



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:47 am GMT

PDB ID : 2Q3R  
Title : Ensemble refinement of the protein crystal structure of At1g76680 from *Arabidopsis thaliana*  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

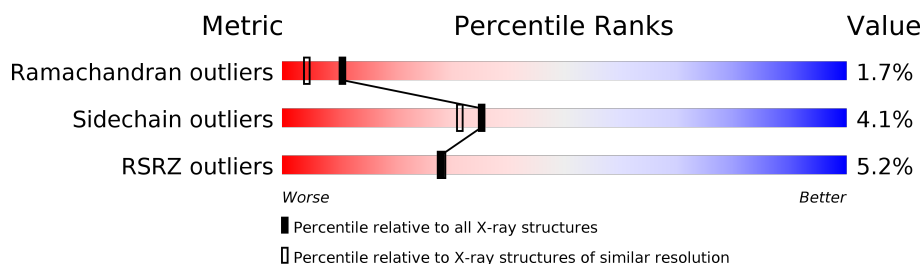
# 1 Overall quality at a glance

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))
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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  $\geq 3$ , 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	372	
1	10-A	372	
1	11-A	372	
1	12-A	372	
1	13-A	372	
1	14-A	372	
1	15-A	372	
1	16-A	372	

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Mol	Chain	Length	Quality of chain
1	2-A	372	
1	3-A	372	
1	4-A	372	
1	5-A	372	
1	6-A	372	
1	7-A	372	
1	8-A	372	
1	9-A	372	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FMN	1-A	373	-	-	-	X
2	FMN	10-A	373	-	-	-	X
2	FMN	11-A	373	-	-	-	X
2	FMN	12-A	373	-	-	-	X
2	FMN	13-A	373	-	-	-	X
2	FMN	14-A	373	-	-	-	X
2	FMN	15-A	373	-	-	-	X
2	FMN	16-A	373	-	-	-	X
2	FMN	2-A	373	-	-	-	X
2	FMN	3-A	373	-	-	-	X
2	FMN	4-A	373	-	-	-	X
2	FMN	5-A	373	-	-	-	X
2	FMN	6-A	373	-	-	-	X
2	FMN	8-A	373	-	-	-	X
2	FMN	9-A	373	-	-	-	X

## 2 Entry composition

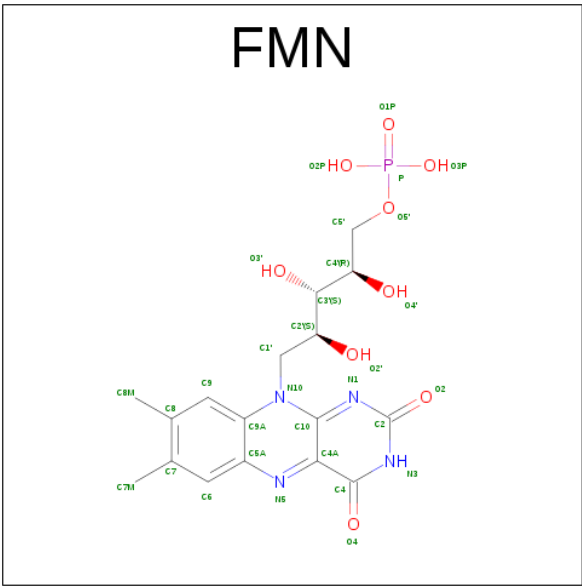
There are 3 unique types of molecules in this entry. The entry contains 46176 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	2-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	3-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	4-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	5-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	6-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	7-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	8-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	9-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	10-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	11-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	12-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	13-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	14-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	15-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			
1	16-A	351	Total	C	N	O	S	0	0	0
			2748	1749	478	508	13			

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	14-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	15-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	16-A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

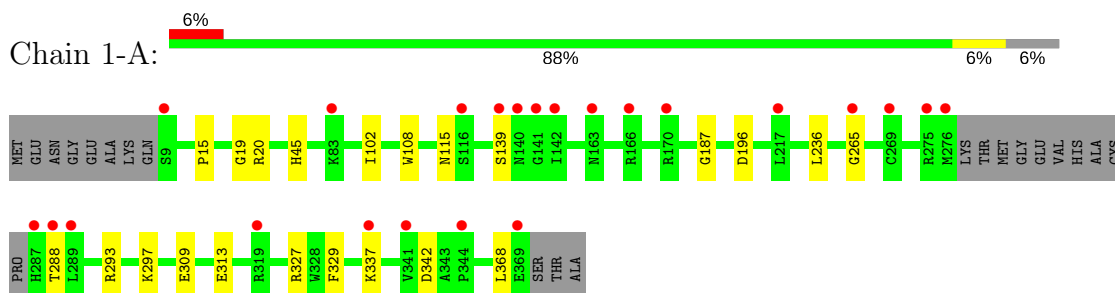
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	107	Total	O	0	0
			107	107		
3	2-A	107	Total	O	0	0
			107	107		
3	3-A	107	Total	O	0	0
			107	107		
3	4-A	107	Total	O	0	0
			107	107		
3	5-A	107	Total	O	0	0
			107	107		
3	6-A	107	Total	O	0	0
			107	107		
3	7-A	107	Total	O	0	0
			107	107		
3	8-A	107	Total	O	0	0
			107	107		
3	9-A	107	Total	O	0	0
			107	107		
3	10-A	107	Total	O	0	0
			107	107		
3	11-A	107	Total	O	0	0
			107	107		
3	12-A	107	Total	O	0	0
			107	107		
3	13-A	107	Total	O	0	0
			107	107		
3	14-A	107	Total	O	0	0
			107	107		
3	15-A	107	Total	O	0	0
			107	107		
3	16-A	107	Total	O	0	0
			107	107		

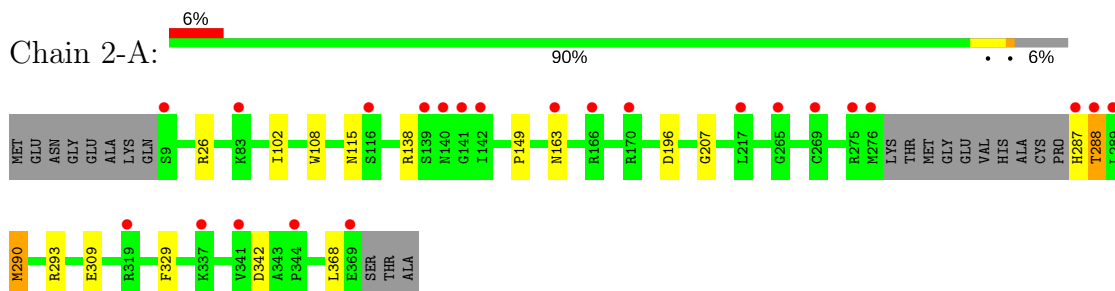
### 3 Residue-property plots [i](#)

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.

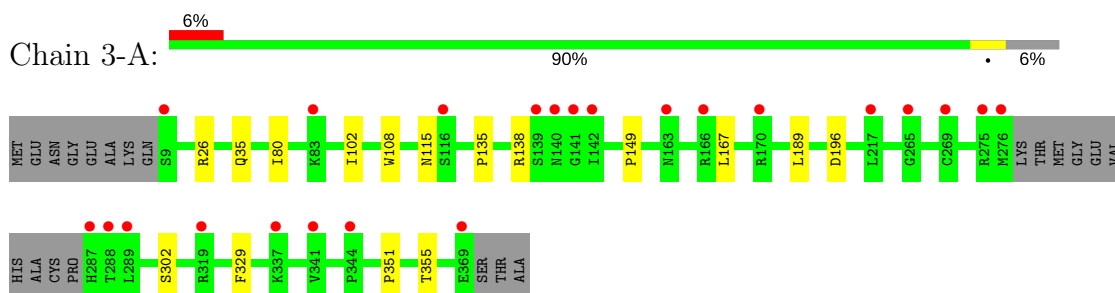
#### • Molecule 1: 12-oxophytodienoate reductase 1



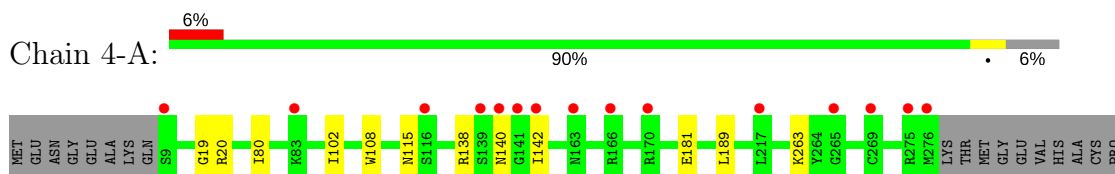
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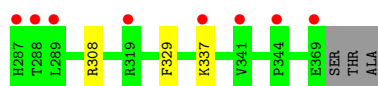


#### • Molecule 1: 12-oxophytodienoate reductase 1

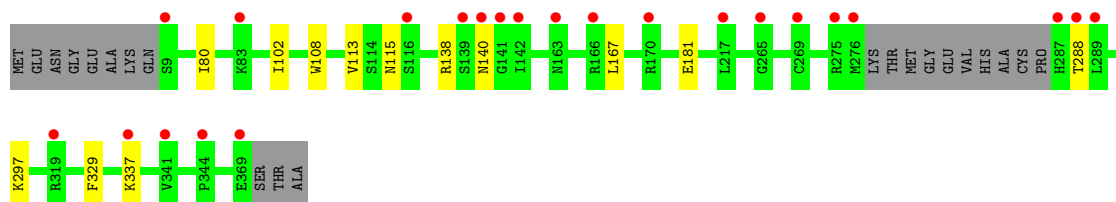


#### • Molecule 1: 12-oxophytodienoate reductase 1

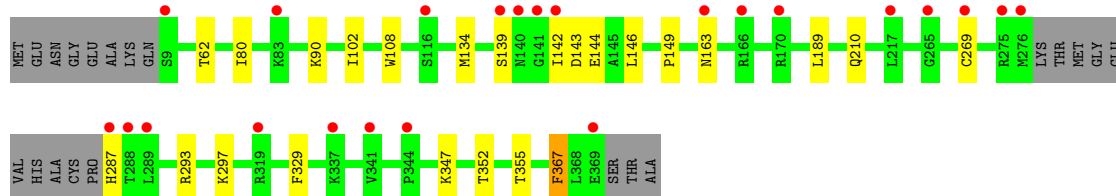
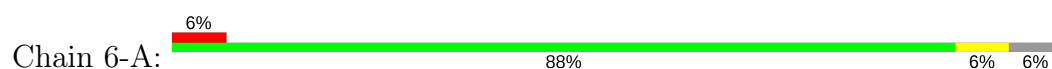




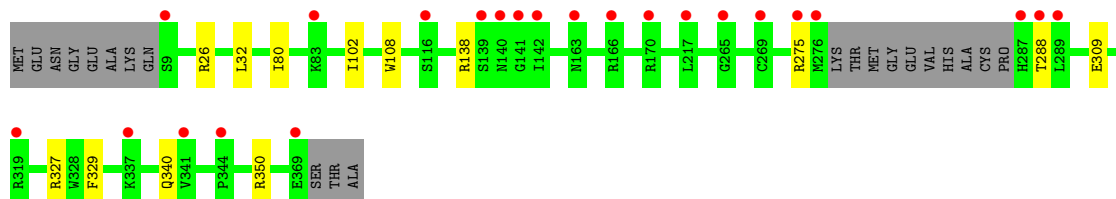
- Molecule 1: 12-oxophytodienoate reductase 1



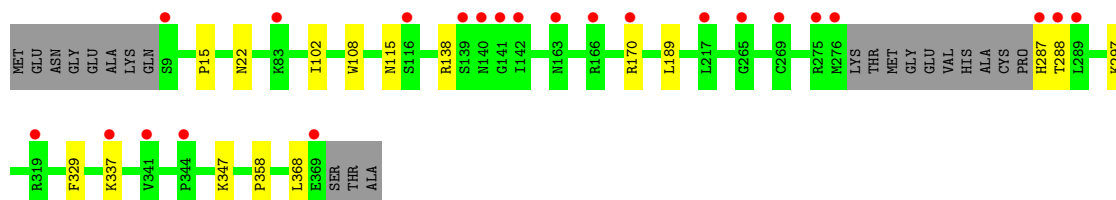
- Molecule 1: 12-oxophytodienoate reductase 1



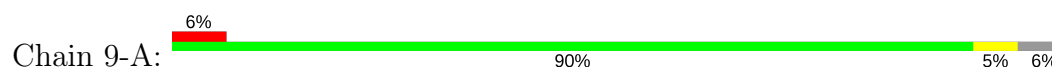
- Molecule 1: 12-oxophytodienoate reductase 1



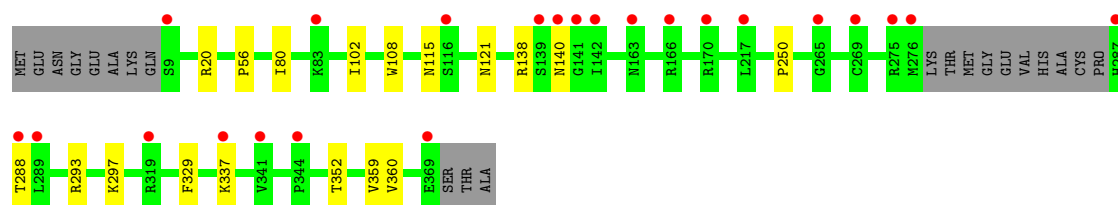
- Molecule 1: 12-oxophytodienoate reductase 1



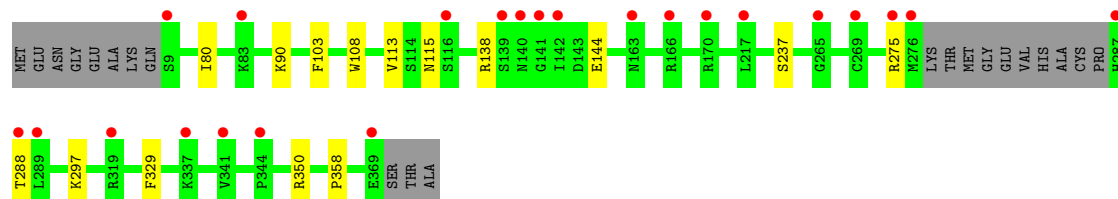
- Molecule 1: 12-oxophytodienoate reductase 1



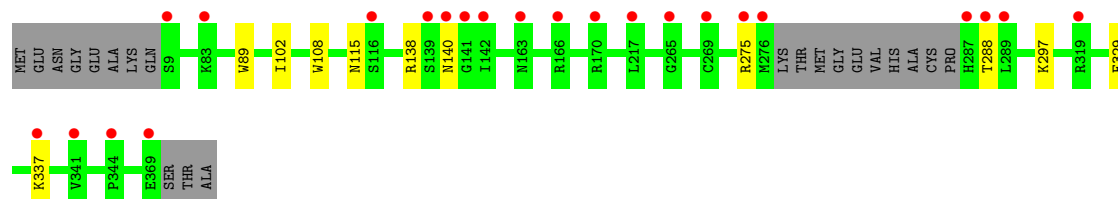




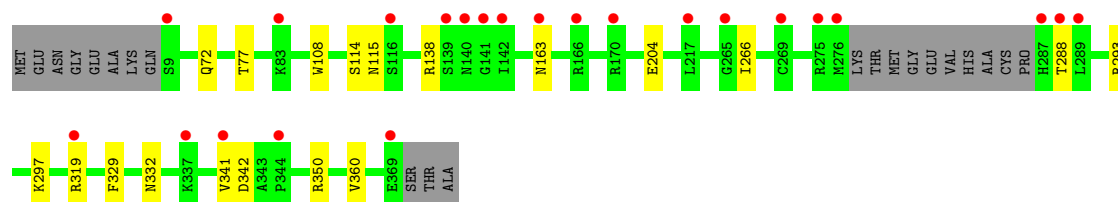
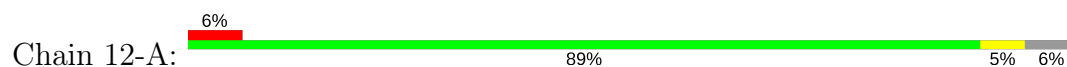
- Molecule 1: 12-oxophytodienoate reductase 1



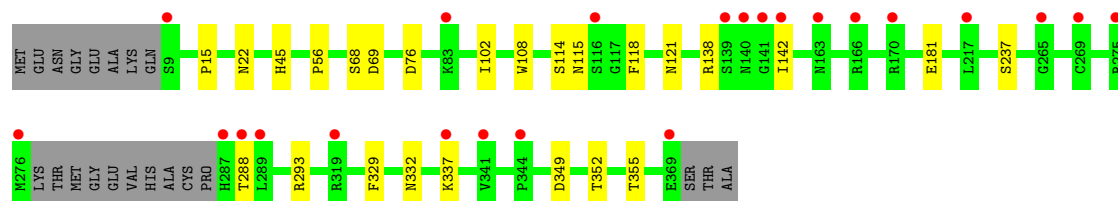
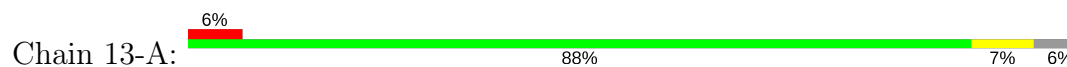
- Molecule 1: 12-oxophytodienoate reductase 1



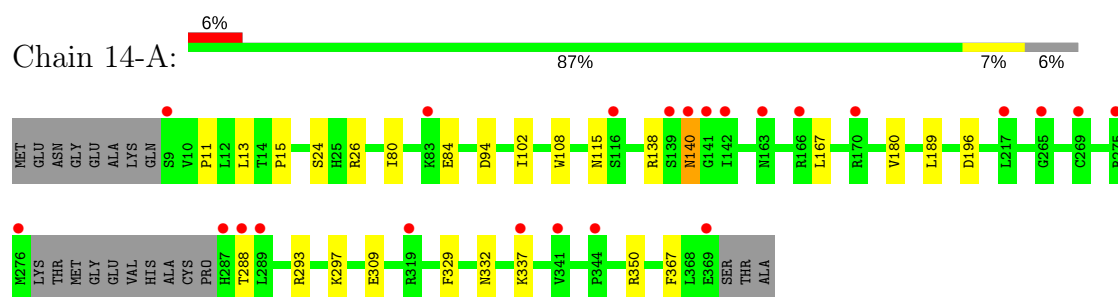
- Molecule 1: 12-oxophytodienoate reductase 1



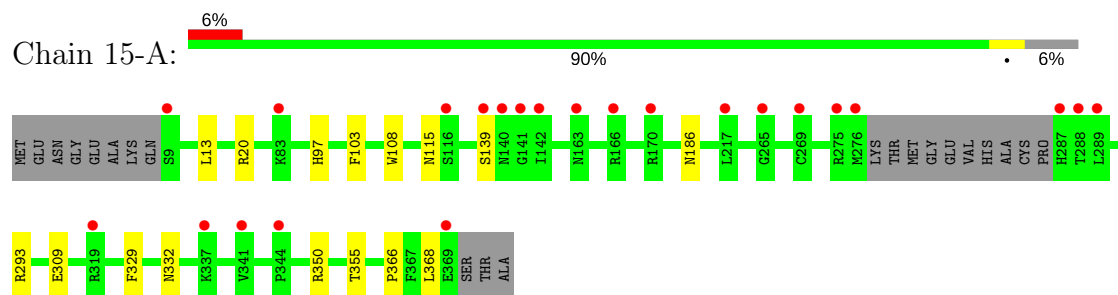
- Molecule 1: 12-oxophytodienoate reductase 1



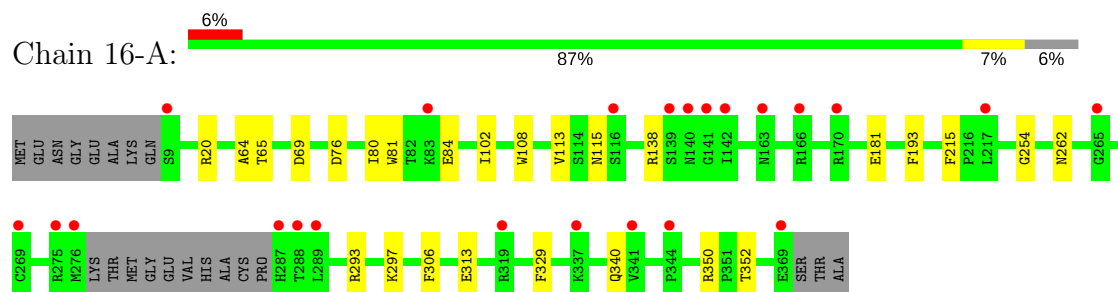
- Molecule 1: 12-oxophytodienoate reductase 1



- Molecule 1: 12-oxophytodienoate reductase 1



- Molecule 1: 12-oxophytodienoate reductase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.69Å 88.07Å 149.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.24 – 2.00 44.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (42.24-2.00) 98.1 (44.03-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.195 , 0.282 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 75.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	46176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.48	0/2822	0.70	1/3831 (0.0%)
1	2-A	0.48	0/2822	0.69	1/3831 (0.0%)
1	3-A	0.50	0/2822	0.69	1/3831 (0.0%)
1	4-A	0.49	0/2822	0.69	1/3831 (0.0%)
1	5-A	0.49	0/2822	0.69	1/3831 (0.0%)
1	6-A	0.49	0/2822	0.69	1/3831 (0.0%)
1	7-A	0.48	0/2822	0.68	1/3831 (0.0%)
1	8-A	0.48	0/2822	0.69	1/3831 (0.0%)
1	9-A	0.49	0/2822	0.69	1/3831 (0.0%)
1	10-A	0.49	0/2822	0.68	0/3831
1	11-A	0.49	0/2822	0.68	1/3831 (0.0%)
1	12-A	0.48	0/2822	0.69	0/3831
1	13-A	0.57	0/2822	0.75	0/3831
1	14-A	0.55	0/2822	0.75	1/3831 (0.0%)
1	15-A	0.54	0/2822	0.75	0/3831
1	16-A	0.55	0/2822	0.75	1/3831 (0.0%)
All	All	0.50	0/45152	0.71	12/61296 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	14-A	102	ILE	N-CA-C	-5.80	95.35	111.00
1	16-A	102	ILE	N-CA-C	-5.73	95.54	111.00
1	1-A	102	ILE	N-CA-C	-5.63	95.79	111.00
1	8-A	102	ILE	N-CA-C	-5.19	96.99	111.00
1	7-A	102	ILE	N-CA-C	-5.16	97.07	111.00
1	9-A	102	ILE	N-CA-C	-5.15	97.09	111.00
1	4-A	102	ILE	N-CA-C	-5.13	97.16	111.00
1	6-A	102	ILE	N-CA-C	-5.10	97.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5-A	102	ILE	N-CA-C	-5.08	97.28	111.00
1	2-A	102	ILE	N-CA-C	-5.08	97.29	111.00
1	11-A	102	ILE	N-CA-C	-5.05	97.36	111.00
1	3-A	102	ILE	N-CA-C	-5.00	97.49	111.00

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	2748	0	2676	0	0
1	2-A	2748	0	2676	0	0
1	3-A	2748	0	2676	0	0
1	4-A	2748	0	2676	0	0
1	5-A	2748	0	2676	0	0
1	6-A	2748	0	2676	0	0
1	7-A	2748	0	2676	0	0
1	8-A	2748	0	2676	0	0
1	9-A	2748	0	2676	0	0
1	10-A	2748	0	2676	0	0
1	11-A	2748	0	2676	0	0
1	12-A	2748	0	2676	0	0
1	13-A	2748	0	2676	0	0
1	14-A	2748	0	2676	0	0
1	15-A	2748	0	2676	0	0
1	16-A	2748	0	2676	0	0
2	1-A	31	0	19	0	0
2	2-A	31	0	19	0	0
2	3-A	31	0	19	0	0
2	4-A	31	0	19	0	0
2	5-A	31	0	19	0	0
2	6-A	31	0	19	0	0
2	7-A	31	0	19	0	0
2	8-A	31	0	19	0	0
2	9-A	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	10-A	31	0	19	0	0
2	11-A	31	0	19	0	0
2	12-A	31	0	19	0	0
2	13-A	31	0	19	0	0
2	14-A	31	0	19	0	0
2	15-A	31	0	18	0	0
2	16-A	31	0	18	0	0
3	1-A	107	0	0	0	0
3	2-A	107	0	0	0	0
3	3-A	107	0	0	0	0
3	4-A	107	0	0	0	0
3	5-A	107	0	0	0	0
3	6-A	107	0	0	0	0
3	7-A	107	0	0	0	0
3	8-A	107	0	0	0	0
3	9-A	107	0	0	0	0
3	10-A	107	0	0	0	0
3	11-A	107	0	0	0	0
3	12-A	107	0	0	0	0
3	13-A	107	0	0	0	0
3	14-A	107	0	0	0	0
3	15-A	107	0	0	0	0
3	16-A	107	0	0	0	0
All	All	46176	0	43118	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	347/372 (93%)	300 (86%)	40 (12%)	7 (2%)	9	3
1	2-A	347/372 (93%)	307 (88%)	34 (10%)	6 (2%)	11	4
1	3-A	347/372 (93%)	313 (90%)	28 (8%)	6 (2%)	11	4
1	4-A	347/372 (93%)	298 (86%)	41 (12%)	8 (2%)	7	3
1	5-A	347/372 (93%)	315 (91%)	29 (8%)	3 (1%)	20	12
1	6-A	347/372 (93%)	304 (88%)	35 (10%)	8 (2%)	7	3
1	7-A	347/372 (93%)	315 (91%)	27 (8%)	5 (1%)	13	6
1	8-A	347/372 (93%)	318 (92%)	24 (7%)	5 (1%)	13	6
1	9-A	347/372 (93%)	311 (90%)	28 (8%)	8 (2%)	7	3
1	10-A	347/372 (93%)	315 (91%)	25 (7%)	7 (2%)	9	3
1	11-A	347/372 (93%)	321 (92%)	24 (7%)	2 (1%)	28	21
1	12-A	347/372 (93%)	301 (87%)	39 (11%)	7 (2%)	9	3
1	13-A	347/372 (93%)	312 (90%)	27 (8%)	8 (2%)	7	3
1	14-A	347/372 (93%)	312 (90%)	30 (9%)	5 (1%)	13	6
1	15-A	347/372 (93%)	312 (90%)	33 (10%)	2 (1%)	28	21
1	16-A	347/372 (93%)	292 (84%)	47 (14%)	8 (2%)	7	3
All	All	5552/5952 (93%)	4946 (89%)	511 (9%)	95 (2%)	11	4

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	139	SER
1	1-A	368	LEU
1	4-A	140	ASN
1	4-A	189	LEU
1	4-A	308	ARG
1	5-A	288	THR
1	6-A	142	ILE
1	6-A	144	GLU
1	6-A	189	LEU
1	8-A	189	LEU
1	9-A	360	VAL
1	12-A	288	THR
1	12-A	319	ARG
1	12-A	342	ASP
1	15-A	139	SER
1	15-A	368	LEU

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Mol	Chain	Res	Type
1	1-A	20	ARG
1	1-A	187	GLY
1	1-A	265	GLY
1	1-A	342	ASP
1	2-A	290	MET
1	2-A	368	LEU
1	3-A	355	THR
1	6-A	139	SER
1	7-A	275	ARG
1	7-A	327	ARG
1	8-A	337	LYS
1	8-A	368	LEU
1	9-A	288	THR
1	10-A	275	ARG
1	10-A	288	THR
1	11-A	275	ARG
1	11-A	288	THR
1	12-A	204	GLU
1	12-A	360	VAL
1	13-A	102	ILE
1	13-A	121	ASN
1	14-A	140	ASN
1	14-A	288	THR
1	16-A	64	ALA
1	16-A	69	ASP
1	16-A	76	ASP
1	16-A	80	ILE
1	3-A	35	GLN
1	4-A	20	ARG
1	5-A	80	ILE
1	6-A	146	LEU
1	8-A	288	THR
1	9-A	56	PRO
1	10-A	144	GLU
1	13-A	69	ASP
1	13-A	114	SER
1	13-A	118	PHE
1	13-A	288	THR
1	14-A	189	LEU
1	2-A	288	THR
1	2-A	342	ASP
1	3-A	189	LEU

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Mol	Chain	Res	Type
1	6-A	143	ASP
1	6-A	367	PHE
1	7-A	340	GLN
1	9-A	140	ASN
1	13-A	68	SER
1	14-A	80	ILE
1	3-A	80	ILE
1	3-A	135	PRO
1	4-A	142	ILE
1	4-A	263	LYS
1	7-A	80	ILE
1	9-A	250	PRO
1	10-A	90	LYS
1	10-A	358	PRO
1	16-A	340	GLN
1	4-A	80	ILE
1	6-A	80	ILE
1	7-A	288	THR
1	9-A	121	ASN
1	9-A	359	VAL
1	12-A	114	SER
1	1-A	19	GLY
1	3-A	351	PRO
1	4-A	19	GLY
1	8-A	358	PRO
1	9-A	80	ILE
1	10-A	80	ILE
1	16-A	113	VAL
1	16-A	215	PHE
1	2-A	149	PRO
1	2-A	207	GLY
1	16-A	254	GLY
1	12-A	341	VAL
1	5-A	113	VAL
1	10-A	113	VAL
1	13-A	56	PRO
1	14-A	11	PRO

### 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	290/306 (95%)	276 (95%)	14 (5%)	30	25
1	2-A	290/306 (95%)	278 (96%)	12 (4%)	35	31
1	3-A	290/306 (95%)	281 (97%)	9 (3%)	45	44
1	4-A	290/306 (95%)	284 (98%)	6 (2%)	59	62
1	5-A	290/306 (95%)	281 (97%)	9 (3%)	45	44
1	6-A	290/306 (95%)	274 (94%)	16 (6%)	25	20
1	7-A	290/306 (95%)	283 (98%)	7 (2%)	54	56
1	8-A	290/306 (95%)	280 (97%)	10 (3%)	42	40
1	9-A	290/306 (95%)	281 (97%)	9 (3%)	45	44
1	10-A	290/306 (95%)	282 (97%)	8 (3%)	49	49
1	11-A	290/306 (95%)	282 (97%)	8 (3%)	49	49
1	12-A	290/306 (95%)	278 (96%)	12 (4%)	35	31
1	13-A	290/306 (95%)	273 (94%)	17 (6%)	23	17
1	14-A	290/306 (95%)	269 (93%)	21 (7%)	17	11
1	15-A	290/306 (95%)	276 (95%)	14 (5%)	30	25
1	16-A	290/306 (95%)	273 (94%)	17 (6%)	23	17
All	All	4640/4896 (95%)	4451 (96%)	189 (4%)	35	31

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	15	PRO
1	1-A	45	HIS
1	1-A	108	TRP
1	1-A	115	ASN
1	1-A	196	ASP
1	1-A	236	LEU
1	1-A	288	THR
1	1-A	293	ARG
1	1-A	297	LYS
1	1-A	309	GLU
1	1-A	313	GLU
1	1-A	327	ARG

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Mol	Chain	Res	Type
1	1-A	329	PHE
1	1-A	337	LYS
1	2-A	26	ARG
1	2-A	108	TRP
1	2-A	115	ASN
1	2-A	138	ARG
1	2-A	163	ASN
1	2-A	196	ASP
1	2-A	287	HIS
1	2-A	288	THR
1	2-A	290	MET
1	2-A	293	ARG
1	2-A	309	GLU
1	2-A	329	PHE
1	3-A	26	ARG
1	3-A	108	TRP
1	3-A	115	ASN
1	3-A	138	ARG
1	3-A	149	PRO
1	3-A	167	LEU
1	3-A	196	ASP
1	3-A	302	SER
1	3-A	329	PHE
1	4-A	108	TRP
1	4-A	115	ASN
1	4-A	138	ARG
1	4-A	181	GLU
1	4-A	329	PHE
1	4-A	337	LYS
1	5-A	108	TRP
1	5-A	115	ASN
1	5-A	138	ARG
1	5-A	140	ASN
1	5-A	167	LEU
1	5-A	181	GLU
1	5-A	297	LYS
1	5-A	329	PHE
1	5-A	337	LYS
1	6-A	62	THR
1	6-A	90	LYS
1	6-A	108	TRP
1	6-A	134	MET

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Mol	Chain	Res	Type
1	6-A	149	PRO
1	6-A	163	ASN
1	6-A	210	GLN
1	6-A	269	CYS
1	6-A	287	HIS
1	6-A	293	ARG
1	6-A	297	LYS
1	6-A	329	PHE
1	6-A	347	LYS
1	6-A	352	THR
1	6-A	355	THR
1	6-A	367	PHE
1	7-A	26	ARG
1	7-A	32	LEU
1	7-A	108	TRP
1	7-A	138	ARG
1	7-A	309	GLU
1	7-A	329	PHE
1	7-A	350	ARG
1	8-A	15	PRO
1	8-A	22	ASN
1	8-A	108	TRP
1	8-A	115	ASN
1	8-A	138	ARG
1	8-A	170	ARG
1	8-A	287	HIS
1	8-A	297	LYS
1	8-A	329	PHE
1	8-A	347	LYS
1	9-A	20	ARG
1	9-A	108	TRP
1	9-A	115	ASN
1	9-A	138	ARG
1	9-A	293	ARG
1	9-A	297	LYS
1	9-A	329	PHE
1	9-A	337	LYS
1	9-A	352	THR
1	10-A	103	PHE
1	10-A	108	TRP
1	10-A	115	ASN
1	10-A	138	ARG

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Mol	Chain	Res	Type
1	10-A	237	SER
1	10-A	297	LYS
1	10-A	329	PHE
1	10-A	350	ARG
1	11-A	89	TRP
1	11-A	108	TRP
1	11-A	115	ASN
1	11-A	138	ARG
1	11-A	140	ASN
1	11-A	297	LYS
1	11-A	329	PHE
1	11-A	337	LYS
1	12-A	72	GLN
1	12-A	77	THR
1	12-A	108	TRP
1	12-A	115	ASN
1	12-A	138	ARG
1	12-A	163	ASN
1	12-A	266	ILE
1	12-A	293	ARG
1	12-A	297	LYS
1	12-A	329	PHE
1	12-A	332	ASN
1	12-A	350	ARG
1	13-A	15	PRO
1	13-A	22	ASN
1	13-A	45	HIS
1	13-A	76	ASP
1	13-A	108	TRP
1	13-A	115	ASN
1	13-A	138	ARG
1	13-A	142	ILE
1	13-A	181	GLU
1	13-A	237	SER
1	13-A	293	ARG
1	13-A	329	PHE
1	13-A	332	ASN
1	13-A	337	LYS
1	13-A	349	ASP
1	13-A	352	THR
1	13-A	355	THR
1	14-A	13	LEU

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Mol	Chain	Res	Type
1	14-A	15	PRO
1	14-A	24	SER
1	14-A	26	ARG
1	14-A	84	GLU
1	14-A	94	ASP
1	14-A	108	TRP
1	14-A	115	ASN
1	14-A	138	ARG
1	14-A	140	ASN
1	14-A	167	LEU
1	14-A	180	VAL
1	14-A	196	ASP
1	14-A	293	ARG
1	14-A	297	LYS
1	14-A	309	GLU
1	14-A	329	PHE
1	14-A	332	ASN
1	14-A	337	LYS
1	14-A	350	ARG
1	14-A	367	PHE
1	15-A	13	LEU
1	15-A	20	ARG
1	15-A	97	HIS
1	15-A	103	PHE
1	15-A	108	TRP
1	15-A	115	ASN
1	15-A	186	ASN
1	15-A	293	ARG
1	15-A	309	GLU
1	15-A	329	PHE
1	15-A	332	ASN
1	15-A	350	ARG
1	15-A	355	THR
1	15-A	366	PRO
1	16-A	20	ARG
1	16-A	65	THR
1	16-A	81	TRP
1	16-A	84	GLU
1	16-A	108	TRP
1	16-A	115	ASN
1	16-A	138	ARG
1	16-A	181	GLU

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Mol	Chain	Res	Type
1	16-A	193	PHE
1	16-A	262	ASN
1	16-A	293	ARG
1	16-A	297	LYS
1	16-A	306	PHE
1	16-A	313	GLU
1	16-A	329	PHE
1	16-A	350	ARG
1	16-A	352	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	40	ASN
1	1-A	43	GLN
1	1-A	75	GLN
1	1-A	97	HIS
1	1-A	199	ASN
1	1-A	210	GLN
1	2-A	43	GLN
1	2-A	97	HIS
1	2-A	115	ASN
1	2-A	163	ASN
1	2-A	199	ASN
1	2-A	211	ASN
1	2-A	346	ASN
1	3-A	40	ASN
1	3-A	97	HIS
1	3-A	121	ASN
1	3-A	312	ASN
1	3-A	346	ASN
1	4-A	35	GLN
1	4-A	43	GLN
1	4-A	97	HIS
1	4-A	115	ASN
1	4-A	140	ASN
1	4-A	171	ASN
1	4-A	199	ASN
1	4-A	211	ASN
1	5-A	43	GLN
1	5-A	75	GLN
1	5-A	97	HIS

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Mol	Chain	Res	Type
1	5-A	115	ASN
1	5-A	312	ASN
1	6-A	43	GLN
1	6-A	97	HIS
1	6-A	115	ASN
1	6-A	210	GLN
1	6-A	211	ASN
1	7-A	35	GLN
1	7-A	43	GLN
1	7-A	97	HIS
1	8-A	35	GLN
1	8-A	40	ASN
1	8-A	43	GLN
1	8-A	97	HIS
1	8-A	115	ASN
1	8-A	312	ASN
1	8-A	340	GLN
1	9-A	43	GLN
1	9-A	97	HIS
1	9-A	115	ASN
1	9-A	140	ASN
1	9-A	171	ASN
1	9-A	186	ASN
1	10-A	35	GLN
1	10-A	43	GLN
1	10-A	115	ASN
1	11-A	35	GLN
1	11-A	43	GLN
1	11-A	97	HIS
1	11-A	115	ASN
1	11-A	171	ASN
1	11-A	262	ASN
1	12-A	35	GLN
1	12-A	40	ASN
1	12-A	45	HIS
1	12-A	72	GLN
1	12-A	97	HIS
1	12-A	115	ASN
1	12-A	163	ASN
1	13-A	35	GLN
1	13-A	43	GLN
1	13-A	97	HIS

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Mol	Chain	Res	Type
1	13-A	115	ASN
1	13-A	119	GLN
1	13-A	140	ASN
1	13-A	262	ASN
1	14-A	35	GLN
1	14-A	43	GLN
1	14-A	97	HIS
1	14-A	115	ASN
1	14-A	211	ASN
1	15-A	35	GLN
1	15-A	43	GLN
1	15-A	115	ASN
1	15-A	121	ASN
1	15-A	199	ASN
1	15-A	346	ASN
1	16-A	22	ASN
1	16-A	43	GLN
1	16-A	75	GLN
1	16-A	85	HIS
1	16-A	115	ASN
1	16-A	140	ASN
1	16-A	211	ASN
1	16-A	262	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 ⓘ

16 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	373	-	31,33,33	2.23	8 (25%)	38,50,50	3.91	19 (50%)
2	FMN	10-A	373	-	31,33,33	2.32	7 (22%)	38,50,50	3.76	17 (44%)
2	FMN	11-A	373	-	31,33,33	2.38	7 (22%)	38,50,50	3.67	16 (42%)
2	FMN	12-A	373	-	31,33,33	2.26	7 (22%)	38,50,50	3.82	17 (44%)
2	FMN	13-A	373	-	31,33,33	2.53	12 (38%)	38,50,50	4.75	17 (44%)
2	FMN	14-A	373	-	31,33,33	2.62	9 (29%)	38,50,50	3.98	13 (34%)
2	FMN	15-A	373	-	31,33,33	2.58	14 (45%)	38,50,50	4.87	17 (44%)
2	FMN	16-A	373	-	31,33,33	2.56	12 (38%)	38,50,50	4.78	16 (42%)
2	FMN	2-A	373	-	31,33,33	2.33	7 (22%)	38,50,50	3.74	17 (44%)
2	FMN	3-A	373	-	31,33,33	2.45	7 (22%)	38,50,50	3.42	19 (50%)
2	FMN	4-A	373	-	31,33,33	2.27	8 (25%)	38,50,50	3.77	15 (39%)
2	FMN	5-A	373	-	31,33,33	2.45	9 (29%)	38,50,50	3.61	16 (42%)
2	FMN	6-A	373	-	31,33,33	2.29	7 (22%)	38,50,50	3.39	19 (50%)
2	FMN	7-A	373	-	31,33,33	2.64	9 (29%)	38,50,50	3.45	14 (36%)
2	FMN	8-A	373	-	31,33,33	2.39	7 (22%)	38,50,50	3.66	16 (42%)
2	FMN	9-A	373	-	31,33,33	1.97	6 (19%)	38,50,50	3.60	15 (39%)

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	373	-	-	0/16/18/18	0/3/3/3
2	FMN	10-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	11-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	12-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	13-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	14-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	15-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	16-A	373	-	-	0/16/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	2-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	3-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	4-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	5-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	6-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	7-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	8-A	373	-	-	0/16/18/18	0/3/3/3
2	FMN	9-A	373	-	-	0/16/18/18	0/3/3/3

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-A	373	FMN	C5'-C4'	-6.96	1.41	1.51
2	7-A	373	FMN	C2-N1	-6.79	1.24	1.38
2	1-A	373	FMN	C1'-N10	-6.40	1.41	1.48
2	6-A	373	FMN	C5'-C4'	-6.03	1.42	1.51
2	15-A	373	FMN	C4'-C3'	-4.53	1.44	1.53
2	16-A	373	FMN	C4'-C3'	-4.49	1.44	1.53
2	13-A	373	FMN	C4'-C3'	-4.49	1.44	1.53
2	14-A	373	FMN	C4'-C3'	-4.22	1.45	1.53
2	11-A	373	FMN	P-O5'	-3.76	1.48	1.60
2	8-A	373	FMN	P-O5'	-3.64	1.48	1.60
2	15-A	373	FMN	C2-N1	-3.64	1.31	1.38
2	2-A	373	FMN	P-O5'	-3.61	1.48	1.60
2	10-A	373	FMN	P-O5'	-3.56	1.48	1.60
2	13-A	373	FMN	C2-N1	-3.49	1.31	1.38
2	11-A	373	FMN	C4'-C3'	-3.26	1.47	1.53
2	8-A	373	FMN	C4'-C3'	-3.25	1.47	1.53
2	16-A	373	FMN	C2-N1	-3.20	1.31	1.38
2	7-A	373	FMN	C2-N3	-3.15	1.31	1.38
2	5-A	373	FMN	P-O5'	-3.09	1.50	1.60
2	2-A	373	FMN	C4'-C3'	-3.07	1.47	1.53
2	14-A	373	FMN	C2-N1	-2.99	1.32	1.38
2	10-A	373	FMN	C4'-C3'	-2.99	1.47	1.53
2	5-A	373	FMN	C4'-C3'	-2.95	1.47	1.53
2	16-A	373	FMN	O5'-C5'	-2.94	1.33	1.44
2	16-A	373	FMN	O3'-C3'	-2.87	1.36	1.43
2	12-A	373	FMN	C4'-C3'	-2.84	1.47	1.53
2	15-A	373	FMN	O3'-C3'	-2.77	1.36	1.43
2	16-A	373	FMN	P-O5'	-2.75	1.51	1.60
2	15-A	373	FMN	O5'-C5'	-2.73	1.34	1.44
2	4-A	373	FMN	C4'-C3'	-2.72	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5-A	373	FMN	C5'-C4'	-2.54	1.48	1.51
2	13-A	373	FMN	O5'-C5'	-2.50	1.34	1.44
2	15-A	373	FMN	P-O5'	-2.39	1.52	1.60
2	10-A	373	FMN	C2-N1	-2.29	1.33	1.38
2	15-A	373	FMN	O4-C4	-2.28	1.18	1.24
2	15-A	373	FMN	C2-N3	-2.25	1.33	1.38
2	8-A	373	FMN	C2-N1	-2.24	1.33	1.38
2	2-A	373	FMN	C2-N1	-2.24	1.33	1.38
2	13-A	373	FMN	O4-C4	-2.23	1.18	1.24
2	11-A	373	FMN	C2-N1	-2.22	1.33	1.38
2	5-A	373	FMN	C2-N1	-2.20	1.33	1.38
2	4-A	373	FMN	C2-N1	-2.17	1.33	1.38
2	3-A	373	FMN	C2-N1	-2.16	1.33	1.38
2	13-A	373	FMN	C2-N3	-2.12	1.34	1.38
2	9-A	373	FMN	C2-N1	-2.10	1.34	1.38
2	12-A	373	FMN	C2-N1	-2.10	1.34	1.38
2	16-A	373	FMN	C2-N3	-2.09	1.34	1.38
2	13-A	373	FMN	O3'-C3'	-2.03	1.38	1.43
2	14-A	373	FMN	P-O1P	-2.02	1.43	1.50
2	16-A	373	FMN	C4-N3	2.01	1.36	1.33
2	16-A	373	FMN	P-O2P	2.01	1.63	1.54
2	15-A	373	FMN	P-O2P	2.02	1.63	1.54
2	4-A	373	FMN	C4-N3	2.09	1.36	1.33
2	7-A	373	FMN	C4-N3	2.10	1.36	1.33
2	9-A	373	FMN	O3'-C3'	2.13	1.47	1.43
2	7-A	373	FMN	C6-C5A	2.14	1.45	1.41
2	6-A	373	FMN	C6-C5A	2.19	1.45	1.41
2	13-A	373	FMN	C9A-C5A	2.20	1.47	1.42
2	15-A	373	FMN	C9A-C5A	2.20	1.47	1.42
2	12-A	373	FMN	C1'-N10	2.20	1.50	1.48
2	1-A	373	FMN	C4-N3	2.21	1.37	1.33
2	15-A	373	FMN	C1'-N10	2.21	1.50	1.48
2	5-A	373	FMN	P-O2P	2.21	1.63	1.54
2	13-A	373	FMN	C2'-C3'	2.27	1.58	1.53
2	4-A	373	FMN	P-O3P	2.31	1.64	1.54
2	9-A	373	FMN	C4-N3	2.34	1.37	1.33
2	4-A	373	FMN	C1'-N10	2.35	1.50	1.48
2	6-A	373	FMN	C9-C9A	2.36	1.45	1.40
2	12-A	373	FMN	P-O3P	2.38	1.64	1.54
2	1-A	373	FMN	O3'-C3'	2.49	1.48	1.43
2	15-A	373	FMN	C5'-C4'	2.53	1.55	1.51
2	6-A	373	FMN	C4-N3	2.63	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	13-A	373	FMN	C4-C4A	2.64	1.46	1.41
2	1-A	373	FMN	O2'-C2'	2.64	1.49	1.43
2	15-A	373	FMN	C4-C4A	2.64	1.46	1.41
2	7-A	373	FMN	P-O3P	2.65	1.65	1.54
2	3-A	373	FMN	C4-N3	2.66	1.37	1.33
2	16-A	373	FMN	C1'-N10	2.77	1.51	1.48
2	14-A	373	FMN	C5'-C4'	2.91	1.56	1.51
2	14-A	373	FMN	C4-C4A	2.96	1.47	1.41
2	13-A	373	FMN	C5'-C4'	3.07	1.56	1.51
2	10-A	373	FMN	C1'-N10	3.11	1.51	1.48
2	7-A	373	FMN	C1'-N10	3.20	1.51	1.48
2	2-A	373	FMN	C1'-N10	3.26	1.51	1.48
2	2-A	373	FMN	C4-C4A	3.33	1.47	1.41
2	1-A	373	FMN	C4-C4A	3.33	1.47	1.41
2	11-A	373	FMN	C1'-N10	3.34	1.51	1.48
2	3-A	373	FMN	C4-C4A	3.35	1.47	1.41
2	1-A	373	FMN	C2'-C3'	3.36	1.60	1.53
2	8-A	373	FMN	C1'-N10	3.36	1.51	1.48
2	10-A	373	FMN	C4-C4A	3.39	1.47	1.41
2	11-A	373	FMN	C4-C4A	3.41	1.47	1.41
2	3-A	373	FMN	C1'-N10	3.47	1.52	1.48
2	8-A	373	FMN	C4-C4A	3.47	1.48	1.41
2	5-A	373	FMN	C4-C4A	3.59	1.48	1.41
2	1-A	373	FMN	C9A-N10	3.67	1.43	1.38
2	5-A	373	FMN	C1'-N10	3.71	1.52	1.48
2	4-A	373	FMN	C4-C4A	3.79	1.48	1.41
2	12-A	373	FMN	C4-C4A	3.83	1.48	1.41
2	7-A	373	FMN	C4-C4A	3.89	1.48	1.41
2	13-A	373	FMN	C4A-C10	3.95	1.48	1.41
2	9-A	373	FMN	C4-C4A	3.96	1.48	1.41
2	15-A	373	FMN	C4A-C10	4.03	1.48	1.41
2	16-A	373	FMN	C4-C4A	4.06	1.49	1.41
2	14-A	373	FMN	C2'-C3'	4.17	1.61	1.53
2	6-A	373	FMN	C4-C4A	4.21	1.49	1.41
2	16-A	373	FMN	C4A-C10	4.29	1.48	1.41
2	14-A	373	FMN	C4A-C10	4.34	1.48	1.41
2	14-A	373	FMN	O2'-C2'	4.58	1.53	1.43
2	10-A	373	FMN	C4A-C10	5.09	1.49	1.41
2	12-A	373	FMN	C4A-C10	5.09	1.49	1.41
2	6-A	373	FMN	C4A-C10	5.18	1.50	1.41
2	2-A	373	FMN	C4A-C10	5.19	1.50	1.41
2	4-A	373	FMN	C4A-C10	5.27	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	11-A	373	FMN	C4A-C10	5.32	1.50	1.41
2	8-A	373	FMN	C4A-C10	5.32	1.50	1.41
2	1-A	373	FMN	C4A-C10	5.47	1.50	1.41
2	9-A	373	FMN	C4A-C10	5.56	1.50	1.41
2	5-A	373	FMN	C4A-C10	5.57	1.50	1.41
2	9-A	373	FMN	C9A-N10	5.83	1.46	1.38
2	3-A	373	FMN	C4A-C10	5.94	1.51	1.41
2	6-A	373	FMN	C9A-N10	6.32	1.47	1.38
2	3-A	373	FMN	C9A-N10	6.51	1.47	1.38
2	7-A	373	FMN	C4A-C10	6.56	1.52	1.41
2	7-A	373	FMN	C9A-N10	7.36	1.48	1.38
2	2-A	373	FMN	C9A-N10	7.94	1.49	1.38
2	10-A	373	FMN	C9A-N10	7.96	1.49	1.38
2	11-A	373	FMN	C9A-N10	7.98	1.49	1.38
2	16-A	373	FMN	C9A-N10	8.00	1.49	1.38
2	12-A	373	FMN	C9A-N10	8.01	1.49	1.38
2	4-A	373	FMN	C9A-N10	8.04	1.49	1.38
2	8-A	373	FMN	C9A-N10	8.07	1.49	1.38
2	5-A	373	FMN	C9A-N10	8.31	1.49	1.38
2	15-A	373	FMN	C9A-N10	8.44	1.49	1.38
2	13-A	373	FMN	C9A-N10	8.51	1.49	1.38
2	14-A	373	FMN	C9A-N10	8.65	1.50	1.38

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9-A	373	FMN	O3P-P-O5'	-12.43	73.66	106.73
2	12-A	373	FMN	O3P-P-O5'	-11.38	76.45	106.73
2	4-A	373	FMN	O3P-P-O5'	-11.29	76.69	106.73
2	16-A	373	FMN	O5'-C5'-C4'	-11.16	79.58	109.36
2	15-A	373	FMN	O5'-C5'-C4'	-11.11	79.69	109.36
2	13-A	373	FMN	O5'-C5'-C4'	-10.41	81.58	109.36
2	7-A	373	FMN	O3P-P-O5'	-10.03	80.05	106.73
2	5-A	373	FMN	O3P-P-O5'	-10.01	80.09	106.73
2	1-A	373	FMN	O3P-P-O5'	-9.79	80.67	106.73
2	8-A	373	FMN	O3P-P-O5'	-9.75	80.78	106.73
2	11-A	373	FMN	O3P-P-O5'	-9.68	80.98	106.73
2	10-A	373	FMN	O3P-P-O5'	-9.67	80.99	106.73
2	2-A	373	FMN	O3P-P-O5'	-9.60	81.19	106.73
2	16-A	373	FMN	O3P-P-O1P	-8.89	75.73	110.50
2	13-A	373	FMN	O3P-P-O1P	-8.81	76.01	110.50
2	15-A	373	FMN	O3P-P-O1P	-8.74	76.30	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	6-A	373	FMN	O3P-P-O1P	-8.34	77.85	110.50
2	3-A	373	FMN	O3P-P-O1P	-8.30	78.02	110.50
2	14-A	373	FMN	O3P-P-O5'	-8.06	85.28	106.73
2	16-A	373	FMN	O3P-P-O5'	-8.02	85.39	106.73
2	14-A	373	FMN	O3P-P-O1P	-8.00	79.21	110.50
2	15-A	373	FMN	C1'-N10-C10	-7.90	110.41	118.50
2	15-A	373	FMN	O3P-P-O5'	-7.80	85.97	106.73
2	13-A	373	FMN	O3P-P-O5'	-7.58	86.56	106.73
2	14-A	373	FMN	O5'-C5'-C4'	-7.54	89.23	109.36
2	3-A	373	FMN	O3P-P-O5'	-7.52	86.73	106.73
2	13-A	373	FMN	C1'-N10-C10	-7.52	110.80	118.50
2	13-A	373	FMN	C4'-C3'-C2'	-7.35	97.60	113.41
2	14-A	373	FMN	C4'-C3'-C2'	-7.22	97.87	113.41
2	16-A	373	FMN	C4'-C3'-C2'	-7.10	98.13	113.41
2	7-A	373	FMN	O3P-P-O1P	-7.09	82.75	110.50
2	6-A	373	FMN	O3P-P-O5'	-7.04	87.99	106.73
2	15-A	373	FMN	C4'-C3'-C2'	-7.02	98.30	113.41
2	10-A	373	FMN	O3P-P-O1P	-6.82	83.81	110.50
2	2-A	373	FMN	O3P-P-O1P	-6.77	83.99	110.50
2	1-A	373	FMN	O3P-P-O1P	-6.73	84.15	110.50
2	12-A	373	FMN	O3P-P-O1P	-6.71	84.23	110.50
2	16-A	373	FMN	C1'-N10-C10	-6.71	111.62	118.50
2	4-A	373	FMN	O3P-P-O1P	-6.70	84.28	110.50
2	1-A	373	FMN	O3P-P-O2P	-6.55	81.20	107.61
2	11-A	373	FMN	O3P-P-O1P	-6.51	85.04	110.50
2	8-A	373	FMN	O3P-P-O1P	-6.43	85.34	110.50
2	5-A	373	FMN	O3P-P-O1P	-6.31	85.82	110.50
2	9-A	373	FMN	O3P-P-O1P	-5.89	87.44	110.50
2	15-A	373	FMN	C4-C4A-C10	-5.79	115.28	119.96
2	7-A	373	FMN	O3P-P-O2P	-5.76	84.38	107.61
2	6-A	373	FMN	O3P-P-O2P	-5.62	84.92	107.61
2	3-A	373	FMN	P-O5'-C5'	-5.56	102.98	118.30
2	13-A	373	FMN	C4-C4A-C10	-5.54	115.48	119.96
2	11-A	373	FMN	O3P-P-O2P	-5.49	85.46	107.61
2	2-A	373	FMN	O3P-P-O2P	-5.47	85.54	107.61
2	6-A	373	FMN	C4'-C3'-C2'	-5.45	101.68	113.41
2	10-A	373	FMN	O3P-P-O2P	-5.41	85.79	107.61
2	8-A	373	FMN	O3P-P-O2P	-5.37	85.94	107.61
2	14-A	373	FMN	O3P-P-O2P	-5.36	85.99	107.61
2	16-A	373	FMN	C4-C4A-C10	-5.32	115.66	119.96
2	7-A	373	FMN	C4-C4A-C10	-5.26	115.70	119.96
2	3-A	373	FMN	O3P-P-O2P	-5.24	86.49	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	10-A	373	FMN	O5'-C5'-C4'	-5.20	95.47	109.36
2	2-A	373	FMN	C4'-C3'-C2'	-5.20	102.22	113.41
2	2-A	373	FMN	O5'-C5'-C4'	-5.19	95.50	109.36
2	1-A	373	FMN	P-O5'-C5'	-5.18	104.04	118.30
2	4-A	373	FMN	P-O5'-C5'	-5.17	104.04	118.30
2	10-A	373	FMN	C4'-C3'-C2'	-5.15	102.33	113.41
2	8-A	373	FMN	C4'-C3'-C2'	-5.08	102.48	113.41
2	11-A	373	FMN	C4'-C3'-C2'	-5.02	102.60	113.41
2	7-A	373	FMN	C4A-C4-N3	-5.01	116.35	123.48
2	5-A	373	FMN	O3P-P-O2P	-5.00	87.45	107.61
2	14-A	373	FMN	C4-C4A-C10	-4.98	115.93	119.96
2	5-A	373	FMN	C4'-C3'-C2'	-4.90	102.86	113.41
2	3-A	373	FMN	C4'-C3'-C2'	-4.88	102.91	113.41
2	7-A	373	FMN	P-O5'-C5'	-4.85	104.95	118.30
2	9-A	373	FMN	C4A-C4-N3	-4.82	116.62	123.48
2	5-A	373	FMN	P-O5'-C5'	-4.80	105.06	118.30
2	1-A	373	FMN	C4A-C10-N10	-4.79	117.19	120.52
2	10-A	373	FMN	C4-C4A-C10	-4.66	116.19	119.96
2	12-A	373	FMN	C4-C4A-C10	-4.63	116.22	119.96
2	9-A	373	FMN	O3P-P-O2P	-4.62	88.97	107.61
2	12-A	373	FMN	P-O5'-C5'	-4.61	105.61	118.30
2	6-A	373	FMN	C4A-C4-N3	-4.58	116.96	123.48
2	4-A	373	FMN	C4-C4A-C10	-4.58	116.26	119.96
2	2-A	373	FMN	C4-C4A-C10	-4.58	116.26	119.96
2	8-A	373	FMN	C4-C4A-C10	-4.57	116.27	119.96
2	3-A	373	FMN	C4A-C4-N3	-4.56	116.98	123.48
2	11-A	373	FMN	C4-C4A-C10	-4.54	116.29	119.96
2	12-A	373	FMN	O3P-P-O2P	-4.54	89.32	107.61
2	4-A	373	FMN	C4'-C3'-C2'	-4.52	103.68	113.41
2	5-A	373	FMN	C4-C4A-C10	-4.50	116.32	119.96
2	4-A	373	FMN	O3P-P-O2P	-4.50	89.47	107.61
2	13-A	373	FMN	O3P-P-O2P	-4.49	89.50	107.61
2	11-A	373	FMN	O5'-C5'-C4'	-4.49	97.38	109.36
2	16-A	373	FMN	C4A-C4-N3	-4.47	117.11	123.48
2	12-A	373	FMN	C4'-C3'-C2'	-4.44	103.86	113.41
2	15-A	373	FMN	O3P-P-O2P	-4.41	89.81	107.61
2	8-A	373	FMN	O5'-C5'-C4'	-4.32	97.83	109.36
2	14-A	373	FMN	C4A-C4-N3	-4.24	117.45	123.48
2	1-A	373	FMN	C1'-N10-C9A	-4.21	114.49	118.35
2	16-A	373	FMN	O3P-P-O2P	-4.19	90.72	107.61
2	1-A	373	FMN	O3'-C3'-C4'	-4.18	98.46	108.82
2	5-A	373	FMN	C4A-C4-N3	-4.18	117.54	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1-A	373	FMN	C4A-C4-N3	-4.13	117.60	123.48
2	9-A	373	FMN	P-O5'-C5'	-4.12	106.95	118.30
2	8-A	373	FMN	C4A-C4-N3	-4.06	117.71	123.48
2	11-A	373	FMN	C4A-C4-N3	-4.03	117.74	123.48
2	4-A	373	FMN	C4A-C4-N3	-4.03	117.75	123.48
2	1-A	373	FMN	C4-C4A-C10	-3.99	116.73	119.96
2	12-A	373	FMN	C4A-C4-N3	-3.99	117.80	123.48
2	1-A	373	FMN	C1'-C2'-C3'	-3.99	98.41	109.82
2	10-A	373	FMN	C4A-C4-N3	-3.93	117.88	123.48
2	2-A	373	FMN	C4A-C4-N3	-3.93	117.89	123.48
2	9-A	373	FMN	C4-C4A-C10	-3.87	116.83	119.96
2	6-A	373	FMN	P-O5'-C5'	-3.85	107.70	118.30
2	13-A	373	FMN	C4A-C4-N3	-3.80	118.07	123.48
2	15-A	373	FMN	C4A-C4-N3	-3.72	118.19	123.48
2	3-A	373	FMN	C4-C4A-C10	-3.71	116.96	119.96
2	8-A	373	FMN	P-O5'-C5'	-3.59	108.42	118.30
2	14-A	373	FMN	C1'-N10-C10	-3.56	114.86	118.50
2	9-A	373	FMN	C4'-C3'-C2'	-3.48	105.92	113.41
2	11-A	373	FMN	P-O5'-C5'	-3.44	108.81	118.30
2	3-A	373	FMN	C4A-C10-N10	-3.27	118.25	120.52
2	6-A	373	FMN	C4A-C10-N10	-3.20	118.30	120.52
2	6-A	373	FMN	C4-C4A-C10	-3.16	117.41	119.96
2	6-A	373	FMN	O5'-C5'-C4'	-2.96	101.45	109.36
2	9-A	373	FMN	C4A-C10-N10	-2.96	118.47	120.52
2	5-A	373	FMN	O5'-C5'-C4'	-2.64	102.32	109.36
2	12-A	373	FMN	C1'-N10-C10	-2.60	115.83	118.50
2	13-A	373	FMN	O2'-C2'-C1'	-2.58	103.83	109.79
2	3-A	373	FMN	O4'-C4'-C5'	-2.46	104.51	110.00
2	15-A	373	FMN	O2'-C2'-C1'	-2.40	104.23	109.79
2	5-A	373	FMN	O2'-C2'-C1'	-2.36	104.33	109.79
2	6-A	373	FMN	O4'-C4'-C5'	-2.32	104.84	110.00
2	2-A	373	FMN	P-O5'-C5'	-2.25	112.09	118.30
2	15-A	373	FMN	O4'-C4'-C5'	-2.19	105.13	110.00
2	8-A	373	FMN	O2'-C2'-C1'	-2.18	104.75	109.79
2	11-A	373	FMN	O2'-C2'-C1'	-2.15	104.83	109.79
2	10-A	373	FMN	P-O5'-C5'	-2.14	112.39	118.30
2	16-A	373	FMN	O4'-C4'-C5'	-2.13	105.25	110.00
2	10-A	373	FMN	C1'-N10-C10	-2.11	116.33	118.50
2	2-A	373	FMN	O2'-C2'-C1'	-2.09	104.97	109.79
2	2-A	373	FMN	C1'-N10-C10	-2.05	116.40	118.50
2	13-A	373	FMN	O4'-C4'-C5'	-2.04	105.46	110.00
2	10-A	373	FMN	O2'-C2'-C1'	-2.04	105.08	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3-A	373	FMN	O2'-C2'-C1'	-2.02	105.12	109.79
2	4-A	373	FMN	O4'-C4'-C3'	2.01	114.08	109.09
2	6-A	373	FMN	C1'-N10-C9A	2.04	120.22	118.35
2	6-A	373	FMN	O2P-P-O1P	2.06	118.55	110.50
2	9-A	373	FMN	C5A-C9A-N10	2.15	119.26	117.66
2	12-A	373	FMN	O4'-C4'-C3'	2.20	114.55	109.09
2	3-A	373	FMN	C5A-C9A-N10	2.28	119.35	117.66
2	12-A	373	FMN	O3'-C3'-C2'	2.34	114.60	108.82
2	3-A	373	FMN	C1'-N10-C9A	2.48	120.61	118.35
2	3-A	373	FMN	C4-C4A-N5	2.53	121.45	118.68
2	3-A	373	FMN	C1'-N10-C10	2.62	121.19	118.50
2	16-A	373	FMN	C1'-C2'-C3'	2.77	117.74	109.82
2	10-A	373	FMN	O2P-P-O5'	2.79	114.17	106.73
2	6-A	373	FMN	O2P-P-O5'	2.79	114.17	106.73
2	6-A	373	FMN	C4-C4A-N5	2.80	121.75	118.68
2	9-A	373	FMN	C1'-N10-C9A	2.81	120.92	118.35
2	7-A	373	FMN	C5A-C9A-N10	2.83	119.76	117.66
2	1-A	373	FMN	C5A-C9A-N10	2.87	119.79	117.66
2	2-A	373	FMN	O2P-P-O5'	2.88	114.40	106.73
2	15-A	373	FMN	C1'-C2'-C3'	2.91	118.13	109.82
2	6-A	373	FMN	C1'-N10-C10	2.92	121.50	118.50
2	6-A	373	FMN	C1'-C2'-C3'	2.94	118.22	109.82
2	3-A	373	FMN	O2P-P-O5'	2.97	114.64	106.73
2	3-A	373	FMN	C1'-C2'-C3'	3.03	118.49	109.82
2	13-A	373	FMN	C1'-C2'-C3'	3.05	118.54	109.82
2	12-A	373	FMN	C1'-C2'-C3'	3.12	118.74	109.82
2	5-A	373	FMN	C4-C4A-N5	3.14	122.12	118.68
2	7-A	373	FMN	C1'-N10-C10	3.17	121.75	118.50
2	12-A	373	FMN	O2P-P-O5'	3.19	115.23	106.73
2	4-A	373	FMN	O2P-P-O5'	3.22	115.31	106.73
2	4-A	373	FMN	C1'-C2'-C3'	3.23	119.04	109.82
2	11-A	373	FMN	O2P-P-O5'	3.24	115.35	106.73
2	8-A	373	FMN	C4-C4A-N5	3.26	122.26	118.68
2	8-A	373	FMN	O2P-P-O5'	3.30	115.51	106.73
2	1-A	373	FMN	C4'-C3'-C2'	3.31	120.54	113.41
2	14-A	373	FMN	C4-C4A-N5	3.32	122.32	118.68
2	11-A	373	FMN	C4-C4A-N5	3.33	122.33	118.68
2	2-A	373	FMN	C4-C4A-N5	3.36	122.37	118.68
2	10-A	373	FMN	C4-C4A-N5	3.36	122.37	118.68
2	9-A	373	FMN	C4-C4A-N5	3.39	122.40	118.68
2	1-A	373	FMN	C4-C4A-N5	3.41	122.42	118.68
2	5-A	373	FMN	O2P-P-O5'	3.44	115.89	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	373	FMN	O2P-P-O5'	3.49	116.03	106.73
2	2-A	373	FMN	C1'-C2'-C3'	3.50	119.83	109.82
2	10-A	373	FMN	C1'-C2'-C3'	3.53	119.90	109.82
2	11-A	373	FMN	C1'-C2'-C3'	3.56	120.00	109.82
2	8-A	373	FMN	C1'-C2'-C3'	3.61	120.15	109.82
2	4-A	373	FMN	C4-C4A-N5	3.62	122.65	118.68
2	12-A	373	FMN	C4-C4A-N5	3.69	122.72	118.68
2	13-A	373	FMN	C4-C4A-N5	3.80	122.85	118.68
2	5-A	373	FMN	C1'-C2'-C3'	3.86	120.85	109.82
2	7-A	373	FMN	C1'-N10-C9A	3.86	121.89	118.35
2	16-A	373	FMN	C4-C4A-N5	3.87	122.92	118.68
2	15-A	373	FMN	C4-C4A-N5	3.94	123.00	118.68
2	9-A	373	FMN	O2P-P-O5'	4.21	117.93	106.73
2	1-A	373	FMN	O2P-P-O5'	4.21	117.93	106.73
2	16-A	373	FMN	C4A-N5-C5A	4.57	121.59	116.76
2	7-A	373	FMN	C4-C4A-N5	4.60	123.72	118.68
2	15-A	373	FMN	C4A-N5-C5A	4.63	121.65	116.76
2	13-A	373	FMN	C4A-N5-C5A	4.68	121.70	116.76
2	7-A	373	FMN	C4A-N5-C5A	5.00	122.04	116.76
2	2-A	373	FMN	C4A-N5-C5A	5.04	122.08	116.76
2	10-A	373	FMN	C4A-N5-C5A	5.07	122.11	116.76
2	8-A	373	FMN	C4A-N5-C5A	5.10	122.14	116.76
2	5-A	373	FMN	C4A-N5-C5A	5.11	122.15	116.76
2	1-A	373	FMN	C4A-N5-C5A	5.12	122.17	116.76
2	14-A	373	FMN	C4A-N5-C5A	5.13	122.18	116.76
2	11-A	373	FMN	C4A-N5-C5A	5.15	122.20	116.76
2	13-A	373	FMN	P-O5'-C5'	5.15	132.48	118.30
2	3-A	373	FMN	C4A-N5-C5A	5.16	122.21	116.76
2	9-A	373	FMN	C4A-N5-C5A	5.19	122.24	116.76
2	4-A	373	FMN	C4A-N5-C5A	5.21	122.26	116.76
2	12-A	373	FMN	C4A-N5-C5A	5.21	122.27	116.76
2	1-A	373	FMN	O2'-C2'-C3'	5.27	122.17	109.09
2	16-A	373	FMN	P-O5'-C5'	5.29	132.87	118.30
2	15-A	373	FMN	P-O5'-C5'	5.44	133.28	118.30
2	7-A	373	FMN	O5'-P-O1P	5.73	122.53	106.47
2	5-A	373	FMN	C1'-N10-C9A	5.88	123.73	118.35
2	6-A	373	FMN	C4A-N5-C5A	6.04	123.14	116.76
2	6-A	373	FMN	O5'-P-O1P	6.05	123.44	106.47
2	3-A	373	FMN	O5'-P-O1P	6.07	123.50	106.47
2	1-A	373	FMN	O5'-P-O1P	6.14	123.70	106.47
2	1-A	373	FMN	C1'-N10-C10	6.63	125.30	118.50
2	9-A	373	FMN	O5'-P-O1P	6.72	125.33	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5-A	373	FMN	O5'-P-O1P	6.82	125.60	106.47
2	11-A	373	FMN	O5'-P-O1P	6.87	125.74	106.47
2	8-A	373	FMN	O5'-P-O1P	6.87	125.75	106.47
2	8-A	373	FMN	C1'-N10-C9A	7.15	124.90	118.35
2	12-A	373	FMN	O5'-P-O1P	7.22	126.73	106.47
2	11-A	373	FMN	C1'-N10-C9A	7.27	125.01	118.35
2	4-A	373	FMN	O5'-P-O1P	7.27	126.87	106.47
2	2-A	373	FMN	O5'-P-O1P	7.30	126.94	106.47
2	10-A	373	FMN	O5'-P-O1P	7.38	127.17	106.47
2	7-A	373	FMN	C4-N3-C2	7.39	121.62	115.16
2	3-A	373	FMN	C4-N3-C2	7.56	121.78	115.16
2	6-A	373	FMN	C4-N3-C2	7.62	121.83	115.16
2	13-A	373	FMN	C4-N3-C2	7.64	121.84	115.16
2	15-A	373	FMN	C4-N3-C2	7.64	121.84	115.16
2	4-A	373	FMN	C1'-N10-C9A	7.72	125.42	118.35
2	2-A	373	FMN	C4-N3-C2	7.79	121.97	115.16
2	11-A	373	FMN	C4-N3-C2	7.81	121.99	115.16
2	1-A	373	FMN	C4-N3-C2	7.83	122.01	115.16
2	10-A	373	FMN	C4-N3-C2	7.84	122.02	115.16
2	4-A	373	FMN	C4-N3-C2	7.87	122.04	115.16
2	8-A	373	FMN	C4-N3-C2	7.88	122.05	115.16
2	14-A	373	FMN	C4-N3-C2	7.93	122.09	115.16
2	16-A	373	FMN	C4-N3-C2	7.97	122.13	115.16
2	12-A	373	FMN	C4-N3-C2	7.97	122.13	115.16
2	5-A	373	FMN	C4-N3-C2	7.97	122.13	115.16
2	14-A	373	FMN	O5'-P-O1P	8.20	129.49	106.47
2	2-A	373	FMN	C1'-N10-C9A	8.31	125.96	118.35
2	9-A	373	FMN	C4-N3-C2	8.33	122.44	115.16
2	12-A	373	FMN	C1'-N10-C9A	8.36	126.01	118.35
2	10-A	373	FMN	C1'-N10-C9A	8.49	126.13	118.35
2	14-A	373	FMN	C1'-N10-C9A	9.13	126.71	118.35
2	13-A	373	FMN	O5'-P-O1P	9.41	132.87	106.47
2	15-A	373	FMN	O5'-P-O1P	9.47	133.04	106.47
2	16-A	373	FMN	O5'-P-O1P	9.55	133.25	106.47
2	16-A	373	FMN	C1'-N10-C9A	13.87	131.06	118.35
2	13-A	373	FMN	C1'-N10-C9A	13.88	131.06	118.35
2	15-A	373	FMN	C1'-N10-C9A	14.65	131.77	118.35

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	1-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	2-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	3-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	4-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	5-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	6-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	7-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	8-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	9-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	10-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	11-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	12-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	13-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	14-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	15-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
1	16-A	351/372 (94%)	0.38	23 (6%)	19	19	13, 27, 45, 64	351 (100%)
All	All	5616/5952 (94%)	0.38	368 (6%)	28	19	13, 27, 46, 64	5616 (100%)

All (368) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	141	GLY	7.3
1	2-A	141	GLY	7.3
1	3-A	141	GLY	7.3
1	4-A	141	GLY	7.3
1	5-A	141	GLY	7.3

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Mol	Chain	Res	Type	RSRZ
1	6-A	141	GLY	7.3
1	7-A	141	GLY	7.3
1	8-A	141	GLY	7.3
1	9-A	141	GLY	7.3
1	10-A	141	GLY	7.3
1	11-A	141	GLY	7.3
1	12-A	141	GLY	7.3
1	13-A	141	GLY	7.3
1	14-A	141	GLY	7.3
1	15-A	141	GLY	7.3
1	16-A	141	GLY	7.3
1	1-A	140	ASN	5.2
1	2-A	140	ASN	5.2
1	3-A	140	ASN	5.2
1	4-A	140	ASN	5.2
1	5-A	140	ASN	5.2
1	6-A	140	ASN	5.2
1	7-A	140	ASN	5.2
1	8-A	140	ASN	5.2
1	9-A	140	ASN	5.2
1	10-A	140	ASN	5.2
1	11-A	140	ASN	5.2
1	12-A	140	ASN	5.2
1	13-A	140	ASN	5.2
1	14-A	140	ASN	5.2
1	15-A	140	ASN	5.2
1	16-A	140	ASN	5.2
1	1-A	142	ILE	4.8
1	2-A	142	ILE	4.8
1	3-A	142	ILE	4.8
1	4-A	142	ILE	4.8
1	5-A	142	ILE	4.8
1	6-A	142	ILE	4.8
1	7-A	142	ILE	4.8
1	8-A	142	ILE	4.8
1	9-A	142	ILE	4.8
1	10-A	142	ILE	4.8
1	11-A	142	ILE	4.8
1	12-A	142	ILE	4.8
1	13-A	142	ILE	4.8
1	14-A	142	ILE	4.8
1	15-A	142	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	16-A	142	ILE	4.8
1	1-A	288	THR	4.5
1	2-A	288	THR	4.5
1	3-A	288	THR	4.5
1	4-A	288	THR	4.5
1	5-A	288	THR	4.5
1	6-A	288	THR	4.5
1	7-A	288	THR	4.5
1	8-A	288	THR	4.5
1	9-A	288	THR	4.5
1	10-A	288	THR	4.5
1	11-A	288	THR	4.5
1	12-A	288	THR	4.5
1	13-A	288	THR	4.5
1	14-A	288	THR	4.5
1	15-A	288	THR	4.5
1	16-A	288	THR	4.5
1	1-A	166	ARG	4.0
1	2-A	166	ARG	4.0
1	3-A	166	ARG	4.0
1	4-A	166	ARG	4.0
1	5-A	166	ARG	4.0
1	6-A	166	ARG	4.0
1	7-A	166	ARG	4.0
1	8-A	166	ARG	4.0
1	9-A	166	ARG	4.0
1	10-A	166	ARG	4.0
1	11-A	166	ARG	4.0
1	12-A	166	ARG	4.0
1	13-A	166	ARG	4.0
1	14-A	166	ARG	4.0
1	15-A	166	ARG	4.0
1	16-A	166	ARG	4.0
1	1-A	319	ARG	3.8
1	2-A	319	ARG	3.8
1	3-A	319	ARG	3.8
1	4-A	319	ARG	3.8
1	5-A	319	ARG	3.8
1	6-A	319	ARG	3.8
1	7-A	319	ARG	3.8
1	8-A	319	ARG	3.8
1	9-A	319	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	10-A	319	ARG	3.8
1	11-A	319	ARG	3.8
1	12-A	319	ARG	3.8
1	13-A	319	ARG	3.8
1	14-A	319	ARG	3.8
1	15-A	319	ARG	3.8
1	16-A	319	ARG	3.8
1	1-A	9	SER	3.6
1	2-A	9	SER	3.6
1	3-A	9	SER	3.6
1	4-A	9	SER	3.6
1	5-A	9	SER	3.6
1	6-A	9	SER	3.6
1	7-A	9	SER	3.6
1	8-A	9	SER	3.6
1	9-A	9	SER	3.6
1	10-A	9	SER	3.6
1	11-A	9	SER	3.6
1	12-A	9	SER	3.6
1	13-A	9	SER	3.6
1	14-A	9	SER	3.6
1	15-A	9	SER	3.6
1	16-A	9	SER	3.6
1	1-A	116	SER	3.5
1	2-A	116	SER	3.5
1	3-A	116	SER	3.5
1	4-A	116	SER	3.5
1	5-A	116	SER	3.5
1	6-A	116	SER	3.5
1	7-A	116	SER	3.5
1	8-A	116	SER	3.5
1	9-A	116	SER	3.5
1	10-A	116	SER	3.5
1	11-A	116	SER	3.5
1	12-A	116	SER	3.5
1	13-A	116	SER	3.5
1	14-A	116	SER	3.5
1	15-A	116	SER	3.5
1	16-A	116	SER	3.5
1	1-A	139	SER	3.5
1	2-A	139	SER	3.5
1	3-A	139	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	4-A	139	SER	3.5
1	5-A	139	SER	3.5
1	6-A	139	SER	3.5
1	7-A	139	SER	3.5
1	8-A	139	SER	3.5
1	9-A	139	SER	3.5
1	10-A	139	SER	3.5
1	11-A	139	SER	3.5
1	12-A	139	SER	3.5
1	13-A	139	SER	3.5
1	14-A	139	SER	3.5
1	15-A	139	SER	3.5
1	16-A	139	SER	3.5
1	1-A	83	LYS	3.2
1	2-A	83	LYS	3.2
1	3-A	83	LYS	3.2
1	4-A	83	LYS	3.2
1	5-A	83	LYS	3.2
1	6-A	83	LYS	3.2
1	7-A	83	LYS	3.2
1	8-A	83	LYS	3.2
1	9-A	83	LYS	3.2
1	10-A	83	LYS	3.2
1	11-A	83	LYS	3.2
1	12-A	83	LYS	3.2
1	13-A	83	LYS	3.2
1	14-A	83	LYS	3.2
1	15-A	83	LYS	3.2
1	16-A	83	LYS	3.2
1	1-A	337	LYS	3.2
1	2-A	337	LYS	3.2
1	3-A	337	LYS	3.2
1	4-A	337	LYS	3.2
1	5-A	337	LYS	3.2
1	6-A	337	LYS	3.2
1	7-A	337	LYS	3.2
1	8-A	337	LYS	3.2
1	9-A	337	LYS	3.2
1	10-A	337	LYS	3.2
1	11-A	337	LYS	3.2
1	12-A	337	LYS	3.2
1	13-A	337	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	14-A	337	LYS	3.2
1	15-A	337	LYS	3.2
1	16-A	337	LYS	3.2
1	1-A	369	GLU	3.1
1	2-A	369	GLU	3.1
1	3-A	369	GLU	3.1
1	4-A	369	GLU	3.1
1	5-A	369	GLU	3.1
1	6-A	369	GLU	3.1
1	7-A	369	GLU	3.1
1	8-A	369	GLU	3.1
1	9-A	369	GLU	3.1
1	10-A	369	GLU	3.1
1	11-A	369	GLU	3.1
1	12-A	369	GLU	3.1
1	13-A	369	GLU	3.1
1	14-A	369	GLU	3.1
1	15-A	369	GLU	3.1
1	16-A	369	GLU	3.1
1	1-A	276	MET	3.0
1	2-A	276	MET	3.0
1	3-A	276	MET	3.0
1	4-A	276	MET	3.0
1	5-A	276	MET	3.0
1	6-A	276	MET	3.0
1	7-A	276	MET	3.0
1	8-A	276	MET	3.0
1	9-A	276	MET	3.0
1	10-A	276	MET	3.0
1	11-A	276	MET	3.0
1	12-A	276	MET	3.0
1	13-A	276	MET	3.0
1	14-A	276	MET	3.0
1	15-A	276	MET	3.0
1	16-A	276	MET	3.0
1	1-A	217	LEU	2.9
1	2-A	217	LEU	2.9
1	3-A	217	LEU	2.9
1	4-A	217	LEU	2.9
1	5-A	217	LEU	2.9
1	6-A	217	LEU	2.9
1	7-A	217	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	8-A	217	LEU	2.9
1	9-A	217	LEU	2.9
1	10-A	217	LEU	2.9
1	11-A	217	LEU	2.9
1	12-A	217	LEU	2.9
1	13-A	217	LEU	2.9
1	14-A	217	LEU	2.9
1	15-A	217	LEU	2.9
1	16-A	217	LEU	2.9
1	1-A	341	VAL	2.9
1	2-A	341	VAL	2.9
1	3-A	341	VAL	2.9
1	4-A	341	VAL	2.9
1	5-A	341	VAL	2.9
1	6-A	341	VAL	2.9
1	7-A	341	VAL	2.9
1	8-A	341	VAL	2.9
1	9-A	341	VAL	2.9
1	10-A	341	VAL	2.9
1	11-A	341	VAL	2.9
1	12-A	341	VAL	2.9
1	13-A	341	VAL	2.9
1	14-A	341	VAL	2.9
1	15-A	341	VAL	2.9
1	16-A	341	VAL	2.9
1	1-A	269	CYS	2.6
1	2-A	269	CYS	2.6
1	3-A	269	CYS	2.6
1	4-A	269	CYS	2.6
1	5-A	269	CYS	2.6
1	6-A	269	CYS	2.6
1	7-A	269	CYS	2.6
1	8-A	269	CYS	2.6
1	9-A	269	CYS	2.6
1	10-A	269	CYS	2.6
1	11-A	269	CYS	2.6
1	12-A	269	CYS	2.6
1	13-A	269	CYS	2.6
1	14-A	269	CYS	2.6
1	15-A	269	CYS	2.6
1	16-A	269	CYS	2.6
1	1-A	287	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	2-A	287	HIS	2.6
1	3-A	287	HIS	2.6
1	4-A	287	HIS	2.6
1	5-A	287	HIS	2.6
1	6-A	287	HIS	2.6
1	7-A	287	HIS	2.6
1	8-A	287	HIS	2.6
1	9-A	287	HIS	2.6
1	10-A	287	HIS	2.6
1	11-A	287	HIS	2.6
1	12-A	287	HIS	2.6
1	13-A	287	HIS	2.6
1	14-A	287	HIS	2.6
1	15-A	287	HIS	2.6
1	16-A	287	HIS	2.6
1	1-A	265	GLY	2.6
1	2-A	265	GLY	2.6
1	3-A	265	GLY	2.6
1	4-A	265	GLY	2.6
1	5-A	265	GLY	2.6
1	6-A	265	GLY	2.6
1	7-A	265	GLY	2.6
1	8-A	265	GLY	2.6
1	9-A	265	GLY	2.6
1	10-A	265	GLY	2.6
1	11-A	265	GLY	2.6
1	12-A	265	GLY	2.6
1	13-A	265	GLY	2.6
1	14-A	265	GLY	2.6
1	15-A	265	GLY	2.6
1	16-A	265	GLY	2.6
1	1-A	163	ASN	2.3
1	2-A	163	ASN	2.3
1	3-A	163	ASN	2.3
1	4-A	163	ASN	2.3
1	5-A	163	ASN	2.3
1	6-A	163	ASN	2.3
1	7-A	163	ASN	2.3
1	8-A	163	ASN	2.3
1	9-A	163	ASN	2.3
1	10-A	163	ASN	2.3
1	11-A	163	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	12-A	163	ASN	2.3
1	13-A	163	ASN	2.3
1	14-A	163	ASN	2.3
1	15-A	163	ASN	2.3
1	16-A	163	ASN	2.3
1	1-A	344	PRO	2.1
1	2-A	344	PRO	2.1
1	3-A	344	PRO	2.1
1	4-A	344	PRO	2.1
1	5-A	344	PRO	2.1
1	6-A	344	PRO	2.1
1	7-A	344	PRO	2.1
1	8-A	344	PRO	2.1
1	9-A	344	PRO	2.1
1	10-A	344	PRO	2.1
1	11-A	344	PRO	2.1
1	12-A	344	PRO	2.1
1	13-A	344	PRO	2.1
1	14-A	344	PRO	2.1
1	15-A	344	PRO	2.1
1	16-A	344	PRO	2.1
1	1-A	289	LEU	2.1
1	2-A	289	LEU	2.1
1	3-A	289	LEU	2.1
1	4-A	289	LEU	2.1
1	5-A	289	LEU	2.1
1	6-A	289	LEU	2.1
1	7-A	289	LEU	2.1
1	8-A	289	LEU	2.1
1	9-A	289	LEU	2.1
1	10-A	289	LEU	2.1
1	11-A	289	LEU	2.1
1	12-A	289	LEU	2.1
1	13-A	289	LEU	2.1
1	14-A	289	LEU	2.1
1	15-A	289	LEU	2.1
1	16-A	289	LEU	2.1
1	1-A	170	ARG	2.1
1	2-A	170	ARG	2.1
1	3-A	170	ARG	2.1
1	4-A	170	ARG	2.1
1	5-A	170	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	6-A	170	ARG	2.1
1	7-A	170	ARG	2.1
1	8-A	170	ARG	2.1
1	9-A	170	ARG	2.1
1	10-A	170	ARG	2.1
1	11-A	170	ARG	2.1
1	12-A	170	ARG	2.1
1	13-A	170	ARG	2.1
1	14-A	170	ARG	2.1
1	15-A	170	ARG	2.1
1	16-A	170	ARG	2.1
1	1-A	275	ARG	2.1
1	2-A	275	ARG	2.1
1	3-A	275	ARG	2.1
1	4-A	275	ARG	2.1
1	5-A	275	ARG	2.1
1	6-A	275	ARG	2.1
1	7-A	275	ARG	2.1
1	8-A	275	ARG	2.1
1	9-A	275	ARG	2.1
1	10-A	275	ARG	2.1
1	11-A	275	ARG	2.1
1	12-A	275	ARG	2.1
1	13-A	275	ARG	2.1
1	14-A	275	ARG	2.1
1	15-A	275	ARG	2.1
1	16-A	275	ARG	2.1

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FMN	2-A	373	31/31	0.92	0.18	2.96	9,17,24,27	31
2	FMN	14-A	373	31/31	0.92	0.18	2.96	0,16,22,26	31
2	FMN	10-A	373	31/31	0.92	0.18	2.95	9,16,24,27	31
2	FMN	13-A	373	31/31	0.92	0.18	2.93	4,17,20,25	31
2	FMN	15-A	373	31/31	0.92	0.18	2.93	4,17,20,26	31
2	FMN	16-A	373	31/31	0.92	0.18	2.93	4,16,22,25	31
2	FMN	8-A	373	31/31	0.92	0.18	2.92	9,17,25,25	31
2	FMN	1-A	373	31/31	0.92	0.18	2.92	0,16,21,25	31
2	FMN	5-A	373	31/31	0.92	0.18	2.88	9,16,24,25	31
2	FMN	12-A	373	31/31	0.92	0.18	2.87	11,16,22,25	31
2	FMN	11-A	373	31/31	0.92	0.18	2.87	9,17,25,26	31
2	FMN	9-A	373	31/31	0.92	0.18	2.87	8,16,20,24	31
2	FMN	6-A	373	31/31	0.92	0.18	2.86	1,17,20,26	31
2	FMN	4-A	373	31/31	0.92	0.18	2.82	11,16,21,25	31
2	FMN	3-A	373	31/31	0.92	0.18	2.60	7,16,21,24	31
2	FMN	7-A	373	31/31	0.92	0.18	1.30	0,17,21,21	31

## 6.5 Other polymers

There are no such residues in this entry.