Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2020 – 11:03 PM BST

PDB ID	:	6Z7T
Title	:	Nucleotide-free Myosin-II motor domain
Authors	:	Ewert, W.; Preller, M.
Deposited on	:	2020-06-01
Resolution	:	1.88 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 24654 atoms, of which 11696 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 Myosin-2 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	726	Total	C	H	N	O	S	0	8	0
			11523	3695	5711	995	1105	17			
1	B	730	Total	C	H	N	O	S	0	4	0
			11613	3719	5763	1001	1113	17			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP P08799
A	-9	HIS	-	expression tag	UNP P08799
A	-8	HIS	-	expression tag	UNP P08799
A	-7	HIS	-	expression tag	UNP P08799
A	-6	HIS	-	expression tag	UNP P08799
A	-5	HIS	-	expression tag	UNP P08799
A	-4	HIS	-	expression tag	UNP P08799
A	-3	HIS	-	expression tag	UNP P08799
A	-2	ASP	-	expression tag	UNP P08799
A	-1	GLY	-	expression tag	UNP P08799
A	0	THR	-	expression tag	UNP P08799
A	1	GLU	-	expression tag	UNP P08799
A	762	LEU	-	expression tag	UNP P08799
A	763	GLU	-	expression tag	UNP P08799
A	764	SER	-	expression tag	UNP P08799
A	765	ASN	-	expression tag	UNP P08799
A	766	GLU	-	expression tag	UNP P08799
A	767	PRO	-	expression tag	UNP P08799
A	768	PRO	-	expression tag	UNP P08799
A	769	MET	-	expression tag	UNP P08799
A	770	ASP	-	expression tag	UNP P08799
A	771	PHE	-	expression tag	UNP P08799
A	772	ASP	-	expression tag	UNP P08799
A	773	ASP	-	expression tag	UNP P08799
A	774	ASP	-	expression tag	UNP P08799

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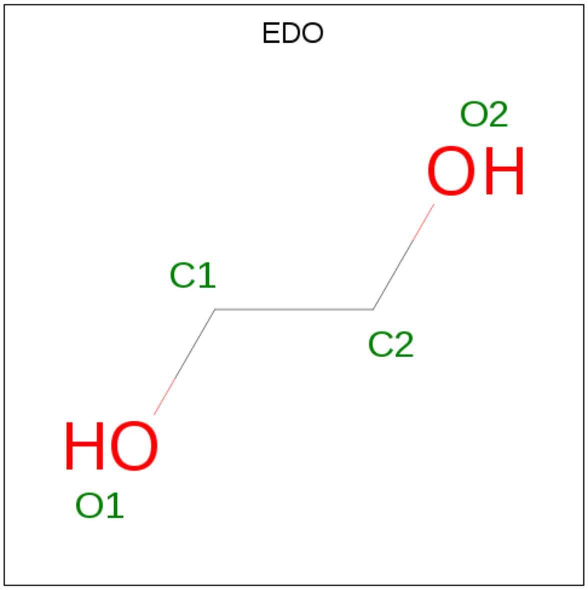
Chain	Residue	Modelled	Actual	Comment	Reference
A	775	ILE	-	expression tag	UNP P08799
A	776	PRO	-	expression tag	UNP P08799
A	777	PHE	-	expression tag	UNP P08799
B	-10	MET	-	initiating methionine	UNP P08799
B	-9	HIS	-	expression tag	UNP P08799
B	-8	HIS	-	expression tag	UNP P08799
B	-7	HIS	-	expression tag	UNP P08799
B	-6	HIS	-	expression tag	UNP P08799
B	-5	HIS	-	expression tag	UNP P08799
B	-4	HIS	-	expression tag	UNP P08799
B	-3	HIS	-	expression tag	UNP P08799
B	-2	ASP	-	expression tag	UNP P08799
B	-1	GLY	-	expression tag	UNP P08799
B	0	THR	-	expression tag	UNP P08799
B	1	GLU	-	expression tag	UNP P08799
B	762	LEU	-	expression tag	UNP P08799
B	763	GLU	-	expression tag	UNP P08799
B	764	SER	-	expression tag	UNP P08799
B	765	ASN	-	expression tag	UNP P08799
B	766	GLU	-	expression tag	UNP P08799
B	767	PRO	-	expression tag	UNP P08799
B	768	PRO	-	expression tag	UNP P08799
B	769	MET	-	expression tag	UNP P08799
B	770	ASP	-	expression tag	UNP P08799
B	771	PHE	-	expression tag	UNP P08799
B	772	ASP	-	expression tag	UNP P08799
B	773	ASP	-	expression tag	UNP P08799
B	774	ASP	-	expression tag	UNP P08799
B	775	ILE	-	expression tag	UNP P08799
B	776	PRO	-	expression tag	UNP P08799
B	777	PHE	-	expression tag	UNP P08799

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

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0

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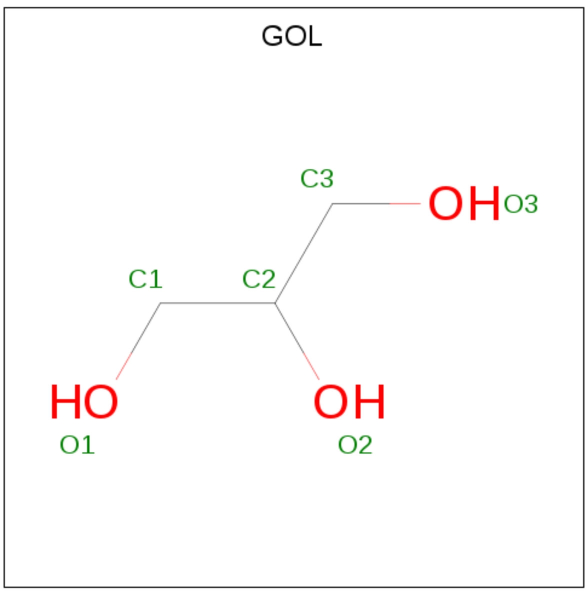
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 13 3 7 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0
4	A	1	Total C H O 14 3 8 3	0	0

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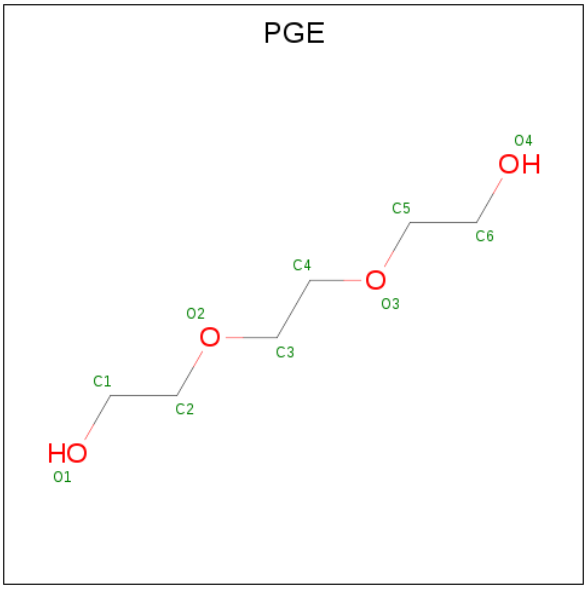
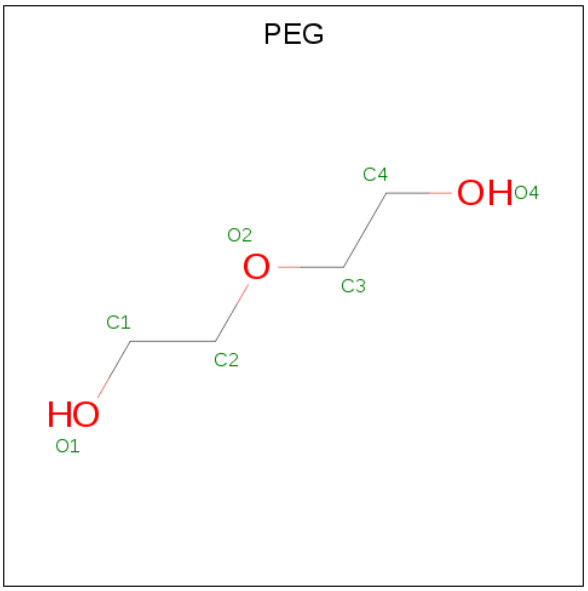
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			13	3	7	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	555	Total	O	0	0
			555	555		
7	B	580	Total	O	0	0
			580	580		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.68Å 174.40Å 100.25Å 90.00° 106.38° 90.00°	Depositor
Resolution (Å)	46.36 – 1.88	Depositor
% Data completeness (in resolution range)	98.5 (46.36-1.88)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.80 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.191 , 0.217	Depositor
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.571	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.249 for h,-k,-h-l	Xtriage
Total number of atoms	24654	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	EDO	A	805	-	3,3,3	0.38	0	2,2,2	0.55	0
3	EDO	A	812	-	3,3,3	0.45	0	2,2,2	0.15	0
3	EDO	B	812	-	3,3,3	0.35	0	2,2,2	0.62	0
3	EDO	B	808	-	3,3,3	0.47	0	2,2,2	0.35	0
4	GOL	A	813	-	5,5,5	0.77	0	5,5,5	1.49	1 (20%)
4	GOL	A	817	-	5,5,5	0.76	0	5,5,5	0.53	0
3	EDO	B	803	-	3,3,3	0.52	0	2,2,2	0.14	0
3	EDO	A	811	-	3,3,3	0.68	0	2,2,2	0.18	0
5	PGE	B	818	-	9,9,9	0.26	0	8,8,8	0.70	0
3	EDO	B	805	-	3,3,3	0.47	0	2,2,2	0.35	0
4	GOL	B	815	-	5,5,5	1.10	0	5,5,5	1.26	1 (20%)
4	GOL	A	815	-	5,5,5	1.21	0	5,5,5	1.06	0
3	EDO	B	811	-	3,3,3	0.61	0	2,2,2	0.57	0
3	EDO	B	810	-	3,3,3	0.42	0	2,2,2	0.52	0
4	GOL	A	814	-	5,5,5	1.62	1 (20%)	5,5,5	2.54	2 (40%)
4	GOL	B	816	-	5,5,5	1.17	0	5,5,5	1.42	1 (20%)
4	GOL	A	816	-	5,5,5	1.93	3 (60%)	5,5,5	1.97	1 (20%)
4	GOL	B	813	-	5,5,5	1.14	1 (20%)	5,5,5	1.10	0
4	GOL	B	814	-	5,5,5	0.59	0	5,5,5	0.96	0
3	EDO	A	810	-	3,3,3	0.49	0	2,2,2	0.30	0
3	EDO	B	804	-	3,3,3	0.50	0	2,2,2	0.41	0
3	EDO	A	806	-	3,3,3	0.50	0	2,2,2	0.27	0
3	EDO	B	809	-	3,3,3	0.49	0	2,2,2	0.41	0
3	EDO	A	804	-	3,3,3	0.46	0	2,2,2	0.40	0
3	EDO	B	806	-	3,3,3	0.53	0	2,2,2	0.70	0
3	EDO	B	807	-	3,3,3	0.63	0	2,2,2	0.36	0
3	EDO	A	809	-	3,3,3	0.44	0	2,2,2	0.36	0
3	EDO	A	803	-	3,3,3	0.33	0	2,2,2	0.48	0
3	EDO	A	807	-	3,3,3	0.62	0	2,2,2	0.11	0
3	EDO	A	808	-	3,3,3	0.70	0	2,2,2	0.55	0
4	GOL	B	817	-	5,5,5	0.82	0	5,5,5	1.15	0
6	PEG	B	819	-	6,6,6	0.50	0	5,5,5	0.27	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
3	EDO	A	805	-	-	1/1/1/1	-
3	EDO	A	812	-	-	1/1/1/1	-
3	EDO	B	812	-	-	1/1/1/1	-
3	EDO	B	808	-	-	1/1/1/1	-
4	GOL	A	813	-	-	4/4/4/4	-
4	GOL	A	817	-	-	2/4/4/4	-
3	EDO	B	803	-	-	0/1/1/1	-
3	EDO	A	811	-	-	0/1/1/1	-
5	PGE	B	818	-	-	4/7/7/7	-
3	EDO	B	805	-	-	0/1/1/1	-
4	GOL	B	815	-	-	0/4/4/4	-
4	GOL	A	815	-	-	4/4/4/4	-
3	EDO	B	811	-	-	1/1/1/1	-
3	EDO	B	810	-	-	1/1/1/1	-
4	GOL	A	814	-	-	0/4/4/4	-
4	GOL	B	816	-	-	0/4/4/4	-
4	GOL	A	816	-	-	0/4/4/4	-
4	GOL	B	813	-	-	0/4/4/4	-
4	GOL	B	814	-	-	0/4/4/4	-
3	EDO	A	810	-	-	0/1/1/1	-
3	EDO	B	804	-	-	1/1/1/1	-
3	EDO	A	806	-	-	0/1/1/1	-
3	EDO	B	809	-	-	1/1/1/1	-
3	EDO	A	804	-	-	1/1/1/1	-
3	EDO	B	806	-	-	1/1/1/1	-
3	EDO	B	807	-	-	1/1/1/1	-
3	EDO	A	809	-	-	1/1/1/1	-
3	EDO	A	803	-	-	0/1/1/1	-
3	EDO	A	807	-	-	1/1/1/1	-
3	EDO	A	808	-	-	1/1/1/1	-
4	GOL	B	817	-	-	2/4/4/4	-
6	PEG	B	819	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	814	GOL	O2-C2	-2.80	1.35	1.43
4	A	816	GOL	C1-C2	2.74	1.63	1.51
4	A	816	GOL	O2-C2	-2.59	1.35	1.43
4	B	813	GOL	O2-C2	-2.43	1.36	1.43
4	A	816	GOL	C3-C2	2.02	1.60	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	814	GOL	C3-C2-C1	-4.73	93.31	111.70
4	A	816	GOL	C3-C2-C1	-3.79	96.96	111.70
4	B	816	GOL	C3-C2-C1	-2.84	100.67	111.70
4	A	813	GOL	O1-C1-C2	-2.69	97.31	110.20
4	A	814	GOL	O2-C2-C3	2.27	119.14	109.12
4	B	815	GOL	C3-C2-C1	-2.18	103.24	111.70

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	813	GOL	O1-C1-C2-C3
4	A	813	GOL	C1-C2-C3-O3
4	A	815	GOL	O1-C1-C2-C3
4	A	815	GOL	C1-C2-C3-O3
4	B	817	GOL	O1-C1-C2-C3
5	B	818	PGE	O2-C3-C4-O3
5	B	818	PGE	O3-C5-C6-O4
4	A	817	GOL	O1-C1-C2-C3
5	B	818	PGE	O1-C1-C2-O2
4	A	817	GOL	O1-C1-C2-O2
4	A	813	GOL	O2-C2-C3-O3
4	B	817	GOL	O1-C1-C2-O2
3	A	805	EDO	O1-C1-C2-O2
3	A	812	EDO	O1-C1-C2-O2
3	B	809	EDO	O1-C1-C2-O2
3	A	809	EDO	O1-C1-C2-O2
4	A	815	GOL	O1-C1-C2-O2
4	A	815	GOL	O2-C2-C3-O3
3	A	804	EDO	O1-C1-C2-O2
6	B	819	PEG	O1-C1-C2-O2
3	B	812	EDO	O1-C1-C2-O2
3	B	804	EDO	O1-C1-C2-O2
4	A	813	GOL	O1-C1-C2-O2
3	B	808	EDO	O1-C1-C2-O2
3	B	807	EDO	O1-C1-C2-O2
3	A	807	EDO	O1-C1-C2-O2
5	B	818	PGE	C4-C3-O2-C2
3	B	811	EDO	O1-C1-C2-O2
3	B	810	EDO	O1-C1-C2-O2
3	B	806	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	808	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.