



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:30 AM GMT

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

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

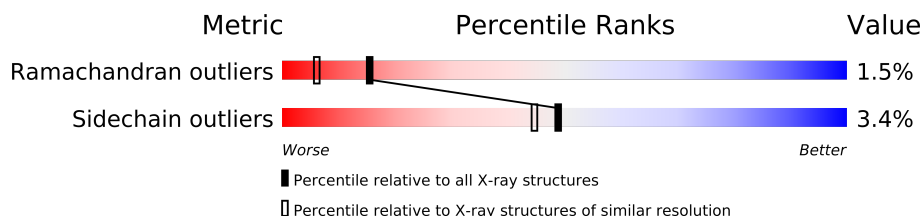
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

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



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

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

Note EDS failed to run properly.

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

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

2 Entry composition

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

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

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

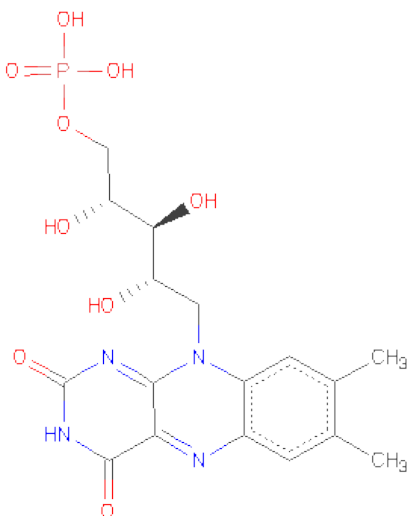
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	1-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	2-A	365	Total	C	N	O	S	0	0	0
			2810	1779	495	524	12			
1	2-B	367	Total	C	N	O	S	0	0	0
			2839	1799	499	529	12			
1	3-A	365	Total	C	N	O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

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

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



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

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

- Molecule 3 is water.

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

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

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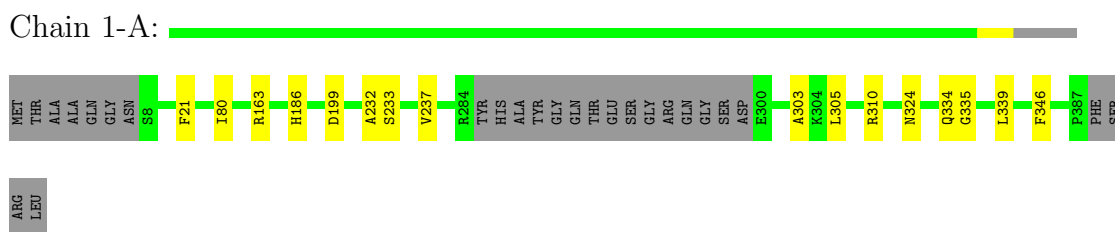
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	12-A	206	Total 206	O 206	0	0
3	12-B	204	Total 204	O 204	0	0
3	13-A	206	Total 206	O 206	0	0
3	13-B	204	Total 204	O 204	0	0
3	14-A	202	Total 202	O 202	0	0
3	14-B	208	Total 208	O 208	0	0
3	15-A	200	Total 200	O 200	0	0
3	15-B	210	Total 210	O 210	0	0
3	16-A	204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

3 Residue-property plots

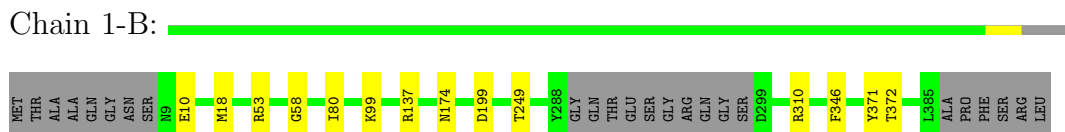
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS failed to run properly.

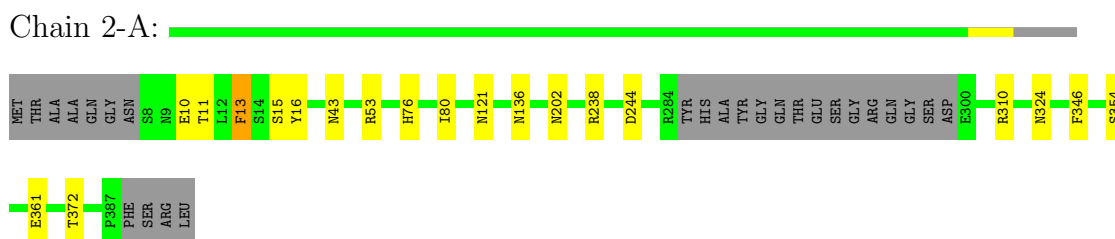
- Molecule 1: 12-oxophytodienoate reductase 3



- Molecule 1: 12-oxophytodienoate reductase 3



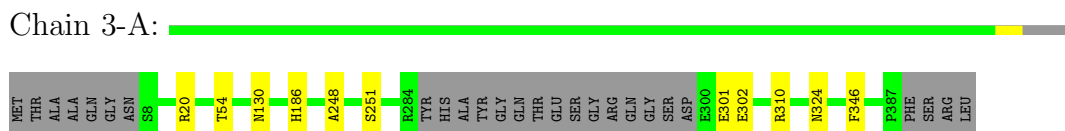
- Molecule 1: 12-oxophytodienoate reductase 3



- Molecule 1: 12-oxophytodienoate reductase 3



- Molecule 1: 12-oxophytodienoate reductase 3



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 3-B:

- Molecule 1: 12-oxophytodienoate reductase 3

Chain 4-A:

LEU

- Molecule 1: 12-oxophytodienoate reductase 3

Chain 4-B:

- Molecule 1: 12-oxophytodienoate reductase 3

Chain 5-A:

- Molecule 1: 12-oxophytodienoate reductase 3

Chain 5-B:

- Molecule 1: 12-oxophytodienoate reductase 3

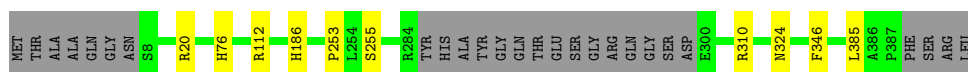
Chain 6-A:

- Molecule 1: 12-oxophytodienoate reductase 3

Chain 6-B:

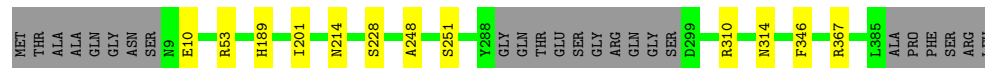
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 7-A:



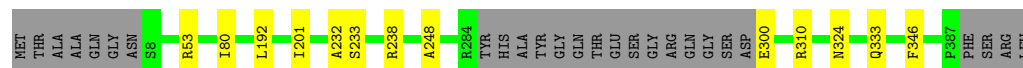
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 7-B:



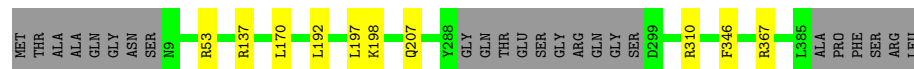
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 8-B:



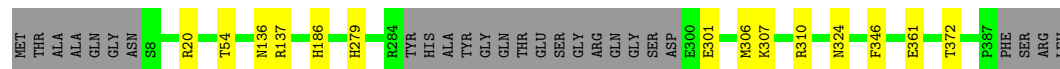
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 9-B:



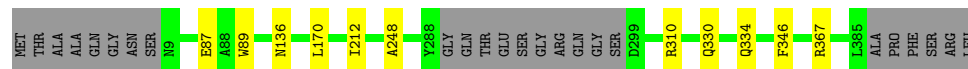
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 10-B:



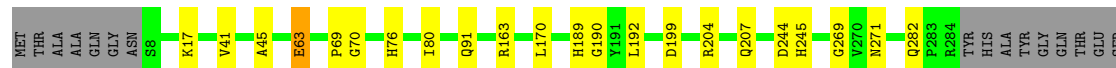
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 11-B:



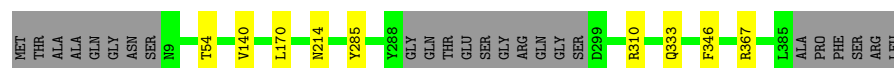
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 12-B:



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 13-B:



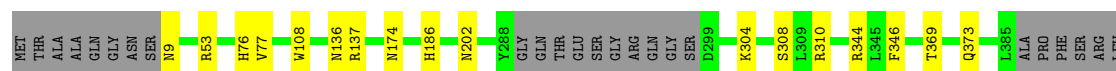
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 11-A: 



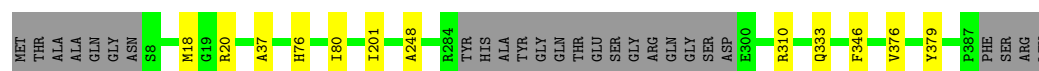
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 11-B: 



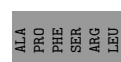
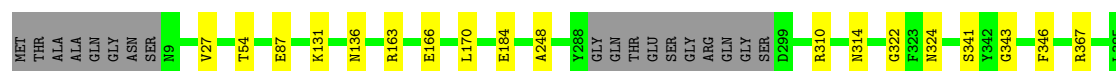
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 12-A: 



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 12-B: 



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 13-A: 



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 13-B: 



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 14-A: 





- Molecule 1: 12-oxophytodienoate reductase 3

Chain 14-B:



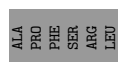
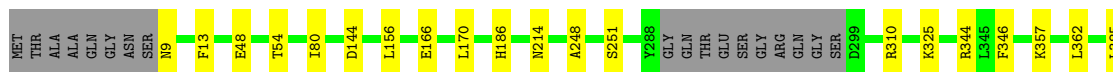
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 15-A:



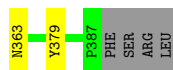
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 15-B:



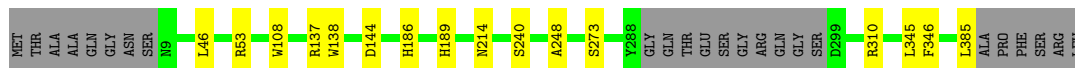
- Molecule 1: 12-oxophytodienoate reductase 3

Chain 16-A:



- Molecule 1: 12-oxophytodienoate reductase 3

Chain 16-B:



4 Data and refinement statistics

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

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

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

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

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

There are no bond length outliers.

All (3) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

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

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

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

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

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

There are no clashes within the asymmetric unit.

The worst 5 of 16 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

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

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	361/391 (92%)	317 (88%)	35 (10%)	9 (2%)	9	2
1	1-B	363/391 (93%)	333 (92%)	25 (7%)	5 (1%)	16	7
1	2-A	361/391 (92%)	300 (83%)	51 (14%)	10 (3%)	8	2
1	2-B	363/391 (93%)	337 (93%)	24 (7%)	2 (1%)	33	24
1	3-A	361/391 (92%)	336 (93%)	22 (6%)	3 (1%)	27	17
1	3-B	363/391 (93%)	339 (93%)	18 (5%)	6 (2%)	14	5
1	4-A	361/391 (92%)	322 (89%)	33 (9%)	6 (2%)	14	5
1	4-B	363/391 (93%)	338 (93%)	20 (6%)	5 (1%)	16	7
1	5-A	361/391 (92%)	331 (92%)	29 (8%)	1 (0%)	50	44
1	5-B	363/391 (93%)	341 (94%)	20 (6%)	2 (1%)	33	24
1	6-A	361/391 (92%)	338 (94%)	22 (6%)	1 (0%)	50	44
1	6-B	363/391 (93%)	341 (94%)	22 (6%)	0	100	100
1	7-A	361/391 (92%)	333 (92%)	24 (7%)	4 (1%)	21	10
1	7-B	363/391 (93%)	334 (92%)	23 (6%)	6 (2%)	14	5
1	8-A	361/391 (92%)	324 (90%)	31 (9%)	6 (2%)	14	5
1	8-B	363/391 (93%)	332 (92%)	28 (8%)	3 (1%)	27	17
1	9-A	361/391 (92%)	330 (91%)	23 (6%)	8 (2%)	10	3
1	9-B	363/391 (93%)	335 (92%)	26 (7%)	2 (1%)	33	24

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

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%)	63	63
1	1-B	300/317 (95%)	291 (97%)	9 (3%)	53	50
1	2-A	298/317 (94%)	287 (96%)	11 (4%)	45	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-B	300/317 (95%)	293 (98%)	7 (2%)	63	63
1	3-A	298/317 (94%)	290 (97%)	8 (3%)	57	56
1	3-B	300/317 (95%)	291 (97%)	9 (3%)	53	50
1	4-A	298/317 (94%)	288 (97%)	10 (3%)	49	45
1	4-B	300/317 (95%)	291 (97%)	9 (3%)	53	50
1	5-A	298/317 (94%)	292 (98%)	6 (2%)	68	69
1	5-B	300/317 (95%)	292 (97%)	8 (3%)	57	56
1	6-A	298/317 (94%)	291 (98%)	7 (2%)	63	63
1	6-B	300/317 (95%)	295 (98%)	5 (2%)	73	75
1	7-A	298/317 (94%)	292 (98%)	6 (2%)	68	69
1	7-B	300/317 (95%)	294 (98%)	6 (2%)	68	69
1	8-A	298/317 (94%)	291 (98%)	7 (2%)	63	63
1	8-B	300/317 (95%)	293 (98%)	7 (2%)	63	63
1	9-A	298/317 (94%)	292 (98%)	6 (2%)	68	69
1	9-B	300/317 (95%)	291 (97%)	9 (3%)	53	50
1	10-A	298/317 (94%)	284 (95%)	14 (5%)	36	29
1	10-B	300/317 (95%)	292 (97%)	8 (3%)	57	56
1	11-A	298/317 (94%)	289 (97%)	9 (3%)	53	50
1	11-B	300/317 (95%)	287 (96%)	13 (4%)	40	33
1	12-A	298/317 (94%)	294 (99%)	4 (1%)	80	82
1	12-B	300/317 (95%)	287 (96%)	13 (4%)	40	33
1	13-A	298/317 (94%)	285 (96%)	13 (4%)	39	32
1	13-B	300/317 (95%)	284 (95%)	16 (5%)	32	24
1	14-A	298/317 (94%)	276 (93%)	22 (7%)	20	12
1	14-B	300/317 (95%)	277 (92%)	23 (8%)	18	11
1	15-A	298/317 (94%)	282 (95%)	16 (5%)	31	24
1	15-B	300/317 (95%)	287 (96%)	13 (4%)	40	33
1	16-A	298/317 (94%)	285 (96%)	13 (4%)	39	32
1	16-B	300/317 (95%)	290 (97%)	10 (3%)	50	46
All	All	9568/10144 (94%)	9244 (97%)	324 (3%)	49	45

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 chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FMN	1-A	7401	-	33,33,33	2.49	6 (18%)	46,50,50	3.27	17 (36%)
2	FMN	1-B	9401	-	33,33,33	2.06	6 (18%)	46,50,50	4.04	17 (36%)
2	FMN	10-A	7401	-	33,33,33	2.16	6 (18%)	46,50,50	2.93	16 (34%)
2	FMN	10-B	9401	-	33,33,33	2.39	7 (21%)	46,50,50	4.00	18 (39%)
2	FMN	11-A	7401	-	33,33,33	2.41	7 (21%)	46,50,50	3.45	17 (36%)
2	FMN	11-B	9401	-	33,33,33	2.14	5 (15%)	46,50,50	4.12	17 (36%)
2	FMN	12-A	7401	-	33,33,33	2.26	9 (27%)	46,50,50	3.03	15 (32%)
2	FMN	12-B	9401	-	33,33,33	2.74	9 (27%)	46,50,50	3.83	17 (36%)
2	FMN	13-A	7401	-	33,33,33	2.81	9 (27%)	46,50,50	3.81	19 (41%)
2	FMN	13-B	9401	-	33,33,33	3.33	11 (33%)	46,50,50	4.33	20 (43%)
2	FMN	14-A	7401	-	33,33,33	2.43	14 (42%)	46,50,50	3.30	18 (39%)
2	FMN	14-B	9401	-	33,33,33	2.68	10 (30%)	46,50,50	3.84	18 (39%)
2	FMN	15-A	7401	-	33,33,33	2.23	8 (24%)	46,50,50	3.52	20 (43%)
2	FMN	15-B	9401	-	33,33,33	3.37	12 (36%)	46,50,50	4.36	22 (47%)
2	FMN	16-A	7401	-	33,33,33	2.75	10 (30%)	46,50,50	3.76	19 (41%)
2	FMN	16-B	9401	-	33,33,33	2.37	9 (27%)	46,50,50	3.91	17 (36%)
2	FMN	2-A	7401	-	33,33,33	2.18	8 (24%)	46,50,50	2.96	13 (28%)
2	FMN	2-B	9401	-	33,33,33	2.57	12 (36%)	46,50,50	3.94	19 (41%)
2	FMN	3-A	7401	-	33,33,33	2.45	7 (21%)	46,50,50	3.17	17 (36%)
2	FMN	3-B	9401	-	33,33,33	2.43	5 (15%)	46,50,50	4.02	18 (39%)
2	FMN	4-A	7401	-	33,33,33	2.32	7 (21%)	46,50,50	3.32	17 (36%)
2	FMN	4-B	9401	-	33,33,33	2.08	6 (18%)	46,50,50	3.69	17 (36%)
2	FMN	5-A	7401	-	33,33,33	2.42	7 (21%)	46,50,50	3.47	17 (36%)
2	FMN	5-B	9401	-	33,33,33	2.38	8 (24%)	46,50,50	4.01	19 (41%)
2	FMN	6-A	7401	-	33,33,33	2.35	7 (21%)	46,50,50	3.83	19 (41%)
2	FMN	6-B	9401	-	33,33,33	2.52	14 (42%)	46,50,50	3.87	19 (41%)
2	FMN	7-A	7401	-	33,33,33	2.98	11 (33%)	46,50,50	3.81	18 (39%)
2	FMN	7-B	9401	-	33,33,33	2.95	9 (27%)	46,50,50	4.18	18 (39%)
2	FMN	8-A	7401	-	33,33,33	2.59	10 (30%)	46,50,50	3.35	18 (39%)
2	FMN	8-B	9401	-	33,33,33	2.29	6 (18%)	46,50,50	4.12	21 (45%)
2	FMN	9-A	7401	-	33,33,33	2.41	7 (21%)	46,50,50	3.36	18 (39%)
2	FMN	9-B	9401	-	33,33,33	2.38	12 (36%)	46,50,50	3.78	17 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

The worst 5 of 274 bond length outliers are listed below:

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

The worst 5 of 572 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7-A	7401	FMN	C1'-N10-C9A	12.56	131.09	118.87
2	15-B	9401	FMN	C1'-N10-C9A	12.47	131.01	118.87
2	13-B	9401	FMN	C1'-N10-C9A	12.19	130.73	118.87
2	13-A	7401	FMN	C1'-N10-C9A	11.51	130.06	118.87
2	12-B	9401	FMN	O2P-P-O1P	-11.43	73.07	110.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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