



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:46 am BST

PDB ID : 2C21
Title : Specificity of the Trypanothione-dependent Leishmania major Glyoxalase I: Structure and biochemical comparison with the human enzyme
Authors : Ariza, A.; Vickers, T.J.; Greig, N.; Armour, K.A.; Eggleston, I.M.; Fairlamb, A.H.; Bond, C.S.
Deposited on : 2005-09-23
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

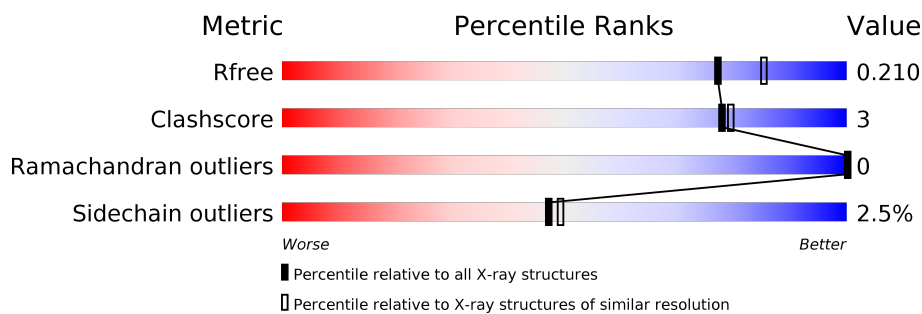
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 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	144	90% 6% . .
1	B	144	89% 7% . .
1	C	144	90% 6% . .
1	D	144	92% 5% .
1	E	144	90% 6% .
1	F	144	92% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7851 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 TRYPANOTHIONE-DEPENDENT GLYOXALASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	7	0
			1158	738	186	223	11			
1	B	139	Total	C	N	O	S	0	7	0
			1160	741	186	222	11			
1	C	139	Total	C	N	O	S	0	7	0
			1159	740	186	222	11			
1	D	139	Total	C	N	O	S	0	7	0
			1159	740	186	222	11			
1	E	139	Total	C	N	O	S	0	5	0
			1149	734	183	221	11			
1	F	139	Total	C	N	O	S	0	6	0
			1155	737	186	221	11			

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

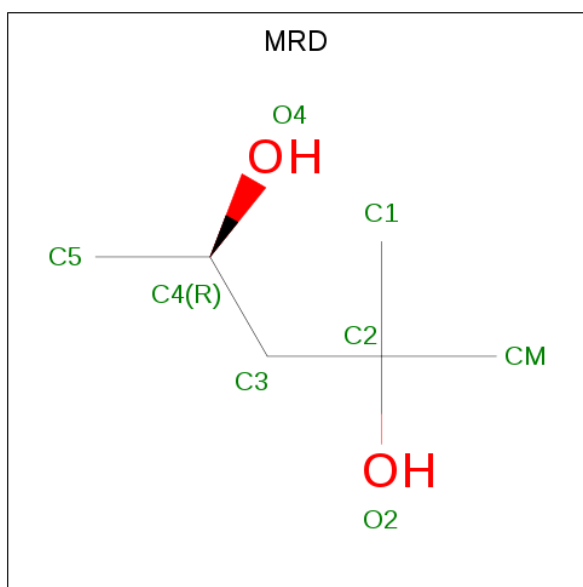
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ni	0	0
			2	2		
2	C	2	Total	Ni	0	0
			2	2		
2	E	2	Total	Ni	0	0
			2	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	1
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			8	6	2		
4	D	1	Total	C	O	0	1
			8	6	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	139	Total	O	0	0
			139	139		
6	B	156	Total	O	0	0
			156	156		
6	C	210	Total	O	0	0
			210	210		
6	D	164	Total	O	0	0
			164	164		
6	E	110	Total	O	0	0
			110	110		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	60	Total	O	0	0
			60	60		

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. 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: TRYPANOTHIONE-DEPENDENT GLYOXALASE I

Chain A:  90% 6% . .




- Molecule 1: TRYPANOTHIONE-DEPENDENT GLYOXALASE I

Chain B:  89% 7% . .



- Molecule 1: TRYPANOTHIONE-DEPENDENT GLYOXALASE I

Chain C:  90% 6% . .



- Molecule 1: TRYPANOTHIONE-DEPENDENT GLYOXALASE I

Chain D:  92% 5% .



- Molecule 1: TRYPANOTHIONE-DEPENDENT GLYOXALASE I

Chain E:  90% 6% .



- Molecule 1: TRYPANOTHIONE-DEPENDENT GLYOXALASE I

Chain F:  92% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	130.19 Å 148.96 Å 50.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	129.10 – 2.00 40.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (129.10-2.00) 99.6 (40.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.155 , 0.201 0.166 , 0.210	Depositor DCC
R_{free} test set	3376 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7851	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRD, NI, MPD, NA

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	0.50	0/1207	0.68	1/1621 (0.1%)
1	B	0.53	0/1209	0.66	0/1624
1	C	0.58	0/1209	0.70	0/1624
1	D	0.55	0/1209	0.70	1/1624 (0.1%)
1	E	0.47	0/1192	0.62	0/1602
1	F	0.48	1/1203 (0.1%)	0.59	0/1616
All	All	0.52	1/7229 (0.0%)	0.66	2/9711 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	132	GLU	C-O	7.36	1.37	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	72	ASP	CB-CG-OD1	7.04	124.64	118.30
1	A	15	ASP	CB-CG-OD1	5.58	123.32	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	1158	0	1140	13	0
1	B	1160	0	1145	15	0
1	C	1159	0	1145	9	0
1	D	1159	0	1145	10	0
1	E	1149	0	1131	3	0
1	F	1155	0	1137	1	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0
2	E	2	0	0	0	0
3	A	8	0	14	1	0
3	B	8	0	14	0	0
3	C	8	0	14	0	0
3	D	16	0	28	3	0
3	E	8	0	14	1	0
4	A	8	0	14	1	0
4	D	8	0	14	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	139	0	0	1	0
6	B	156	0	0	3	0
6	C	210	0	0	3	0
6	D	164	0	0	0	0
6	E	110	0	0	1	0
6	F	60	0	0	0	0
All	All	7851	0	6955	41	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 3.

All (41) 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:C:78[B]:ILE:HG21	1:D:6[B]:MET:HE1	1.22	1.17
1:C:78[B]:ILE:CG2	1:D:6[B]:MET:HE1	1.84	1.07
1:A:6[B]:MET:HE1	1:B:78[B]:ILE:HG21	1.39	1.01
1:A:6[B]:MET:CE	1:B:78[B]:ILE:CG2	2.41	0.99
6:C:2026:HOH:O	1:D:6[A]:MET:SD	2.25	0.94
1:A:6[B]:MET:CE	1:B:78[B]:ILE:HG21	1.99	0.92
1:A:6[B]:MET:HE3	1:B:78[B]:ILE:CG2	2.01	0.91
1:A:6[B]:MET:HE1	1:B:78[B]:ILE:CG2	2.01	0.88
1:C:78[B]:ILE:CG2	1:D:6[B]:MET:CE	2.56	0.84
1:A:6[B]:MET:CE	1:B:78[B]:ILE:HG23	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6[A]:MET:SD	6:B:2017:HOH:O	2.43	0.75
1:A:6[B]:MET:HE3	1:B:78[B]:ILE:HG23	1.70	0.74
3:D:1143:MPD:HM1	3:D:1143:MPD:H53	1.78	0.65
6:A:2020:HOH:O	1:B:6[A]:MET:SD	2.56	0.63
1:B:123:ASN:HD22	1:B:126:THR:H	1.46	0.62
1:B:93[B]:ARG:NH2	1:B:102:GLU:OE2	2.31	0.59
1:E:78[B]:ILE:HG12	1:E:119[B]:ILE:HD13	1.84	0.58
1:C:93[A]:ARG:NH1	6:C:2159:HOH:O	2.38	0.55
1:F:123:ASN:HD22	1:F:126:THR:H	1.54	0.55
1:E:138:GLN:OE1	6:E:2107:HOH:O	2.18	0.53
1:C:78[B]:ILE:HG23	1:D:6[B]:MET:CE	2.39	0.51
1:B:123:ASN:ND2	1:B:126:THR:H	2.08	0.51
1:C:95:HIS:HE1	6:C:2153:HOH:O	1.95	0.49
1:D:100:ASP:OD2	3:D:1143:MPD:H13	2.13	0.49
1:B:6[B]:MET:HE2	1:B:6[B]:MET:HB3	1.70	0.48
1:A:6[B]:MET:HB3	1:A:6[B]:MET:HE2	1.75	0.46
1:D:35:TRP:CD2	3:D:1141[A]:MPD:H12	2.51	0.46
1:D:35:TRP:CD2	4:D:1142[B]:MRD:H1C2	2.51	0.46
1:C:6[B]:MET:HE2	1:C:6[B]:MET:HB3	1.65	0.45
1:C:30:LYS:NZ	1:C:31:VAL:O	2.50	0.45
1:B:30:LYS:NZ	6:B:2047:HOH:O	2.26	0.45
1:B:34:LYS:HG2	1:B:45:VAL:HG22	1.98	0.44
1:C:12:ARG:HD2	1:D:73:GLU:O	2.18	0.43
3:E:1144:MPD:H53	3:E:1144:MPD:O2	2.18	0.43
1:A:123:ASN:HD22	1:A:126:THR:H	1.65	0.43
1:D:6[B]:MET:HB3	1:D:6[B]:MET:HE2	1.85	0.43
1:E:37:VAL:HG21	1:E:42:TYR:CZ	2.54	0.42
1:A:86[B]:LYS:NZ	1:A:103:ASP:O	2.52	0.42
1:A:35:TRP:CD2	4:A:2144[B]:MRD:H1C2	2.55	0.42
1:A:35:TRP:CD2	3:A:1144[A]:MPD:H12	2.55	0.41
1:B:137:GLU:OE1	6:B:2152:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/144 (100%)	140 (97%)	4 (3%)	0	100	100
1	B	144/144 (100%)	142 (99%)	2 (1%)	0	100	100
1	C	144/144 (100%)	141 (98%)	3 (2%)	0	100	100
1	D	144/144 (100%)	141 (98%)	3 (2%)	0	100	100
1	E	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
1	F	143/144 (99%)	140 (98%)	3 (2%)	0	100	100
All	All	861/864 (100%)	842 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	129/126 (102%)	125 (97%)	4 (3%)	40	40
1	B	129/126 (102%)	127 (98%)	2 (2%)	62	67
1	C	129/126 (102%)	126 (98%)	3 (2%)	50	53
1	D	129/126 (102%)	127 (98%)	2 (2%)	62	67
1	E	127/126 (101%)	123 (97%)	4 (3%)	40	40
1	F	128/126 (102%)	125 (98%)	3 (2%)	50	53
All	All	771/756 (102%)	753 (98%)	18 (2%)	47	53

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	104	GLU
1	A	113	ASP
1	A	123	ASN

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Mol	Chain	Res	Type
1	B	108	MET
1	B	123	ASN
1	C	30	LYS
1	C	104	GLU
1	C	113	ASP
1	D	3	SER
1	D	113	ASP
1	E	70	LYS
1	E	87	GLU
1	E	104	GLU
1	E	113	ASP
1	F	16	LEU
1	F	47	LEU
1	F	113	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
1	B	123	ASN
1	F	123	ASN

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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
4	MRD	A	2144[B]	-	7,7,7	0.27	0	9,10,10	0.42	0
3	MPD	E	1144	-	7,7,7	0.42	0	9,10,10	0.49	0
3	MPD	D	1141[A]	-	7,7,7	0.33	0	9,10,10	0.69	0
3	MPD	D	1143	-	7,7,7	0.47	0	9,10,10	0.72	0
3	MPD	B	1142	-	7,7,7	0.43	0	9,10,10	0.29	0
3	MPD	A	1144[A]	-	7,7,7	0.29	0	9,10,10	0.40	0
3	MPD	C	1144	-	7,7,7	0.38	0	9,10,10	0.39	0
4	MRD	D	1142[B]	-	7,7,7	0.32	0	9,10,10	0.70	0

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
4	MRD	A	2144[B]	-	-	0/5/5/5	-
3	MPD	E	1144	-	-	4/5/5/5	-
3	MPD	D	1141[A]	-	-	2/5/5/5	-
3	MPD	D	1143	-	-	1/5/5/5	-
3	MPD	B	1142	-	-	1/5/5/5	-
3	MPD	A	1144[A]	-	-	2/5/5/5	-
3	MPD	C	1144	-	-	1/5/5/5	-
4	MRD	D	1142[B]	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1144	MPD	O2-C2-C3-C4
3	D	1143	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	1144[A]	MPD	C2-C3-C4-O4
3	E	1144	MPD	C1-C2-C3-C4
3	E	1144	MPD	CM-C2-C3-C4
3	B	1142	MPD	O2-C2-C3-C4
3	D	1141[A]	MPD	C2-C3-C4-C5
3	E	1144	MPD	C2-C3-C4-C5
3	A	1144[A]	MPD	C2-C3-C4-C5
3	D	1141[A]	MPD	C2-C3-C4-O4
3	C	1144	MPD	C2-C3-C4-O4

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2144[B]	MRD	1	0
3	E	1144	MPD	1	0
3	D	1141[A]	MPD	1	0
3	D	1143	MPD	2	0
3	A	1144[A]	MPD	1	0
4	D	1142[B]	MRD	1	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.