



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:48 PM UTC

PDB ID : 4LNC / pdb_00004lnc
Title : Neutron structure of the cyclic glucose bound Xylose Isomerase E186Q mutant
Authors : Munshi, P.; Meilleur, F.; Myles, D.
Deposited on : 2013-07-11
Resolution : 2.19 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

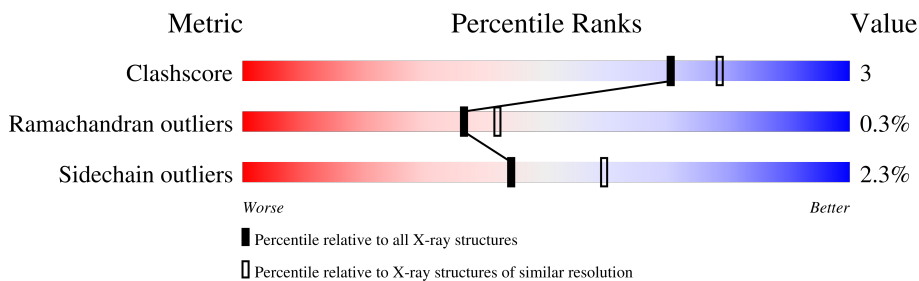
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

NEUTRON DIFFRACTION, X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 ≥ 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	388	 81% 17% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7245 atoms, of which 2759 are hydrogens and 1155 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.

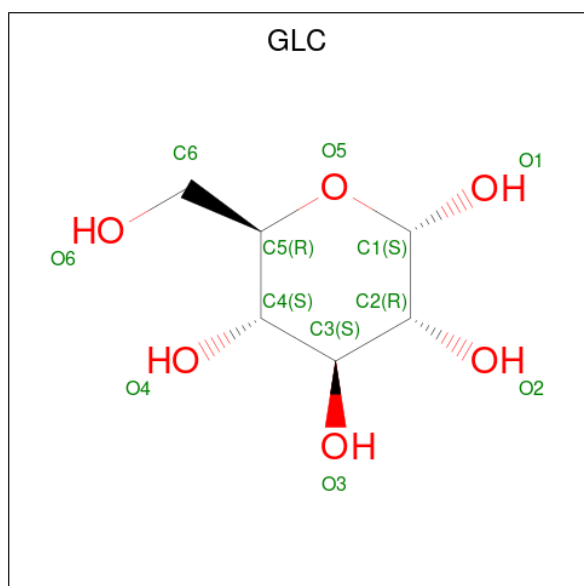
- Molecule 1 is a protein called Xylose isomerase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	385	6381	1905	606	2748	547	567	8	0	366	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	ALA	GLN	engineered mutation	UNP P24300
A	8	VAL	GLU	engineered mutation	UNP P24300
A	186	GLN	GLU	engineered mutation	UNP P24300

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	D	H	O		
2	A	1	27	6	4	11	6	0	1

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	Mn		0	0
			2	2			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

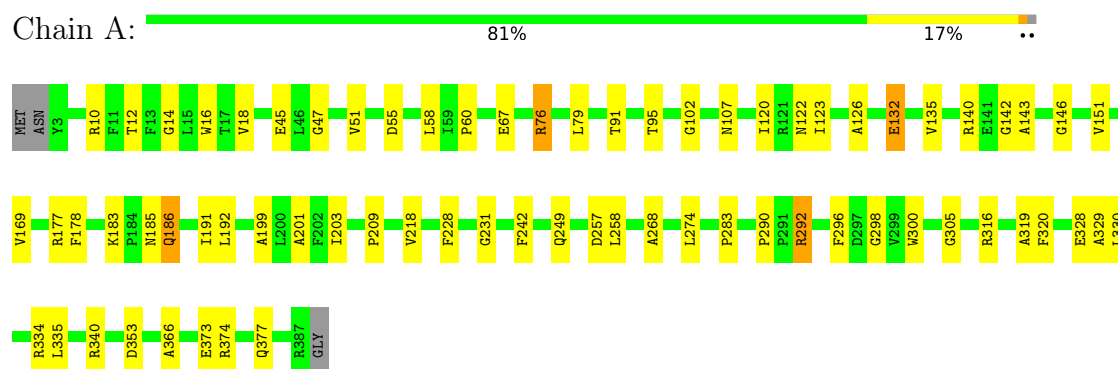
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	289	Total	D	O	0	0
			834	545	289		

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.

Note EDS failed to run properly.

- Molecule 1: Xylose isomerase



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.97Å 99.52Å 102.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.10 – 2.19	Depositor
% Data completeness (in resolution range)	93.1 (41.10-2.19)	Depositor
R_{merge}	0.28	Depositor
R_{sym}	0.28	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 1.84Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.284 , 0.322	Depositor
Wilson B-factor (Å ²)	17.2	Xtriage
Anisotropy	0.588	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for -h,-l,-k	Xtriage
Total number of atoms	7245	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: GLC, MN, DOD, MG

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	1.92	76/5425 (1.4%)	1.57	54/7331 (0.7%)

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169[A]	VAL	CA-CB	11.62	1.69	1.54
1	A	151[A]	VAL	CA-CB	7.98	1.64	1.54
1	A	151[B]	VAL	CA-CB	7.98	1.64	1.54
1	A	300[A]	TRP	CA-C	7.36	1.62	1.52
1	A	300[B]	TRP	CA-C	7.36	1.62	1.52
1	A	201[A]	ALA	CA-CB	6.91	1.64	1.53
1	A	95[A]	THR	CA-CB	6.74	1.64	1.53
1	A	95[B]	THR	CA-CB	6.74	1.64	1.53
1	A	373[B]	GLU	C-O	-6.63	1.16	1.24
1	A	14[B]	GLY	CA-C	6.37	1.58	1.52
1	A	191[A]	ILE	CA-CB	-6.37	1.46	1.54
1	A	203[A]	ILE	CA-CB	-6.36	1.46	1.54
1	A	199[A]	ALA	C-O	6.29	1.31	1.24
1	A	274[A]	LEU	CA-C	6.26	1.60	1.52
1	A	274[B]	LEU	CA-C	6.26	1.60	1.52
1	A	366[B]	ALA	CA-CB	-6.18	1.43	1.53
1	A	292[A]	ARG	CB-CG	-6.12	1.34	1.52
1	A	292[B]	ARG	CB-CG	-6.12	1.34	1.52
1	A	305[A]	GLY	C-O	6.11	1.31	1.23
1	A	305[B]	GLY	C-O	6.11	1.31	1.23
1	A	123[A]	ILE	C-O	-6.00	1.17	1.24
1	A	123[B]	ILE	C-O	-6.00	1.17	1.24
1	A	334[A]	ARG	CD-NE	-5.99	1.37	1.46
1	A	334[B]	ARG	CD-NE	-5.99	1.37	1.46
1	A	209	PRO	CA-C	-5.95	1.41	1.52
1	A	107[A]	ASN	CA-C	5.92	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107[B]	ASN	CA-C	5.92	1.60	1.52
1	A	186[A]	GLN	CD-NE2	-5.88	1.21	1.33
1	A	218[A]	VAL	CA-CB	5.84	1.60	1.54
1	A	185[A]	ASN	N-CA	-5.82	1.38	1.46
1	A	185[B]	ASN	N-CA	-5.82	1.38	1.46
1	A	340[A]	ARG	CZ-NH1	5.70	1.40	1.32
1	A	340[B]	ARG	CZ-NH1	5.70	1.40	1.32
1	A	257[A]	ASP	C-O	5.69	1.31	1.23
1	A	257[B]	ASP	C-O	5.69	1.31	1.23
1	A	249[A]	GLN	CA-C	-5.66	1.45	1.52
1	A	249[B]	GLN	CA-C	-5.66	1.45	1.52
1	A	328[A]	GLU	CG-CD	5.63	1.66	1.52
1	A	328[B]	GLU	CG-CD	5.63	1.66	1.52
1	A	328[A]	GLU	N-CA	5.61	1.53	1.46
1	A	328[B]	GLU	N-CA	5.61	1.53	1.46
1	A	102[A]	GLY	C-O	5.53	1.28	1.23
1	A	102[B]	GLY	C-O	5.53	1.28	1.23
1	A	120[A]	ILE	N-CA	5.51	1.53	1.46
1	A	120[B]	ILE	N-CA	5.51	1.53	1.46
1	A	374[A]	ARG	N-CA	-5.51	1.39	1.46
1	A	374[B]	ARG	N-CA	-5.51	1.39	1.46
1	A	140[A]	ARG	CA-C	5.50	1.59	1.52
1	A	140[B]	ARG	CA-C	5.50	1.59	1.52
1	A	242[A]	PHE	C-O	-5.50	1.16	1.24
1	A	242[B]	PHE	C-O	-5.50	1.16	1.24
1	A	12[A]	THR	C-O	-5.46	1.17	1.23
1	A	12[B]	THR	C-O	-5.46	1.17	1.23
1	A	126[A]	ALA	CA-CB	-5.28	1.45	1.53
1	A	126[B]	ALA	CA-CB	-5.28	1.45	1.53
1	A	377[A]	GLN	C-O	-5.25	1.17	1.24
1	A	377[B]	GLN	C-O	-5.25	1.17	1.24
1	A	55[B]	ASP	CA-C	-5.25	1.45	1.52
1	A	51[A]	VAL	CB-CG1	-5.18	1.35	1.52
1	A	51[B]	VAL	CB-CG1	-5.18	1.35	1.52
1	A	18[B]	VAL	CB-CG2	5.16	1.69	1.52
1	A	329[B]	ALA	CA-CB	-5.14	1.45	1.53
1	A	122[A]	ASN	C-O	-5.13	1.17	1.24
1	A	122[B]	ASN	C-O	-5.13	1.17	1.24
1	A	298[B]	GLY	C-O	5.12	1.29	1.23
1	A	135[A]	VAL	N-CA	5.12	1.52	1.46
1	A	320[A]	PHE	C-O	-5.11	1.18	1.24
1	A	320[B]	PHE	C-O	-5.11	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178[A]	PHE	C-O	-5.07	1.18	1.23
1	A	178[B]	PHE	C-O	-5.07	1.18	1.23
1	A	353[A]	ASP	CA-C	-5.06	1.46	1.52
1	A	353[B]	ASP	CA-C	-5.06	1.46	1.52
1	A	319[B]	ALA	CA-CB	5.03	1.61	1.53
1	A	231[B]	GLY	C-O	-5.02	1.17	1.23
1	A	132[A]	GLU	CG-CD	5.01	1.64	1.52
1	A	132[B]	GLU	CG-CD	5.01	1.64	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334[A]	ARG	NE-CZ-NH2	13.24	131.11	119.20
1	A	334[B]	ARG	NE-CZ-NH2	13.24	131.11	119.20
1	A	334[A]	ARG	NE-CZ-NH1	-9.18	112.33	121.50
1	A	334[B]	ARG	NE-CZ-NH1	-9.18	112.33	121.50
1	A	76[A]	ARG	NE-CZ-NH2	-6.90	112.99	119.20
1	A	76[B]	ARG	NE-CZ-NH2	-6.90	112.99	119.20
1	A	340[A]	ARG	CG-CD-NE	6.76	126.86	112.00
1	A	340[B]	ARG	CG-CD-NE	6.76	126.86	112.00
1	A	95[A]	THR	N-CA-C	6.69	119.92	111.69
1	A	95[B]	THR	N-CA-C	6.69	119.92	111.69
1	A	123[A]	ILE	N-CA-C	-6.50	104.18	110.42
1	A	123[B]	ILE	N-CA-C	-6.50	104.18	110.42
1	A	334[A]	ARG	CD-NE-CZ	6.17	133.03	124.40
1	A	334[B]	ARG	CD-NE-CZ	6.17	133.03	124.40
1	A	268[A]	ALA	N-CA-C	-6.11	104.18	111.69
1	A	16[B]	TRP	N-CA-C	5.83	120.13	113.19
1	A	47[B]	GLY	CA-C-O	5.73	124.68	118.95
1	A	296[A]	PHE	N-CA-C	5.69	117.48	111.28
1	A	296[B]	PHE	N-CA-C	5.69	117.48	111.28
1	A	334[A]	ARG	CG-CD-NE	-5.64	99.60	112.00
1	A	334[B]	ARG	CG-CD-NE	-5.64	99.60	112.00
1	A	142[A]	GLY	N-CA-C	5.56	117.67	110.45
1	A	142[B]	GLY	N-CA-C	5.56	117.67	110.45
1	A	177[B]	ARG	NE-CZ-NH1	-5.48	116.02	121.50
1	A	177[A]	ARG	NE-CZ-NH1	-5.48	116.02	121.50
1	A	274[A]	LEU	N-CA-C	5.47	116.94	110.97
1	A	274[B]	LEU	N-CA-C	5.47	116.94	110.97
1	A	330[A]	LEU	N-CA-C	-5.47	105.32	111.28
1	A	330[B]	LEU	N-CA-C	-5.47	105.32	111.28
1	A	67[A]	GLU	N-CA-C	-5.44	105.44	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67[B]	GLU	N-CA-C	-5.44	105.44	111.36
1	A	76[A]	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	A	76[B]	ARG	NH1-CZ-NH2	5.41	126.33	119.30
1	A	146[A]	GLY	N-CA-C	5.40	119.21	112.73
1	A	146[B]	GLY	N-CA-C	5.40	119.21	112.73
1	A	290	PRO	CA-C-N	-5.34	114.21	119.92
1	A	290	PRO	C-N-CA	-5.34	114.21	119.92
1	A	45[A]	GLU	N-CA-C	5.30	117.80	111.71
1	A	45[B]	GLU	N-CA-C	5.30	117.80	111.71
1	A	143[A]	ALA	N-CA-CB	-5.29	103.36	111.56
1	A	143[B]	ALA	N-CA-CB	-5.29	103.36	111.56
1	A	316[A]	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	316[B]	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	183[B]	LYS	CA-C-N	-5.24	113.29	119.84
1	A	183[B]	LYS	C-N-CA	-5.24	113.29	119.84
1	A	228[A]	PHE	O-C-N	5.24	124.52	120.38
1	A	228[B]	PHE	O-C-N	5.24	124.52	120.38
1	A	258[A]	LEU	N-CA-C	-5.22	103.50	110.55
1	A	258[B]	LEU	N-CA-C	-5.22	103.50	110.55
1	A	79[A]	LEU	N-CA-C	-5.21	105.68	111.36
1	A	192[A]	LEU	CD1-CG-CD2	-5.02	99.75	110.80
1	A	192[B]	LEU	CD1-CG-CD2	-5.02	99.75	110.80
1	A	374[A]	ARG	CA-C-O	5.02	125.87	120.55
1	A	374[B]	ARG	CA-C-O	5.02	125.87	120.55

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	3633	2748	133	2	0
2	A	16	11	0	0	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	834	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4486	2759	133	15	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 (15) 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)
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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	660/388 (170%)	646 (98%)	13 (2%)	1 (0%)	43 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186[A]	GLN

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	528/303 (174%)	516 (98%)	12 (2%)	44 59

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10[B]	ARG
1	A	10[A]	ARG
1	A	58[B]	LEU
1	A	76[A]	ARG
1	A	76[B]	ARG
1	A	91[A]	THR
1	A	91[B]	THR
1	A	132[A]	GLU
1	A	132[B]	GLU
1	A	292[A]	ARG
1	A	292[B]	ARG
1	A	335[A]	LEU

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

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 failed to run properly - this section is therefore empty.

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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