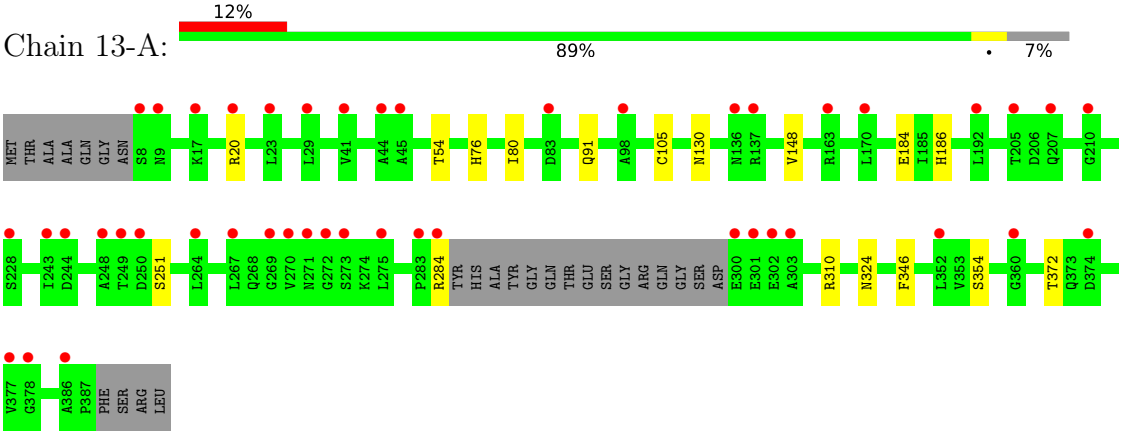
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 12-B:



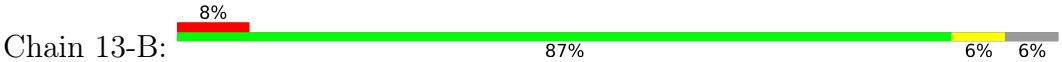
• Molecule 1: 12-oxophytodienoate reductase 3

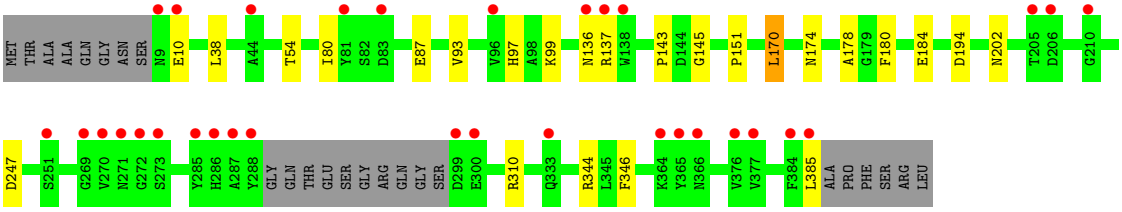
Chain 13-A:



• Molecule 1: 12-oxophytodienoate reductase 3

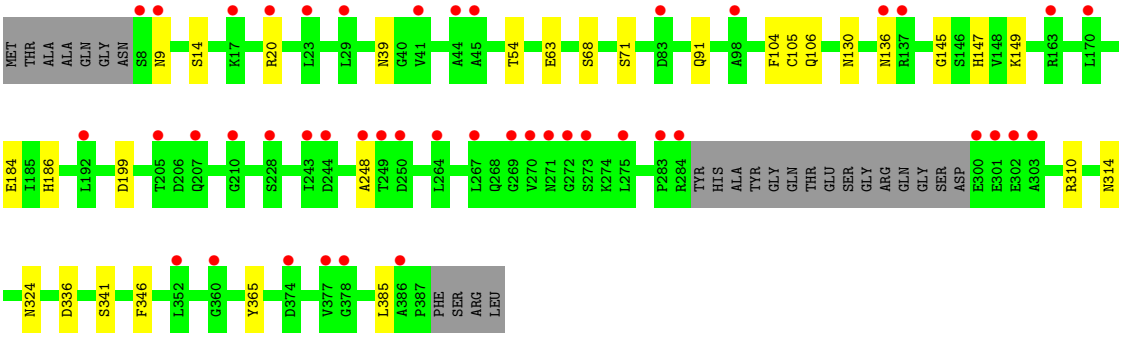
Chain 13-B:





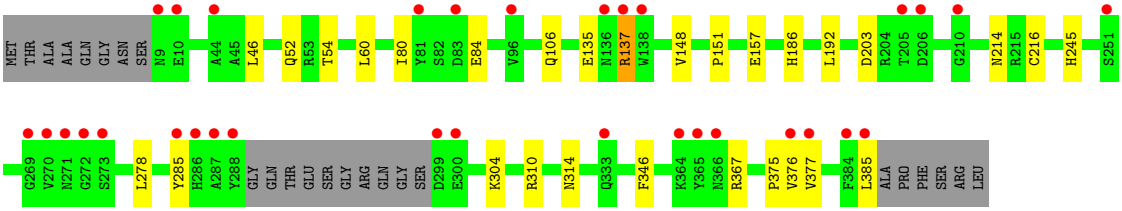
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 14-A:



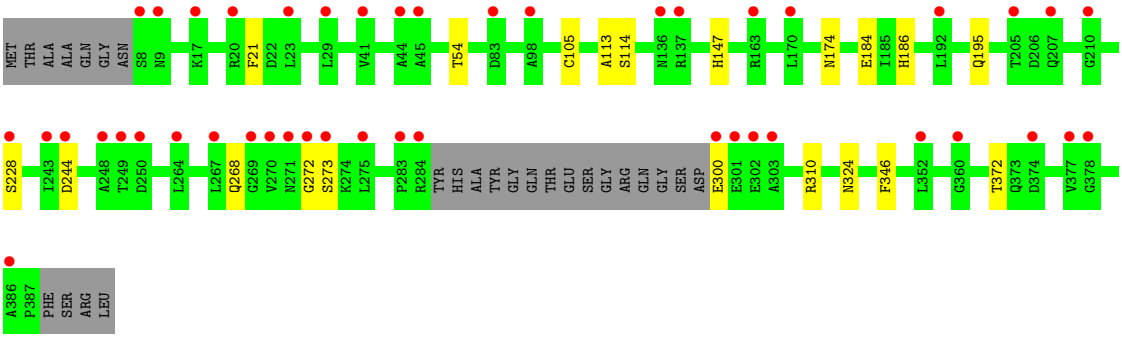
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 14-B:



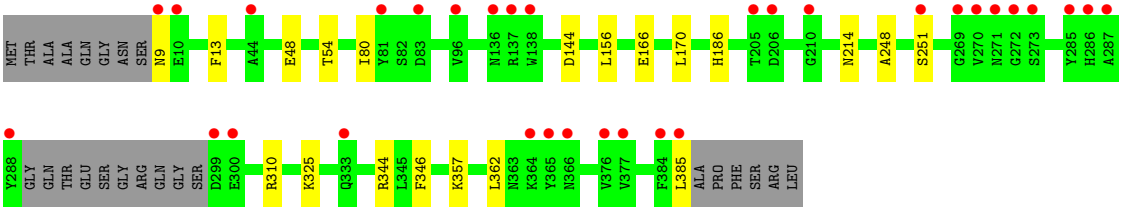
• Molecule 1: 12-oxophytodienoate reductase 3

Chain 15-A:

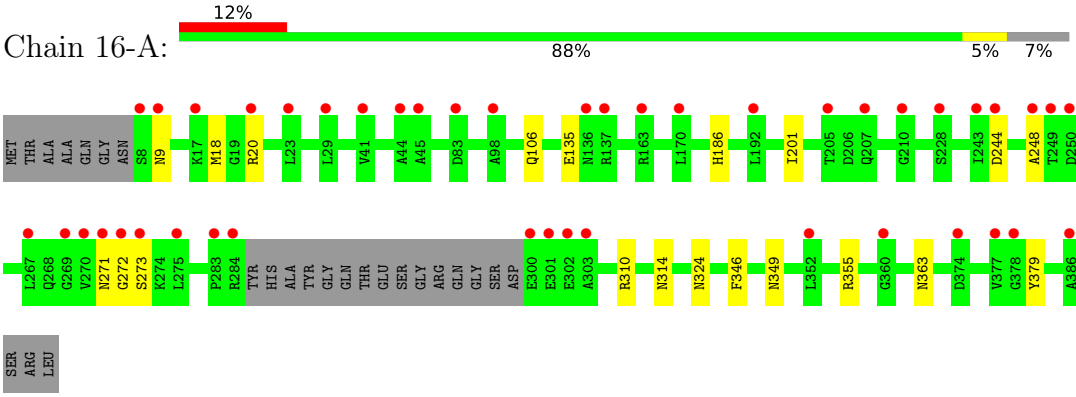


• Molecule 1: 12-oxophytodienoate reductase 3

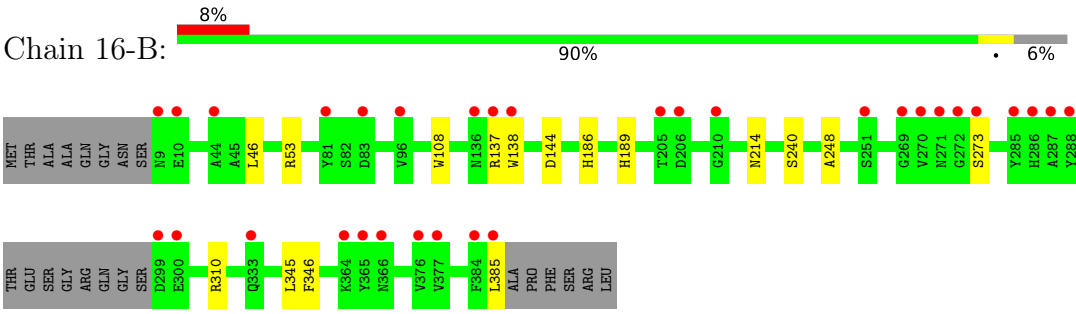
Chain 15-B:



• Molecule 1: 12-oxophytodienoate reductase 3



• Molecule 1: 12-oxophytodienoate reductase 3



4 Data and refinement statistics (i)

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) 91.3 (24.90-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.235 0.186 , 0.238	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)	0.23 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.41	0/2875	0.64	0/3895
1	1-B	0.40	0/2906	0.64	0/3937
1	2-A	0.43	0/2875	0.65	0/3895
1	2-B	0.41	0/2906	0.63	0/3937
1	3-A	0.41	0/2875	0.64	0/3895
1	3-B	0.42	0/2906	0.65	0/3937
1	4-A	0.42	0/2875	0.64	0/3895
1	4-B	0.41	0/2906	0.64	0/3937
1	5-A	0.41	0/2875	0.64	0/3895
1	5-B	0.41	0/2906	0.64	0/3937
1	6-A	0.41	0/2875	0.64	0/3895
1	6-B	0.41	0/2906	0.64	0/3937
1	7-A	0.41	0/2875	0.64	0/3895
1	7-B	0.41	0/2906	0.65	0/3937
1	8-A	0.41	0/2875	0.65	0/3895
1	8-B	0.42	0/2906	0.64	0/3937
1	9-A	0.41	0/2875	0.63	0/3895
1	9-B	0.41	0/2906	0.63	0/3937
1	10-A	0.41	0/2875	0.66	0/3895
1	10-B	0.41	0/2906	0.64	0/3937
1	11-A	0.41	0/2875	0.65	0/3895
1	11-B	0.41	0/2906	0.64	0/3937
1	12-A	0.41	0/2875	0.64	0/3895
1	12-B	0.41	0/2906	0.64	0/3937
1	13-A	0.46	0/2875	0.70	0/3895
1	13-B	0.47	0/2906	0.72	1/3937 (0.0%)
1	14-A	0.46	0/2875	0.70	0/3895
1	14-B	0.48	0/2906	0.71	0/3937
1	15-A	0.46	0/2875	0.72	0/3895
1	15-B	0.46	0/2906	0.71	1/3937 (0.0%)
1	16-A	0.45	0/2875	0.71	0/3895
1	16-B	0.46	0/2906	0.71	1/3937 (0.0%)

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1-A	361/391 (92%)	317 (88%)	35 (10%)	9 (2%)	5 2
1	1-B	363/391 (93%)	333 (92%)	25 (7%)	5 (1%)	11 5
1	2-A	361/391 (92%)	300 (83%)	51 (14%)	10 (3%)	5 1
1	2-B	363/391 (93%)	337 (93%)	24 (7%)	2 (1%)	25 19
1	3-A	361/391 (92%)	336 (93%)	22 (6%)	3 (1%)	19 13
1	3-B	363/391 (93%)	339 (93%)	18 (5%)	6 (2%)	9 4
1	4-A	361/391 (92%)	322 (89%)	33 (9%)	6 (2%)	9 4
1	4-B	363/391 (93%)	338 (93%)	20 (6%)	5 (1%)	11 5
1	5-A	361/391 (92%)	331 (92%)	29 (8%)	1 (0%)	41 37
1	5-B	363/391 (93%)	341 (94%)	20 (6%)	2 (1%)	25 19
1	6-A	361/391 (92%)	338 (94%)	22 (6%)	1 (0%)	41 37
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%)	14 8
1	7-B	363/391 (93%)	334 (92%)	23 (6%)	6 (2%)	9 4
1	8-A	361/391 (92%)	324 (90%)	31 (9%)	6 (2%)	9 4
1	8-B	363/391 (93%)	332 (92%)	28 (8%)	3 (1%)	19 13
1	9-A	361/391 (92%)	330 (91%)	23 (6%)	8 (2%)	6 2
1	9-B	363/391 (93%)	335 (92%)	26 (7%)	2 (1%)	25 19
1	10-A	361/391 (92%)	309 (86%)	33 (9%)	19 (5%)	2 0
1	10-B	363/391 (93%)	338 (93%)	24 (7%)	1 (0%)	41 37
1	11-A	361/391 (92%)	336 (93%)	22 (6%)	3 (1%)	19 13
1	11-B	363/391 (93%)	337 (93%)	22 (6%)	4 (1%)	14 8
1	12-A	361/391 (92%)	328 (91%)	25 (7%)	8 (2%)	6 2
1	12-B	363/391 (93%)	326 (90%)	32 (9%)	5 (1%)	11 5
1	13-A	361/391 (92%)	322 (89%)	35 (10%)	4 (1%)	14 8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	13-B	363/391 (93%)	327 (90%)	27 (7%)	9 (2%)	5 2
1	14-A	361/391 (92%)	312 (86%)	42 (12%)	7 (2%)	8 3
1	14-B	363/391 (93%)	311 (86%)	45 (12%)	7 (2%)	8 3
1	15-A	361/391 (92%)	324 (90%)	33 (9%)	4 (1%)	14 8
1	15-B	363/391 (93%)	326 (90%)	31 (8%)	6 (2%)	9 4
1	16-A	361/391 (92%)	324 (90%)	30 (8%)	7 (2%)	8 3
1	16-B	363/391 (93%)	332 (92%)	26 (7%)	5 (1%)	11 5
All	All	11584/12512 (93%)	10513 (91%)	903 (8%)	168 (2%)	10 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	298/317 (94%)	291 (98%)	7 (2%)	50	53
1	1-B	300/317 (95%)	291 (97%)	9 (3%)	41	41
1	2-A	298/317 (94%)	287 (96%)	11 (4%)	34	32
1	2-B	300/317 (95%)	293 (98%)	7 (2%)	50	53
1	3-A	298/317 (94%)	290 (97%)	8 (3%)	44	46
1	3-B	300/317 (95%)	291 (97%)	9 (3%)	41	41
1	4-A	298/317 (94%)	288 (97%)	10 (3%)	37	36
1	4-B	300/317 (95%)	291 (97%)	9 (3%)	41	41
1	5-A	298/317 (94%)	292 (98%)	6 (2%)	55	58
1	5-B	300/317 (95%)	292 (97%)	8 (3%)	44	46
1	6-A	298/317 (94%)	291 (98%)	7 (2%)	50	53
1	6-B	300/317 (95%)	295 (98%)	5 (2%)	60	65
1	7-A	298/317 (94%)	292 (98%)	6 (2%)	55	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	7-B	300/317 (95%)	294 (98%)	6 (2%)	55	58
1	8-A	298/317 (94%)	291 (98%)	7 (2%)	50	53
1	8-B	300/317 (95%)	293 (98%)	7 (2%)	50	53
1	9-A	298/317 (94%)	292 (98%)	6 (2%)	55	58
1	9-B	300/317 (95%)	291 (97%)	9 (3%)	41	41
1	10-A	298/317 (94%)	284 (95%)	14 (5%)	26	22
1	10-B	300/317 (95%)	292 (97%)	8 (3%)	44	46
1	11-A	298/317 (94%)	289 (97%)	9 (3%)	41	41
1	11-B	300/317 (95%)	287 (96%)	13 (4%)	29	26
1	12-A	298/317 (94%)	294 (99%)	4 (1%)	69	74
1	12-B	300/317 (95%)	287 (96%)	13 (4%)	29	26
1	13-A	298/317 (94%)	285 (96%)	13 (4%)	28	25
1	13-B	300/317 (95%)	284 (95%)	16 (5%)	22	18
1	14-A	298/317 (94%)	276 (93%)	22 (7%)	13	9
1	14-B	300/317 (95%)	277 (92%)	23 (8%)	13	8
1	15-A	298/317 (94%)	282 (95%)	16 (5%)	22	18
1	15-B	300/317 (95%)	287 (96%)	13 (4%)	29	26
1	16-A	298/317 (94%)	285 (96%)	13 (4%)	28	25
1	16-B	300/317 (95%)	290 (97%)	10 (3%)	38	37
All	All	9568/10144 (94%)	9244 (97%)	324 (3%)	37	36

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

Mol	Chain	Res	Type
1	1-A	21	PHE
1	1-A	163	ARG
1	1-A	186	HIS
1	1-A	199	ASP
1	1-A	310	ARG
1	1-A	324	ASN
1	1-A	346	PHE
1	1-B	53	ARG
1	1-B	99	LYS
1	1-B	137	ARG
1	1-B	174	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1-B	199	ASP
1	1-B	249	THR
1	1-B	310	ARG
1	1-B	346	PHE
1	1-B	371	TYR
1	2-A	10	GLU
1	2-A	13	PHE
1	2-A	43	ASN
1	2-A	53	ARG
1	2-A	238	ARG
1	2-A	244	ASP
1	2-A	310	ARG
1	2-A	324	ASN
1	2-A	346	PHE
1	2-A	354	SER
1	2-A	372	THR
1	2-B	105	CYS
1	2-B	137	ARG
1	2-B	170	LEU
1	2-B	181	ASP
1	2-B	310	ARG
1	2-B	346	PHE
1	2-B	367	ARG
1	3-A	20	ARG
1	3-A	54	THR
1	3-A	130	ASN
1	3-A	186	HIS
1	3-A	302	GLU
1	3-A	310	ARG
1	3-A	324	ASN
1	3-A	346	PHE
1	3-B	54	THR
1	3-B	77	VAL
1	3-B	109	HIS
1	3-B	181	ASP
1	3-B	186	HIS
1	3-B	310	ARG
1	3-B	326	GLU
1	3-B	346	PHE
1	3-B	367	ARG
1	4-A	38	LEU
1	4-A	54	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-A	94	GLU
1	4-A	144	ASP
1	4-A	186	HIS
1	4-A	310	ARG
1	4-A	324	ASN
1	4-A	346	PHE
1	4-A	349	ASN
1	4-A	354	SER
1	4-B	22	ASP
1	4-B	53	ARG
1	4-B	60	LEU
1	4-B	137	ARG
1	4-B	174	ASN
1	4-B	207	GLN
1	4-B	244	ASP
1	4-B	310	ARG
1	4-B	346	PHE
1	5-A	21	PHE
1	5-A	54	THR
1	5-A	302	GLU
1	5-A	310	ARG
1	5-A	324	ASN
1	5-A	346	PHE
1	5-B	54	THR
1	5-B	136	ASN
1	5-B	146	SER
1	5-B	186	HIS
1	5-B	199	ASP
1	5-B	212	ILE
1	5-B	310	ARG
1	5-B	346	PHE
1	6-A	54	THR
1	6-A	174	ASN
1	6-A	244	ASP
1	6-A	310	ARG
1	6-A	324	ASN
1	6-A	336	ASP
1	6-A	346	PHE
1	6-B	137	ARG
1	6-B	170	LEU
1	6-B	199	ASP
1	6-B	310	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	6-B	346	PHE
1	7-A	20	ARG
1	7-A	186	HIS
1	7-A	310	ARG
1	7-A	324	ASN
1	7-A	346	PHE
1	7-A	385	LEU
1	7-B	53	ARG
1	7-B	214	ASN
1	7-B	310	ARG
1	7-B	314	ASN
1	7-B	346	PHE
1	7-B	367	ARG
1	8-A	53	ARG
1	8-A	238	ARG
1	8-A	300	GLU
1	8-A	310	ARG
1	8-A	324	ASN
1	8-A	333	GLN
1	8-A	346	PHE
1	8-B	53	ARG
1	8-B	137	ARG
1	8-B	170	LEU
1	8-B	207	GLN
1	8-B	310	ARG
1	8-B	346	PHE
1	8-B	367	ARG
1	9-A	20	ARG
1	9-A	54	THR
1	9-A	310	ARG
1	9-A	324	ASN
1	9-A	346	PHE
1	9-A	372	THR
1	9-B	87	GLU
1	9-B	89	TRP
1	9-B	170	LEU
1	9-B	212	ILE
1	9-B	310	ARG
1	9-B	330	GLN
1	9-B	334	GLN
1	9-B	346	PHE
1	9-B	367	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	10-A	17	LYS
1	10-A	41	VAL
1	10-A	63	GLU
1	10-A	163	ARG
1	10-A	170	LEU
1	10-A	199	ASP
1	10-A	244	ASP
1	10-A	282	GLN
1	10-A	310	ARG
1	10-A	311	MET
1	10-A	324	ASN
1	10-A	326	GLU
1	10-A	330	GLN
1	10-A	346	PHE
1	10-B	54	THR
1	10-B	170	LEU
1	10-B	214	ASN
1	10-B	285	TYR
1	10-B	310	ARG
1	10-B	333	GLN
1	10-B	346	PHE
1	10-B	367	ARG
1	11-A	21	PHE
1	11-A	60	LEU
1	11-A	134	SER
1	11-A	186	HIS
1	11-A	251	SER
1	11-A	252	ASP
1	11-A	310	ARG
1	11-A	324	ASN
1	11-A	346	PHE
1	11-B	9	ASN
1	11-B	53	ARG
1	11-B	77	VAL
1	11-B	108	TRP
1	11-B	137	ARG
1	11-B	174	ASN
1	11-B	186	HIS
1	11-B	304	LYS
1	11-B	310	ARG
1	11-B	344	ARG
1	11-B	346	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	11-B	369	THR
1	11-B	373	GLN
1	12-A	20	ARG
1	12-A	310	ARG
1	12-A	333	GLN
1	12-A	346	PHE
1	12-B	54	THR
1	12-B	87	GLU
1	12-B	131	LYS
1	12-B	163	ARG
1	12-B	166	GLU
1	12-B	170	LEU
1	12-B	184	GLU
1	12-B	310	ARG
1	12-B	314	ASN
1	12-B	324	ASN
1	12-B	341	SER
1	12-B	346	PHE
1	12-B	367	ARG
1	13-A	20	ARG
1	13-A	54	THR
1	13-A	80	ILE
1	13-A	105	CYS
1	13-A	130	ASN
1	13-A	184	GLU
1	13-A	186	HIS
1	13-A	284	ARG
1	13-A	310	ARG
1	13-A	324	ASN
1	13-A	346	PHE
1	13-A	354	SER
1	13-A	372	THR
1	13-B	54	THR
1	13-B	80	ILE
1	13-B	87	GLU
1	13-B	97	HIS
1	13-B	99	LYS
1	13-B	137	ARG
1	13-B	151	PRO
1	13-B	170	LEU
1	13-B	174	ASN
1	13-B	184	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13-B	194	ASP
1	13-B	247	ASP
1	13-B	310	ARG
1	13-B	344	ARG
1	13-B	346	PHE
1	13-B	385	LEU
1	14-A	14	SER
1	14-A	20	ARG
1	14-A	54	THR
1	14-A	63	GLU
1	14-A	71	SER
1	14-A	104	PHE
1	14-A	105	CYS
1	14-A	106	GLN
1	14-A	130	ASN
1	14-A	147	HIS
1	14-A	149	LYS
1	14-A	184	GLU
1	14-A	186	HIS
1	14-A	199	ASP
1	14-A	310	ARG
1	14-A	314	ASN
1	14-A	324	ASN
1	14-A	336	ASP
1	14-A	341	SER
1	14-A	346	PHE
1	14-A	365	TYR
1	14-A	385	LEU
1	14-B	46	LEU
1	14-B	52	GLN
1	14-B	54	THR
1	14-B	60	LEU
1	14-B	80	ILE
1	14-B	84	GLU
1	14-B	106	GLN
1	14-B	135	GLU
1	14-B	137	ARG
1	14-B	151	PRO
1	14-B	157	GLU
1	14-B	186	HIS
1	14-B	203	ASP
1	14-B	214	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	14-B	216	CYS
1	14-B	278	LEU
1	14-B	285	TYR
1	14-B	304	LYS
1	14-B	310	ARG
1	14-B	314	ASN
1	14-B	346	PHE
1	14-B	367	ARG
1	14-B	385	LEU
1	15-A	21	PHE
1	15-A	54	THR
1	15-A	105	CYS
1	15-A	114	SER
1	15-A	147	HIS
1	15-A	174	ASN
1	15-A	184	GLU
1	15-A	186	HIS
1	15-A	195	GLN
1	15-A	228	SER
1	15-A	244	ASP
1	15-A	300	GLU
1	15-A	310	ARG
1	15-A	324	ASN
1	15-A	346	PHE
1	15-A	372	THR
1	15-B	9	ASN
1	15-B	48	GLU
1	15-B	54	THR
1	15-B	80	ILE
1	15-B	156	LEU
1	15-B	166	GLU
1	15-B	186	HIS
1	15-B	214	ASN
1	15-B	310	ARG
1	15-B	325	LYS
1	15-B	344	ARG
1	15-B	346	PHE
1	15-B	385	LEU
1	16-A	9	ASN
1	16-A	20	ARG
1	16-A	106	GLN
1	16-A	135	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16-A	186	HIS
1	16-A	244	ASP
1	16-A	310	ARG
1	16-A	314	ASN
1	16-A	324	ASN
1	16-A	346	PHE
1	16-A	349	ASN
1	16-A	355	ARG
1	16-A	363	ASN
1	16-B	46	LEU
1	16-B	53	ARG
1	16-B	137	ARG
1	16-B	138	TRP
1	16-B	186	HIS
1	16-B	214	ASN
1	16-B	240	SER
1	16-B	310	ARG
1	16-B	346	PHE
1	16-B	385	LEU

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2-A	43	ASN
1	2-A	52	GLN
1	2-A	97	HIS
1	2-A	195	GLN
1	2-A	214	ASN
1	2-A	221	GLN
1	2-A	268	GLN
1	2-A	271	ASN
1	2-A	324	ASN
1	2-A	334	GLN
1	2-B	39	ASN
1	2-B	76	HIS
1	2-B	119	GLN
1	2-B	174	ASN
1	2-B	195	GLN
1	2-B	214	ASN
1	2-B	268	GLN
1	2-B	271	ASN
1	2-B	282	GLN
1	2-B	314	ASN
1	2-B	334	GLN
1	3-A	39	ASN
1	3-A	52	GLN
1	3-A	97	HIS
1	3-A	195	GLN
1	3-A	221	GLN
1	3-A	268	GLN
1	3-A	271	ASN
1	3-A	282	GLN
1	3-A	324	ASN
1	3-A	334	GLN
1	3-B	39	ASN
1	3-B	91	GLN
1	3-B	109	HIS
1	3-B	119	GLN
1	3-B	174	ASN
1	3-B	195	GLN
1	3-B	214	ASN
1	3-B	268	GLN
1	3-B	314	ASN
1	3-B	334	GLN
1	3-B	373	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	4-A	39	ASN
1	4-A	97	HIS
1	4-A	119	GLN
1	4-A	147	HIS
1	4-A	195	GLN
1	4-A	268	GLN
1	4-A	282	GLN
1	4-A	314	ASN
1	4-A	324	ASN
1	4-B	39	ASN
1	4-B	76	HIS
1	4-B	97	HIS
1	4-B	174	ASN
1	4-B	195	GLN
1	4-B	207	GLN
1	4-B	214	ASN
1	4-B	268	GLN
1	4-B	271	ASN
1	4-B	314	ASN
1	4-B	334	GLN
1	5-A	39	ASN
1	5-A	52	GLN
1	5-A	97	HIS
1	5-A	195	GLN
1	5-A	221	GLN
1	5-A	268	GLN
1	5-A	314	ASN
1	5-A	324	ASN
1	5-A	334	GLN
1	5-B	9	ASN
1	5-B	39	ASN
1	5-B	76	HIS
1	5-B	97	HIS
1	5-B	174	ASN
1	5-B	189	HIS
1	5-B	195	GLN
1	5-B	214	ASN
1	5-B	268	GLN
1	5-B	271	ASN
1	5-B	282	GLN
1	5-B	314	ASN
1	5-B	334	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5-B	373	GLN
1	6-A	39	ASN
1	6-A	52	GLN
1	6-A	97	HIS
1	6-A	195	GLN
1	6-A	221	GLN
1	6-A	268	GLN
1	6-A	282	GLN
1	6-A	324	ASN
1	6-B	39	ASN
1	6-B	76	HIS
1	6-B	97	HIS
1	6-B	174	ASN
1	6-B	195	GLN
1	6-B	214	ASN
1	6-B	268	GLN
1	6-B	271	ASN
1	6-B	282	GLN
1	6-B	314	ASN
1	6-B	334	GLN
1	7-A	39	ASN
1	7-A	52	GLN
1	7-A	97	HIS
1	7-A	119	GLN
1	7-A	195	GLN
1	7-A	221	GLN
1	7-A	268	GLN
1	7-A	282	GLN
1	7-A	314	ASN
1	7-A	324	ASN
1	7-A	334	GLN
1	7-B	39	ASN
1	7-B	76	HIS
1	7-B	97	HIS
1	7-B	174	ASN
1	7-B	189	HIS
1	7-B	195	GLN
1	7-B	214	ASN
1	7-B	265	ASN
1	7-B	286	HIS
1	7-B	314	ASN
1	7-B	333	GLN

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	9-B	330	GLN
1	10-A	52	GLN
1	10-A	147	HIS
1	10-A	189	HIS
1	10-A	195	GLN
1	10-A	268	GLN
1	10-A	271	ASN
1	10-A	324	ASN
1	10-A	330	GLN
1	10-A	334	GLN
1	10-A	373	GLN
1	10-B	39	ASN
1	10-B	76	HIS
1	10-B	97	HIS
1	10-B	147	HIS
1	10-B	174	ASN
1	10-B	189	HIS
1	10-B	195	GLN
1	10-B	214	ASN
1	10-B	268	GLN
1	10-B	271	ASN
1	10-B	282	GLN
1	10-B	314	ASN
1	10-B	333	GLN
1	11-A	39	ASN
1	11-A	195	GLN
1	11-A	221	GLN
1	11-A	268	GLN
1	11-A	271	ASN
1	11-A	314	ASN
1	11-A	324	ASN
1	11-A	333	GLN
1	11-A	334	GLN
1	11-B	39	ASN
1	11-B	97	HIS
1	11-B	106	GLN
1	11-B	174	ASN
1	11-B	195	GLN
1	11-B	214	ASN
1	11-B	268	GLN
1	11-B	271	ASN
1	11-B	314	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	11-B	330	GLN
1	11-B	366	ASN
1	11-B	373	GLN
1	12-A	39	ASN
1	12-A	52	GLN
1	12-A	97	HIS
1	12-A	195	GLN
1	12-A	221	GLN
1	12-A	268	GLN
1	12-A	271	ASN
1	12-A	334	GLN
1	12-B	39	ASN
1	12-B	76	HIS
1	12-B	91	GLN
1	12-B	97	HIS
1	12-B	119	GLN
1	12-B	147	HIS
1	12-B	195	GLN
1	12-B	214	ASN
1	12-B	268	GLN
1	12-B	314	ASN
1	12-B	333	GLN
1	12-B	334	GLN
1	12-B	373	GLN
1	13-A	39	ASN
1	13-A	91	GLN
1	13-A	97	HIS
1	13-A	186	HIS
1	13-A	195	GLN
1	13-A	268	GLN
1	13-A	324	ASN
1	13-A	334	GLN
1	13-A	373	GLN
1	13-B	76	HIS
1	13-B	97	HIS
1	13-B	174	ASN
1	13-B	186	HIS
1	13-B	214	ASN
1	13-B	268	GLN
1	13-B	334	GLN
1	14-A	39	ASN
1	14-A	52	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	14-A	91	GLN
1	14-A	97	HIS
1	14-A	130	ASN
1	14-A	147	HIS
1	14-A	195	GLN
1	14-A	221	GLN
1	14-A	245	HIS
1	14-A	268	GLN
1	14-A	324	ASN
1	14-A	330	GLN
1	14-A	333	GLN
1	14-A	334	GLN
1	14-B	9	ASN
1	14-B	39	ASN
1	14-B	76	HIS
1	14-B	121	ASN
1	14-B	174	ASN
1	14-B	195	GLN
1	14-B	202	ASN
1	14-B	214	ASN
1	14-B	268	GLN
1	14-B	314	ASN
1	14-B	330	GLN
1	14-B	366	ASN
1	15-A	39	ASN
1	15-A	52	GLN
1	15-A	76	HIS
1	15-A	97	HIS
1	15-A	195	GLN
1	15-A	214	ASN
1	15-A	268	GLN
1	15-A	324	ASN
1	15-A	334	GLN
1	15-B	9	ASN
1	15-B	39	ASN
1	15-B	76	HIS
1	15-B	97	HIS
1	15-B	119	GLN
1	15-B	174	ASN
1	15-B	189	HIS
1	15-B	195	GLN
1	15-B	214	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	15-B	268	GLN
1	15-B	314	ASN
1	15-B	333	GLN
1	15-B	334	GLN
1	15-B	363	ASN
1	16-A	9	ASN
1	16-A	39	ASN
1	16-A	52	GLN
1	16-A	97	HIS
1	16-A	189	HIS
1	16-A	195	GLN
1	16-A	214	ASN
1	16-A	221	GLN
1	16-A	268	GLN
1	16-A	271	ASN
1	16-A	282	GLN
1	16-A	324	ASN
1	16-A	330	GLN
1	16-A	333	GLN
1	16-A	334	GLN
1	16-A	349	ASN
1	16-A	373	GLN
1	16-B	39	ASN
1	16-B	136	ASN
1	16-B	174	ASN
1	16-B	195	GLN
1	16-B	207	GLN
1	16-B	214	ASN
1	16-B	221	GLN
1	16-B	245	HIS
1	16-B	268	GLN
1	16-B	286	HIS
1	16-B	330	GLN
1	16-B	363	ASN
1	16-B	373	GLN

5.3.3 RNA

There are no RNA 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 monosaccharides 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	3-B	9401	-	33,33,33	1.96	8 (24%)	48,50,50	3.59	20 (41%)
2	FMN	6-B	9401	-	33,33,33	2.11	13 (39%)	48,50,50	3.64	18 (37%)
2	FMN	1-A	7401	-	33,33,33	2.00	7 (21%)	48,50,50	2.80	15 (31%)
2	FMN	11-A	7401	-	33,33,33	1.92	5 (15%)	48,50,50	2.92	16 (33%)
2	FMN	11-B	9401	-	33,33,33	2.03	4 (12%)	48,50,50	3.63	12 (25%)
2	FMN	5-B	9401	-	33,33,33	1.89	7 (21%)	48,50,50	3.47	18 (37%)
2	FMN	16-A	7401	-	33,33,33	2.21	10 (30%)	48,50,50	3.32	22 (45%)
2	FMN	14-A	7401	-	33,33,33	2.15	12 (36%)	48,50,50	3.00	21 (43%)
2	FMN	4-B	9401	-	33,33,33	1.56	7 (21%)	48,50,50	3.22	14 (29%)
2	FMN	7-A	7401	-	33,33,33	2.29	8 (24%)	48,50,50	3.23	23 (47%)
2	FMN	6-A	7401	-	33,33,33	2.08	6 (18%)	48,50,50	3.21	16 (33%)
2	FMN	2-A	7401	-	33,33,33	1.60	7 (21%)	48,50,50	2.57	15 (31%)
2	FMN	13-B	9401	-	33,33,33	2.57	13 (39%)	48,50,50	3.78	24 (50%)
2	FMN	12-B	9401	-	33,33,33	1.95	12 (36%)	48,50,50	3.26	14 (29%)
2	FMN	9-B	9401	-	33,33,33	2.03	10 (30%)	48,50,50	3.45	15 (31%)
2	FMN	1-B	9401	-	33,33,33	1.92	5 (15%)	48,50,50	3.55	15 (31%)
2	FMN	8-B	9401	-	33,33,33	1.67	7 (21%)	48,50,50	3.42	20 (41%)
2	FMN	13-A	7401	-	33,33,33	2.24	11 (33%)	48,50,50	3.34	24 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FMN	14-B	9401	-	33,33,33	2.03	10 (30%)	48,50,50	3.41	18 (37%)
2	FMN	3-A	7401	-	33,33,33	2.00	9 (27%)	48,50,50	2.89	16 (33%)
2	FMN	2-B	9401	-	33,33,33	2.15	13 (39%)	48,50,50	3.69	19 (39%)
2	FMN	8-A	7401	-	33,33,33	1.90	11 (33%)	48,50,50	2.77	18 (37%)
2	FMN	4-A	7401	-	33,33,33	1.84	5 (15%)	48,50,50	2.88	16 (33%)
2	FMN	15-B	9401	-	33,33,33	2.58	13 (39%)	48,50,50	3.80	23 (47%)
2	FMN	15-A	7401	-	33,33,33	1.89	9 (27%)	48,50,50	2.78	16 (33%)
2	FMN	12-A	7401	-	33,33,33	1.60	8 (24%)	48,50,50	2.67	17 (35%)
2	FMN	7-B	9401	-	33,33,33	2.34	9 (27%)	48,50,50	3.63	23 (47%)
2	FMN	5-A	7401	-	33,33,33	1.93	5 (15%)	48,50,50	2.94	16 (33%)
2	FMN	10-A	7401	-	33,33,33	1.49	7 (21%)	48,50,50	2.62	21 (43%)
2	FMN	9-A	7401	-	33,33,33	1.77	10 (30%)	48,50,50	2.81	17 (35%)
2	FMN	10-B	9401	-	33,33,33	1.97	9 (27%)	48,50,50	3.49	17 (35%)
2	FMN	16-B	9401	-	33,33,33	1.92	10 (30%)	48,50,50	3.56	22 (45%)

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	3-B	9401	-	-	4/18/18/18	0/3/3/3
2	FMN	6-B	9401	-	-	3/18/18/18	0/3/3/3
2	FMN	1-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	11-B	9401	-	-	2/18/18/18	0/3/3/3
2	FMN	5-B	9401	-	-	4/18/18/18	0/3/3/3
2	FMN	16-A	7401	-	-	4/18/18/18	0/3/3/3
2	FMN	14-A	7401	-	-	1/18/18/18	0/3/3/3
2	FMN	4-B	9401	-	-	2/18/18/18	0/3/3/3
2	FMN	7-A	7401	-	-	4/18/18/18	0/3/3/3
2	FMN	6-A	7401	-	-	4/18/18/18	0/3/3/3
2	FMN	2-A	7401	-	-	3/18/18/18	0/3/3/3
2	FMN	13-B	9401	-	-	4/18/18/18	0/3/3/3
2	FMN	12-B	9401	-	-	3/18/18/18	0/3/3/3
2	FMN	9-B	9401	-	-	2/18/18/18	0/3/3/3

Continued on next page...

Continued from previous page...

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

All (280) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7-A	7401	FMN	C1'-C2'	-8.94	1.40	1.52
2	11-B	9401	FMN	C5'-C4'	-8.02	1.40	1.51
2	1-B	9401	FMN	C5'-C4'	-7.65	1.41	1.51
2	7-B	9401	FMN	C1'-C2'	-7.49	1.42	1.52
2	13-B	9401	FMN	C1'-C2'	-7.24	1.42	1.52
2	6-A	7401	FMN	C5'-C4'	-7.24	1.41	1.51
2	15-B	9401	FMN	C1'-C2'	-7.09	1.42	1.52
2	15-B	9401	FMN	C9A-N10	7.03	1.53	1.41
2	13-B	9401	FMN	C9A-N10	6.81	1.53	1.41
2	2-B	9401	FMN	C1'-C2'	-6.71	1.43	1.52
2	13-A	7401	FMN	C1'-C2'	-6.66	1.43	1.52
2	16-A	7401	FMN	C1'-C2'	-6.59	1.43	1.52
2	6-B	9401	FMN	C1'-C2'	-6.36	1.43	1.52
2	1-A	7401	FMN	C1'-C2'	-6.30	1.43	1.52
2	3-A	7401	FMN	C1'-C2'	-6.30	1.43	1.52
2	7-B	9401	FMN	C9A-N10	5.98	1.51	1.41
2	3-B	9401	FMN	C1'-C2'	-5.86	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	11-A	7401	FMN	C1'-C2'	-5.84	1.44	1.52
2	5-A	7401	FMN	C1'-C2'	-5.63	1.44	1.52
2	5-B	9401	FMN	C9A-N10	5.46	1.50	1.41
2	14-A	7401	FMN	C4'-C3'	-5.45	1.43	1.53
2	15-A	7401	FMN	C1'-C2'	-5.33	1.45	1.52
2	4-A	7401	FMN	C1'-C2'	-5.29	1.45	1.52
2	5-A	7401	FMN	C9A-N10	5.28	1.50	1.41
2	13-A	7401	FMN	C9A-N10	5.11	1.50	1.41
2	16-B	9401	FMN	C5'-C4'	5.10	1.59	1.51
2	10-B	9401	FMN	C1'-C2'	-5.09	1.45	1.52
2	7-A	7401	FMN	C9A-N10	5.09	1.50	1.41
2	11-A	7401	FMN	C9A-N10	5.08	1.50	1.41
2	10-B	9401	FMN	C9A-N10	5.08	1.50	1.41
2	6-A	7401	FMN	C9A-N10	4.94	1.49	1.41
2	4-A	7401	FMN	C9A-N10	4.90	1.49	1.41
2	8-A	7401	FMN	C9A-N10	4.89	1.49	1.41
2	16-A	7401	FMN	C9A-N10	4.84	1.49	1.41
2	14-B	9401	FMN	C9A-N10	4.84	1.49	1.41
2	3-B	9401	FMN	C9A-N10	4.84	1.49	1.41
2	9-A	7401	FMN	C9A-N10	4.82	1.49	1.41
2	1-A	7401	FMN	C9A-N10	4.75	1.49	1.41
2	14-B	9401	FMN	C5'-C4'	4.69	1.58	1.51
2	9-B	9401	FMN	C1'-C2'	-4.63	1.46	1.52
2	16-B	9401	FMN	C9A-N10	4.56	1.49	1.41
2	12-B	9401	FMN	C9A-N10	4.48	1.49	1.41
2	12-B	9401	FMN	C1'-C2'	4.48	1.59	1.52
2	3-A	7401	FMN	C9A-N10	4.35	1.48	1.41
2	14-A	7401	FMN	C5'-C4'	-4.34	1.45	1.51
2	9-B	9401	FMN	C9A-N10	4.23	1.48	1.41
2	5-B	9401	FMN	C1'-C2'	-4.21	1.46	1.52
2	15-A	7401	FMN	C5'-C4'	-4.10	1.46	1.51
2	4-B	9401	FMN	C9A-N10	4.04	1.48	1.41
2	15-B	9401	FMN	C5'-C4'	4.02	1.57	1.51
2	7-B	9401	FMN	C5'-C4'	3.99	1.57	1.51
2	9-B	9401	FMN	C4'-C3'	-3.91	1.46	1.53
2	8-B	9401	FMN	C1'-C2'	3.90	1.58	1.52
2	13-B	9401	FMN	C5'-C4'	3.85	1.57	1.51
2	2-B	9401	FMN	C9A-N10	3.82	1.47	1.41
2	13-B	9401	FMN	C6-C5A	3.82	1.46	1.40
2	8-A	7401	FMN	C5A-N5	-3.82	1.32	1.39
2	15-A	7401	FMN	C5A-N5	-3.81	1.32	1.39
2	14-A	7401	FMN	P-O5'	-3.80	1.48	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	11-B	9401	FMN	C9-C9A	3.78	1.45	1.39
2	14-A	7401	FMN	C6-C5A	3.78	1.45	1.40
2	9-A	7401	FMN	C5A-N5	-3.77	1.32	1.39
2	2-A	7401	FMN	C2-N3	-3.77	1.30	1.39
2	15-B	9401	FMN	C6-C5A	3.75	1.45	1.40
2	15-B	9401	FMN	C1'-N10	3.74	1.57	1.48
2	10-B	9401	FMN	C9-C9A	3.74	1.45	1.39
2	1-B	9401	FMN	C9-C9A	3.67	1.45	1.39
2	12-A	7401	FMN	C9A-C5A	3.66	1.47	1.41
2	2-A	7401	FMN	C9A-C5A	3.64	1.47	1.41
2	13-B	9401	FMN	C1'-N10	3.59	1.57	1.48
2	15-A	7401	FMN	C9A-N10	3.59	1.47	1.41
2	6-B	9401	FMN	C9A-N10	3.59	1.47	1.41
2	6-A	7401	FMN	C1'-C2'	-3.57	1.47	1.52
2	14-A	7401	FMN	C9-C9A	3.54	1.45	1.39
2	9-B	9401	FMN	C9-C9A	3.52	1.45	1.39
2	6-A	7401	FMN	C5A-N5	-3.51	1.32	1.39
2	4-A	7401	FMN	C5A-N5	-3.48	1.32	1.39
2	5-B	9401	FMN	C9-C9A	3.47	1.45	1.39
2	11-A	7401	FMN	C5A-N5	-3.47	1.32	1.39
2	1-A	7401	FMN	C5A-N5	-3.45	1.32	1.39
2	5-A	7401	FMN	C5A-N5	-3.44	1.32	1.39
2	10-A	7401	FMN	C2'-C3'	3.44	1.60	1.53
2	16-B	9401	FMN	C2'-C3'	3.43	1.59	1.53
2	3-A	7401	FMN	C5A-N5	-3.42	1.32	1.39
2	13-A	7401	FMN	C5A-N5	-3.42	1.32	1.39
2	12-A	7401	FMN	C2-N3	-3.39	1.31	1.39
2	8-A	7401	FMN	C1'-C2'	3.37	1.57	1.52
2	11-B	9401	FMN	C9A-N10	3.31	1.47	1.41
2	16-A	7401	FMN	C5A-N5	-3.31	1.33	1.39
2	7-B	9401	FMN	C9-C9A	3.30	1.45	1.39
2	12-B	9401	FMN	C5A-N5	-3.27	1.33	1.39
2	12-A	7401	FMN	C4A-C10	3.25	1.53	1.44
2	6-B	9401	FMN	C9-C9A	3.22	1.44	1.39
2	14-B	9401	FMN	C9-C9A	3.22	1.44	1.39
2	3-A	7401	FMN	C4'-C3'	-3.21	1.47	1.53
2	14-B	9401	FMN	C6-C5A	3.19	1.45	1.40
2	9-B	9401	FMN	C6-C5A	3.19	1.45	1.40
2	8-A	7401	FMN	C9A-C5A	3.17	1.46	1.41
2	15-B	9401	FMN	C2-N1	-3.17	1.29	1.36
2	16-A	7401	FMN	C9-C9A	3.16	1.44	1.39
2	9-A	7401	FMN	C9A-C5A	3.16	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2-B	9401	FMN	C2'-C3'	3.16	1.59	1.53
2	8-B	9401	FMN	C6-C5A	3.15	1.44	1.40
2	2-B	9401	FMN	C9-C9A	3.13	1.44	1.39
2	14-B	9401	FMN	O3'-C3'	-3.12	1.35	1.43
2	3-B	9401	FMN	C9-C9A	3.11	1.44	1.39
2	3-A	7401	FMN	P-O5'	-3.11	1.50	1.60
2	13-A	7401	FMN	C9-C9A	3.09	1.44	1.39
2	4-B	9401	FMN	C9-C9A	3.09	1.44	1.39
2	16-A	7401	FMN	O3'-C3'	-3.05	1.35	1.43
2	14-A	7401	FMN	O2'-C2'	3.03	1.49	1.43
2	13-A	7401	FMN	O3'-C3'	-3.03	1.35	1.43
2	7-B	9401	FMN	C9A-C5A	3.02	1.46	1.41
2	13-B	9401	FMN	C2-N1	-3.01	1.29	1.36
2	5-B	9401	FMN	C6-C5A	3.00	1.44	1.40
2	10-B	9401	FMN	C6-C5A	2.99	1.44	1.40
2	6-A	7401	FMN	C9-C9A	2.99	1.44	1.39
2	7-B	9401	FMN	C6-C5A	2.99	1.44	1.40
2	15-B	9401	FMN	C9-C9A	2.99	1.44	1.39
2	14-B	9401	FMN	C9A-C5A	2.98	1.46	1.41
2	13-B	9401	FMN	C9-C9A	2.96	1.44	1.39
2	9-B	9401	FMN	O2'-C2'	2.95	1.49	1.43
2	6-B	9401	FMN	P-O5'	-2.94	1.50	1.60
2	2-A	7401	FMN	C4A-C10	2.94	1.52	1.44
2	7-A	7401	FMN	C2'-C3'	-2.92	1.48	1.53
2	11-B	9401	FMN	C5A-N5	-2.91	1.33	1.39
2	16-B	9401	FMN	C9-C9A	2.90	1.44	1.39
2	16-B	9401	FMN	C9A-C5A	2.89	1.46	1.41
2	4-B	9401	FMN	C6-C5A	2.89	1.44	1.40
2	8-B	9401	FMN	C4A-C10	2.88	1.52	1.44
2	13-B	9401	FMN	P-O5'	-2.87	1.51	1.60
2	6-B	9401	FMN	C6-C5A	2.86	1.44	1.40
2	14-B	9401	FMN	C2'-C3'	2.86	1.58	1.53
2	1-B	9401	FMN	C5A-N5	-2.86	1.34	1.39
2	1-A	7401	FMN	P-O5'	-2.85	1.51	1.60
2	7-A	7401	FMN	C6-C5A	2.85	1.44	1.40
2	2-B	9401	FMN	O2'-C2'	2.82	1.49	1.43
2	1-A	7401	FMN	C9-C9A	2.82	1.44	1.39
2	3-B	9401	FMN	C9A-C5A	2.80	1.45	1.41
2	8-B	9401	FMN	C9A-N10	2.80	1.46	1.41
2	14-B	9401	FMN	C1'-N10	2.80	1.55	1.48
2	3-B	9401	FMN	C6-C5A	2.79	1.44	1.40
2	9-B	9401	FMN	P-O5'	-2.79	1.51	1.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-A	7401	FMN	C9-C9A	2.79	1.44	1.39
2	2-B	9401	FMN	C6-C5A	2.78	1.44	1.40
2	13-A	7401	FMN	C6-C5A	2.77	1.44	1.40
2	10-B	9401	FMN	P-O5'	-2.77	1.51	1.60
2	6-B	9401	FMN	C4'-C3'	-2.77	1.48	1.53
2	7-A	7401	FMN	C2-N1	-2.75	1.30	1.36
2	8-A	7401	FMN	C10-N10	2.75	1.43	1.37
2	16-A	7401	FMN	C6-C5A	2.75	1.44	1.40
2	13-B	9401	FMN	C9A-C5A	2.73	1.45	1.41
2	11-A	7401	FMN	C9-C9A	2.72	1.44	1.39
2	15-B	9401	FMN	C9A-C5A	2.72	1.45	1.41
2	15-B	9401	FMN	P-O5'	-2.71	1.51	1.60
2	3-A	7401	FMN	C9-C9A	2.70	1.44	1.39
2	4-A	7401	FMN	C9-C9A	2.67	1.44	1.39
2	6-B	9401	FMN	O2'-C2'	2.66	1.49	1.43
2	10-A	7401	FMN	C6-C5A	2.64	1.44	1.40
2	15-A	7401	FMN	C9-C9A	2.64	1.43	1.39
2	9-A	7401	FMN	C1'-C2'	2.63	1.56	1.52
2	12-B	9401	FMN	C4A-C10	2.62	1.51	1.44
2	7-A	7401	FMN	C5A-N5	-2.62	1.34	1.39
2	4-B	9401	FMN	C4A-C10	2.61	1.51	1.44
2	12-B	9401	FMN	C2'-C3'	2.60	1.58	1.53
2	8-B	9401	FMN	C9-C9A	2.59	1.43	1.39
2	2-B	9401	FMN	P-O5'	-2.59	1.51	1.60
2	4-B	9401	FMN	C5A-N5	-2.58	1.34	1.39
2	10-A	7401	FMN	C9A-C5A	2.57	1.45	1.41
2	16-A	7401	FMN	C9A-C5A	2.57	1.45	1.41
2	8-B	9401	FMN	C5A-N5	-2.54	1.34	1.39
2	8-A	7401	FMN	C4A-C10	2.53	1.51	1.44
2	13-A	7401	FMN	C9A-C5A	2.52	1.45	1.41
2	16-B	9401	FMN	C1'-C2'	-2.52	1.49	1.52
2	12-B	9401	FMN	C9A-C5A	2.51	1.45	1.41
2	5-B	9401	FMN	C5A-N5	-2.50	1.34	1.39
2	9-A	7401	FMN	C10-N10	2.50	1.42	1.37
2	12-B	9401	FMN	C4'-C3'	2.49	1.58	1.53
2	8-A	7401	FMN	C2'-C3'	2.47	1.58	1.53
2	6-B	9401	FMN	C2'-C3'	2.47	1.58	1.53
2	9-A	7401	FMN	C9-C9A	2.47	1.43	1.39
2	8-A	7401	FMN	C9-C9A	2.45	1.43	1.39
2	16-B	9401	FMN	C6-C5A	2.45	1.43	1.40
2	8-A	7401	FMN	C1'-N10	2.44	1.54	1.48
2	14-A	7401	FMN	C2-N1	-2.43	1.31	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9-A	7401	FMN	C4A-C10	2.42	1.51	1.44
2	12-A	7401	FMN	C9A-N10	2.42	1.45	1.41
2	7-A	7401	FMN	C9A-C5A	2.41	1.45	1.41
2	7-B	9401	FMN	C5A-N5	-2.40	1.34	1.39
2	6-B	9401	FMN	P-O3P	2.38	1.64	1.54
2	2-B	9401	FMN	O3'-C3'	2.38	1.48	1.43
2	2-B	9401	FMN	C4'-C3'	-2.37	1.49	1.53
2	2-B	9401	FMN	C9A-C5A	2.37	1.45	1.41
2	12-B	9401	FMN	C2-N3	-2.36	1.33	1.39
2	4-A	7401	FMN	C6-C5A	2.35	1.43	1.40
2	16-B	9401	FMN	O2'-C2'	2.35	1.48	1.43
2	1-B	9401	FMN	O2-C2	-2.34	1.19	1.24
2	10-A	7401	FMN	C4A-C10	2.34	1.51	1.44
2	12-A	7401	FMN	P-O2P	2.33	1.63	1.54
2	5-B	9401	FMN	C9A-C5A	2.32	1.45	1.41
2	16-A	7401	FMN	C5'-C4'	2.32	1.55	1.51
2	3-B	9401	FMN	C2-N1	-2.31	1.31	1.36
2	12-B	9401	FMN	C1'-N10	2.31	1.54	1.48
2	7-B	9401	FMN	O3'-C3'	2.30	1.48	1.43
2	7-B	9401	FMN	C2-N1	-2.30	1.31	1.36
2	10-B	9401	FMN	C5A-N5	-2.30	1.35	1.39
2	12-B	9401	FMN	C9-C9A	2.29	1.43	1.39
2	1-A	7401	FMN	C6-C5A	2.29	1.43	1.40
2	16-A	7401	FMN	C2-N1	-2.28	1.31	1.36
2	2-B	9401	FMN	C2-N1	-2.28	1.31	1.36
2	3-B	9401	FMN	C5A-N5	-2.27	1.35	1.39
2	15-B	9401	FMN	C4'-C3'	2.27	1.57	1.53
2	13-A	7401	FMN	C2-N1	-2.26	1.31	1.36
2	14-A	7401	FMN	P-O1P	-2.25	1.43	1.50
2	14-A	7401	FMN	C1'-N10	-2.24	1.42	1.48
2	6-B	9401	FMN	O3'-C3'	2.24	1.48	1.43
2	14-B	9401	FMN	C5A-N5	-2.24	1.35	1.39
2	5-A	7401	FMN	C6-C5A	2.22	1.43	1.40
2	2-A	7401	FMN	C1'-N10	2.22	1.53	1.48
2	7-A	7401	FMN	C9-C9A	2.22	1.43	1.39
2	2-B	9401	FMN	P-O3P	2.21	1.63	1.54
2	14-A	7401	FMN	C10-N10	-2.21	1.32	1.37
2	10-A	7401	FMN	C1'-N10	2.21	1.53	1.48
2	13-A	7401	FMN	C5'-C4'	2.21	1.54	1.51
2	9-B	9401	FMN	P-O3P	2.20	1.63	1.54
2	5-B	9401	FMN	C4A-C10	2.20	1.50	1.44
2	3-A	7401	FMN	C6-C5A	2.20	1.43	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	10-A	7401	FMN	O2-C2	-2.20	1.20	1.24
2	14-B	9401	FMN	C4A-C10	2.19	1.50	1.44
2	2-B	9401	FMN	C5A-N5	-2.19	1.35	1.39
2	9-B	9401	FMN	C5A-N5	-2.18	1.35	1.39
2	13-B	9401	FMN	C4'-C3'	2.18	1.57	1.53
2	9-A	7401	FMN	C6-C5A	2.18	1.43	1.40
2	15-A	7401	FMN	C10-N10	-2.17	1.32	1.37
2	14-A	7401	FMN	P-O2P	2.17	1.63	1.54
2	8-A	7401	FMN	C6-C5A	2.16	1.43	1.40
2	11-A	7401	FMN	C6-C5A	2.14	1.43	1.40
2	12-B	9401	FMN	C4-N3	-2.13	1.34	1.38
2	4-B	9401	FMN	C9A-C5A	2.13	1.44	1.41
2	10-B	9401	FMN	C9A-C5A	2.13	1.44	1.41
2	12-B	9401	FMN	C6-C5A	2.13	1.43	1.40
2	16-A	7401	FMN	C4'-C3'	-2.13	1.49	1.53
2	10-B	9401	FMN	O2'-C2'	2.12	1.47	1.43
2	15-B	9401	FMN	P-O3P	2.12	1.63	1.54
2	15-A	7401	FMN	C6-C5A	2.11	1.43	1.40
2	3-B	9401	FMN	O2'-C2'	2.11	1.47	1.43
2	3-A	7401	FMN	C2-N1	-2.11	1.31	1.36
2	9-A	7401	FMN	C1'-N10	2.10	1.53	1.48
2	9-A	7401	FMN	P-O2P	2.10	1.63	1.54
2	13-B	9401	FMN	C2'-C3'	-2.10	1.49	1.53
2	6-B	9401	FMN	C5A-N5	-2.10	1.35	1.39
2	6-B	9401	FMN	C9A-C5A	2.10	1.44	1.41
2	1-A	7401	FMN	C4'-C3'	-2.09	1.49	1.53
2	6-A	7401	FMN	C6-C5A	2.09	1.43	1.40
2	15-A	7401	FMN	P-O5'	-2.09	1.53	1.60
2	3-A	7401	FMN	C9A-C5A	2.09	1.44	1.41
2	13-A	7401	FMN	O2-C2	-2.09	1.20	1.24
2	6-B	9401	FMN	C2-N1	-2.08	1.31	1.36
2	16-B	9401	FMN	C4A-C10	2.08	1.50	1.44
2	13-B	9401	FMN	C4A-N5	2.07	1.34	1.30
2	12-A	7401	FMN	O2'-C2'	-2.07	1.39	1.43
2	9-B	9401	FMN	C2-N1	-2.06	1.31	1.36
2	1-B	9401	FMN	C9A-N10	2.06	1.44	1.41
2	14-A	7401	FMN	O5'-C5'	-2.06	1.36	1.44
2	2-A	7401	FMN	P-O2P	2.05	1.62	1.54
2	2-A	7401	FMN	O2'-C2'	-2.05	1.39	1.43
2	15-A	7401	FMN	C2-N1	-2.05	1.31	1.36
2	8-B	9401	FMN	C2-N3	-2.05	1.34	1.39
2	10-B	9401	FMN	C4A-C10	2.05	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-B	9401	FMN	P-O3P	2.04	1.62	1.54
2	15-B	9401	FMN	C4A-N5	2.04	1.34	1.30
2	16-B	9401	FMN	C2-N1	-2.03	1.31	1.36
2	15-B	9401	FMN	C2'-C3'	-2.03	1.49	1.53
2	2-A	7401	FMN	C5A-N5	-2.03	1.35	1.39
2	10-A	7401	FMN	C9-C9A	2.03	1.42	1.39
2	12-A	7401	FMN	C1'-N10	2.02	1.53	1.48
2	12-A	7401	FMN	C5A-N5	-2.02	1.35	1.39
2	13-A	7401	FMN	C4'-C3'	-2.01	1.49	1.53
2	4-B	9401	FMN	C1'-C2'	2.01	1.55	1.52
2	8-A	7401	FMN	P-O2P	2.00	1.62	1.54

All (581) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	11-B	9401	FMN	O3P-P-O5'	-11.52	76.08	106.73
2	4-A	7401	FMN	O3P-P-O5'	-11.34	76.56	106.73
2	1-B	9401	FMN	O3P-P-O5'	-11.07	77.27	106.73
2	6-A	7401	FMN	P-O5'-C5'	-11.02	87.95	118.30
2	5-A	7401	FMN	O3P-P-O5'	-10.95	77.60	106.73
2	11-A	7401	FMN	O3P-P-O5'	-10.92	77.67	106.73
2	7-A	7401	FMN	O3P-P-O5'	-10.82	77.94	106.73
2	14-A	7401	FMN	O3P-P-O5'	-10.82	77.95	106.73
2	15-B	9401	FMN	O5'-P-O1P	-10.77	76.25	106.47
2	13-B	9401	FMN	O5'-P-O1P	-10.72	76.40	106.47
2	8-B	9401	FMN	O5'-P-O1P	-10.65	76.59	106.47
2	14-B	9401	FMN	O3P-P-O2P	-10.63	67.00	107.64
2	14-B	9401	FMN	O3P-P-O5'	-10.61	78.50	106.73
2	10-B	9401	FMN	O5'-P-O1P	-10.41	77.27	106.47
2	7-B	9401	FMN	O5'-P-O1P	-10.41	77.27	106.47
2	1-B	9401	FMN	O2P-P-O5'	10.38	134.36	106.73
2	3-B	9401	FMN	O2P-P-O5'	10.33	134.21	106.73
2	16-B	9401	FMN	O3P-P-O2P	-10.31	68.22	107.64
2	9-A	7401	FMN	O3P-P-O5'	-10.30	79.33	106.73
2	11-B	9401	FMN	O2P-P-O5'	10.24	133.98	106.73
2	10-B	9401	FMN	O2P-P-O5'	10.08	133.55	106.73
2	9-B	9401	FMN	O5'-P-O1P	-10.07	78.23	106.47
2	9-B	9401	FMN	O2P-P-O5'	10.04	133.46	106.73
2	5-B	9401	FMN	O5'-P-O1P	-10.03	78.34	106.47
2	13-B	9401	FMN	O2P-P-O5'	9.97	133.28	106.73
2	9-B	9401	FMN	O3P-P-O5'	-9.97	80.20	106.73
2	10-B	9401	FMN	O3P-P-O5'	-9.94	80.28	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6-B	9401	FMN	O5'-P-O1P	-9.94	78.60	106.47
2	1-B	9401	FMN	O5'-P-O1P	-9.93	78.61	106.47
2	11-B	9401	FMN	O5'-P-O1P	-9.91	78.68	106.47
2	3-B	9401	FMN	O3P-P-O5'	-9.89	80.41	106.73
2	8-A	7401	FMN	O3P-P-O5'	-9.86	80.48	106.73
2	5-B	9401	FMN	O2P-P-O5'	9.84	132.93	106.73
2	14-B	9401	FMN	O2P-P-O5'	9.84	132.92	106.73
2	15-B	9401	FMN	O2P-P-O5'	9.83	132.90	106.73
2	12-A	7401	FMN	O3P-P-O5'	-9.78	80.72	106.73
2	11-B	9401	FMN	P-O5'-C5'	-9.76	91.40	118.30
2	4-B	9401	FMN	O2P-P-O5'	9.70	132.54	106.73
2	16-B	9401	FMN	O3P-P-O5'	-9.67	81.00	106.73
2	12-B	9401	FMN	O2P-P-O1P	-9.61	73.07	110.68
2	7-B	9401	FMN	O3P-P-O5'	-9.60	81.19	106.73
2	13-B	9401	FMN	O3P-P-O5'	-9.56	81.29	106.73
2	15-B	9401	FMN	O3P-P-O5'	-9.52	81.39	106.73
2	8-B	9401	FMN	O2P-P-O1P	-9.52	73.41	110.68
2	1-A	7401	FMN	O3P-P-O5'	-9.48	81.52	106.73
2	2-B	9401	FMN	C4'-C3'-C2'	-9.46	93.68	113.36
2	12-B	9401	FMN	O2P-P-O5'	9.42	131.79	106.73
2	2-B	9401	FMN	O5'-P-O1P	-9.38	80.15	106.47
2	2-A	7401	FMN	O3P-P-O5'	-9.36	81.82	106.73
2	7-B	9401	FMN	O2P-P-O5'	9.35	131.62	106.73
2	2-B	9401	FMN	O2P-P-O1P	-9.35	74.08	110.68
2	8-B	9401	FMN	O2P-P-O5'	9.28	131.43	106.73
2	3-B	9401	FMN	O5'-P-O1P	-9.26	80.50	106.47
2	6-B	9401	FMN	O2P-P-O1P	-9.15	74.87	110.68
2	12-B	9401	FMN	O5'-P-O1P	-9.09	80.98	106.47
2	3-B	9401	FMN	O2P-P-O1P	-9.05	75.24	110.68
2	6-B	9401	FMN	C4'-C3'-C2'	-9.04	94.56	113.36
2	13-A	7401	FMN	O3P-P-O1P	-9.04	75.30	110.68
2	6-A	7401	FMN	O3P-P-O5'	-9.01	82.75	106.73
2	4-B	9401	FMN	O2P-P-O1P	-9.00	75.45	110.68
2	1-B	9401	FMN	P-O5'-C5'	-8.99	93.52	118.30
2	9-B	9401	FMN	O2P-P-O1P	-8.96	75.60	110.68
2	16-A	7401	FMN	O3P-P-O1P	-8.92	75.76	110.68
2	4-B	9401	FMN	O3P-P-O5'	-8.83	83.24	106.73
2	5-B	9401	FMN	O3P-P-O5'	-8.77	83.39	106.73
2	16-B	9401	FMN	O2P-P-O5'	8.64	129.72	106.73
2	4-B	9401	FMN	O5'-P-O1P	-8.50	82.62	106.47
2	3-A	7401	FMN	O3P-P-O5'	-8.36	84.47	106.73
2	2-B	9401	FMN	O2P-P-O5'	8.33	128.91	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	13-A	7401	FMN	O5'-C5'-C4'	-8.27	87.30	109.36
2	6-B	9401	FMN	O2P-P-O5'	8.25	128.69	106.73
2	16-A	7401	FMN	O5'-C5'-C4'	-8.24	87.36	109.36
2	12-B	9401	FMN	O3P-P-O5'	-8.20	84.92	106.73
2	10-A	7401	FMN	O3P-P-O5'	-8.17	85.00	106.73
2	15-A	7401	FMN	O3P-P-O1P	-8.06	79.14	110.68
2	10-B	9401	FMN	O2P-P-O1P	-7.98	79.45	110.68
2	2-B	9401	FMN	O3P-P-O2P	-7.96	77.20	107.64
2	1-B	9401	FMN	O2P-P-O1P	-7.94	79.60	110.68
2	16-A	7401	FMN	O5'-P-O1P	7.80	128.35	106.47
2	5-B	9401	FMN	O2P-P-O1P	-7.79	80.16	110.68
2	8-B	9401	FMN	O3P-P-O5'	-7.79	86.01	106.73
2	6-B	9401	FMN	O3P-P-O2P	-7.78	77.91	107.64
2	7-B	9401	FMN	O2P-P-O1P	-7.58	81.01	110.68
2	13-A	7401	FMN	O5'-P-O1P	7.57	127.70	106.47
2	3-B	9401	FMN	C4'-C3'-C2'	-7.55	97.67	113.36
2	11-B	9401	FMN	O2P-P-O1P	-7.49	81.35	110.68
2	7-A	7401	FMN	C4'-C3'-C2'	-7.47	97.83	113.36
2	15-B	9401	FMN	O3P-P-O2P	-7.43	79.22	107.64
2	13-B	9401	FMN	O3P-P-O2P	-7.41	79.32	107.64
2	6-B	9401	FMN	O3P-P-O5'	-7.34	87.20	106.73
2	13-B	9401	FMN	O2P-P-O1P	-7.33	81.97	110.68
2	15-B	9401	FMN	O2P-P-O1P	-7.30	82.08	110.68
2	2-B	9401	FMN	O3P-P-O5'	-7.29	87.34	106.73
2	7-A	7401	FMN	O5'-P-O1P	7.24	126.79	106.47
2	16-B	9401	FMN	O2P-P-O1P	-7.20	82.51	110.68
2	5-B	9401	FMN	O3P-P-O2P	-7.19	80.15	107.64
2	15-A	7401	FMN	O3P-P-O5'	-7.17	87.65	106.73
2	4-B	9401	FMN	O3P-P-O2P	-7.13	80.38	107.64
2	7-A	7401	FMN	O3P-P-O1P	-7.12	82.83	110.68
2	12-A	7401	FMN	O3P-P-O1P	-7.08	82.97	110.68
2	16-B	9401	FMN	C4'-C3'-C2'	-7.03	98.74	113.36
2	15-A	7401	FMN	C4'-C3'-C2'	-6.94	98.92	113.36
2	7-B	9401	FMN	O3P-P-O2P	-6.93	81.14	107.64
2	6-B	9401	FMN	O5'-C5'-C4'	-6.91	90.91	109.36
2	15-A	7401	FMN	O5'-P-O1P	6.90	125.84	106.47
2	14-A	7401	FMN	O3P-P-O1P	-6.89	83.71	110.68
2	3-A	7401	FMN	O3P-P-O1P	-6.87	83.79	110.68
2	13-A	7401	FMN	C4'-C3'-C2'	-6.84	99.13	113.36
2	2-B	9401	FMN	O5'-C5'-C4'	-6.81	91.18	109.36
2	10-B	9401	FMN	P-O5'-C5'	-6.80	99.57	118.30
2	7-B	9401	FMN	C4'-C3'-C2'	-6.78	99.26	113.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3-A	7401	FMN	O5'-P-O1P	6.78	125.48	106.47
2	10-A	7401	FMN	O3P-P-O1P	-6.77	84.16	110.68
2	2-A	7401	FMN	O3P-P-O1P	-6.77	84.16	110.68
2	3-A	7401	FMN	O5'-C5'-C4'	-6.72	91.41	109.36
2	12-B	9401	FMN	O3P-P-O2P	-6.72	81.97	107.64
2	16-A	7401	FMN	C4'-C3'-C2'	-6.69	99.44	113.36
2	9-A	7401	FMN	O3P-P-O1P	-6.69	84.50	110.68
2	8-A	7401	FMN	O3P-P-O1P	-6.64	84.69	110.68
2	5-B	9401	FMN	P-O5'-C5'	-6.58	100.17	118.30
2	3-A	7401	FMN	C4'-C3'-C2'	-6.58	99.68	113.36
2	11-A	7401	FMN	P-O5'-C5'	-6.48	100.43	118.30
2	3-A	7401	FMN	O3P-P-O2P	-6.48	82.86	107.64
2	14-B	9401	FMN	O2P-P-O1P	-6.47	85.35	110.68
2	6-A	7401	FMN	O3P-P-O1P	-6.47	85.36	110.68
2	6-A	7401	FMN	O3P-P-O2P	-6.46	82.93	107.64
2	14-A	7401	FMN	O5'-P-O1P	6.41	124.47	106.47
2	10-A	7401	FMN	O3P-P-O2P	-6.41	83.12	107.64
2	8-A	7401	FMN	O3P-P-O2P	-6.40	83.17	107.64
2	1-A	7401	FMN	O3P-P-O1P	-6.39	85.66	110.68
2	5-A	7401	FMN	P-O5'-C5'	-6.36	100.77	118.30
2	8-A	7401	FMN	O5'-P-O1P	6.36	124.30	106.47
2	5-A	7401	FMN	O3P-P-O1P	-6.35	85.82	110.68
2	7-A	7401	FMN	C1'-N10-C9A	6.34	131.09	120.51
2	14-A	7401	FMN	O5'-C5'-C4'	-6.33	92.45	109.36
2	15-B	9401	FMN	C1'-N10-C9A	6.29	131.01	120.51
2	10-B	9401	FMN	O3P-P-O2P	-6.26	83.69	107.64
2	16-B	9401	FMN	O5'-P-O1P	-6.25	88.93	106.47
2	11-A	7401	FMN	O3P-P-O1P	-6.24	86.26	110.68
2	9-A	7401	FMN	O3P-P-O2P	-6.23	83.82	107.64
2	2-A	7401	FMN	O5'-P-O1P	6.23	123.95	106.47
2	16-A	7401	FMN	O3P-P-O5'	-6.21	90.20	106.73
2	12-A	7401	FMN	O3P-P-O2P	-6.21	83.90	107.64
2	13-A	7401	FMN	O3P-P-O2P	-6.17	84.03	107.64
2	1-A	7401	FMN	O5'-P-O1P	6.16	123.75	106.47
2	1-A	7401	FMN	O3P-P-O2P	-6.13	84.21	107.64
2	13-B	9401	FMN	C1'-N10-C9A	6.13	130.73	120.51
2	5-A	7401	FMN	O5'-P-O1P	6.13	123.66	106.47
2	9-A	7401	FMN	O5'-P-O1P	6.11	123.61	106.47
2	2-A	7401	FMN	O3P-P-O2P	-6.06	84.48	107.64
2	3-B	9401	FMN	O3P-P-O2P	-6.06	84.48	107.64
2	16-A	7401	FMN	O3P-P-O2P	-6.03	84.58	107.64
2	12-A	7401	FMN	O5'-P-O1P	6.02	123.37	106.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	9-B	9401	FMN	O3P-P-O2P	-6.01	84.67	107.64
2	13-A	7401	FMN	O3P-P-O5'	-5.94	90.92	106.73
2	1-A	7401	FMN	C4'-C3'-C2'	-5.92	101.04	113.36
2	15-B	9401	FMN	C4'-C3'-C2'	-5.92	101.05	113.36
2	4-A	7401	FMN	O3P-P-O1P	-5.90	87.59	110.68
2	11-A	7401	FMN	O5'-P-O1P	5.87	122.95	106.47
2	10-A	7401	FMN	O5'-P-O1P	5.87	122.93	106.47
2	14-A	7401	FMN	O3P-P-O2P	-5.87	85.22	107.64
2	13-B	9401	FMN	C4'-C3'-C2'	-5.86	101.17	113.36
2	8-B	9401	FMN	O3P-P-O2P	-5.86	85.24	107.64
2	4-A	7401	FMN	O5'-P-O1P	5.81	122.77	106.47
2	9-B	9401	FMN	C4'-C3'-C2'	-5.74	101.43	113.36
2	13-A	7401	FMN	C1'-N10-C9A	5.73	130.06	120.51
2	14-A	7401	FMN	C4'-C3'-C2'	-5.70	101.51	113.36
2	14-B	9401	FMN	O5'-P-O1P	-5.68	90.55	106.47
2	16-A	7401	FMN	C5'-C4'-C3'	5.64	123.10	112.20
2	7-B	9401	FMN	C1'-N10-C9A	5.61	129.87	120.51
2	6-A	7401	FMN	O2P-P-O5'	5.59	121.61	106.73
2	15-A	7401	FMN	O3P-P-O2P	-5.57	86.37	107.64
2	13-A	7401	FMN	C5'-C4'-C3'	5.56	122.94	112.20
2	4-A	7401	FMN	O3P-P-O2P	-5.55	86.43	107.64
2	1-B	9401	FMN	O3P-P-O2P	-5.53	86.49	107.64
2	11-B	9401	FMN	O3P-P-O2P	-5.53	86.50	107.64
2	16-A	7401	FMN	C1'-N10-C9A	5.44	129.58	120.51
2	16-B	9401	FMN	O5'-C5'-C4'	-5.37	95.04	109.36
2	11-A	7401	FMN	O3P-P-O2P	-5.30	87.36	107.64
2	2-B	9401	FMN	C5'-C4'-C3'	5.25	122.34	112.20
2	5-B	9401	FMN	O3P-P-O1P	5.23	131.16	110.68
2	16-B	9401	FMN	C5'-C4'-C3'	5.15	122.16	112.20
2	4-B	9401	FMN	O3P-P-O1P	5.14	130.79	110.68
2	15-B	9401	FMN	C1'-C2'-C3'	5.11	124.08	109.79
2	5-A	7401	FMN	O3P-P-O2P	-5.10	88.15	107.64
2	7-B	9401	FMN	O3P-P-O1P	5.08	130.59	110.68
2	4-A	7401	FMN	P-O5'-C5'	-5.07	104.33	118.30
2	6-A	7401	FMN	O5'-C5'-C4'	5.07	122.89	109.36
2	7-A	7401	FMN	O3P-P-O2P	-5.06	88.30	107.64
2	4-A	7401	FMN	C4'-C3'-C2'	-5.06	102.84	113.36
2	4-A	7401	FMN	O2P-P-O5'	5.05	120.16	106.73
2	11-B	9401	FMN	O3P-P-O1P	5.04	130.42	110.68
2	8-B	9401	FMN	O3P-P-O1P	5.00	130.27	110.68
2	16-B	9401	FMN	O3P-P-O1P	4.98	130.18	110.68
2	13-B	9401	FMN	C1'-C2'-C3'	4.97	123.67	109.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6-B	9401	FMN	O3P-P-O1P	4.96	130.12	110.68
2	5-A	7401	FMN	C4'-C3'-C2'	-4.96	103.04	113.36
2	12-B	9401	FMN	O3P-P-O1P	4.96	130.10	110.68
2	2-B	9401	FMN	O3P-P-O1P	4.92	129.93	110.68
2	11-A	7401	FMN	C4'-C3'-C2'	-4.92	103.14	113.36
2	11-A	7401	FMN	O2P-P-O5'	4.90	119.76	106.73
2	5-B	9401	FMN	C4'-C3'-C2'	-4.85	103.28	113.36
2	10-B	9401	FMN	C4'-C3'-C2'	-4.82	103.34	113.36
2	1-B	9401	FMN	O3P-P-O1P	4.73	129.22	110.68
2	14-B	9401	FMN	C4'-C3'-C2'	-4.64	103.70	113.36
2	5-A	7401	FMN	O2P-P-O5'	4.64	119.09	106.73
2	6-A	7401	FMN	O5'-P-O1P	4.61	119.42	106.47
2	9-A	7401	FMN	O2P-P-O5'	4.61	119.00	106.73
2	8-B	9401	FMN	C1'-N10-C9A	-4.60	112.85	120.51
2	6-A	7401	FMN	C5'-C4'-C3'	-4.58	103.35	112.20
2	8-A	7401	FMN	O2P-P-O5'	4.58	118.92	106.73
2	10-B	9401	FMN	O3P-P-O1P	4.54	128.44	110.68
2	6-B	9401	FMN	C5'-C4'-C3'	4.51	120.92	112.20
2	7-B	9401	FMN	C1'-C2'-C3'	4.42	122.15	109.79
2	1-A	7401	FMN	P-O5'-C5'	-4.39	106.19	118.30
2	9-B	9401	FMN	O5'-C5'-C4'	-4.36	97.73	109.36
2	3-B	9401	FMN	O3P-P-O1P	4.32	127.61	110.68
2	13-B	9401	FMN	O5'-C5'-C4'	-4.32	97.83	109.36
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	6-A	7401	FMN	C4'-C3'-C2'	-4.26	104.51	113.36
2	8-B	9401	FMN	C5'-C4'-C3'	-4.21	104.07	112.20
2	15-B	9401	FMN	O3P-P-O1P	4.17	127.01	110.68
2	15-A	7401	FMN	P-O5'-C5'	-4.17	106.82	118.30
2	16-A	7401	FMN	P-O5'-C5'	4.16	129.75	118.30
2	15-B	9401	FMN	O2'-C2'-C3'	-4.14	99.02	109.10
2	13-B	9401	FMN	O3P-P-O1P	4.07	126.63	110.68
2	13-A	7401	FMN	P-O5'-C5'	4.06	129.49	118.30
2	12-B	9401	FMN	P-O5'-C5'	-4.06	107.12	118.30
2	13-B	9401	FMN	O2'-C2'-C3'	-4.05	99.25	109.10
2	9-B	9401	FMN	P-O5'-C5'	-4.01	107.25	118.30
2	1-A	7401	FMN	O2P-P-O5'	3.98	117.31	106.73
2	14-B	9401	FMN	O3P-P-O1P	3.97	126.24	110.68
2	8-B	9401	FMN	P-O5'-C5'	-3.94	107.44	118.30
2	14-A	7401	FMN	C4-C4A-N5	3.92	123.81	118.23
2	3-B	9401	FMN	C1'-N10-C9A	3.92	127.04	120.51
2	4-B	9401	FMN	P-O5'-C5'	-3.83	107.74	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	9-B	9401	FMN	O3P-P-O1P	3.81	125.59	110.68
2	10-A	7401	FMN	O2P-P-O5'	3.79	116.82	106.73
2	15-B	9401	FMN	C4-C4A-N5	3.76	123.58	118.23
2	11-B	9401	FMN	C4'-C3'-C2'	-3.73	105.60	113.36
2	2-A	7401	FMN	O2P-P-O5'	3.72	116.62	106.73
2	6-A	7401	FMN	C1'-C2'-C3'	3.65	120.00	109.79
2	13-B	9401	FMN	C4-C4A-N5	3.65	123.42	118.23
2	3-B	9401	FMN	O5'-C5'-C4'	-3.64	99.65	109.36
2	12-A	7401	FMN	O2P-P-O5'	3.61	116.35	106.73
2	8-A	7401	FMN	C9A-N10-C10	-3.56	115.22	120.77
2	9-A	7401	FMN	C9A-N10-C10	-3.50	115.31	120.77
2	2-A	7401	FMN	P-O5'-C5'	-3.48	108.72	118.30
2	13-A	7401	FMN	C1'-C2'-C3'	3.47	119.48	109.79
2	16-A	7401	FMN	O4'-C4'-C5'	-3.45	102.16	109.92
2	13-A	7401	FMN	O4'-C4'-C5'	-3.44	102.19	109.92
2	5-A	7401	FMN	C1'-C2'-C3'	3.41	119.33	109.79
2	12-A	7401	FMN	C4-C4A-N5	3.37	123.03	118.23
2	14-B	9401	FMN	O5'-C5'-C4'	-3.37	100.37	109.36
2	12-B	9401	FMN	C4A-C10-N1	-3.35	116.96	124.73
2	14-B	9401	FMN	C5'-C4'-C3'	3.33	118.64	112.20
2	14-B	9401	FMN	C1'-C2'-C3'	3.33	119.09	109.79
2	15-B	9401	FMN	O2'-C2'-C1'	-3.33	101.75	109.80
2	5-B	9401	FMN	C1'-C2'-C3'	3.31	119.04	109.79
2	11-A	7401	FMN	C1'-C2'-C3'	3.31	119.03	109.79
2	7-A	7401	FMN	O2P-P-O5'	3.31	115.53	106.73
2	6-B	9401	FMN	C4-C4A-N5	3.30	122.93	118.23
2	2-A	7401	FMN	C4-C4A-N5	3.30	122.92	118.23
2	8-A	7401	FMN	C4A-C10-N1	-3.28	117.11	124.73
2	7-A	7401	FMN	C4-C4A-N5	3.28	122.89	118.23
2	10-A	7401	FMN	O5'-C5'-C4'	-3.28	100.62	109.36
2	5-B	9401	FMN	C1'-N10-C9A	3.26	125.95	120.51
2	15-A	7401	FMN	O5'-C5'-C4'	-3.26	100.66	109.36
2	9-A	7401	FMN	P-O5'-C5'	-3.26	109.32	118.30
2	10-A	7401	FMN	C4'-C3'-C2'	-3.24	106.63	113.36
2	13-A	7401	FMN	C9-C9A-N10	3.23	126.20	121.84
2	2-B	9401	FMN	C4-C4A-N5	3.22	122.81	118.23
2	16-A	7401	FMN	C1'-C2'-C3'	3.22	118.77	109.79
2	7-A	7401	FMN	C1'-C2'-C3'	3.20	118.74	109.79
2	10-A	7401	FMN	C4-C4A-N5	3.20	122.78	118.23
2	9-A	7401	FMN	C4A-C10-N1	-3.19	117.32	124.73
2	16-B	9401	FMN	C1'-N10-C9A	3.19	125.83	120.51
2	13-B	9401	FMN	O2'-C2'-C1'	-3.18	102.10	109.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3-B	9401	FMN	C4-C4A-N5	3.18	122.75	118.23
2	1-A	7401	FMN	O5'-C5'-C4'	-3.15	100.94	109.36
2	8-A	7401	FMN	C1'-C2'-C3'	3.14	118.57	109.79
2	13-A	7401	FMN	C5A-N5-C4A	3.12	123.26	118.07
2	15-B	9401	FMN	C10-N1-C2	3.11	123.11	116.90
2	13-B	9401	FMN	C10-N1-C2	3.10	123.11	116.90
2	2-B	9401	FMN	O4'-C4'-C3'	-3.09	101.59	109.10
2	9-B	9401	FMN	C4-C4A-N5	3.07	122.61	118.23
2	7-B	9401	FMN	C4-C4A-N5	3.05	122.58	118.23
2	8-B	9401	FMN	O3'-C3'-C2'	-3.05	101.44	108.81
2	10-A	7401	FMN	O2-C2-N1	-3.05	116.78	121.83
2	14-A	7401	FMN	O2-C2-N1	-3.05	116.78	121.83
2	16-A	7401	FMN	C9-C9A-N10	3.05	125.95	121.84
2	6-B	9401	FMN	O4'-C4'-C3'	-3.03	101.73	109.10
2	3-B	9401	FMN	P-O5'-C5'	-3.03	109.96	118.30
2	16-A	7401	FMN	C5A-N5-C4A	3.02	123.09	118.07
2	16-A	7401	FMN	C4-C4A-N5	3.01	122.51	118.23
2	8-B	9401	FMN	C5A-C9A-N10	3.01	121.06	117.95
2	14-B	9401	FMN	C4-C4A-N5	3.00	122.51	118.23
2	16-B	9401	FMN	C4-C4A-N5	2.99	122.49	118.23
2	15-A	7401	FMN	O4-C4-C4A	-2.97	118.72	126.60
2	14-A	7401	FMN	C9A-C5A-N5	-2.96	119.22	122.43
2	7-A	7401	FMN	O2-C2-N1	-2.96	116.93	121.83
2	9-A	7401	FMN	C1'-C2'-C3'	2.95	118.03	109.79
2	12-A	7401	FMN	P-O5'-C5'	-2.95	110.17	118.30
2	3-B	9401	FMN	C5'-C4'-C3'	2.95	117.91	112.20
2	12-B	9401	FMN	C9A-N10-C10	-2.95	116.18	120.77
2	13-A	7401	FMN	O2P-P-O1P	2.94	122.19	110.68
2	3-A	7401	FMN	C5'-C4'-C3'	2.92	117.84	112.20
2	8-A	7401	FMN	C5A-N5-C4A	2.91	122.90	118.07
2	5-A	7401	FMN	C1'-N10-C9A	2.90	125.35	120.51
2	15-A	7401	FMN	C9A-C5A-N5	-2.90	119.28	122.43
2	10-B	9401	FMN	C4-C4A-N5	2.88	122.34	118.23
2	9-A	7401	FMN	C5A-N5-C4A	2.87	122.85	118.07
2	6-A	7401	FMN	C5A-N5-C4A	2.86	122.83	118.07
2	13-A	7401	FMN	C4-C4A-N5	2.86	122.31	118.23
2	16-B	9401	FMN	C10-N1-C2	2.86	122.62	116.90
2	15-B	9401	FMN	C4A-C10-N10	2.86	120.66	116.48
2	7-A	7401	FMN	C10-N1-C2	2.84	122.58	116.90
2	14-B	9401	FMN	C4A-C10-N1	-2.83	118.16	124.73
2	5-A	7401	FMN	C5A-N5-C4A	2.83	122.77	118.07
2	16-A	7401	FMN	O2'-C2'-C1'	-2.81	103.00	109.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2-A	7401	FMN	C4A-C10-N1	-2.81	118.22	124.73
2	7-B	9401	FMN	O5'-C5'-C4'	-2.81	101.87	109.36
2	15-B	9401	FMN	C9A-N10-C10	-2.80	116.40	120.77
2	8-A	7401	FMN	P-O5'-C5'	-2.80	110.58	118.30
2	9-A	7401	FMN	C10-N1-C2	2.79	122.48	116.90
2	15-B	9401	FMN	O2-C2-N1	-2.78	117.22	121.83
2	11-B	9401	FMN	C5A-N5-C4A	2.78	122.69	118.07
2	3-A	7401	FMN	O2-C2-N1	-2.78	117.22	121.83
2	11-A	7401	FMN	C5A-N5-C4A	2.78	122.69	118.07
2	12-B	9401	FMN	C5A-N5-C4A	2.77	122.68	118.07
2	16-A	7401	FMN	O2P-P-O1P	2.77	121.51	110.68
2	14-A	7401	FMN	O2P-P-O5'	2.76	114.08	106.73
2	12-A	7401	FMN	C4A-C10-N1	-2.76	118.33	124.73
2	13-B	9401	FMN	C9A-N10-C10	-2.75	116.48	120.77
2	16-B	9401	FMN	O2-C2-N1	-2.75	117.28	121.83
2	14-B	9401	FMN	C5A-N5-C4A	2.75	122.64	118.07
2	16-B	9401	FMN	C1'-C2'-C3'	2.74	117.45	109.79
2	13-B	9401	FMN	C4A-C10-N10	2.74	120.48	116.48
2	14-B	9401	FMN	C10-N1-C2	2.74	122.37	116.90
2	1-B	9401	FMN	C4-C4A-N5	2.73	122.12	118.23
2	4-A	7401	FMN	C5A-N5-C4A	2.73	122.60	118.07
2	8-B	9401	FMN	C1'-C2'-C3'	-2.72	102.17	109.79
2	1-B	9401	FMN	C5A-N5-C4A	2.71	122.58	118.07
2	13-A	7401	FMN	O2'-C2'-C1'	-2.71	103.25	109.80
2	4-A	7401	FMN	C1'-C2'-C3'	2.71	117.35	109.79
2	6-A	7401	FMN	O4-C4-C4A	-2.70	119.44	126.60
2	8-B	9401	FMN	C4A-C10-N1	-2.70	118.48	124.73
2	8-A	7401	FMN	C10-N1-C2	2.69	122.29	116.90
2	1-A	7401	FMN	O2-C2-N1	-2.69	117.37	121.83
2	11-A	7401	FMN	O4-C4-C4A	-2.69	119.47	126.60
2	13-B	9401	FMN	O2-C2-N1	-2.69	117.38	121.83
2	7-B	9401	FMN	C9-C9A-N10	2.68	125.46	121.84
2	5-B	9401	FMN	C4-C4A-N5	2.68	122.05	118.23
2	15-B	9401	FMN	C9-C9A-N10	2.68	125.45	121.84
2	3-B	9401	FMN	O2-C2-N1	-2.68	117.39	121.83
2	7-A	7401	FMN	C9-C9A-N10	2.67	125.45	121.84
2	2-B	9401	FMN	C1'-N10-C9A	2.67	124.97	120.51
2	14-A	7401	FMN	O4'-C4'-C5'	-2.67	103.91	109.92
2	8-B	9401	FMN	C4'-C3'-C2'	2.67	118.92	113.36
2	7-B	9401	FMN	O2-C2-N1	-2.67	117.40	121.83
2	8-A	7401	FMN	O4-C4-C4A	-2.66	119.55	126.60
2	5-A	7401	FMN	O4-C4-C4A	-2.65	119.57	126.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1-A	7401	FMN	O4-C4-C4A	-2.65	119.58	126.60
2	9-A	7401	FMN	O4-C4-C4A	-2.65	119.58	126.60
2	1-A	7401	FMN	C5A-N5-C4A	2.64	122.46	118.07
2	12-A	7401	FMN	N3-C2-N1	2.62	124.52	119.38
2	15-A	7401	FMN	C5A-N5-C4A	2.62	122.42	118.07
2	2-B	9401	FMN	O2-C2-N1	-2.61	117.50	121.83
2	11-A	7401	FMN	C1'-N10-C9A	2.61	124.87	120.51
2	4-A	7401	FMN	O4-C4-C4A	-2.61	119.67	126.60
2	16-A	7401	FMN	O2-C2-N1	-2.61	117.50	121.83
2	6-B	9401	FMN	O2-C2-N1	-2.61	117.50	121.83
2	7-B	9401	FMN	C10-N1-C2	2.61	122.12	116.90
2	13-B	9401	FMN	C9-C9A-N10	2.61	125.36	121.84
2	3-A	7401	FMN	C5A-N5-C4A	2.61	122.41	118.07
2	3-A	7401	FMN	O4-C4-C4A	-2.61	119.68	126.60
2	3-B	9401	FMN	C1'-C2'-C3'	2.60	117.05	109.79
2	4-A	7401	FMN	O2-C2-N1	-2.60	117.52	121.83
2	1-A	7401	FMN	C1'-C2'-C3'	2.59	117.03	109.79
2	9-B	9401	FMN	C9A-C5A-N5	-2.59	119.62	122.43
2	12-B	9401	FMN	C10-N1-C2	2.58	122.06	116.90
2	8-B	9401	FMN	C9A-C5A-N5	-2.58	119.63	122.43
2	2-B	9401	FMN	O3'-C3'-C4'	2.58	115.04	108.81
2	10-A	7401	FMN	P-O5'-C5'	-2.56	111.24	118.30
2	9-A	7401	FMN	C4'-C3'-C2'	-2.56	108.03	113.36
2	16-A	7401	FMN	C10-N1-C2	2.56	122.02	116.90
2	5-B	9401	FMN	C5A-N5-C4A	2.55	122.32	118.07
2	7-A	7401	FMN	C5A-N5-C4A	2.55	122.32	118.07
2	11-B	9401	FMN	C4-C4A-N5	2.55	121.85	118.23
2	4-B	9401	FMN	C4A-C10-N1	-2.54	118.84	124.73
2	3-A	7401	FMN	O2P-P-O5'	2.54	113.48	106.73
2	11-A	7401	FMN	O2-C2-N1	-2.53	117.64	121.83
2	10-A	7401	FMN	C5'-C4'-C3'	2.52	117.07	112.20
2	2-A	7401	FMN	N3-C2-N1	2.51	124.32	119.38
2	13-A	7401	FMN	O2-C2-N1	-2.51	117.66	121.83
2	16-B	9401	FMN	C4A-C10-N1	-2.50	118.92	124.73
2	13-B	9401	FMN	C5A-N5-C4A	2.50	122.23	118.07
2	13-A	7401	FMN	C10-N1-C2	2.50	121.90	116.90
2	10-B	9401	FMN	C5A-N5-C4A	2.50	122.22	118.07
2	14-A	7401	FMN	O4-C4-C4A	-2.50	119.98	126.60
2	15-A	7401	FMN	O2-C2-N1	-2.49	117.70	121.83
2	16-B	9401	FMN	C4A-C10-N10	2.49	120.12	116.48
2	15-B	9401	FMN	C5A-N5-C4A	2.48	122.20	118.07
2	10-B	9401	FMN	C1'-C2'-C3'	2.47	116.69	109.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3-B	9401	FMN	C10-N1-C2	2.47	121.84	116.90
2	5-A	7401	FMN	O2-C2-N1	-2.46	117.75	121.83
2	14-A	7401	FMN	C10-N1-C2	2.46	121.83	116.90
2	4-B	9401	FMN	C5A-N5-C4A	2.46	122.16	118.07
2	15-A	7401	FMN	C1'-C2'-C3'	2.46	116.65	109.79
2	16-B	9401	FMN	C5A-N5-C4A	2.45	122.15	118.07
2	6-B	9401	FMN	O3'-C3'-C4'	2.44	114.71	108.81
2	15-A	7401	FMN	O2P-P-O5'	2.44	113.23	106.73
2	9-B	9401	FMN	O2-C2-N1	-2.44	117.79	121.83
2	7-A	7401	FMN	C5'-C4'-C3'	2.43	116.91	112.20
2	7-B	9401	FMN	O3'-C3'-C2'	2.43	114.68	108.81
2	7-B	9401	FMN	C5A-N5-C4A	2.42	122.10	118.07
2	11-B	9401	FMN	C4A-C10-N1	-2.42	119.11	124.73
2	9-A	7401	FMN	O2-C2-N1	-2.42	117.82	121.83
2	12-A	7401	FMN	O2-C2-N1	-2.41	117.83	121.83
2	1-B	9401	FMN	C4'-C3'-C2'	-2.40	108.36	113.36
2	2-B	9401	FMN	O4-C4-C4A	-2.40	120.22	126.60
2	12-A	7401	FMN	C4'-C3'-C2'	-2.40	108.38	113.36
2	9-B	9401	FMN	O4-C4-C4A	-2.40	120.24	126.60
2	10-A	7401	FMN	O4'-C4'-C5'	-2.39	104.54	109.92
2	12-A	7401	FMN	C10-N1-C2	2.39	121.68	116.90
2	6-B	9401	FMN	C5A-N5-C4A	2.39	122.05	118.07
2	15-B	9401	FMN	C9-C9A-C5A	-2.39	115.60	120.11
2	7-B	9401	FMN	C4A-C10-N10	2.38	119.96	116.48
2	6-B	9401	FMN	O4-C4-C4A	-2.38	120.29	126.60
2	2-B	9401	FMN	C5A-N5-C4A	2.38	122.03	118.07
2	7-A	7401	FMN	C4A-C10-N10	2.38	119.95	116.48
2	1-B	9401	FMN	O4-C4-C4A	-2.37	120.31	126.60
2	11-B	9401	FMN	O4-C4-C4A	-2.37	120.32	126.60
2	8-A	7401	FMN	C4'-C3'-C2'	-2.36	108.45	113.36
2	16-B	9401	FMN	C4-N3-C2	-2.36	121.28	125.64
2	10-B	9401	FMN	O4-C4-C4A	-2.36	120.34	126.60
2	2-A	7401	FMN	C1'-N10-C9A	2.36	124.44	120.51
2	10-A	7401	FMN	C10-N1-C2	2.35	121.61	116.90
2	7-A	7401	FMN	O3'-C3'-C4'	2.35	114.49	108.81
2	13-B	9401	FMN	C9-C9A-C5A	-2.35	115.67	120.11
2	15-A	7401	FMN	C5'-C4'-C3'	2.33	116.71	112.20
2	3-B	9401	FMN	C5A-N5-C4A	2.33	121.95	118.07
2	9-B	9401	FMN	C5A-N5-C4A	2.33	121.95	118.07
2	1-B	9401	FMN	C4A-C10-N1	-2.33	119.32	124.73
2	2-B	9401	FMN	C10-N1-C2	2.33	121.56	116.90
2	6-B	9401	FMN	C9A-C5A-N5	-2.33	119.90	122.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3-A	7401	FMN	C1'-N10-C9A	2.32	124.38	120.51
2	10-A	7401	FMN	C1'-N10-C9A	2.32	124.38	120.51
2	5-A	7401	FMN	C10-N1-C2	2.32	121.54	116.90
2	14-A	7401	FMN	O4'-C4'-C3'	-2.32	103.47	109.10
2	8-B	9401	FMN	C5A-N5-C4A	2.30	121.91	118.07
2	4-B	9401	FMN	C9A-C5A-N5	-2.30	119.93	122.43
2	10-B	9401	FMN	C9A-C5A-N5	-2.30	119.93	122.43
2	7-A	7401	FMN	O2'-C2'-C3'	-2.30	103.51	109.10
2	7-A	7401	FMN	O4-C4-C4A	-2.30	120.50	126.60
2	12-A	7401	FMN	C5A-C9A-N10	2.30	120.33	117.95
2	2-A	7401	FMN	C10-N1-C2	2.29	121.49	116.90
2	14-B	9401	FMN	C9A-N10-C10	-2.29	117.19	120.77
2	3-A	7401	FMN	C10-N1-C2	2.29	121.49	116.90
2	8-B	9401	FMN	N10-C10-N1	2.29	124.94	118.35
2	5-B	9401	FMN	O4-C4-C4A	-2.29	120.52	126.60
2	16-B	9401	FMN	O4'-C4'-C5'	-2.28	104.79	109.92
2	10-A	7401	FMN	C4A-C10-N1	-2.28	119.44	124.73
2	4-B	9401	FMN	C4-C4A-N5	2.28	121.47	118.23
2	4-A	7401	FMN	C10-N1-C2	2.28	121.45	116.90
2	2-B	9401	FMN	C9A-C5A-N5	-2.28	119.96	122.43
2	10-B	9401	FMN	C1'-N10-C9A	2.28	124.31	120.51
2	6-A	7401	FMN	O2-C2-N1	-2.27	118.06	121.83
2	15-B	9401	FMN	C9A-C9-C8	2.27	123.87	119.30
2	1-A	7401	FMN	C10-N1-C2	2.27	121.44	116.90
2	2-A	7401	FMN	C4A-C10-N10	2.27	119.80	116.48
2	14-A	7401	FMN	C5'-C4'-C3'	2.27	116.58	112.20
2	3-B	9401	FMN	O4-C4-C4A	-2.26	120.59	126.60
2	6-B	9401	FMN	C10-N1-C2	2.26	121.42	116.90
2	6-A	7401	FMN	C10-N1-C2	2.26	121.42	116.90
2	9-A	7401	FMN	O2'-C2'-C1'	-2.25	104.35	109.80
2	2-B	9401	FMN	O4'-C4'-C5'	-2.25	104.86	109.92
2	12-A	7401	FMN	O4'-C4'-C5'	-2.25	104.86	109.92
2	8-A	7401	FMN	O2'-C2'-C1'	-2.25	104.37	109.80
2	1-B	9401	FMN	O4'-C4'-C5'	-2.25	104.87	109.92
2	11-A	7401	FMN	C10-N1-C2	2.24	121.39	116.90
2	13-B	9401	FMN	C9A-C9-C8	2.24	123.82	119.30
2	4-B	9401	FMN	O4-C4-C4A	-2.23	120.68	126.60
2	14-A	7401	FMN	C5A-N5-C4A	2.23	121.78	118.07
2	5-B	9401	FMN	C4A-C10-N1	-2.23	119.56	124.73
2	12-B	9401	FMN	N10-C10-N1	2.22	124.75	118.35
2	12-B	9401	FMN	N3-C2-N1	2.22	123.74	119.38
2	14-B	9401	FMN	C1'-N10-C9A	2.22	124.22	120.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	10-A	7401	FMN	N3-C2-N1	2.22	123.74	119.38
2	7-B	9401	FMN	O4-C4-C4A	-2.22	120.71	126.60
2	16-B	9401	FMN	C9A-N10-C10	-2.21	117.31	120.77
2	4-A	7401	FMN	C4A-C10-N1	-2.21	119.59	124.73
2	14-A	7401	FMN	P-O5'-C5'	-2.21	112.20	118.30
2	6-A	7401	FMN	C4A-C10-N1	-2.20	119.62	124.73
2	4-B	9401	FMN	O3'-C3'-C2'	-2.20	103.50	108.81
2	14-B	9401	FMN	C4-N3-C2	-2.20	121.58	125.64
2	16-B	9401	FMN	N3-C2-N1	2.20	123.69	119.38
2	14-B	9401	FMN	N3-C2-N1	2.19	123.69	119.38
2	7-B	9401	FMN	O2'-C2'-C1'	-2.19	104.50	109.80
2	5-A	7401	FMN	C4A-C10-N1	-2.19	119.65	124.73
2	9-A	7401	FMN	C4-N3-C2	-2.19	121.60	125.64
2	12-A	7401	FMN	C9A-N10-C10	-2.19	117.36	120.77
2	13-A	7401	FMN	N3-C2-N1	2.18	123.66	119.38
2	8-A	7401	FMN	O2-C2-N1	-2.18	118.22	121.83
2	10-A	7401	FMN	C4-N3-C2	-2.18	121.62	125.64
2	8-B	9401	FMN	C4-C4A-N5	2.17	121.32	118.23
2	13-A	7401	FMN	C4A-C10-N10	2.17	119.65	116.48
2	11-A	7401	FMN	C4A-C10-N1	-2.17	119.70	124.73
2	5-A	7401	FMN	C9A-N10-C10	-2.17	117.39	120.77
2	6-A	7401	FMN	C9A-C5A-N5	-2.17	120.08	122.43
2	13-A	7401	FMN	C4A-C10-N1	-2.17	119.70	124.73
2	4-A	7401	FMN	C9A-N10-C10	-2.17	117.39	120.77
2	5-B	9401	FMN	C10-N1-C2	2.17	121.23	116.90
2	7-A	7401	FMN	O3'-C3'-C2'	2.16	114.03	108.81
2	10-A	7401	FMN	C4A-C10-N10	2.16	119.63	116.48
2	7-A	7401	FMN	C9A-C5A-N5	-2.16	120.09	122.43
2	7-B	9401	FMN	C4A-C10-N1	-2.16	119.73	124.73
2	3-A	7401	FMN	O4'-C4'-C5'	-2.15	105.08	109.92
2	8-A	7401	FMN	C9-C9A-C5A	-2.15	116.05	120.11
2	9-A	7401	FMN	C9-C9A-C5A	-2.15	116.05	120.11
2	10-B	9401	FMN	C10-N1-C2	2.15	121.20	116.90
2	12-A	7401	FMN	C4A-C10-N10	2.14	119.62	116.48
2	14-A	7401	FMN	C10-C4A-N5	-2.14	120.31	124.86
2	14-A	7401	FMN	O3'-C3'-C2'	-2.13	103.65	108.81
2	15-A	7401	FMN	O4-C4-N3	2.12	124.19	120.12
2	15-B	9401	FMN	O3'-C3'-C2'	2.12	113.93	108.81
2	4-A	7401	FMN	C1'-N10-C9A	2.12	124.05	120.51
2	7-B	9401	FMN	C9A-N10-C10	-2.12	117.47	120.77
2	10-B	9401	FMN	O2-C2-N1	-2.12	118.32	121.83
2	1-A	7401	FMN	C9A-C5A-N5	-2.12	120.13	122.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	16-A	7401	FMN	C4A-C10-N10	2.12	119.58	116.48
2	16-B	9401	FMN	C9-C9A-N10	2.12	124.70	121.84
2	8-A	7401	FMN	C4-N3-C2	-2.10	121.75	125.64
2	8-A	7401	FMN	N10-C10-N1	2.10	124.40	118.35
2	13-A	7401	FMN	C4-N3-C2	-2.10	121.76	125.64
2	8-B	9401	FMN	N3-C2-N1	2.10	123.50	119.38
2	3-B	9401	FMN	C4A-C10-N10	2.10	119.55	116.48
2	5-A	7401	FMN	C9A-C5A-N5	-2.09	120.16	122.43
2	10-A	7401	FMN	C5A-N5-C4A	2.09	121.55	118.07
2	1-A	7401	FMN	C4A-C10-N1	-2.09	119.88	124.73
2	2-A	7401	FMN	C9A-N10-C10	-2.09	117.51	120.77
2	8-B	9401	FMN	O4-C4-C4A	-2.09	121.06	126.60
2	3-A	7401	FMN	C9A-C5A-N5	-2.09	120.16	122.43
2	13-B	9401	FMN	C4A-C10-N1	-2.08	119.90	124.73
2	13-A	7401	FMN	C9-C9A-C5A	-2.08	116.18	120.11
2	15-B	9401	FMN	C4A-C10-N1	-2.08	119.91	124.73
2	14-A	7401	FMN	C6-C5A-N5	2.07	122.14	118.51
2	12-B	9401	FMN	O4-C4-C4A	-2.07	121.10	126.60
2	7-A	7401	FMN	C9A-C9-C8	2.07	123.47	119.30
2	2-A	7401	FMN	O2-C2-N1	-2.07	118.40	121.83
2	3-B	9401	FMN	C9-C9A-N10	2.07	124.63	121.84
2	9-B	9401	FMN	C10-N1-C2	2.06	121.03	116.90
2	11-A	7401	FMN	C9A-N10-C10	-2.06	117.55	120.77
2	5-B	9401	FMN	C9A-C5A-N5	-2.06	120.19	122.43
2	16-A	7401	FMN	C4-N3-C2	-2.06	121.83	125.64
2	7-B	9401	FMN	C9-C9A-C5A	-2.06	116.22	120.11
2	10-A	7401	FMN	C10-C4A-N5	-2.06	120.49	124.86
2	16-A	7401	FMN	C4A-C10-N1	-2.06	119.95	124.73
2	11-A	7401	FMN	C9A-C5A-N5	-2.06	120.19	122.43
2	2-A	7401	FMN	C5A-C9A-N10	2.06	120.08	117.95
2	14-A	7401	FMN	C4-N3-C2	-2.05	121.86	125.64
2	5-B	9401	FMN	O2-C2-N1	-2.05	118.44	121.83
2	6-B	9401	FMN	O2'-C2'-C3'	2.05	114.07	109.10
2	13-B	9401	FMN	O3'-C3'-C2'	2.04	113.75	108.81
2	1-B	9401	FMN	N3-C2-N1	2.04	123.39	119.38
2	10-B	9401	FMN	C4A-C10-N1	-2.03	120.01	124.73
2	12-A	7401	FMN	C1'-C2'-C3'	2.03	115.47	109.79
2	3-A	7401	FMN	C4A-C10-N1	-2.03	120.02	124.73
2	13-A	7401	FMN	C9A-N10-C10	-2.03	117.60	120.77
2	15-A	7401	FMN	C10-N1-C2	2.03	120.96	116.90
2	16-A	7401	FMN	N3-C2-N1	2.03	123.36	119.38
2	4-A	7401	FMN	C9A-C5A-N5	-2.03	120.23	122.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3-B	9401	FMN	C4A-C10-N1	-2.02	120.03	124.73
2	5-B	9401	FMN	C9-C9A-N10	2.02	124.57	121.84
2	10-A	7401	FMN	C9A-C5A-N5	-2.01	120.25	122.43
2	7-B	9401	FMN	O4'-C4'-C3'	2.01	113.98	109.10
2	4-B	9401	FMN	C10-N1-C2	2.01	120.92	116.90
2	7-A	7401	FMN	C9-C9A-C5A	-2.01	116.32	120.11
2	1-B	9401	FMN	C9A-C5A-N5	-2.00	120.26	122.43
2	13-B	9401	FMN	C4-N3-C2	-2.00	121.95	125.64

There are no chirality outliers.

All (105) 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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
2	12-A	7401	FMN	C2'-C1'-N10-C10
2	15-A	7401	FMN	C2'-C1'-N10-C10
2	6-B	9401	FMN	C2'-C1'-N10-C10

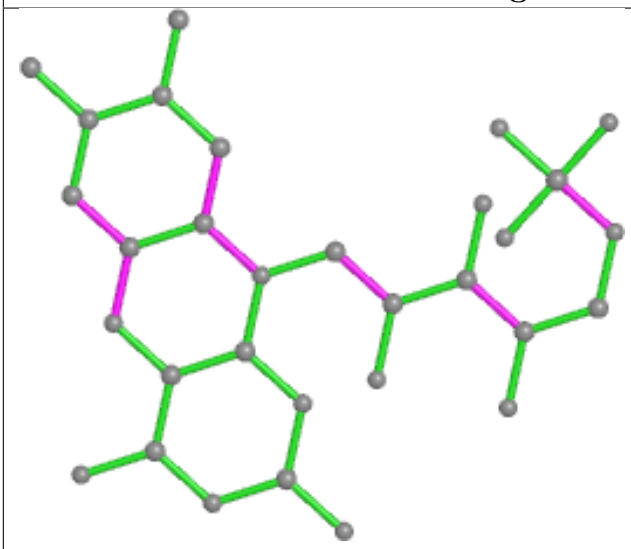
There are no ring outliers.

No monomer is involved in short contacts.

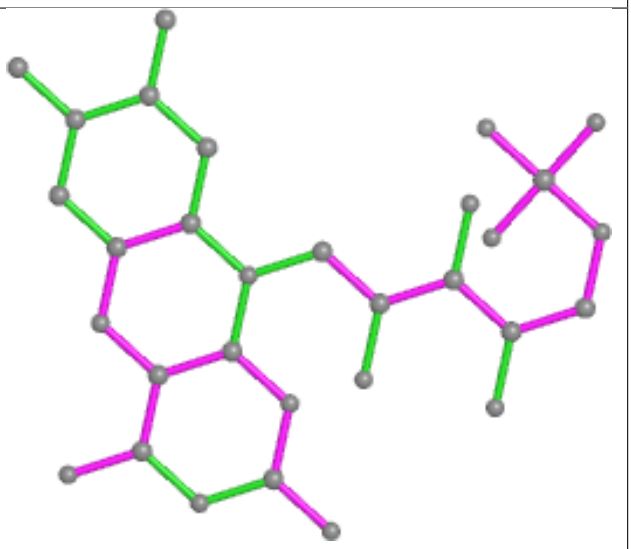
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

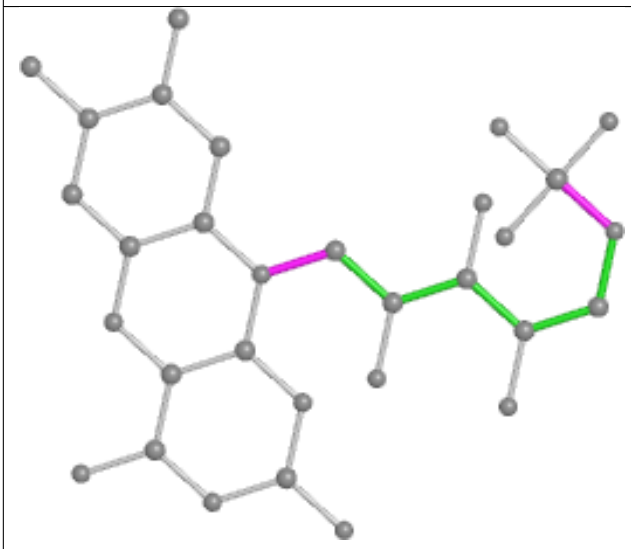
Ligand FMN A 7401



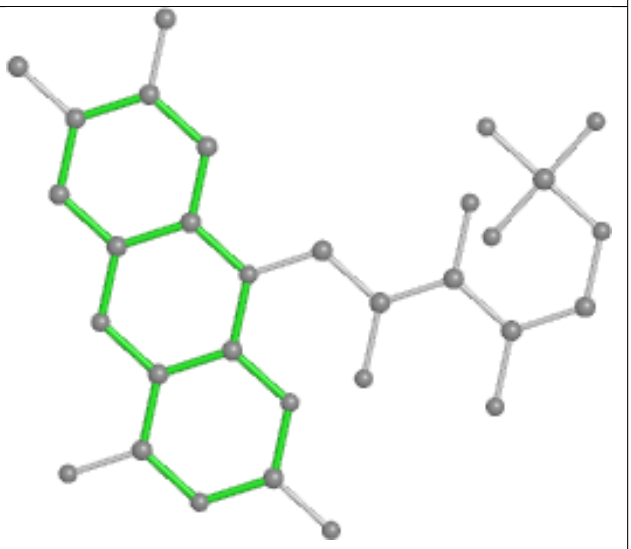
Bond lengths



Bond angles

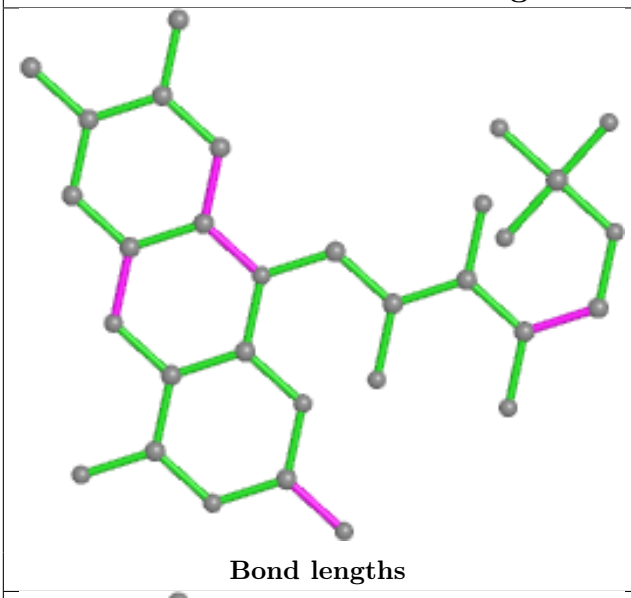


Torsions

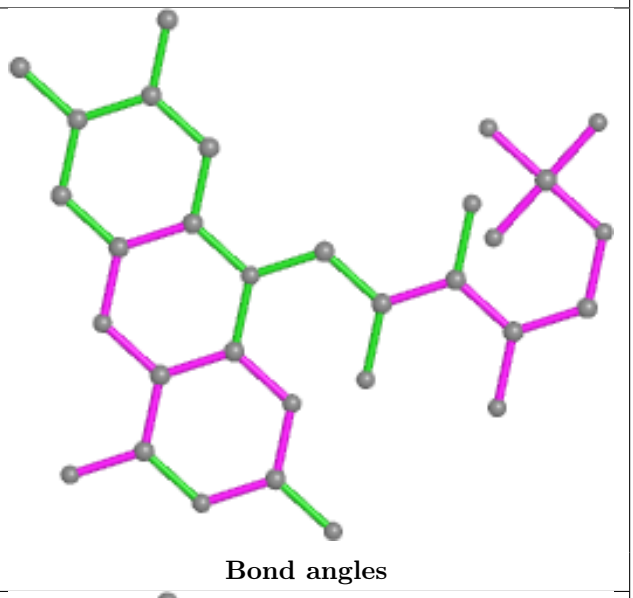


Rings

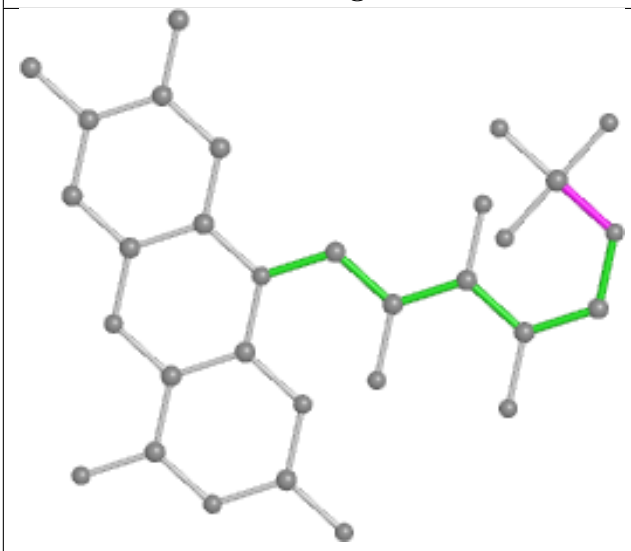
Ligand FMN B 9401



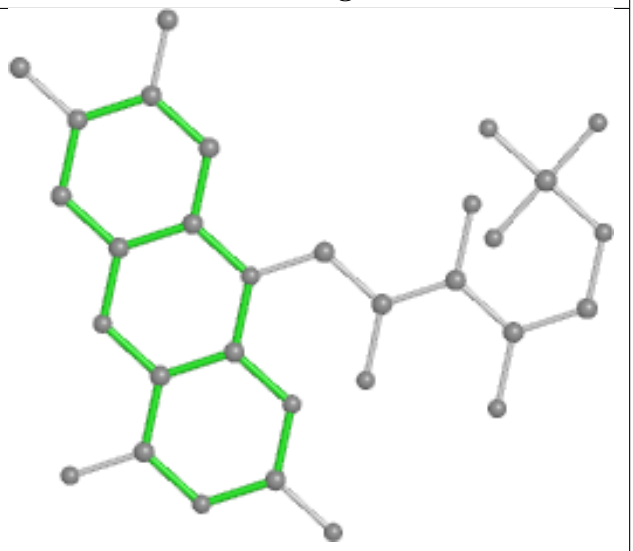
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	1-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	2-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	2-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	3-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	3-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	4-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	4-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	5-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	5-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	6-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	6-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	7-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	7-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	8-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	8-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	9-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	9-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	10-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	10-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	11-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	11-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)
1	12-A	365/391 (93%)	0.88	45 (12%)	4	3	9, 20, 35, 53	365 (100%)
1	12-B	367/391 (93%)	0.60	32 (8%)	10	9	7, 18, 30, 51	367 (100%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	13-A	365/391 (93%)	0.88	45 (12%) 4 3	9, 20, 35, 53	365 (100%)
1	13-B	367/391 (93%)	0.60	32 (8%) 10 9	7, 18, 30, 51	367 (100%)
1	14-A	365/391 (93%)	0.88	45 (12%) 4 3	9, 20, 35, 53	365 (100%)
1	14-B	367/391 (93%)	0.60	32 (8%) 10 9	7, 18, 30, 51	367 (100%)
1	15-A	365/391 (93%)	0.88	45 (12%) 4 3	9, 20, 35, 53	365 (100%)
1	15-B	367/391 (93%)	0.60	32 (8%) 10 9	7, 18, 30, 51	367 (100%)
1	16-A	365/391 (93%)	0.88	45 (12%) 4 3	9, 20, 35, 53	365 (100%)
1	16-B	367/391 (93%)	0.60	32 (8%) 10 9	7, 18, 30, 51	367 (100%)
All	All	11712/12512 (93%)	0.74	1232 (10%) 7 5	7, 18, 33, 53	11712 (100%)

All (1232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	272	GLY	13.1
1	2-A	272	GLY	13.1
1	3-A	272	GLY	13.1
1	4-A	272	GLY	13.1
1	5-A	272	GLY	13.1
1	6-A	272	GLY	13.1
1	7-A	272	GLY	13.1
1	8-A	272	GLY	13.1
1	9-A	272	GLY	13.1
1	10-A	272	GLY	13.1
1	11-A	272	GLY	13.1
1	12-A	272	GLY	13.1
1	13-A	272	GLY	13.1
1	14-A	272	GLY	13.1
1	15-A	272	GLY	13.1
1	16-A	272	GLY	13.1
1	1-A	271	ASN	10.3
1	2-A	271	ASN	10.3
1	3-A	271	ASN	10.3
1	4-A	271	ASN	10.3
1	5-A	271	ASN	10.3
1	6-A	271	ASN	10.3
1	7-A	271	ASN	10.3
1	8-A	271	ASN	10.3
1	9-A	271	ASN	10.3
1	10-A	271	ASN	10.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	11-A	271	ASN	10.3
1	12-A	271	ASN	10.3
1	13-A	271	ASN	10.3
1	14-A	271	ASN	10.3
1	15-A	271	ASN	10.3
1	16-A	271	ASN	10.3
1	1-B	269	GLY	9.2
1	2-B	269	GLY	9.2
1	3-B	269	GLY	9.2
1	4-B	269	GLY	9.2
1	5-B	269	GLY	9.2
1	6-B	269	GLY	9.2
1	7-B	269	GLY	9.2
1	8-B	269	GLY	9.2
1	9-B	269	GLY	9.2
1	10-B	269	GLY	9.2
1	11-B	269	GLY	9.2
1	12-B	269	GLY	9.2
1	13-B	269	GLY	9.2
1	14-B	269	GLY	9.2
1	15-B	269	GLY	9.2
1	16-B	269	GLY	9.2
1	1-A	273	SER	8.9
1	2-A	273	SER	8.9
1	3-A	273	SER	8.9
1	4-A	273	SER	8.9
1	5-A	273	SER	8.9
1	6-A	273	SER	8.9
1	7-A	273	SER	8.9
1	8-A	273	SER	8.9
1	9-A	273	SER	8.9
1	10-A	273	SER	8.9
1	11-A	273	SER	8.9
1	12-A	273	SER	8.9
1	13-A	273	SER	8.9
1	14-A	273	SER	8.9
1	15-A	273	SER	8.9
1	16-A	273	SER	8.9
1	1-B	270	VAL	8.1
1	2-B	270	VAL	8.1
1	3-B	270	VAL	8.1
1	4-B	270	VAL	8.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	5-B	270	VAL	8.1
1	6-B	270	VAL	8.1
1	7-B	270	VAL	8.1
1	8-B	270	VAL	8.1
1	9-B	270	VAL	8.1
1	10-B	270	VAL	8.1
1	11-B	270	VAL	8.1
1	12-B	270	VAL	8.1
1	13-B	270	VAL	8.1
1	14-B	270	VAL	8.1
1	15-B	270	VAL	8.1
1	16-B	270	VAL	8.1
1	1-B	287	ALA	6.0
1	2-B	287	ALA	6.0
1	3-B	287	ALA	6.0
1	4-B	287	ALA	6.0
1	5-B	287	ALA	6.0
1	6-B	287	ALA	6.0
1	7-B	287	ALA	6.0
1	8-B	287	ALA	6.0
1	9-B	287	ALA	6.0
1	10-B	287	ALA	6.0
1	11-B	287	ALA	6.0
1	12-B	287	ALA	6.0
1	13-B	287	ALA	6.0
1	14-B	287	ALA	6.0
1	15-B	287	ALA	6.0
1	16-B	287	ALA	6.0
1	1-A	20	ARG	4.9
1	2-A	20	ARG	4.9
1	3-A	20	ARG	4.9
1	4-A	20	ARG	4.9
1	5-A	20	ARG	4.9
1	6-A	20	ARG	4.9
1	7-A	20	ARG	4.9
1	8-A	20	ARG	4.9
1	9-A	20	ARG	4.9
1	10-A	20	ARG	4.9
1	11-A	20	ARG	4.9
1	12-A	20	ARG	4.9
1	13-A	20	ARG	4.9
1	14-A	20	ARG	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	15-A	20	ARG	4.9
1	16-A	20	ARG	4.9
1	1-A	137	ARG	4.9
1	2-A	137	ARG	4.9
1	3-A	137	ARG	4.9
1	4-A	137	ARG	4.9
1	5-A	137	ARG	4.9
1	6-A	137	ARG	4.9
1	7-A	137	ARG	4.9
1	8-A	137	ARG	4.9
1	9-A	137	ARG	4.9
1	10-A	137	ARG	4.9
1	11-A	137	ARG	4.9
1	12-A	137	ARG	4.9
1	13-A	137	ARG	4.9
1	14-A	137	ARG	4.9
1	15-A	137	ARG	4.9
1	16-A	137	ARG	4.9
1	1-B	285	TYR	4.8
1	2-B	285	TYR	4.8
1	3-B	285	TYR	4.8
1	4-B	285	TYR	4.8
1	5-B	285	TYR	4.8
1	6-B	285	TYR	4.8
1	7-B	285	TYR	4.8
1	8-B	285	TYR	4.8
1	9-B	285	TYR	4.8
1	10-B	285	TYR	4.8
1	11-B	285	TYR	4.8
1	12-B	285	TYR	4.8
1	13-B	285	TYR	4.8
1	14-B	285	TYR	4.8
1	15-B	285	TYR	4.8
1	16-B	285	TYR	4.8
1	1-A	300	GLU	4.8
1	2-A	300	GLU	4.8
1	3-A	300	GLU	4.8
1	4-A	300	GLU	4.8
1	5-A	300	GLU	4.8
1	6-A	300	GLU	4.8
1	7-A	300	GLU	4.8
1	8-A	300	GLU	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	9-A	300	GLU	4.8
1	10-A	300	GLU	4.8
1	11-A	300	GLU	4.8
1	12-A	300	GLU	4.8
1	13-A	300	GLU	4.8
1	14-A	300	GLU	4.8
1	15-A	300	GLU	4.8
1	16-A	300	GLU	4.8
1	1-A	377	VAL	4.7
1	2-A	377	VAL	4.7
1	3-A	377	VAL	4.7
1	4-A	377	VAL	4.7
1	5-A	377	VAL	4.7
1	6-A	377	VAL	4.7
1	7-A	377	VAL	4.7
1	8-A	377	VAL	4.7
1	9-A	377	VAL	4.7
1	10-A	377	VAL	4.7
1	11-A	377	VAL	4.7
1	12-A	377	VAL	4.7
1	13-A	377	VAL	4.7
1	14-A	377	VAL	4.7
1	15-A	377	VAL	4.7
1	16-A	377	VAL	4.7
1	1-A	269	GLY	4.7
1	2-A	269	GLY	4.7
1	3-A	269	GLY	4.7
1	4-A	269	GLY	4.7
1	5-A	269	GLY	4.7
1	6-A	269	GLY	4.7
1	7-A	269	GLY	4.7
1	8-A	269	GLY	4.7
1	9-A	269	GLY	4.7
1	10-A	269	GLY	4.7
1	11-A	269	GLY	4.7
1	12-A	269	GLY	4.7
1	13-A	269	GLY	4.7
1	14-A	269	GLY	4.7
1	15-A	269	GLY	4.7
1	16-A	269	GLY	4.7
1	1-B	9	ASN	4.7
1	2-B	9	ASN	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	3-B	9	ASN	4.7
1	4-B	9	ASN	4.7
1	5-B	9	ASN	4.7
1	6-B	9	ASN	4.7
1	7-B	9	ASN	4.7
1	8-B	9	ASN	4.7
1	9-B	9	ASN	4.7
1	10-B	9	ASN	4.7
1	11-B	9	ASN	4.7
1	12-B	9	ASN	4.7
1	13-B	9	ASN	4.7
1	14-B	9	ASN	4.7
1	15-B	9	ASN	4.7
1	16-B	9	ASN	4.7
1	1-A	8	SER	4.6
1	2-A	8	SER	4.6
1	3-A	8	SER	4.6
1	4-A	8	SER	4.6
1	5-A	8	SER	4.6
1	6-A	8	SER	4.6
1	7-A	8	SER	4.6
1	8-A	8	SER	4.6
1	9-A	8	SER	4.6
1	10-A	8	SER	4.6
1	11-A	8	SER	4.6
1	12-A	8	SER	4.6
1	13-A	8	SER	4.6
1	14-A	8	SER	4.6
1	15-A	8	SER	4.6
1	16-A	8	SER	4.6
1	1-B	272	GLY	4.6
1	2-B	272	GLY	4.6
1	3-B	272	GLY	4.6
1	4-B	272	GLY	4.6
1	5-B	272	GLY	4.6
1	6-B	272	GLY	4.6
1	7-B	272	GLY	4.6
1	8-B	272	GLY	4.6
1	9-B	272	GLY	4.6
1	10-B	272	GLY	4.6
1	11-B	272	GLY	4.6
1	12-B	272	GLY	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	13-B	272	GLY	4.6
1	14-B	272	GLY	4.6
1	15-B	272	GLY	4.6
1	16-B	272	GLY	4.6
1	1-A	378	GLY	4.3
1	2-A	378	GLY	4.3
1	3-A	378	GLY	4.3
1	4-A	378	GLY	4.3
1	5-A	378	GLY	4.3
1	6-A	378	GLY	4.3
1	7-A	378	GLY	4.3
1	8-A	378	GLY	4.3
1	9-A	378	GLY	4.3
1	10-A	378	GLY	4.3
1	11-A	378	GLY	4.3
1	12-A	378	GLY	4.3
1	13-A	378	GLY	4.3
1	14-A	378	GLY	4.3
1	15-A	378	GLY	4.3
1	16-A	378	GLY	4.3
1	1-B	210	GLY	4.1
1	2-B	210	GLY	4.1
1	3-B	210	GLY	4.1
1	4-B	210	GLY	4.1
1	5-B	210	GLY	4.1
1	6-B	210	GLY	4.1
1	7-B	210	GLY	4.1
1	8-B	210	GLY	4.1
1	9-B	210	GLY	4.1
1	10-B	210	GLY	4.1
1	11-B	210	GLY	4.1
1	12-B	210	GLY	4.1
1	13-B	210	GLY	4.1
1	14-B	210	GLY	4.1
1	15-B	210	GLY	4.1
1	16-B	210	GLY	4.1
1	1-B	205	THR	4.0
1	2-B	205	THR	4.0
1	3-B	205	THR	4.0
1	4-B	205	THR	4.0
1	5-B	205	THR	4.0
1	6-B	205	THR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	7-B	205	THR	4.0
1	8-B	205	THR	4.0
1	9-B	205	THR	4.0
1	10-B	205	THR	4.0
1	11-B	205	THR	4.0
1	12-B	205	THR	4.0
1	13-B	205	THR	4.0
1	14-B	205	THR	4.0
1	15-B	205	THR	4.0
1	16-B	205	THR	4.0
1	1-B	136	ASN	4.0
1	2-B	136	ASN	4.0
1	3-B	136	ASN	4.0
1	4-B	136	ASN	4.0
1	5-B	136	ASN	4.0
1	6-B	136	ASN	4.0
1	7-B	136	ASN	4.0
1	8-B	136	ASN	4.0
1	9-B	136	ASN	4.0
1	10-B	136	ASN	4.0
1	11-B	136	ASN	4.0
1	12-B	136	ASN	4.0
1	13-B	136	ASN	4.0
1	14-B	136	ASN	4.0
1	15-B	136	ASN	4.0
1	16-B	136	ASN	4.0
1	1-B	273	SER	3.9
1	2-B	273	SER	3.9
1	3-B	273	SER	3.9
1	4-B	273	SER	3.9
1	5-B	273	SER	3.9
1	6-B	273	SER	3.9
1	7-B	273	SER	3.9
1	8-B	273	SER	3.9
1	9-B	273	SER	3.9
1	10-B	273	SER	3.9
1	11-B	273	SER	3.9
1	12-B	273	SER	3.9
1	13-B	273	SER	3.9
1	14-B	273	SER	3.9
1	15-B	273	SER	3.9
1	16-B	273	SER	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-B	271	ASN	3.9
1	2-B	271	ASN	3.9
1	3-B	271	ASN	3.9
1	4-B	271	ASN	3.9
1	5-B	271	ASN	3.9
1	6-B	271	ASN	3.9
1	7-B	271	ASN	3.9
1	8-B	271	ASN	3.9
1	9-B	271	ASN	3.9
1	10-B	271	ASN	3.9
1	11-B	271	ASN	3.9
1	12-B	271	ASN	3.9
1	13-B	271	ASN	3.9
1	14-B	271	ASN	3.9
1	15-B	271	ASN	3.9
1	16-B	271	ASN	3.9
1	1-A	205	THR	3.7
1	2-A	205	THR	3.7
1	3-A	205	THR	3.7
1	4-A	205	THR	3.7
1	5-A	205	THR	3.7
1	6-A	205	THR	3.7
1	7-A	205	THR	3.7
1	8-A	205	THR	3.7
1	9-A	205	THR	3.7
1	10-A	205	THR	3.7
1	11-A	205	THR	3.7
1	12-A	205	THR	3.7
1	13-A	205	THR	3.7
1	14-A	205	THR	3.7
1	15-A	205	THR	3.7
1	16-A	205	THR	3.7
1	1-A	270	VAL	3.7
1	2-A	270	VAL	3.7
1	3-A	270	VAL	3.7
1	4-A	270	VAL	3.7
1	5-A	270	VAL	3.7
1	6-A	270	VAL	3.7
1	7-A	270	VAL	3.7
1	8-A	270	VAL	3.7
1	9-A	270	VAL	3.7
1	10-A	270	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	11-A	270	VAL	3.7
1	12-A	270	VAL	3.7
1	13-A	270	VAL	3.7
1	14-A	270	VAL	3.7
1	15-A	270	VAL	3.7
1	16-A	270	VAL	3.7
1	1-B	286	HIS	3.7
1	2-B	286	HIS	3.7
1	3-B	286	HIS	3.7
1	4-B	286	HIS	3.7
1	5-B	286	HIS	3.7
1	6-B	286	HIS	3.7
1	7-B	286	HIS	3.7
1	8-B	286	HIS	3.7
1	9-B	286	HIS	3.7
1	10-B	286	HIS	3.7
1	11-B	286	HIS	3.7
1	12-B	286	HIS	3.7
1	13-B	286	HIS	3.7
1	14-B	286	HIS	3.7
1	15-B	286	HIS	3.7
1	16-B	286	HIS	3.7
1	1-A	243	ILE	3.5
1	2-A	243	ILE	3.5
1	3-A	243	ILE	3.5
1	4-A	243	ILE	3.5
1	5-A	243	ILE	3.5
1	6-A	243	ILE	3.5
1	7-A	243	ILE	3.5
1	8-A	243	ILE	3.5
1	9-A	243	ILE	3.5
1	10-A	243	ILE	3.5
1	11-A	243	ILE	3.5
1	12-A	243	ILE	3.5
1	13-A	243	ILE	3.5
1	14-A	243	ILE	3.5
1	15-A	243	ILE	3.5
1	16-A	243	ILE	3.5
1	1-A	302	GLU	3.5
1	2-A	302	GLU	3.5
1	3-A	302	GLU	3.5
1	4-A	302	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	5-A	302	GLU	3.5
1	6-A	302	GLU	3.5
1	7-A	302	GLU	3.5
1	8-A	302	GLU	3.5
1	9-A	302	GLU	3.5
1	10-A	302	GLU	3.5
1	11-A	302	GLU	3.5
1	12-A	302	GLU	3.5
1	13-A	302	GLU	3.5
1	14-A	302	GLU	3.5
1	15-A	302	GLU	3.5
1	16-A	302	GLU	3.5
1	1-A	301	GLU	3.5
1	2-A	301	GLU	3.5
1	3-A	301	GLU	3.5
1	4-A	301	GLU	3.5
1	5-A	301	GLU	3.5
1	6-A	301	GLU	3.5
1	7-A	301	GLU	3.5
1	8-A	301	GLU	3.5
1	9-A	301	GLU	3.5
1	10-A	301	GLU	3.5
1	11-A	301	GLU	3.5
1	12-A	301	GLU	3.5
1	13-A	301	GLU	3.5
1	14-A	301	GLU	3.5
1	15-A	301	GLU	3.5
1	16-A	301	GLU	3.5
1	1-A	228	SER	3.5
1	2-A	228	SER	3.5
1	3-A	228	SER	3.5
1	4-A	228	SER	3.5
1	5-A	228	SER	3.5
1	6-A	228	SER	3.5
1	7-A	228	SER	3.5
1	8-A	228	SER	3.5
1	9-A	228	SER	3.5
1	10-A	228	SER	3.5
1	11-A	228	SER	3.5
1	12-A	228	SER	3.5
1	13-A	228	SER	3.5
1	14-A	228	SER	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	15-A	228	SER	3.5
1	16-A	228	SER	3.5
1	1-B	376	VAL	3.5
1	2-B	376	VAL	3.5
1	3-B	376	VAL	3.5
1	4-B	376	VAL	3.5
1	5-B	376	VAL	3.5
1	6-B	376	VAL	3.5
1	7-B	376	VAL	3.5
1	8-B	376	VAL	3.5
1	9-B	376	VAL	3.5
1	10-B	376	VAL	3.5
1	11-B	376	VAL	3.5
1	12-B	376	VAL	3.5
1	13-B	376	VAL	3.5
1	14-B	376	VAL	3.5
1	15-B	376	VAL	3.5
1	16-B	376	VAL	3.5
1	1-B	333	GLN	3.4
1	2-B	333	GLN	3.4
1	3-B	333	GLN	3.4
1	4-B	333	GLN	3.4
1	5-B	333	GLN	3.4
1	6-B	333	GLN	3.4
1	7-B	333	GLN	3.4
1	8-B	333	GLN	3.4
1	9-B	333	GLN	3.4
1	10-B	333	GLN	3.4
1	11-B	333	GLN	3.4
1	12-B	333	GLN	3.4
1	13-B	333	GLN	3.4
1	14-B	333	GLN	3.4
1	15-B	333	GLN	3.4
1	16-B	333	GLN	3.4
1	1-A	303	ALA	3.3
1	2-A	303	ALA	3.3
1	3-A	303	ALA	3.3
1	4-A	303	ALA	3.3
1	5-A	303	ALA	3.3
1	6-A	303	ALA	3.3
1	7-A	303	ALA	3.3
1	8-A	303	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	9-A	303	ALA	3.3
1	10-A	303	ALA	3.3
1	11-A	303	ALA	3.3
1	12-A	303	ALA	3.3
1	13-A	303	ALA	3.3
1	14-A	303	ALA	3.3
1	15-A	303	ALA	3.3
1	16-A	303	ALA	3.3
1	1-A	9	ASN	3.3
1	2-A	9	ASN	3.3
1	3-A	9	ASN	3.3
1	4-A	9	ASN	3.3
1	5-A	9	ASN	3.3
1	6-A	9	ASN	3.3
1	7-A	9	ASN	3.3
1	8-A	9	ASN	3.3
1	9-A	9	ASN	3.3
1	10-A	9	ASN	3.3
1	11-A	9	ASN	3.3
1	12-A	9	ASN	3.3
1	13-A	9	ASN	3.3
1	14-A	9	ASN	3.3
1	15-A	9	ASN	3.3
1	16-A	9	ASN	3.3
1	1-A	23	LEU	3.1
1	2-A	23	LEU	3.1
1	3-A	23	LEU	3.1
1	4-A	23	LEU	3.1
1	5-A	23	LEU	3.1
1	6-A	23	LEU	3.1
1	7-A	23	LEU	3.1
1	8-A	23	LEU	3.1
1	9-A	23	LEU	3.1
1	10-A	23	LEU	3.1
1	11-A	23	LEU	3.1
1	12-A	23	LEU	3.1
1	13-A	23	LEU	3.1
1	14-A	23	LEU	3.1
1	15-A	23	LEU	3.1
1	16-A	23	LEU	3.1
1	1-A	170	LEU	3.1
1	2-A	170	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	3-A	170	LEU	3.1
1	4-A	170	LEU	3.1
1	5-A	170	LEU	3.1
1	6-A	170	LEU	3.1
1	7-A	170	LEU	3.1
1	8-A	170	LEU	3.1
1	9-A	170	LEU	3.1
1	10-A	170	LEU	3.1
1	11-A	170	LEU	3.1
1	12-A	170	LEU	3.1
1	13-A	170	LEU	3.1
1	14-A	170	LEU	3.1
1	15-A	170	LEU	3.1
1	16-A	170	LEU	3.1
1	1-A	244	ASP	3.1
1	2-A	244	ASP	3.1
1	3-A	244	ASP	3.1
1	4-A	244	ASP	3.1
1	5-A	244	ASP	3.1
1	6-A	244	ASP	3.1
1	7-A	244	ASP	3.1
1	8-A	244	ASP	3.1
1	9-A	244	ASP	3.1
1	10-A	244	ASP	3.1
1	11-A	244	ASP	3.1
1	12-A	244	ASP	3.1
1	13-A	244	ASP	3.1
1	14-A	244	ASP	3.1
1	15-A	244	ASP	3.1
1	16-A	244	ASP	3.1
1	1-A	45	ALA	2.9
1	2-A	45	ALA	2.9
1	3-A	45	ALA	2.9
1	4-A	45	ALA	2.9
1	5-A	45	ALA	2.9
1	6-A	45	ALA	2.9
1	7-A	45	ALA	2.9
1	8-A	45	ALA	2.9
1	9-A	45	ALA	2.9
1	10-A	45	ALA	2.9
1	11-A	45	ALA	2.9
1	12-A	45	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	13-A	45	ALA	2.9
1	14-A	45	ALA	2.9
1	15-A	45	ALA	2.9
1	16-A	45	ALA	2.9
1	1-B	288	TYR	2.9
1	2-B	288	TYR	2.9
1	3-B	288	TYR	2.9
1	4-B	288	TYR	2.9
1	5-B	288	TYR	2.9
1	6-B	288	TYR	2.9
1	7-B	288	TYR	2.9
1	8-B	288	TYR	2.9
1	9-B	288	TYR	2.9
1	10-B	288	TYR	2.9
1	11-B	288	TYR	2.9
1	12-B	288	TYR	2.9
1	13-B	288	TYR	2.9
1	14-B	288	TYR	2.9
1	15-B	288	TYR	2.9
1	16-B	288	TYR	2.9
1	1-A	136	ASN	2.9
1	2-A	136	ASN	2.9
1	3-A	136	ASN	2.9
1	4-A	136	ASN	2.9
1	5-A	136	ASN	2.9
1	6-A	136	ASN	2.9
1	7-A	136	ASN	2.9
1	8-A	136	ASN	2.9
1	9-A	136	ASN	2.9
1	10-A	136	ASN	2.9
1	11-A	136	ASN	2.9
1	12-A	136	ASN	2.9
1	13-A	136	ASN	2.9
1	14-A	136	ASN	2.9
1	15-A	136	ASN	2.9
1	16-A	136	ASN	2.9
1	1-A	360	GLY	2.9
1	2-A	360	GLY	2.9
1	3-A	360	GLY	2.9
1	4-A	360	GLY	2.9
1	5-A	360	GLY	2.9
1	6-A	360	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	7-A	360	GLY	2.9
1	8-A	360	GLY	2.9
1	9-A	360	GLY	2.9
1	10-A	360	GLY	2.9
1	11-A	360	GLY	2.9
1	12-A	360	GLY	2.9
1	13-A	360	GLY	2.9
1	14-A	360	GLY	2.9
1	15-A	360	GLY	2.9
1	16-A	360	GLY	2.9
1	1-B	300	GLU	2.9
1	2-B	300	GLU	2.9
1	3-B	300	GLU	2.9
1	4-B	300	GLU	2.9
1	5-B	300	GLU	2.9
1	6-B	300	GLU	2.9
1	7-B	300	GLU	2.9
1	8-B	300	GLU	2.9
1	9-B	300	GLU	2.9
1	10-B	300	GLU	2.9
1	11-B	300	GLU	2.9
1	12-B	300	GLU	2.9
1	13-B	300	GLU	2.9
1	14-B	300	GLU	2.9
1	15-B	300	GLU	2.9
1	16-B	300	GLU	2.9
1	1-A	267	LEU	2.9
1	2-A	267	LEU	2.9
1	3-A	267	LEU	2.9
1	4-A	267	LEU	2.9
1	5-A	267	LEU	2.9
1	6-A	267	LEU	2.9
1	7-A	267	LEU	2.9
1	8-A	267	LEU	2.9
1	9-A	267	LEU	2.9
1	10-A	267	LEU	2.9
1	11-A	267	LEU	2.9
1	12-A	267	LEU	2.9
1	13-A	267	LEU	2.9
1	14-A	267	LEU	2.9
1	15-A	267	LEU	2.9
1	16-A	267	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	17	LYS	2.7
1	2-A	17	LYS	2.7
1	3-A	17	LYS	2.7
1	4-A	17	LYS	2.7
1	5-A	17	LYS	2.7
1	6-A	17	LYS	2.7
1	7-A	17	LYS	2.7
1	8-A	17	LYS	2.7
1	9-A	17	LYS	2.7
1	10-A	17	LYS	2.7
1	11-A	17	LYS	2.7
1	12-A	17	LYS	2.7
1	13-A	17	LYS	2.7
1	14-A	17	LYS	2.7
1	15-A	17	LYS	2.7
1	16-A	17	LYS	2.7
1	1-B	385	LEU	2.7
1	2-B	385	LEU	2.7
1	3-B	385	LEU	2.7
1	4-B	385	LEU	2.7
1	5-B	385	LEU	2.7
1	6-B	385	LEU	2.7
1	7-B	385	LEU	2.7
1	8-B	385	LEU	2.7
1	9-B	385	LEU	2.7
1	10-B	385	LEU	2.7
1	11-B	385	LEU	2.7
1	12-B	385	LEU	2.7
1	13-B	385	LEU	2.7
1	14-B	385	LEU	2.7
1	15-B	385	LEU	2.7
1	16-B	385	LEU	2.7
1	1-B	364	LYS	2.7
1	2-B	364	LYS	2.7
1	3-B	364	LYS	2.7
1	4-B	364	LYS	2.7
1	5-B	364	LYS	2.7
1	6-B	364	LYS	2.7
1	7-B	364	LYS	2.7
1	8-B	364	LYS	2.7
1	9-B	364	LYS	2.7
1	10-B	364	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	11-B	364	LYS	2.7
1	12-B	364	LYS	2.7
1	13-B	364	LYS	2.7
1	14-B	364	LYS	2.7
1	15-B	364	LYS	2.7
1	16-B	364	LYS	2.7
1	1-B	365	TYR	2.5
1	2-B	365	TYR	2.5
1	3-B	365	TYR	2.5
1	4-B	365	TYR	2.5
1	5-B	365	TYR	2.5
1	6-B	365	TYR	2.5
1	7-B	365	TYR	2.5
1	8-B	365	TYR	2.5
1	9-B	365	TYR	2.5
1	10-B	365	TYR	2.5
1	11-B	365	TYR	2.5
1	12-B	365	TYR	2.5
1	13-B	365	TYR	2.5
1	14-B	365	TYR	2.5
1	15-B	365	TYR	2.5
1	16-B	365	TYR	2.5
1	1-A	386	ALA	2.5
1	2-A	386	ALA	2.5
1	3-A	386	ALA	2.5
1	4-A	386	ALA	2.5
1	5-A	386	ALA	2.5
1	6-A	386	ALA	2.5
1	7-A	386	ALA	2.5
1	8-A	386	ALA	2.5
1	9-A	386	ALA	2.5
1	10-A	386	ALA	2.5
1	11-A	386	ALA	2.5
1	12-A	386	ALA	2.5
1	13-A	386	ALA	2.5
1	14-A	386	ALA	2.5
1	15-A	386	ALA	2.5
1	16-A	386	ALA	2.5
1	1-B	206	ASP	2.5
1	2-B	206	ASP	2.5
1	3-B	206	ASP	2.5
1	4-B	206	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	5-B	206	ASP	2.5
1	6-B	206	ASP	2.5
1	7-B	206	ASP	2.5
1	8-B	206	ASP	2.5
1	9-B	206	ASP	2.5
1	10-B	206	ASP	2.5
1	11-B	206	ASP	2.5
1	12-B	206	ASP	2.5
1	13-B	206	ASP	2.5
1	14-B	206	ASP	2.5
1	15-B	206	ASP	2.5
1	16-B	206	ASP	2.5
1	1-A	283	PRO	2.5
1	2-A	283	PRO	2.5
1	3-A	283	PRO	2.5
1	4-A	283	PRO	2.5
1	5-A	283	PRO	2.5
1	6-A	283	PRO	2.5
1	7-A	283	PRO	2.5
1	8-A	283	PRO	2.5
1	9-A	283	PRO	2.5
1	10-A	283	PRO	2.5
1	11-A	283	PRO	2.5
1	12-A	283	PRO	2.5
1	13-A	283	PRO	2.5
1	14-A	283	PRO	2.5
1	15-A	283	PRO	2.5
1	16-A	283	PRO	2.5
1	1-A	374	ASP	2.5
1	2-A	374	ASP	2.5
1	3-A	374	ASP	2.5
1	4-A	374	ASP	2.5
1	5-A	374	ASP	2.5
1	6-A	374	ASP	2.5
1	7-A	374	ASP	2.5
1	8-A	374	ASP	2.5
1	9-A	374	ASP	2.5
1	10-A	374	ASP	2.5
1	11-A	374	ASP	2.5
1	12-A	374	ASP	2.5
1	13-A	374	ASP	2.5
1	14-A	374	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	15-A	374	ASP	2.5
1	16-A	374	ASP	2.5
1	1-B	366	ASN	2.4
1	2-B	366	ASN	2.4
1	3-B	366	ASN	2.4
1	4-B	366	ASN	2.4
1	5-B	366	ASN	2.4
1	6-B	366	ASN	2.4
1	7-B	366	ASN	2.4
1	8-B	366	ASN	2.4
1	9-B	366	ASN	2.4
1	10-B	366	ASN	2.4
1	11-B	366	ASN	2.4
1	12-B	366	ASN	2.4
1	13-B	366	ASN	2.4
1	14-B	366	ASN	2.4
1	15-B	366	ASN	2.4
1	16-B	366	ASN	2.4
1	1-B	377	VAL	2.4
1	2-B	377	VAL	2.4
1	3-B	377	VAL	2.4
1	4-B	377	VAL	2.4
1	5-B	377	VAL	2.4
1	6-B	377	VAL	2.4
1	7-B	377	VAL	2.4
1	8-B	377	VAL	2.4
1	9-B	377	VAL	2.4
1	10-B	377	VAL	2.4
1	11-B	377	VAL	2.4
1	12-B	377	VAL	2.4
1	13-B	377	VAL	2.4
1	14-B	377	VAL	2.4
1	15-B	377	VAL	2.4
1	16-B	377	VAL	2.4
1	1-A	264	LEU	2.3
1	2-A	264	LEU	2.3
1	3-A	264	LEU	2.3
1	4-A	264	LEU	2.3
1	5-A	264	LEU	2.3
1	6-A	264	LEU	2.3
1	7-A	264	LEU	2.3
1	8-A	264	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	9-A	264	LEU	2.3
1	10-A	264	LEU	2.3
1	11-A	264	LEU	2.3
1	12-A	264	LEU	2.3
1	13-A	264	LEU	2.3
1	14-A	264	LEU	2.3
1	15-A	264	LEU	2.3
1	16-A	264	LEU	2.3
1	1-B	251	SER	2.3
1	2-B	251	SER	2.3
1	3-B	251	SER	2.3
1	4-B	251	SER	2.3
1	5-B	251	SER	2.3
1	6-B	251	SER	2.3
1	7-B	251	SER	2.3
1	8-B	251	SER	2.3
1	9-B	251	SER	2.3
1	10-B	251	SER	2.3
1	11-B	251	SER	2.3
1	12-B	251	SER	2.3
1	13-B	251	SER	2.3
1	14-B	251	SER	2.3
1	15-B	251	SER	2.3
1	16-B	251	SER	2.3
1	1-B	81	TYR	2.3
1	2-B	81	TYR	2.3
1	3-B	81	TYR	2.3
1	4-B	81	TYR	2.3
1	5-B	81	TYR	2.3
1	6-B	81	TYR	2.3
1	7-B	81	TYR	2.3
1	8-B	81	TYR	2.3
1	9-B	81	TYR	2.3
1	10-B	81	TYR	2.3
1	11-B	81	TYR	2.3
1	12-B	81	TYR	2.3
1	13-B	81	TYR	2.3
1	14-B	81	TYR	2.3
1	15-B	81	TYR	2.3
1	16-B	81	TYR	2.3
1	1-B	44	ALA	2.3
1	2-B	44	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	3-B	44	ALA	2.3
1	4-B	44	ALA	2.3
1	5-B	44	ALA	2.3
1	6-B	44	ALA	2.3
1	7-B	44	ALA	2.3
1	8-B	44	ALA	2.3
1	9-B	44	ALA	2.3
1	10-B	44	ALA	2.3
1	11-B	44	ALA	2.3
1	12-B	44	ALA	2.3
1	13-B	44	ALA	2.3
1	14-B	44	ALA	2.3
1	15-B	44	ALA	2.3
1	16-B	44	ALA	2.3
1	1-B	137	ARG	2.2
1	2-B	137	ARG	2.2
1	3-B	137	ARG	2.2
1	4-B	137	ARG	2.2
1	5-B	137	ARG	2.2
1	6-B	137	ARG	2.2
1	7-B	137	ARG	2.2
1	8-B	137	ARG	2.2
1	9-B	137	ARG	2.2
1	10-B	137	ARG	2.2
1	11-B	137	ARG	2.2
1	12-B	137	ARG	2.2
1	13-B	137	ARG	2.2
1	14-B	137	ARG	2.2
1	15-B	137	ARG	2.2
1	16-B	137	ARG	2.2
1	1-A	98	ALA	2.2
1	2-A	98	ALA	2.2
1	3-A	98	ALA	2.2
1	4-A	98	ALA	2.2
1	5-A	98	ALA	2.2
1	6-A	98	ALA	2.2
1	7-A	98	ALA	2.2
1	8-A	98	ALA	2.2
1	9-A	98	ALA	2.2
1	10-A	98	ALA	2.2
1	11-A	98	ALA	2.2
1	12-A	98	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	13-A	98	ALA	2.2
1	14-A	98	ALA	2.2
1	15-A	98	ALA	2.2
1	16-A	98	ALA	2.2
1	1-B	384	PHE	2.2
1	2-B	384	PHE	2.2
1	3-B	384	PHE	2.2
1	4-B	384	PHE	2.2
1	5-B	384	PHE	2.2
1	6-B	384	PHE	2.2
1	7-B	384	PHE	2.2
1	8-B	384	PHE	2.2
1	9-B	384	PHE	2.2
1	10-B	384	PHE	2.2
1	11-B	384	PHE	2.2
1	12-B	384	PHE	2.2
1	13-B	384	PHE	2.2
1	14-B	384	PHE	2.2
1	15-B	384	PHE	2.2
1	16-B	384	PHE	2.2
1	1-A	249	THR	2.2
1	2-A	249	THR	2.2
1	3-A	249	THR	2.2
1	4-A	249	THR	2.2
1	5-A	249	THR	2.2
1	6-A	249	THR	2.2
1	7-A	249	THR	2.2
1	8-A	249	THR	2.2
1	9-A	249	THR	2.2
1	10-A	249	THR	2.2
1	11-A	249	THR	2.2
1	12-A	249	THR	2.2
1	13-A	249	THR	2.2
1	14-A	249	THR	2.2
1	15-A	249	THR	2.2
1	16-A	249	THR	2.2
1	1-A	248	ALA	2.2
1	2-A	248	ALA	2.2
1	3-A	248	ALA	2.2
1	4-A	248	ALA	2.2
1	5-A	248	ALA	2.2
1	6-A	248	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	7-A	248	ALA	2.2
1	8-A	248	ALA	2.2
1	9-A	248	ALA	2.2
1	10-A	248	ALA	2.2
1	11-A	248	ALA	2.2
1	12-A	248	ALA	2.2
1	13-A	248	ALA	2.2
1	14-A	248	ALA	2.2
1	15-A	248	ALA	2.2
1	16-A	248	ALA	2.2
1	1-A	352	LEU	2.2
1	2-A	352	LEU	2.2
1	3-A	352	LEU	2.2
1	4-A	352	LEU	2.2
1	5-A	352	LEU	2.2
1	6-A	352	LEU	2.2
1	7-A	352	LEU	2.2
1	8-A	352	LEU	2.2
1	9-A	352	LEU	2.2
1	10-A	352	LEU	2.2
1	11-A	352	LEU	2.2
1	12-A	352	LEU	2.2
1	13-A	352	LEU	2.2
1	14-A	352	LEU	2.2
1	15-A	352	LEU	2.2
1	16-A	352	LEU	2.2
1	1-A	250	ASP	2.2
1	2-A	250	ASP	2.2
1	3-A	250	ASP	2.2
1	4-A	250	ASP	2.2
1	5-A	250	ASP	2.2
1	6-A	250	ASP	2.2
1	7-A	250	ASP	2.2
1	8-A	250	ASP	2.2
1	9-A	250	ASP	2.2
1	10-A	250	ASP	2.2
1	11-A	250	ASP	2.2
1	12-A	250	ASP	2.2
1	13-A	250	ASP	2.2
1	14-A	250	ASP	2.2
1	15-A	250	ASP	2.2
1	16-A	250	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1-A	29	LEU	2.1
1	2-A	29	LEU	2.1
1	3-A	29	LEU	2.1
1	4-A	29	LEU	2.1
1	5-A	29	LEU	2.1
1	6-A	29	LEU	2.1
1	7-A	29	LEU	2.1
1	8-A	29	LEU	2.1
1	9-A	29	LEU	2.1
1	10-A	29	LEU	2.1
1	11-A	29	LEU	2.1
1	12-A	29	LEU	2.1
1	13-A	29	LEU	2.1
1	14-A	29	LEU	2.1
1	15-A	29	LEU	2.1
1	16-A	29	LEU	2.1
1	1-A	44	ALA	2.1
1	2-A	44	ALA	2.1
1	3-A	44	ALA	2.1
1	4-A	44	ALA	2.1
1	5-A	44	ALA	2.1
1	6-A	44	ALA	2.1
1	7-A	44	ALA	2.1
1	8-A	44	ALA	2.1
1	9-A	44	ALA	2.1
1	10-A	44	ALA	2.1
1	11-A	44	ALA	2.1
1	12-A	44	ALA	2.1
1	13-A	44	ALA	2.1
1	14-A	44	ALA	2.1
1	15-A	44	ALA	2.1
1	16-A	44	ALA	2.1
1	1-B	10	GLU	2.1
1	2-B	10	GLU	2.1
1	3-B	10	GLU	2.1
1	4-B	10	GLU	2.1
1	5-B	10	GLU	2.1
1	6-B	10	GLU	2.1
1	7-B	10	GLU	2.1
1	8-B	10	GLU	2.1
1	9-B	10	GLU	2.1
1	10-B	10	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	11-B	10	GLU	2.1
1	12-B	10	GLU	2.1
1	13-B	10	GLU	2.1
1	14-B	10	GLU	2.1
1	15-B	10	GLU	2.1
1	16-B	10	GLU	2.1
1	1-A	210	GLY	2.1
1	2-A	210	GLY	2.1
1	3-A	210	GLY	2.1
1	4-A	210	GLY	2.1
1	5-A	210	GLY	2.1
1	6-A	210	GLY	2.1
1	7-A	210	GLY	2.1
1	8-A	210	GLY	2.1
1	9-A	210	GLY	2.1
1	10-A	210	GLY	2.1
1	11-A	210	GLY	2.1
1	12-A	210	GLY	2.1
1	13-A	210	GLY	2.1
1	14-A	210	GLY	2.1
1	15-A	210	GLY	2.1
1	16-A	210	GLY	2.1
1	1-B	83	ASP	2.1
1	2-B	83	ASP	2.1
1	3-B	83	ASP	2.1
1	4-B	83	ASP	2.1
1	5-B	83	ASP	2.1
1	6-B	83	ASP	2.1
1	7-B	83	ASP	2.1
1	8-B	83	ASP	2.1
1	9-B	83	ASP	2.1
1	10-B	83	ASP	2.1
1	11-B	83	ASP	2.1
1	12-B	83	ASP	2.1
1	13-B	83	ASP	2.1
1	14-B	83	ASP	2.1
1	15-B	83	ASP	2.1
1	16-B	83	ASP	2.1
1	1-A	275	LEU	2.1
1	2-A	275	LEU	2.1
1	3-A	275	LEU	2.1
1	4-A	275	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	5-A	275	LEU	2.1
1	6-A	275	LEU	2.1
1	7-A	275	LEU	2.1
1	8-A	275	LEU	2.1
1	9-A	275	LEU	2.1
1	10-A	275	LEU	2.1
1	11-A	275	LEU	2.1
1	12-A	275	LEU	2.1
1	13-A	275	LEU	2.1
1	14-A	275	LEU	2.1
1	15-A	275	LEU	2.1
1	16-A	275	LEU	2.1
1	1-A	41	VAL	2.1
1	2-A	41	VAL	2.1
1	3-A	41	VAL	2.1
1	4-A	41	VAL	2.1
1	5-A	41	VAL	2.1
1	6-A	41	VAL	2.1
1	7-A	41	VAL	2.1
1	8-A	41	VAL	2.1
1	9-A	41	VAL	2.1
1	10-A	41	VAL	2.1
1	11-A	41	VAL	2.1
1	12-A	41	VAL	2.1
1	13-A	41	VAL	2.1
1	14-A	41	VAL	2.1
1	15-A	41	VAL	2.1
1	16-A	41	VAL	2.1
1	1-A	83	ASP	2.1
1	1-A	163	ARG	2.1
1	2-A	83	ASP	2.1
1	2-A	163	ARG	2.1
1	3-A	83	ASP	2.1
1	3-A	163	ARG	2.1
1	4-A	83	ASP	2.1
1	4-A	163	ARG	2.1
1	5-A	83	ASP	2.1
1	5-A	163	ARG	2.1
1	6-A	83	ASP	2.1
1	6-A	163	ARG	2.1
1	7-A	83	ASP	2.1
1	7-A	163	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	8-A	83	ASP	2.1
1	8-A	163	ARG	2.1
1	9-A	83	ASP	2.1
1	9-A	163	ARG	2.1
1	10-A	83	ASP	2.1
1	10-A	163	ARG	2.1
1	11-A	83	ASP	2.1
1	11-A	163	ARG	2.1
1	12-A	83	ASP	2.1
1	12-A	163	ARG	2.1
1	13-A	83	ASP	2.1
1	13-A	163	ARG	2.1
1	14-A	83	ASP	2.1
1	14-A	163	ARG	2.1
1	15-A	83	ASP	2.1
1	15-A	163	ARG	2.1
1	16-A	83	ASP	2.1
1	16-A	163	ARG	2.1
1	1-B	96	VAL	2.1
1	1-B	299	ASP	2.1
1	2-B	96	VAL	2.1
1	2-B	299	ASP	2.1
1	3-B	96	VAL	2.1
1	3-B	299	ASP	2.1
1	4-B	96	VAL	2.1
1	4-B	299	ASP	2.1
1	5-B	96	VAL	2.1
1	5-B	299	ASP	2.1
1	6-B	96	VAL	2.1
1	6-B	299	ASP	2.1
1	7-B	96	VAL	2.1
1	7-B	299	ASP	2.1
1	8-B	96	VAL	2.1
1	8-B	299	ASP	2.1
1	9-B	96	VAL	2.1
1	9-B	299	ASP	2.1
1	10-B	96	VAL	2.1
1	10-B	299	ASP	2.1
1	11-B	96	VAL	2.1
1	11-B	299	ASP	2.1
1	12-B	96	VAL	2.1
1	12-B	299	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	13-B	96	VAL	2.1
1	13-B	299	ASP	2.1
1	14-B	96	VAL	2.1
1	14-B	299	ASP	2.1
1	15-B	96	VAL	2.1
1	15-B	299	ASP	2.1
1	16-B	96	VAL	2.1
1	16-B	299	ASP	2.1
1	1-A	192	LEU	2.0
1	2-A	192	LEU	2.0
1	3-A	192	LEU	2.0
1	4-A	192	LEU	2.0
1	5-A	192	LEU	2.0
1	6-A	192	LEU	2.0
1	7-A	192	LEU	2.0
1	8-A	192	LEU	2.0
1	9-A	192	LEU	2.0
1	10-A	192	LEU	2.0
1	11-A	192	LEU	2.0
1	12-A	192	LEU	2.0
1	13-A	192	LEU	2.0
1	14-A	192	LEU	2.0
1	15-A	192	LEU	2.0
1	16-A	192	LEU	2.0
1	1-A	284	ARG	2.0
1	1-A	207	GLN	2.0
1	1-B	138	TRP	2.0
1	2-A	284	ARG	2.0
1	2-A	207	GLN	2.0
1	2-B	138	TRP	2.0
1	3-A	284	ARG	2.0
1	3-A	207	GLN	2.0
1	3-B	138	TRP	2.0
1	4-A	284	ARG	2.0
1	4-A	207	GLN	2.0
1	4-B	138	TRP	2.0
1	5-A	284	ARG	2.0
1	5-A	207	GLN	2.0
1	5-B	138	TRP	2.0
1	6-A	284	ARG	2.0
1	6-A	207	GLN	2.0
1	6-B	138	TRP	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	7-A	284	ARG	2.0
1	7-A	207	GLN	2.0
1	7-B	138	TRP	2.0
1	8-A	284	ARG	2.0
1	8-A	207	GLN	2.0
1	8-B	138	TRP	2.0
1	9-A	284	ARG	2.0
1	9-A	207	GLN	2.0
1	9-B	138	TRP	2.0
1	10-A	284	ARG	2.0
1	10-A	207	GLN	2.0
1	10-B	138	TRP	2.0
1	11-A	284	ARG	2.0
1	11-A	207	GLN	2.0
1	11-B	138	TRP	2.0
1	12-A	284	ARG	2.0
1	12-A	207	GLN	2.0
1	12-B	138	TRP	2.0
1	13-A	284	ARG	2.0
1	13-A	207	GLN	2.0
1	13-B	138	TRP	2.0
1	14-A	284	ARG	2.0
1	14-A	207	GLN	2.0
1	14-B	138	TRP	2.0
1	15-A	284	ARG	2.0
1	15-A	207	GLN	2.0
1	15-B	138	TRP	2.0
1	16-A	284	ARG	2.0
1	16-A	207	GLN	2.0
1	16-B	138	TRP	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 monosaccharides in this entry.

6.4 Ligands (i)

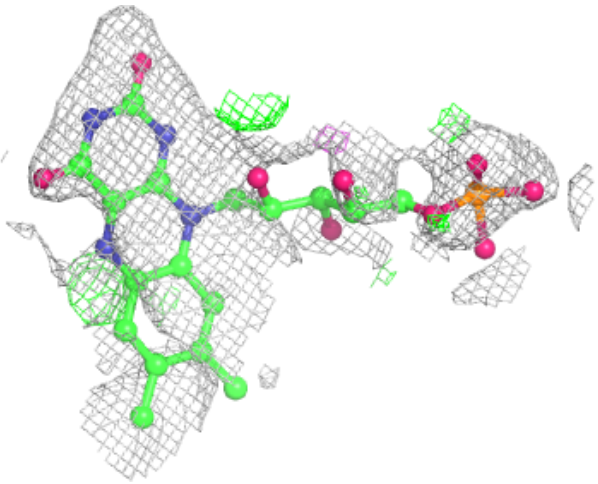
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

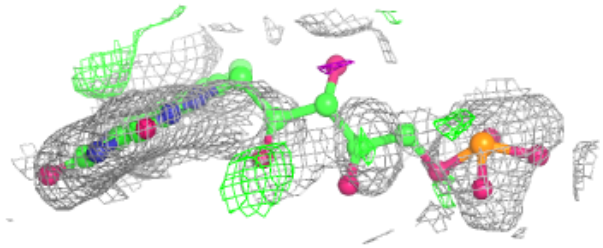
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FMN	1-B	9401	31/31	0.91	0.21	1,12,18,23	31
2	FMN	2-B	9401	31/31	0.91	0.21	1,8,14,19	31
2	FMN	3-B	9401	31/31	0.91	0.21	1,8,18,19	31
2	FMN	4-B	9401	31/31	0.91	0.21	1,8,14,15	31
2	FMN	5-B	9401	31/31	0.91	0.21	1,8,15,16	31
2	FMN	6-B	9401	31/31	0.91	0.21	1,8,15,19	31
2	FMN	7-B	9401	31/31	0.91	0.21	1,7,12,14	31
2	FMN	8-B	9401	31/31	0.91	0.21	1,6,17,20	31
2	FMN	9-B	9401	31/31	0.91	0.21	1,9,16,18	31
2	FMN	10-B	9401	31/31	0.91	0.21	4,10,14,16	31
2	FMN	11-B	9401	31/31	0.91	0.21	1,11,18,21	31
2	FMN	12-B	9401	31/31	0.91	0.21	1,8,16,17	31
2	FMN	13-B	9401	31/31	0.91	0.21	1,8,16,20	31
2	FMN	14-B	9401	31/31	0.91	0.21	1,8,14,15	31
2	FMN	15-B	9401	31/31	0.91	0.21	1,8,15,20	31
2	FMN	16-B	9401	31/31	0.91	0.21	1,9,15,18	31
2	FMN	1-A	7401	31/31	0.93	0.19	1,8,19,24	31
2	FMN	2-A	7401	31/31	0.93	0.19	1,8,20,22	31
2	FMN	3-A	7401	31/31	0.93	0.19	1,6,18,24	31
2	FMN	4-A	7401	31/31	0.93	0.19	1,8,19,24	31
2	FMN	5-A	7401	31/31	0.93	0.19	1,8,18,24	31
2	FMN	6-A	7401	31/31	0.93	0.19	1,7,17,19	31
2	FMN	7-A	7401	31/31	0.93	0.19	1,5,14,20	31
2	FMN	8-A	7401	31/31	0.93	0.19	1,5,21,25	31
2	FMN	9-A	7401	31/31	0.93	0.19	1,4,21,25	31
2	FMN	10-A	7401	31/31	0.93	0.19	1,4,8,15	31
2	FMN	11-A	7401	31/31	0.93	0.19	1,8,18,23	31
2	FMN	12-A	7401	31/31	0.93	0.19	1,9,17,18	31
2	FMN	13-A	7401	31/31	0.93	0.19	1,2,14,16	31
2	FMN	14-A	7401	31/31	0.93	0.19	1,7,10,14	31
2	FMN	15-A	7401	31/31	0.93	0.19	1,6,14,18	31
2	FMN	16-A	7401	31/31	0.93	0.19	1,2,12,16	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:

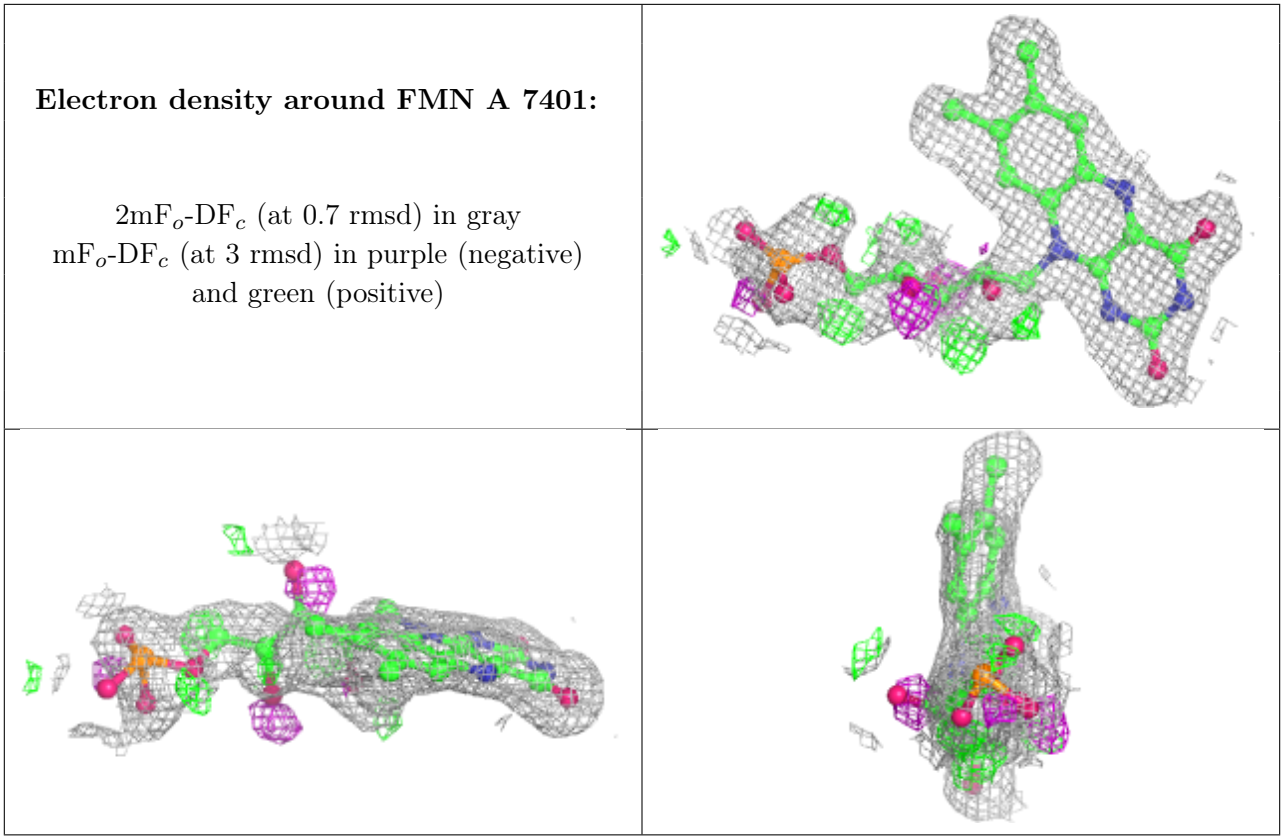
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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 (i)

There are no such residues in this entry.