



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:42 PM GMT

PDB ID : 1Q52
Title : Crystal Structure of Mycobacterium tuberculosis MenB, a Key Enzyme in Vitamin K2 Biosynthesis
Authors : Truglio, J.J.; Theis, K.; Feng, Y.; Gajda, R.; Machutta, C.; Tonge, P.J.; Kisker, C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2003-08-05
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

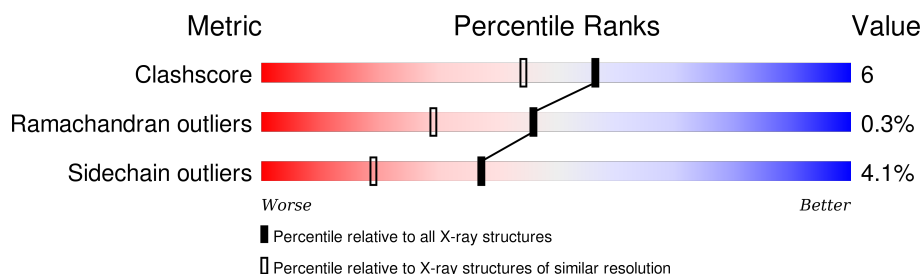
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)






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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	C	314	
1	D	314	
1	E	314	
1	F	314	
1	G	314	

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Mol	Chain	Length	Quality of chain
1	H	314	 73%11% • 14%
1	I	314	 72%11% • 14%
1	J	314	 70%12% • 14%
1	K	314	 70%15% • 14%
1	L	314	 72%13% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28487 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 menB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2118	1344	380	385	9			
1	B	279	Total	C	N	O	S	0	0	0
			2191	1388	396	398	9			
1	C	269	Total	C	N	O	S	0	0	0
			2118	1344	380	385	9			
1	D	269	Total	C	N	O	S	0	0	0
			2118	1344	380	385	9			
1	E	269	Total	C	N	O	S	0	0	0
			2118	1344	380	385	9			
1	F	269	Total	C	N	O	S	0	0	0
			2118	1344	380	385	9			
1	G	269	Total	C	N	O	S	0	0	0
			2118	1344	380	385	9			
1	H	269	Total	C	N	O	S	0	0	0
			2118	1344	380	385	9			
1	I	269	Total	C	N	O	S	0	0	0
			2118	1344	380	385	9			
1	J	269	Total	C	N	O	S	0	0	0
			2118	1344	380	385	9			
1	K	271	Total	C	N	O	S	0	0	0
			2132	1351	382	390	9			
1	L	269	Total	C	N	O	S	0	0	0
			2118	1344	380	385	9			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	231	Total	O	0	0
			231	231		
2	B	244	Total	O	0	0
			244	244		

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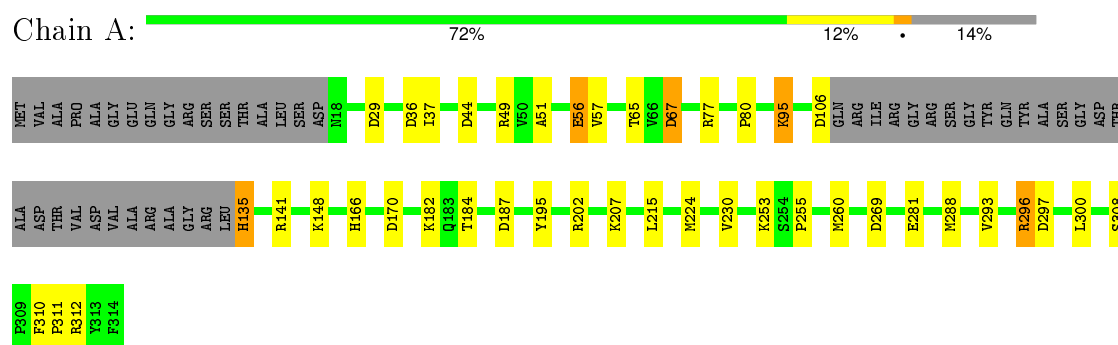
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	253	Total 253	O 253	0	0
2	D	223	Total 223	O 223	0	0
2	E	264	Total 264	O 264	0	0
2	F	237	Total 237	O 237	0	0
2	G	246	Total 246	O 246	0	0
2	H	242	Total 242	O 242	0	0
2	I	214	Total 214	O 214	0	0
2	J	270	Total 270	O 270	0	0
2	K	275	Total 275	O 275	0	0
2	L	285	Total 285	O 285	0	0

3 Residue-property plots [i](#)

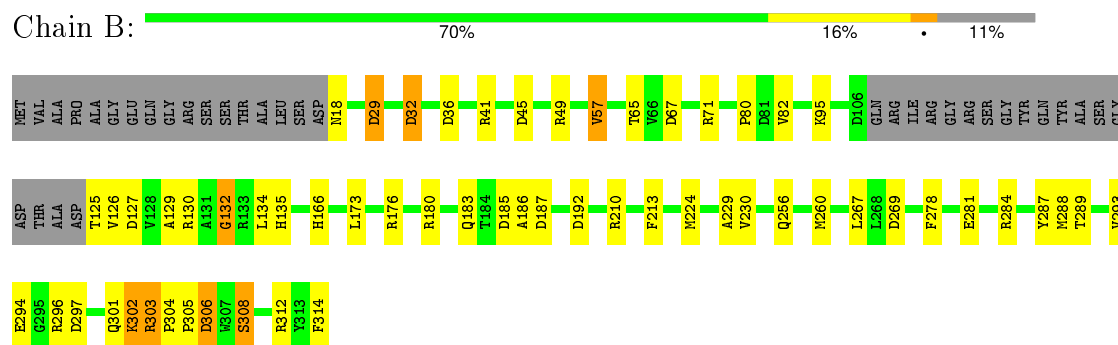
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 was not executed.

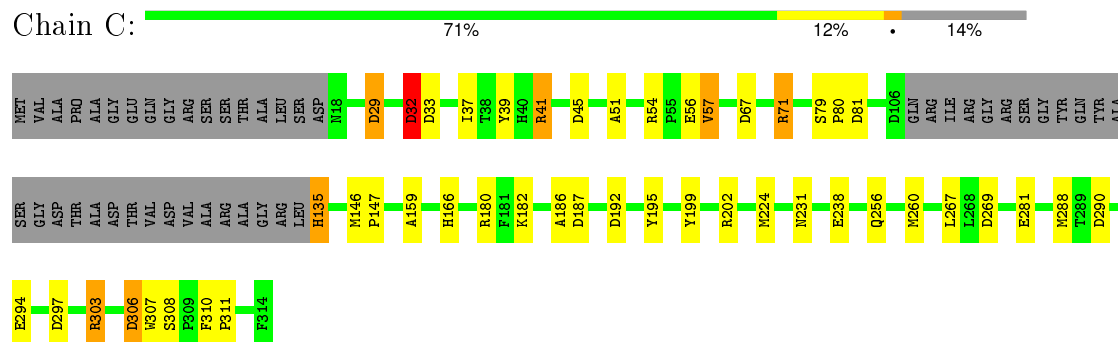
- Molecule 1: menB



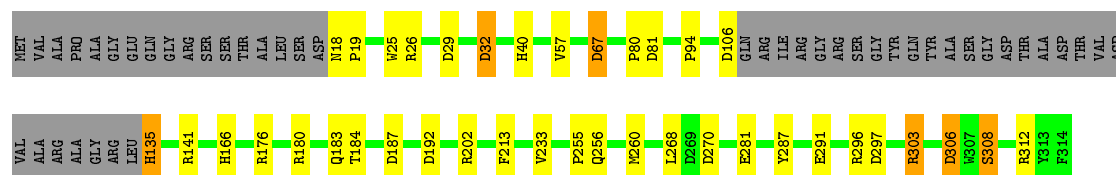
- Molecule 1: menB



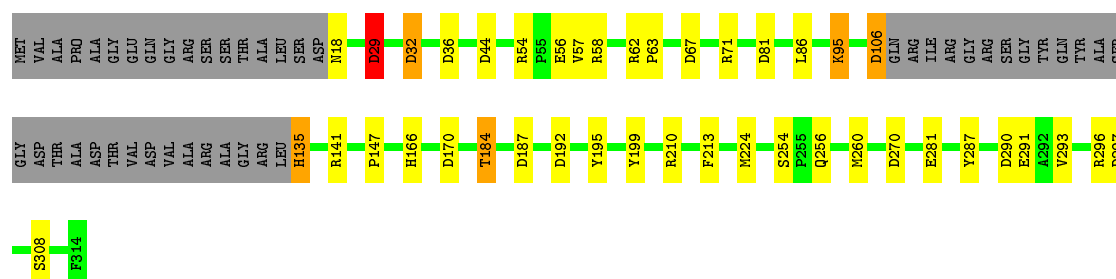
- Molecule 1: menB



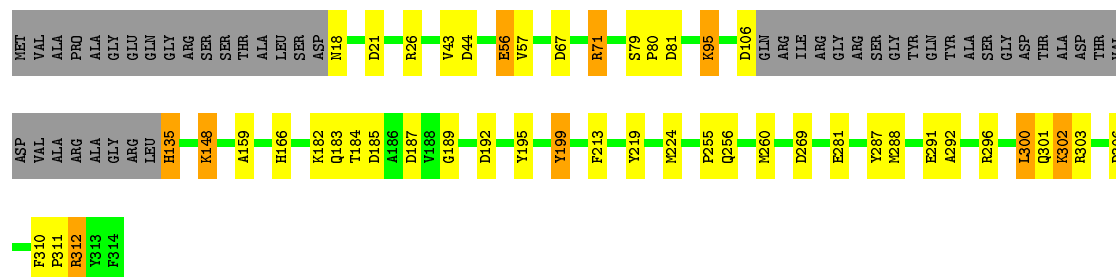
• Molecule 1: menB

Chain H:  73% 11% 14%

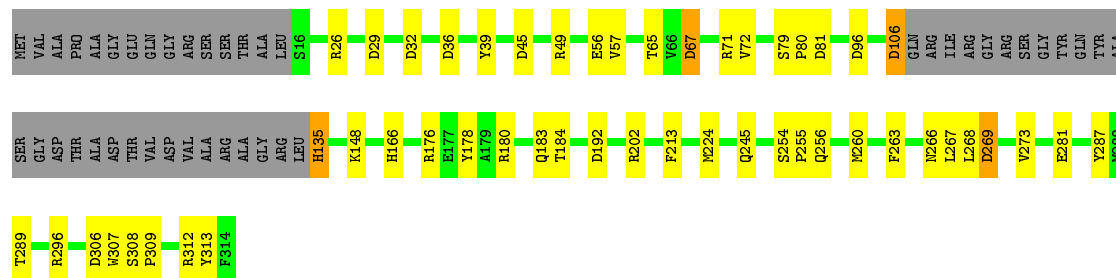
• Molecule 1: menB

Chain I:  72% 11% 14%

• Molecule 1: menB

Chain J:  70% 12% 14%

• Molecule 1: menB

Chain K:  70% 15% 14%

• Molecule 1: menB

Chain L:  72% 13% 14%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.38 Å 139.43 Å 142.03 Å 90.00° 97.29° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80	Depositor
% Data completeness (in resolution range)	97.4 (50.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.195 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28487	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	A	1.05	1/2172 (0.0%)	1.06	9/2945 (0.3%)
1	B	1.09	3/2245 (0.1%)	1.09	14/3044 (0.5%)
1	C	1.01	2/2172 (0.1%)	1.01	8/2945 (0.3%)
1	D	1.02	0/2172	1.00	10/2945 (0.3%)
1	E	1.05	1/2172 (0.0%)	1.06	12/2945 (0.4%)
1	F	1.03	0/2172	1.04	12/2945 (0.4%)
1	G	1.08	1/2172 (0.0%)	1.06	10/2945 (0.3%)
1	H	1.06	0/2172	1.05	13/2945 (0.4%)
1	I	1.01	2/2172 (0.1%)	1.05	16/2945 (0.5%)
1	J	1.04	2/2172 (0.1%)	1.03	9/2945 (0.3%)
1	K	1.13	3/2186 (0.1%)	1.10	13/2964 (0.4%)
1	L	1.09	1/2172 (0.0%)	1.10	11/2945 (0.4%)
All	All	1.06	16/26151 (0.1%)	1.06	137/35458 (0.4%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	178	TYR	CD2-CE2	6.76	1.49	1.39
1	K	273	VAL	CB-CG1	6.44	1.66	1.52
1	I	141	ARG	CG-CD	5.96	1.66	1.51
1	B	229	ALA	CA-CB	5.96	1.65	1.52
1	C	146	MET	CG-SD	5.86	1.96	1.81

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	180	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	G	192	ASP	CB-CG-OD2	11.44	128.60	118.30
1	E	192	ASP	CB-CG-OD2	9.32	126.69	118.30
1	B	224	MET	CG-SD-CE	-9.16	85.54	100.20
1	H	192	ASP	CB-CG-OD2	9.11	126.50	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2118	0	2036	24	0
1	B	2191	0	2115	35	0
1	C	2118	0	2036	35	0
1	D	2118	0	2036	26	0
1	E	2118	0	2036	29	0
1	F	2118	0	2036	24	0
1	G	2118	0	2036	34	0
1	H	2118	0	2036	23	0
1	I	2118	0	2036	21	0
1	J	2118	0	2036	27	0
1	K	2132	0	2045	35	0
1	L	2118	0	2036	23	0
2	A	231	0	0	5	2
2	B	244	0	0	8	0
2	C	253	0	0	13	0
2	D	223	0	0	5	0
2	E	264	0	0	15	0
2	F	237	0	0	4	0
2	G	246	0	0	12	0
2	H	242	0	0	4	0
2	I	214	0	0	8	0
2	J	270	0	0	6	0
2	K	275	0	0	8	0
2	L	285	0	0	8	2
All	All	28487	0	24520	304	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 304 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ASN:N	2:E:567:HOH:O	1.84	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASN:N	2:B:542:HOH:O	1.90	1.04
1:F:185:ASP:HB2	2:F:542:HOH:O	1.56	1.03
1:H:135:HIS:N	2:H:548:HOH:O	1.93	1.00
1:I:18:ASN:N	2:I:521:HOH:O	2.03	0.91

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
2:A:532:HOH:O	2:L:398:HOH:O[1_556]	2.17	0.03
2:A:542:HOH:O	2:L:474:HOH:O[1_556]	2.18	0.02

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	A	265/314 (84%)	256 (97%)	9 (3%)	0	100	100
1	B	275/314 (88%)	264 (96%)	9 (3%)	2 (1%)	26	11
1	C	265/314 (84%)	260 (98%)	4 (2%)	1 (0%)	39	23
1	D	265/314 (84%)	258 (97%)	7 (3%)	0	100	100
1	E	265/314 (84%)	256 (97%)	9 (3%)	0	100	100
1	F	265/314 (84%)	249 (94%)	14 (5%)	2 (1%)	24	8
1	G	265/314 (84%)	254 (96%)	10 (4%)	1 (0%)	39	23
1	H	265/314 (84%)	259 (98%)	6 (2%)	0	100	100
1	I	265/314 (84%)	255 (96%)	10 (4%)	0	100	100
1	J	265/314 (84%)	255 (96%)	8 (3%)	2 (1%)	24	8
1	K	267/314 (85%)	259 (97%)	7 (3%)	1 (0%)	39	23
1	L	265/314 (84%)	258 (97%)	6 (2%)	1 (0%)	39	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3192/3768 (85%)	3083 (97%)	99 (3%)	10 (0%)	46 29

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	302	LYS
1	F	301	GLN
1	G	302	LYS
1	J	302	LYS
1	B	302	LYS

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	A	215/247 (87%)	204 (95%)	11 (5%)	29 12
1	B	222/247 (90%)	213 (96%)	9 (4%)	37 19
1	C	215/247 (87%)	205 (95%)	10 (5%)	32 14
1	D	215/247 (87%)	207 (96%)	8 (4%)	41 23
1	E	215/247 (87%)	207 (96%)	8 (4%)	41 23
1	F	215/247 (87%)	206 (96%)	9 (4%)	36 18
1	G	215/247 (87%)	206 (96%)	9 (4%)	36 18
1	H	215/247 (87%)	208 (97%)	7 (3%)	45 27
1	I	215/247 (87%)	207 (96%)	8 (4%)	41 23
1	J	215/247 (87%)	205 (95%)	10 (5%)	32 14
1	K	217/247 (88%)	211 (97%)	6 (3%)	51 35
1	L	215/247 (87%)	205 (95%)	10 (5%)	32 14
All	All	2589/2964 (87%)	2484 (96%)	105 (4%)	37 19

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	32	ASP
1	G	148	LYS
1	L	135	HIS
1	F	56	GLU
1	F	303	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	256	GLN
1	G	135	HIS
1	J	256	GLN
1	E	256	GLN
1	K	256	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.