



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 09:57 AM EDT

PDB ID : 5H8M  
Title : Crystal structure of Mycobacterium tuberculosis malate synthase C619A, G459A mutant in complex with product malate  
Authors : Krieger, I.V.; Huang, H.-L.; Sacchettini, J.C.  
Deposited on : 2015-12-23  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

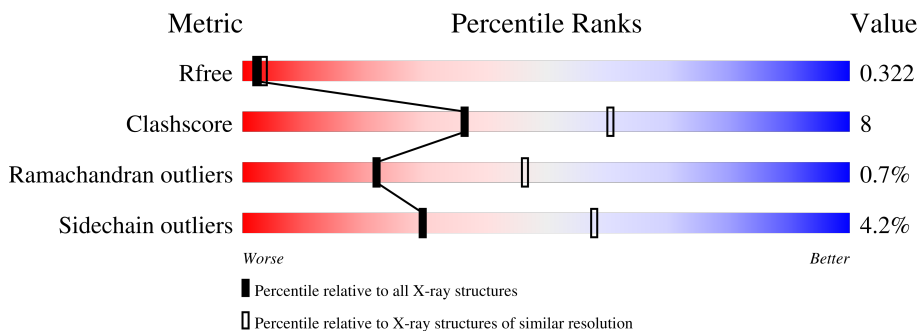
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	741	 75%      19%      • 5%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5489 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 Malate synthase G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	706	5421	3404	956	1039	22	0	3	0

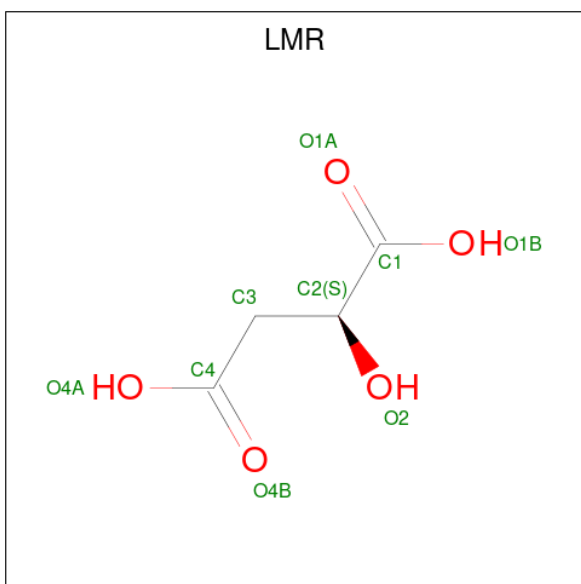
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	459	ALA	GLY	engineered mutation	UNP P9WK17
A	619	ALA	CYS	engineered mutation	UNP P9WK17

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	4	5		

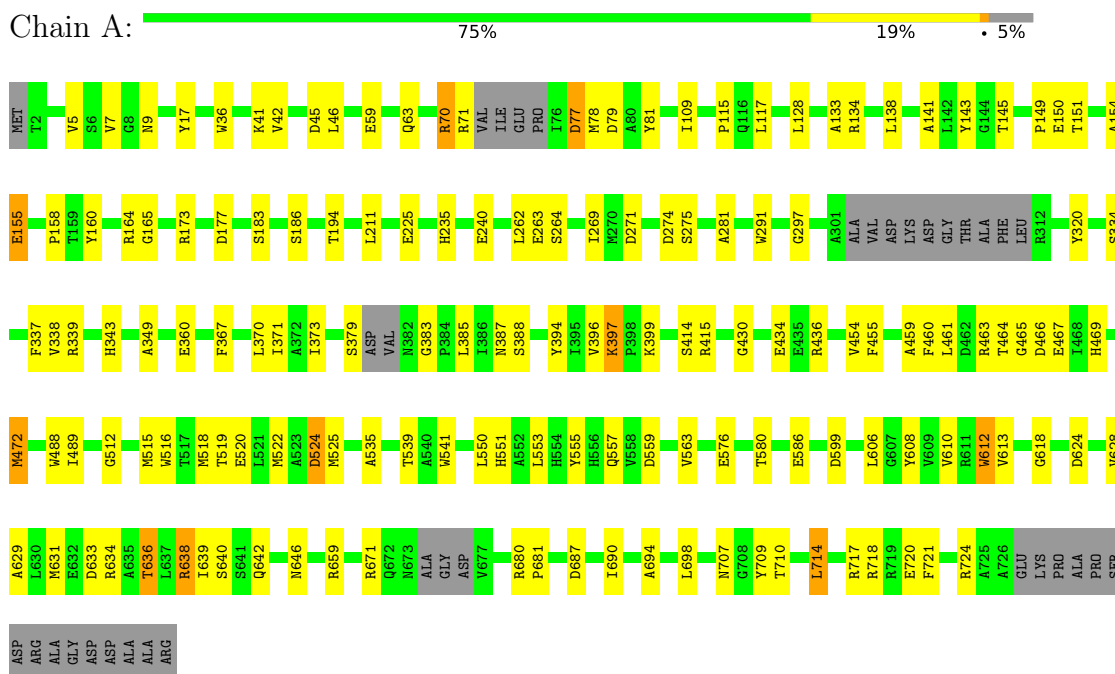
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Malate synthase G



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.26Å 80.26Å 226.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.36 – 2.70 45.36 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.36-2.70) 89.5 (45.36-2.20)	Depositor EDS
$R_{merge}$	0.41	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.226 , 0.322 0.226 , 0.322	Depositor DCC
$R_{free}$ test set	1748 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.3	Xtrriage
Anisotropy	0.473	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 17.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5489	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.38	0/5527	0.55	0/7511

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5421	0	5372	85	0
2	A	1	0	0	0	0
3	A	9	0	4	2	0
4	A	58	0	0	5	0
All	All	5489	0	5376	85	0

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 8.

All (85) 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:A:434:GLU:HB3	1:A:459:ALA:HB3	1.63	0.79
1:A:690:ILE:HD11	1:A:724:ARG:HD2	1.63	0.79
1:A:461:LEU:HA	1:A:639:ILE:HD11	1.72	0.72
1:A:541:TRP:HZ3	3:A:802:LMR:H2	1.54	0.71
1:A:297:GLY:HA3	1:A:385:LEU:HB2	1.73	0.71
1:A:115:PRO:HB3	1:A:551:HIS:HD2	1.59	0.68
1:A:77:ASP:OD1	1:A:79:ASP:N	2.27	0.65
1:A:46:LEU:HD11	1:A:415:ARG:HG3	1.78	0.64
1:A:472:MET:HG2	1:A:646:ASN:HD22	1.64	0.63
1:A:399:LYS:HD3	1:A:709:TYR:CE2	2.34	0.63
1:A:461:LEU:H	1:A:461:LEU:HD22	1.66	0.61
1:A:367:PHE:O	1:A:371:ILE:HG13	2.01	0.60
1:A:281:ALA:HB2	1:A:349:ALA:HA	1.84	0.59
1:A:360:GLU:OE2	4:A:901:HOH:O	2.17	0.59
1:A:430:GLY:HA2	1:A:455:PHE:HB3	1.84	0.59
1:A:77:ASP:OD1	1:A:78:MET:N	2.36	0.59
1:A:379:SER:N	1:A:383:GLY:O	2.29	0.59
1:A:463:ARG:HH22	1:A:467:GLU:HB2	1.69	0.58
1:A:436:ARG:N	1:A:466:ASP:OD1	2.36	0.58
1:A:388:SER:HB2	4:A:908:HOH:O	2.03	0.57
1:A:379:SER:HB3	1:A:383:GLY:H	1.70	0.57
1:A:81:TYR:OH	1:A:436:ARG:NH2	2.36	0.55
1:A:271:ASP:OD2	1:A:275:SER:OG	2.17	0.55
1:A:274:ASP:OD2	1:A:634:ARG:NE	2.40	0.55
1:A:690:ILE:HD13	1:A:720:GLU:O	2.07	0.55
1:A:370:LEU:HD12	1:A:373:ILE:HD12	1.89	0.54
1:A:633:ASP:OD2	3:A:802:LMR:O2	2.22	0.54
1:A:177:ASP:OD2	1:A:186:SER:HB2	2.08	0.54
1:A:7:VAL:HG11	1:A:36:TRP:HB3	1.90	0.54
1:A:145:THR:HG21	1:A:522:MET:HG3	1.89	0.54
1:A:551:HIS:CD2	1:A:555:TYR:HE1	2.26	0.53
1:A:612:TRP:CE2	1:A:714:LEU:HD13	2.44	0.53
1:A:387:ASN:ND2	4:A:908:HOH:O	2.30	0.52
1:A:638:ARG:NH1	1:A:707:ASN:O	2.42	0.52
1:A:379:SER:HB3	1:A:383:GLY:N	2.25	0.52
1:A:512:GLY:HA2	1:A:539:THR:O	2.08	0.52
1:A:141:ALA:HB1	1:A:550:LEU:HD21	1.92	0.51
1:A:463:ARG:NH2	1:A:467:GLU:HB2	2.26	0.50
1:A:339:ARG:HB2	1:A:396:VAL:HB	1.93	0.50
1:A:606:LEU:O	1:A:610:VAL:HG23	2.12	0.50
1:A:613:VAL:O	1:A:718:ARG:NH1	2.44	0.49
1:A:535:ALA:HB1	4:A:950:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:TRP:CE2	1:A:525:MET:HB2	2.48	0.48
1:A:515:MET:CE	1:A:541:TRP:HB3	2.44	0.48
1:A:235:HIS:CD2	1:A:559:ASP:HA	2.49	0.47
1:A:337:PHE:CE2	1:A:394:TYR:HB3	2.49	0.47
1:A:138:LEU:HD13	1:A:262:LEU:HD11	1.97	0.46
1:A:291:TRP:CH2	1:A:338:VAL:HB	2.51	0.46
1:A:59:GLU:O	1:A:63:GLN:HG3	2.15	0.46
1:A:109:ILE:HG21	1:A:454:VAL:HB	1.98	0.46
1:A:698:LEU:HD22	1:A:710:THR:HG22	1.98	0.45
1:A:150:GLU:HB3	1:A:155:GLU:HA	1.96	0.45
1:A:70:ARG:HD2	1:A:71:ARG:NH1	2.32	0.45
1:A:469:HIS:HB2	1:A:642:GLN:OE1	2.17	0.45
1:A:559:ASP:O	1:A:563:VAL:HG23	2.17	0.45
1:A:624:ASP:OD1	1:A:628:VAL:N	2.43	0.45
1:A:134:ARG:O	1:A:263:GLU:HA	2.17	0.44
1:A:608:TYR:OH	1:A:618:GLY:O	2.25	0.44
1:A:524:ASP:OD1	1:A:524:ASP:N	2.50	0.44
1:A:41:LYS:HE2	1:A:45:ASP:OD2	2.17	0.44
1:A:154:ALA:O	1:A:164:ARG:HD2	2.17	0.44
1:A:133:ALA:O	1:A:264:SER:HB2	2.18	0.44
1:A:194:THR:HG22	1:A:225:GLU:O	2.17	0.44
1:A:343:HIS:CE1	1:A:397:LYS:HE2	2.53	0.43
1:A:488:TRP:HB3	1:A:580:THR:O	2.17	0.43
1:A:461:LEU:HD21	4:A:939:HOH:O	2.18	0.43
1:A:519:THR:HG23	1:A:520:GLU:HG3	2.00	0.43
1:A:553:LEU:O	1:A:557:GLN:HG3	2.19	0.43
1:A:149:PRO:HB2	1:A:151:THR:HB	2.01	0.43
1:A:460:PHE:O	1:A:464:THR:N	2.45	0.43
1:A:659:ARG:HA	1:A:659:ARG:HD2	1.87	0.43
1:A:680:ARG:HA	1:A:681:PRO:HD2	1.94	0.43
1:A:436:ARG:HG3	1:A:463:ARG:NH1	2.34	0.42
1:A:465:GLY:HA3	1:A:638:ARG:HG2	2.01	0.42
1:A:143:TYR:O	1:A:164:ARG:NE	2.44	0.42
1:A:633:ASP:O	1:A:636:THR:HG23	2.19	0.42
1:A:488:TRP:CZ3	1:A:489:ILE:HG13	2.54	0.42
1:A:42:VAL:HG22	1:A:415:ARG:HB3	2.02	0.42
1:A:515:MET:HE2	1:A:515:MET:HB2	1.74	0.42
1:A:269:ILE:HA	1:A:337:PHE:HB2	2.02	0.41
1:A:240:GLU:OE2	1:A:320:TYR:OH	2.31	0.41
1:A:460:PHE:HB2	1:A:489:ILE:HD11	2.01	0.41
1:A:5:VAL:HG21	1:A:17:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TYR:OH	1:A:165:GLY:HA3	2.21	0.41
1:A:694:ALA:HB2	1:A:717:ARG:HD2	2.04	0.40

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	A	699/741 (94%)	654 (94%)	40 (6%)	5 (1%)	22 46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	586	GLU
1	A	721	PHE
1	A	77	ASP
1	A	629	ALA
1	A	158	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	571/593 (96%)	546 (96%)	25 (4%)	28 56

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	70	ARG
1	A	117	LEU
1	A	128	LEU
1	A	155	GLU
1	A	173	ARG
1	A	183	SER
1	A	211	LEU
1	A	334	SER
1	A	397	LYS
1	A	414	SER
1	A	472	MET
1	A	518	MET
1	A	524	ASP
1	A	576	GLU
1	A	599	ASP
1	A	612	TRP
1	A	631[A]	MET
1	A	631[B]	MET
1	A	636	THR
1	A	638	ARG
1	A	640	SER
1	A	671	ARG
1	A	687	ASP
1	A	714	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
3	LMR	A	802	2	8,8,8	1.06	0	10,10,10	1.95	3 (30%)

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
3	LMR	A	802	2	-	2/8/8/8	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	LMR	O1B-C1-C2	3.61	120.66	112.72
3	A	802	LMR	O1B-C1-O1A	-2.92	117.45	124.09
3	A	802	LMR	C2-C3-C4	2.49	118.29	112.13

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	LMR	O1B-C1-C2-C3
3	A	802	LMR	O1A-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	LMR	2	0

## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.