



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 12:21 am GMT

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

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

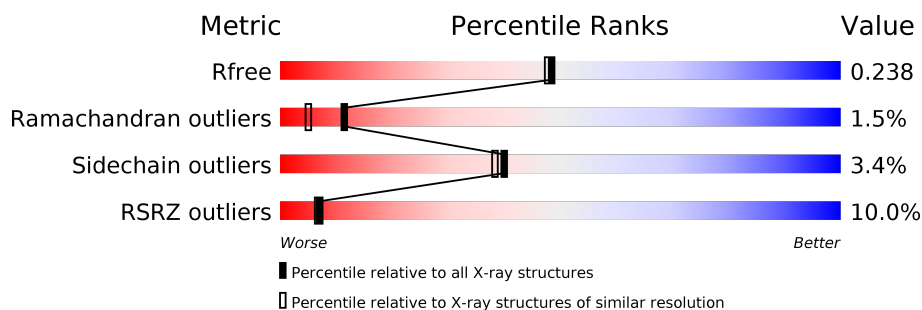
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	7193 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	1-A	391	<div> <div>12%</div> <div>89%</div> <div>7%</div> </div>
1	1-B	391	<div> <div>8%</div> <div>90%</div> <div>6%</div> </div>
1	10-A	391	<div> <div>12%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
1	10-B	391	<div> <div>8%</div> <div>92%</div> <div>6%</div> </div>
1	11-A	391	<div> <div>12%</div> <div>90%</div> <div>7%</div> </div>
1	11-B	391	<div> <div>8%</div> <div>90%</div> <div>6%</div> </div>
1	12-A	391	<div> <div>12%</div> <div>90%</div> <div>7%</div> </div>

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

2 Entry composition

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

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

- Molecule 1 is a protein called 12-oxophytodienoate reductase 3.

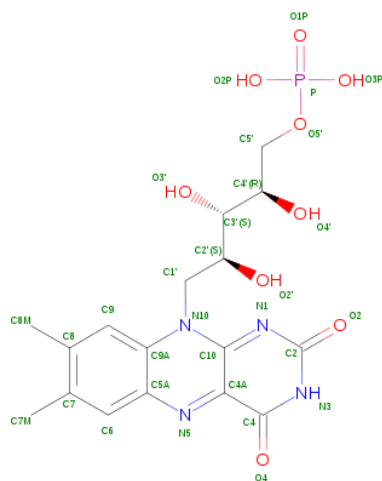
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	2-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	3-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	4-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	5-A	365	Total	C	N	O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

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

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



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	15-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	16-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	1-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	2-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	3-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	4-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	5-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	6-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	7-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	8-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	9-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	10-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	11-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	12-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	13-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	14-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	15-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	16-B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is water.

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

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

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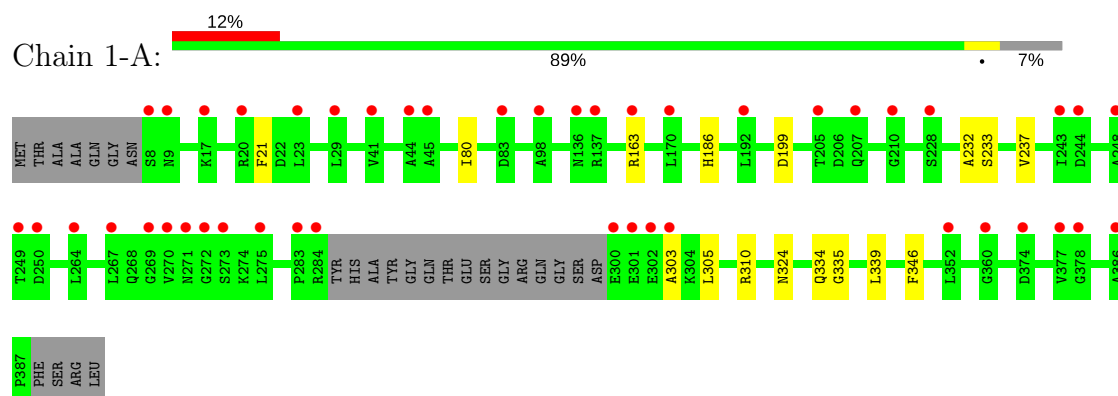
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	7-B	207	Total 207	O 207	0	0
3	8-B	209	Total 209	O 209	0	0
3	9-B	205	Total 205	O 205	0	0
3	10-B	210	Total 210	O 210	0	0
3	11-B	207	Total 207	O 207	0	0
3	12-B	204	Total 204	O 204	0	0
3	13-B	204	Total 204	O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

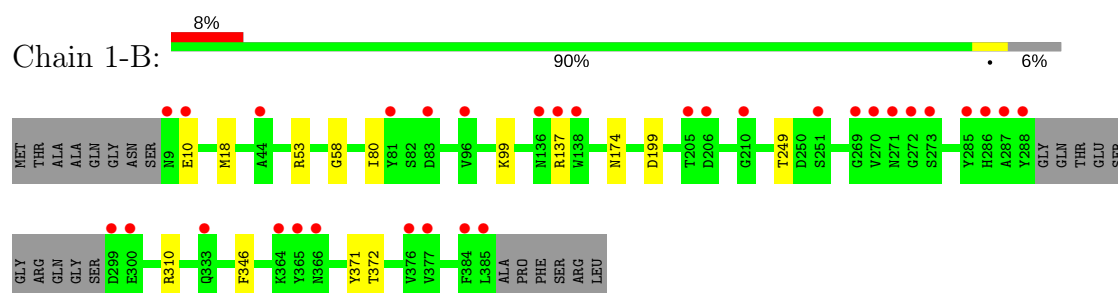
3 Residue-property plots [i](#)

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

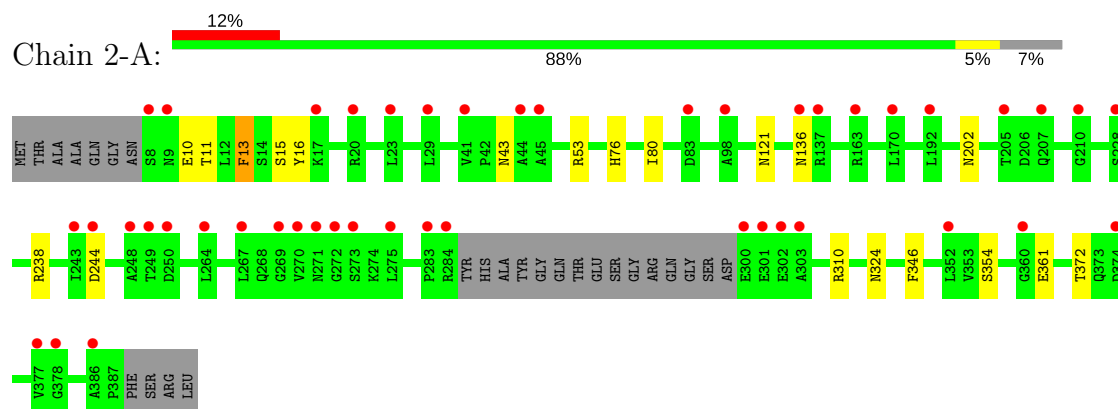
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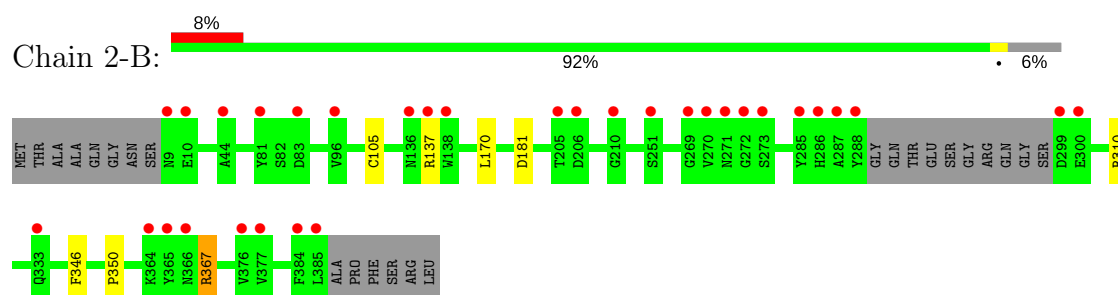
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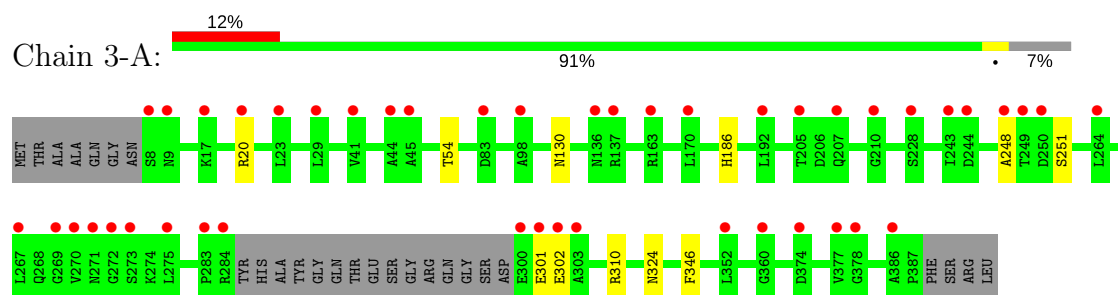
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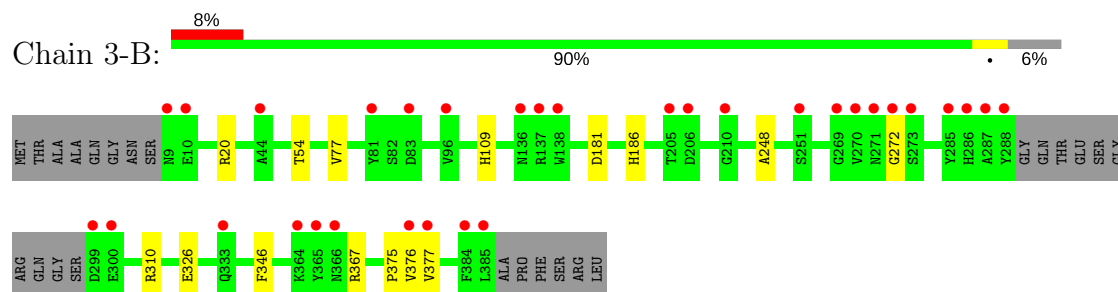
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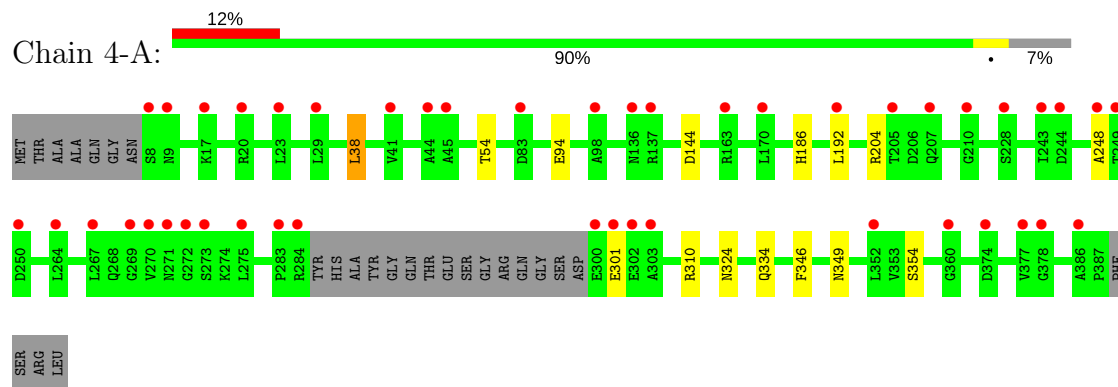
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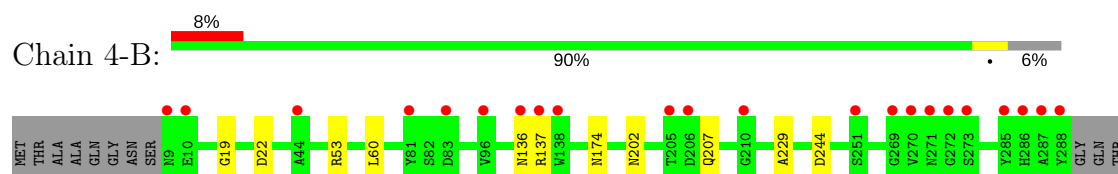
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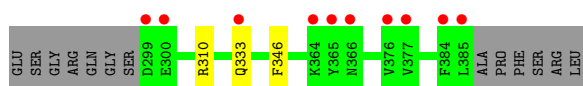


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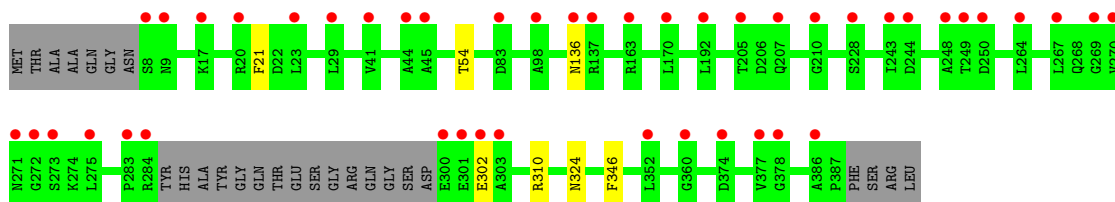


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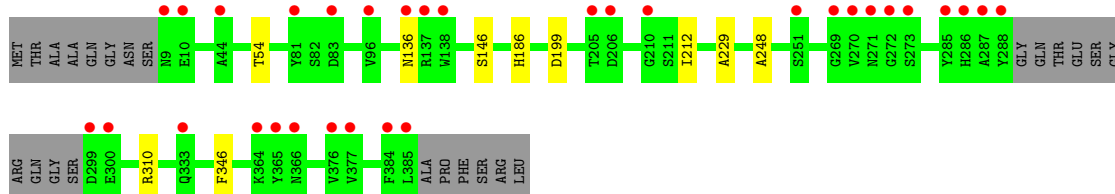




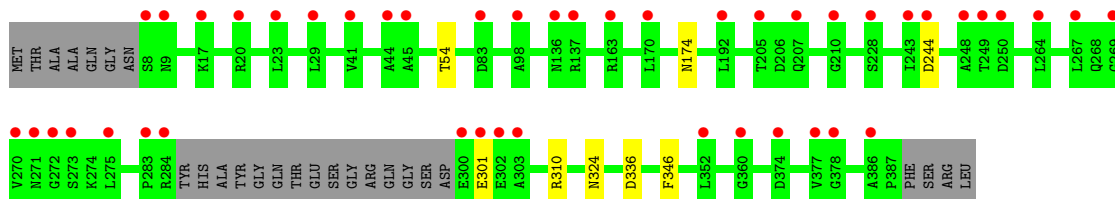
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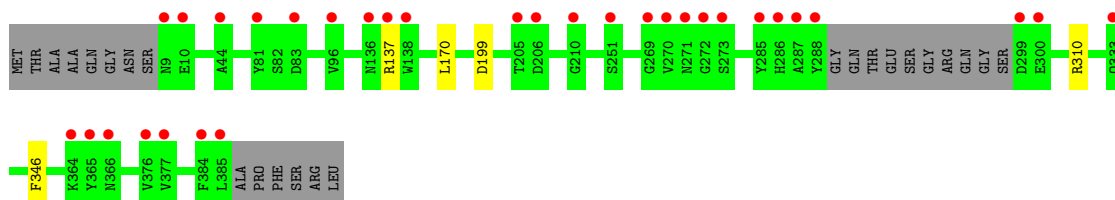
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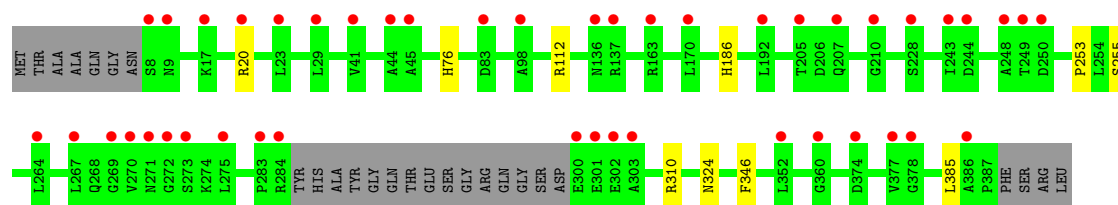


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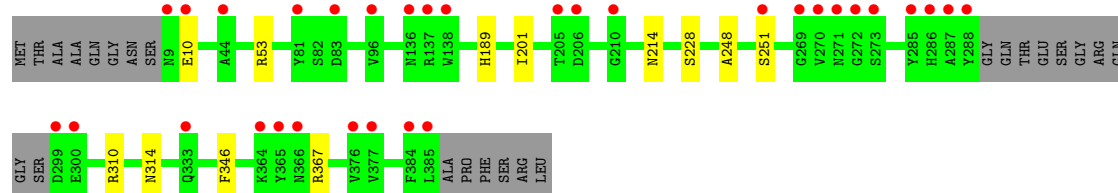


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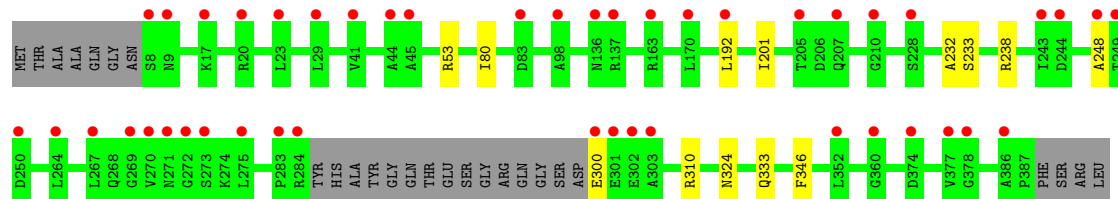




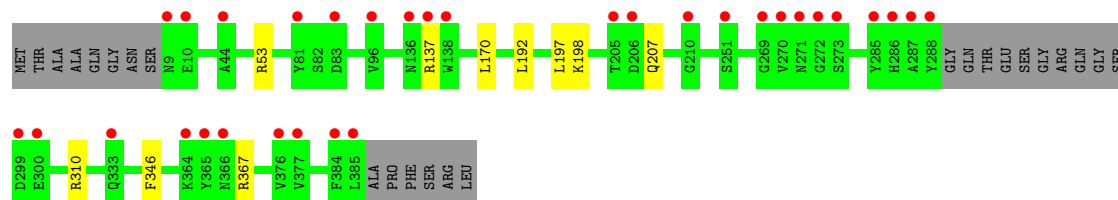
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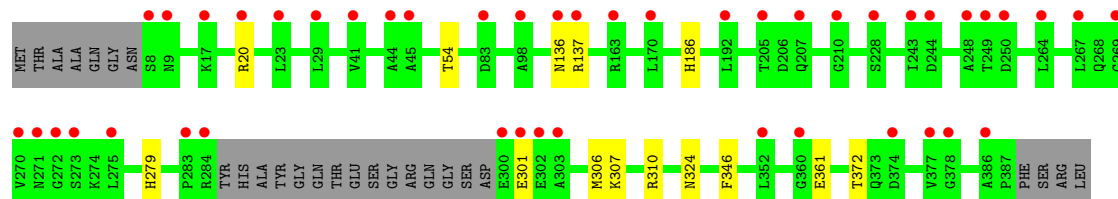
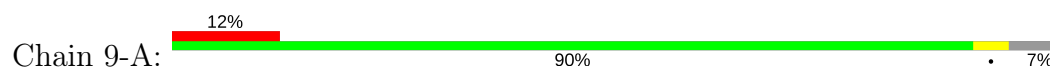
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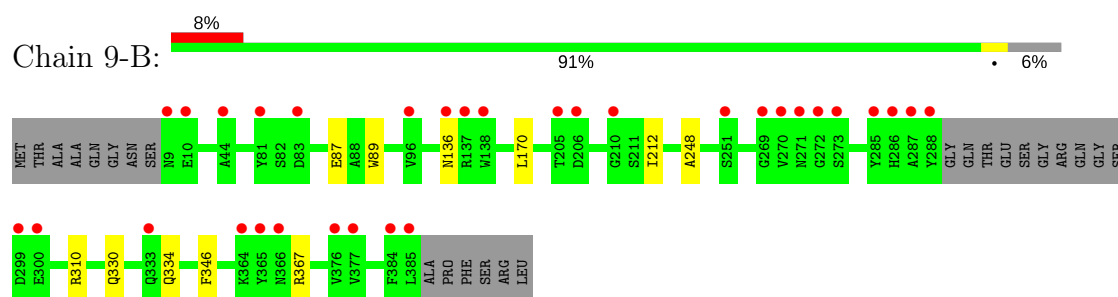
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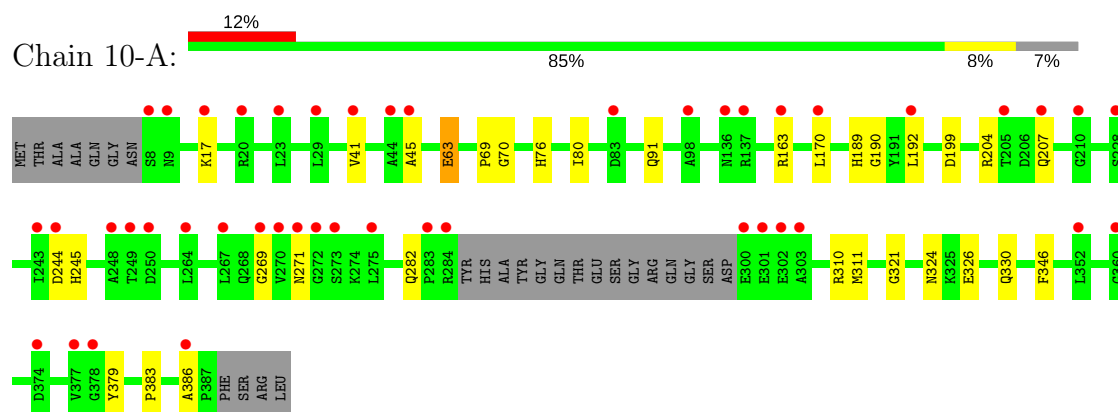
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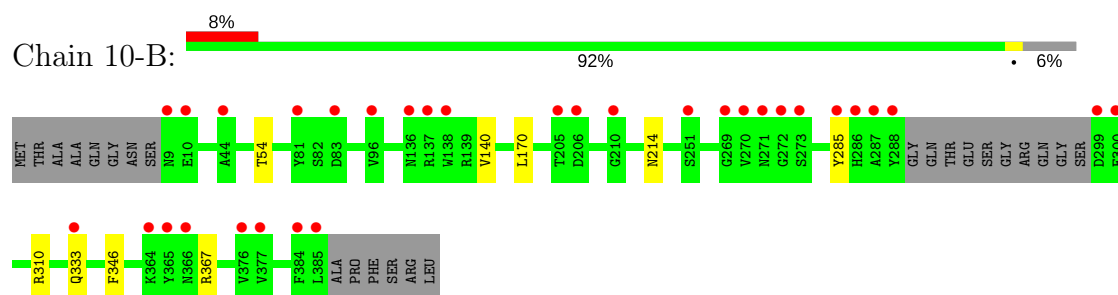
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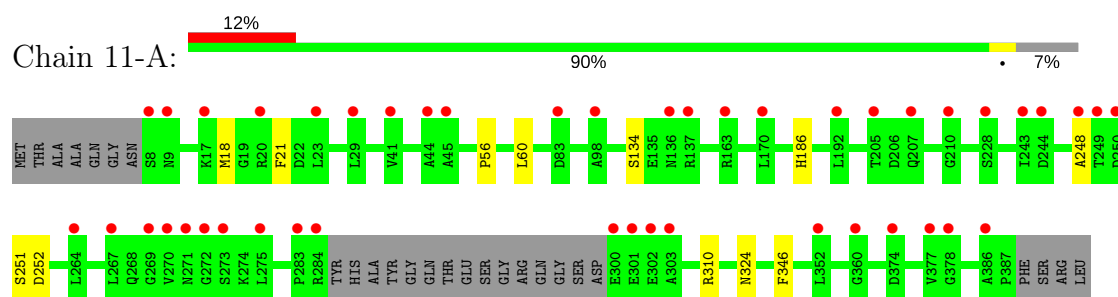
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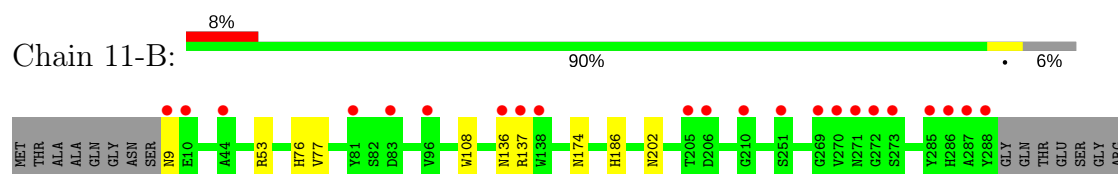
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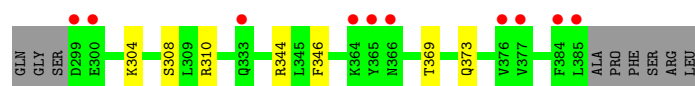


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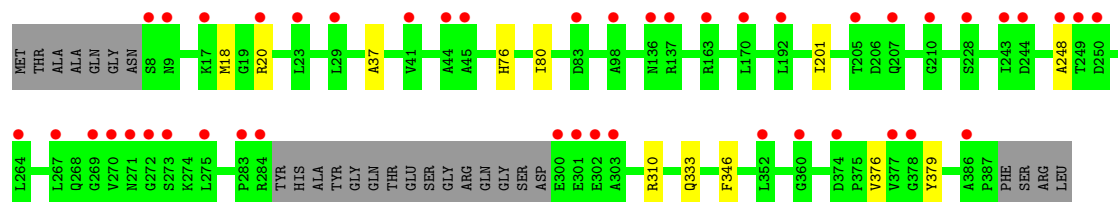


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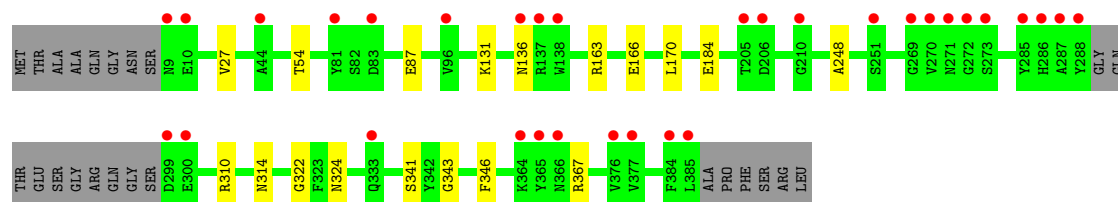




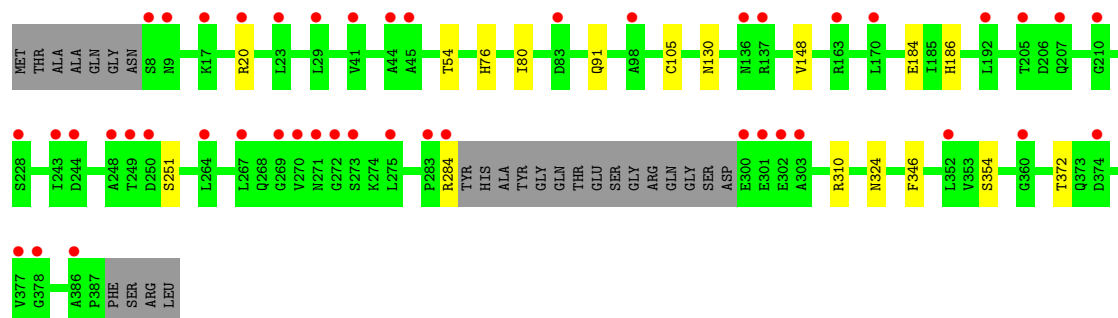
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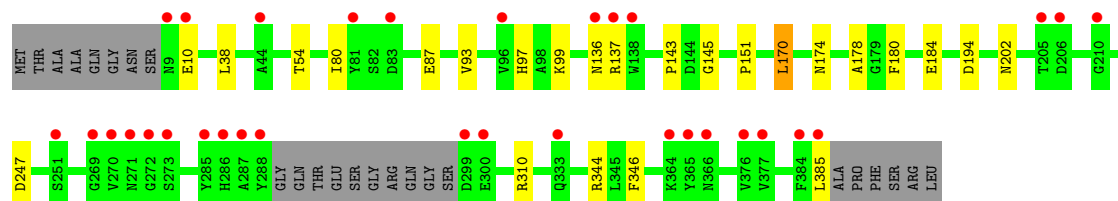
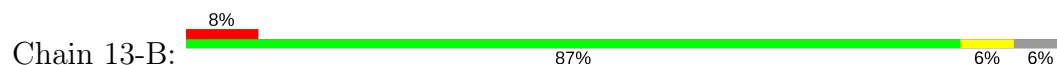
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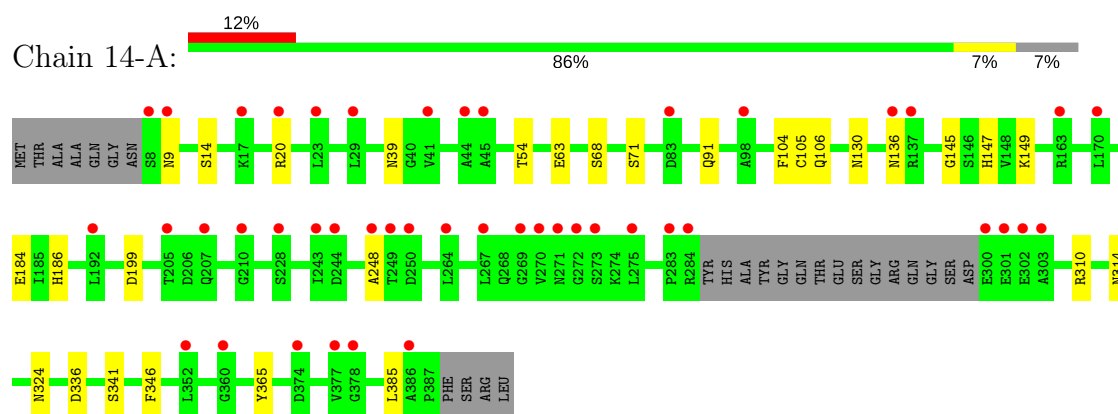
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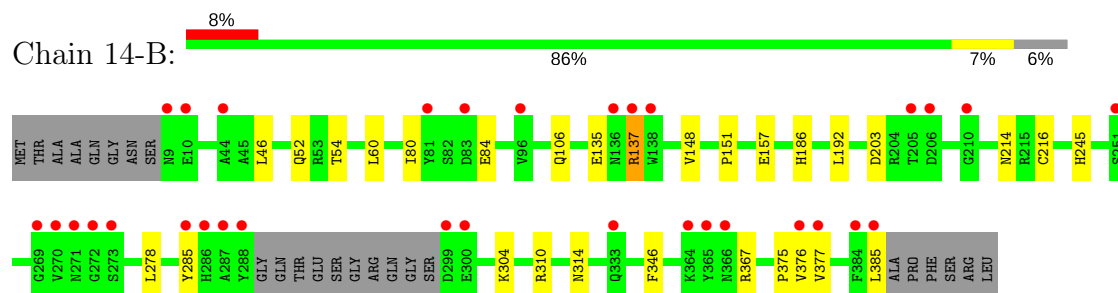
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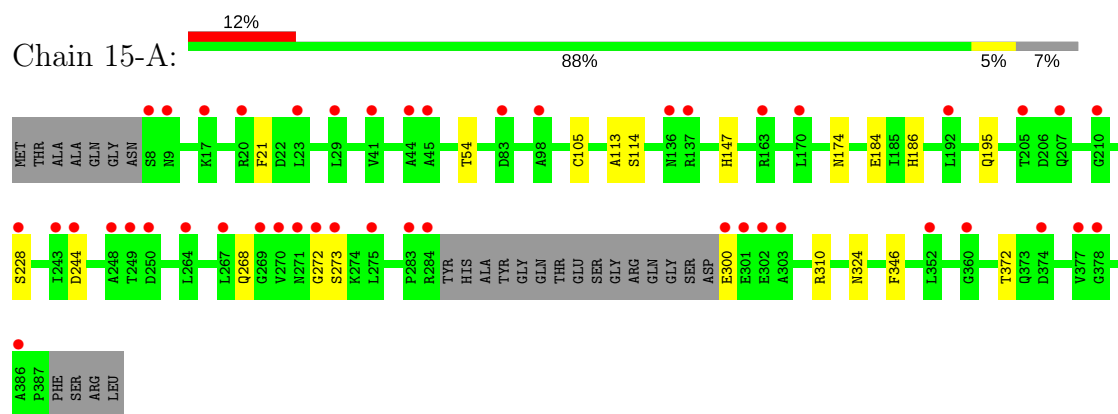
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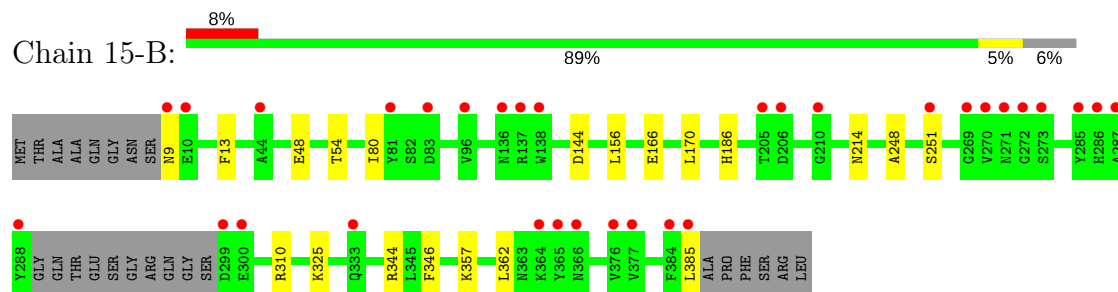
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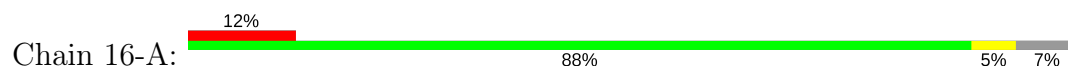
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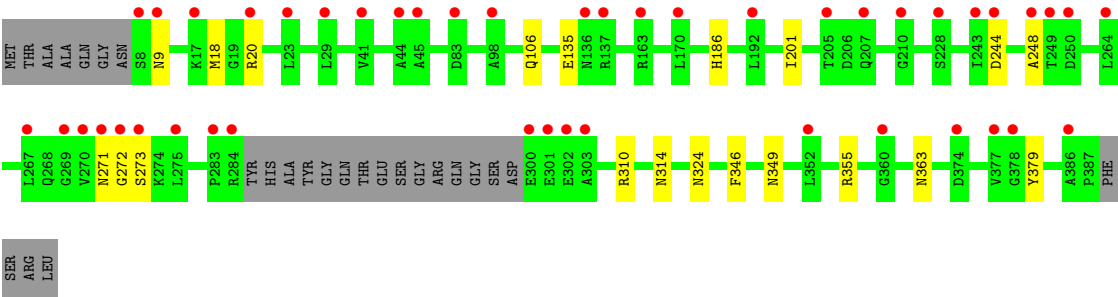


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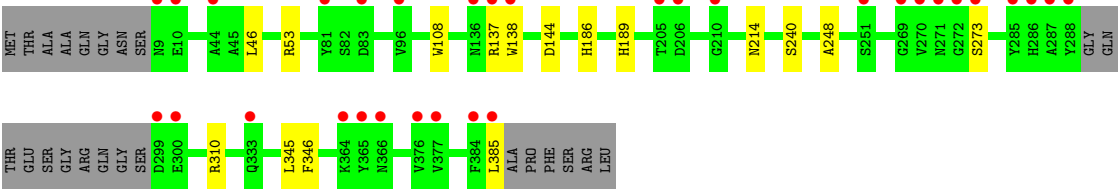


- Molecule 1: 12-oxophytodienoate reductase 3





● Molecule 1: 12-oxophytodienoate reductase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.11Å 85.07Å 121.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.90 – 2.00 24.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.1 (24.90-2.00) 91.3 (24.90-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.180 , 0.235 0.186 , 0.238	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	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1-A	0.41	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(°)	Ideal(°)
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 [i](#)

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

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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

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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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	361/391 (92%)	317 (88%)	35 (10%)	9 (2%)	6	2
1	1-B	363/391 (93%)	333 (92%)	25 (7%)	5 (1%)	12	6
1	2-A	361/391 (92%)	300 (83%)	51 (14%)	10 (3%)	5	2
1	2-B	363/391 (93%)	337 (93%)	24 (7%)	2 (1%)	27	21
1	3-A	361/391 (92%)	336 (93%)	22 (6%)	3 (1%)	21	14
1	3-B	363/391 (93%)	339 (93%)	18 (5%)	6 (2%)	10	4
1	4-A	361/391 (92%)	322 (89%)	33 (9%)	6 (2%)	10	4
1	4-B	363/391 (93%)	338 (93%)	20 (6%)	5 (1%)	12	6
1	5-A	361/391 (92%)	331 (92%)	29 (8%)	1 (0%)	43	39
1	5-B	363/391 (93%)	341 (94%)	20 (6%)	2 (1%)	27	21
1	6-A	361/391 (92%)	338 (94%)	22 (6%)	1 (0%)	43	39
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%)	16	8
1	7-B	363/391 (93%)	334 (92%)	23 (6%)	6 (2%)	10	4
1	8-A	361/391 (92%)	324 (90%)	31 (9%)	6 (2%)	10	4
1	8-B	363/391 (93%)	332 (92%)	28 (8%)	3 (1%)	21	14
1	9-A	361/391 (92%)	330 (91%)	23 (6%)	8 (2%)	7	3
1	9-B	363/391 (93%)	335 (92%)	26 (7%)	2 (1%)	27	21
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%)	43	39
1	11-A	361/391 (92%)	336 (93%)	22 (6%)	3 (1%)	21	14
1	11-B	363/391 (93%)	337 (93%)	22 (6%)	4 (1%)	16	8
1	12-A	361/391 (92%)	328 (91%)	25 (7%)	8 (2%)	7	3
1	12-B	363/391 (93%)	326 (90%)	32 (9%)	5 (1%)	12	6
1	13-A	361/391 (92%)	322 (89%)	35 (10%)	4 (1%)	16	8

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

5 of 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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	298/317 (94%)	291 (98%)	7 (2%)	53	56
1	1-B	300/317 (95%)	291 (97%)	9 (3%)	44	44
1	2-A	298/317 (94%)	287 (96%)	11 (4%)	37	35
1	2-B	300/317 (95%)	293 (98%)	7 (2%)	53	56
1	3-A	298/317 (94%)	290 (97%)	8 (3%)	48	49
1	3-B	300/317 (95%)	291 (97%)	9 (3%)	44	44
1	4-A	298/317 (94%)	288 (97%)	10 (3%)	40	38
1	4-B	300/317 (95%)	291 (97%)	9 (3%)	44	44
1	5-A	298/317 (94%)	292 (98%)	6 (2%)	58	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5-B	300/317 (95%)	292 (97%)	8 (3%)	48	49
1	6-A	298/317 (94%)	291 (98%)	7 (2%)	53	56
1	6-B	300/317 (95%)	295 (98%)	5 (2%)	63	68
1	7-A	298/317 (94%)	292 (98%)	6 (2%)	58	61
1	7-B	300/317 (95%)	294 (98%)	6 (2%)	58	61
1	8-A	298/317 (94%)	291 (98%)	7 (2%)	53	56
1	8-B	300/317 (95%)	293 (98%)	7 (2%)	53	56
1	9-A	298/317 (94%)	292 (98%)	6 (2%)	58	61
1	9-B	300/317 (95%)	291 (97%)	9 (3%)	44	44
1	10-A	298/317 (94%)	284 (95%)	14 (5%)	29	24
1	10-B	300/317 (95%)	292 (97%)	8 (3%)	48	49
1	11-A	298/317 (94%)	289 (97%)	9 (3%)	44	44
1	11-B	300/317 (95%)	287 (96%)	13 (4%)	32	28
1	12-A	298/317 (94%)	294 (99%)	4 (1%)	71	76
1	12-B	300/317 (95%)	287 (96%)	13 (4%)	32	28
1	13-A	298/317 (94%)	285 (96%)	13 (4%)	31	27
1	13-B	300/317 (95%)	284 (95%)	16 (5%)	25	20
1	14-A	298/317 (94%)	276 (93%)	22 (7%)	15	10
1	14-B	300/317 (95%)	277 (92%)	23 (8%)	14	9
1	15-A	298/317 (94%)	282 (95%)	16 (5%)	24	19
1	15-B	300/317 (95%)	287 (96%)	13 (4%)	32	28
1	16-A	298/317 (94%)	285 (96%)	13 (4%)	31	27
1	16-B	300/317 (95%)	290 (97%)	10 (3%)	41	39
All	All	9568/10144 (94%)	9244 (97%)	324 (3%)	40	38

5 of 324 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	10-A	311	MET
1	12-A	20	ARG
1	15-B	346	PHE
1	10-A	346	PHE
1	11-A	252	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 348 such sidechains are listed below:

Mol	Chain	Res	Type
1	8-A	366	ASN
1	10-A	324	ASN
1	16-A	97	HIS
1	8-B	195	GLN
1	9-A	314	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FMN	1-A	7401	-	31,33,33	2.38	7 (22%)	39,50,50	3.57	16 (41%)
2	FMN	1-B	9401	-	31,33,33	2.26	6 (19%)	39,50,50	4.27	16 (41%)
2	FMN	10-A	7401	-	31,33,33	2.24	6 (19%)	39,50,50	3.36	17 (43%)
2	FMN	10-B	9401	-	31,33,33	2.43	8 (25%)	39,50,50	4.37	17 (43%)
2	FMN	11-A	7401	-	31,33,33	2.39	6 (19%)	39,50,50	3.75	15 (38%)
2	FMN	11-B	9401	-	31,33,33	2.42	5 (16%)	39,50,50	4.43	16 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	12-A	7401	-	31,33,33	2.39	9 (29%)	39,50,50	3.51	16 (41%)
2	FMN	12-B	9401	-	31,33,33	2.60	7 (22%)	39,50,50	4.04	17 (43%)
2	FMN	13-A	7401	-	31,33,33	2.67	9 (29%)	39,50,50	4.45	20 (51%)
2	FMN	13-B	9401	-	31,33,33	3.36	11 (35%)	39,50,50	4.98	21 (53%)
2	FMN	14-A	7401	-	31,33,33	2.55	15 (48%)	39,50,50	3.69	19 (48%)
2	FMN	14-B	9401	-	31,33,33	2.92	10 (32%)	39,50,50	4.13	16 (41%)
2	FMN	15-A	7401	-	31,33,33	2.14	7 (22%)	39,50,50	3.52	19 (48%)
2	FMN	15-B	9401	-	31,33,33	3.44	11 (35%)	39,50,50	5.03	22 (56%)
2	FMN	16-A	7401	-	31,33,33	2.62	10 (32%)	39,50,50	4.40	20 (51%)
2	FMN	16-B	9401	-	31,33,33	2.62	9 (29%)	39,50,50	4.25	17 (43%)
2	FMN	2-A	7401	-	31,33,33	2.29	8 (25%)	39,50,50	3.48	14 (35%)
2	FMN	2-B	9401	-	31,33,33	2.34	11 (35%)	39,50,50	4.46	18 (46%)
2	FMN	3-A	7401	-	31,33,33	2.33	7 (22%)	39,50,50	3.66	15 (38%)
2	FMN	3-B	9401	-	31,33,33	2.36	6 (19%)	39,50,50	4.53	19 (48%)
2	FMN	4-A	7401	-	31,33,33	2.35	6 (19%)	39,50,50	3.67	15 (38%)
2	FMN	4-B	9401	-	31,33,33	2.19	3 (9%)	39,50,50	4.05	17 (43%)
2	FMN	5-A	7401	-	31,33,33	2.45	6 (19%)	39,50,50	3.79	15 (38%)
2	FMN	5-B	9401	-	31,33,33	2.53	7 (22%)	39,50,50	4.42	19 (48%)
2	FMN	6-A	7401	-	31,33,33	2.62	7 (22%)	39,50,50	3.91	17 (43%)
2	FMN	6-B	9401	-	31,33,33	2.33	12 (38%)	39,50,50	4.39	19 (48%)
2	FMN	7-A	7401	-	31,33,33	2.50	7 (22%)	39,50,50	4.57	20 (51%)
2	FMN	7-B	9401	-	31,33,33	2.77	9 (29%)	39,50,50	4.77	20 (51%)
2	FMN	8-A	7401	-	31,33,33	2.67	9 (29%)	39,50,50	3.50	19 (48%)
2	FMN	8-B	9401	-	31,33,33	2.13	3 (9%)	39,50,50	4.53	20 (51%)
2	FMN	9-A	7401	-	31,33,33	2.55	7 (22%)	39,50,50	3.53	18 (46%)
2	FMN	9-B	9401	-	31,33,33	2.46	12 (38%)	39,50,50	4.23	16 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	1-A	7401	-	-	0/16/18/18	0/3/3/3
2	FMN	1-B	9401	-	-	0/16/18/18	0/3/3/3
2	FMN	10-A	7401	-	-	0/16/18/18	0/3/3/3
2	FMN	10-B	9401	-	-	0/16/18/18	0/3/3/3

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

The worst 5 of 256 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	11-B	9401	FMN	C5'-C4'	-7.75	1.40	1.51
2	1-B	9401	FMN	C5'-C4'	-7.40	1.41	1.51
2	6-A	7401	FMN	C5'-C4'	-6.99	1.41	1.51
2	14-A	7401	FMN	C1'-N10	-5.76	1.42	1.48
2	14-A	7401	FMN	C4'-C3'	-5.24	1.43	1.53

The worst 5 of 565 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	11-B	9401	FMN	O3P-P-O5'	-11.52	76.08	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	365/391 (93%)	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%)

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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 6	7, 18, 33, 53	11712 (100%)

The worst 5 of 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

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 carbohydrates 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FMN	13-B	9401	31/31	0.91	0.21	1,8,16,20	31
2	FMN	15-B	9401	31/31	0.91	0.21	1,8,15,20	31

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

6.5 Other polymers ⓘ

There are no such residues in this entry.