



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:35 AM UTC

PDB ID : 2XIS / pdb_00002xis
Title : A METAL-MEDIATED HYDRIDE SHIFT MECHANISM FOR XYLOSE ISOMERASE BASED ON THE 1.6 ANGSTROMS STREPTOMYCES RUBIGINOSUS STRUCTURES WITH XYLITOL AND D-XYLOSE
Authors : Whitlow, M.; Howard, A.J.
Deposited on : 1991-03-25
Resolution : 1.71 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

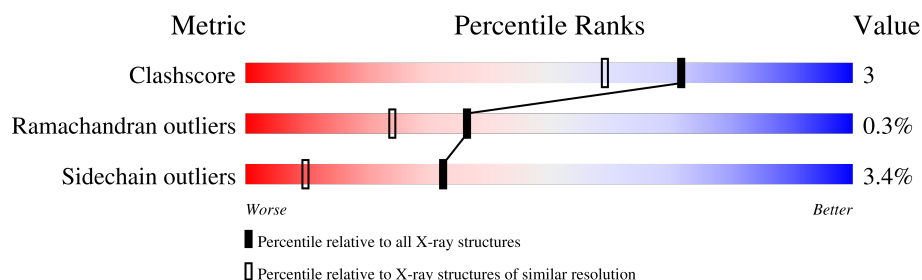
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)

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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	387	

2 Entry composition [i](#)

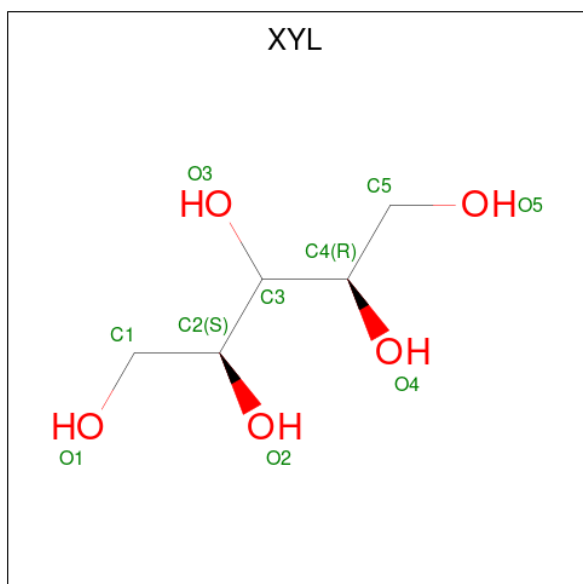
There are 4 unique types of molecules in this entry. The entry contains 3406 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	3049	1910	560	571	8	0	8	1

- Molecule 2 is Xylitol (CCD ID: XYL) (formula: C₅H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	10	5	5	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is water.

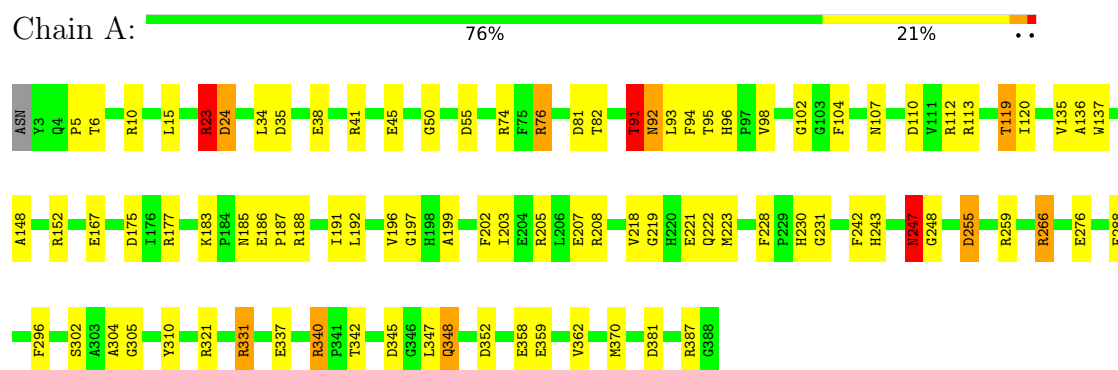
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	345	Total 345	O 345	0	0

3 Residue-property plots

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 was not executed.

• Molecule 1: XYLOSE ISOMERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	94.64Å 99.97Å 103.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.71	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.71)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3406	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.56	26/3171 (0.8%)	1.90	82/4290 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	222	GLN	C-O	7.76	1.34	1.24
1	A	222	GLN	N-CA	7.30	1.55	1.46
1	A	340	ARG	CD-NE	-6.93	1.36	1.46
1	A	228	PHE	N-CA	6.65	1.52	1.46
1	A	137	TRP	N-CA	6.60	1.54	1.46
1	A	247	ASN	N-CA	6.54	1.54	1.46
1	A	247	ASN	CA-C	6.16	1.61	1.52
1	A	192	LEU	N-CA	6.03	1.53	1.45
1	A	135	VAL	N-CA	5.83	1.52	1.46
1	A	113	ARG	CZ-NH2	5.81	1.41	1.33
1	A	302	SER	N-CA	5.63	1.53	1.46
1	A	82	THR	CA-CB	5.62	1.62	1.53
1	A	266	ARG	C-O	5.61	1.30	1.24
1	A	255[A]	ASP	N-CA	5.55	1.53	1.46
1	A	255[B]	ASP	N-CA	5.55	1.53	1.46
1	A	243	HIS	N-CA	5.55	1.52	1.46
1	A	188	ARG	N-CA	5.52	1.52	1.45
1	A	119	THR	CB-OG1	5.49	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	ASN	CG-OD1	5.45	1.33	1.23
1	A	288	PHE	N-CA	5.42	1.53	1.45
1	A	120	ILE	N-CA	5.38	1.52	1.46
1	A	23	ARG	CD-NE	-5.22	1.39	1.46
1	A	102	GLY	N-CA	5.21	1.51	1.45
1	A	6	THR	N-CA	5.15	1.50	1.45
1	A	197	GLY	C-O	5.05	1.29	1.23
1	A	191	ILE	N-CA	5.02	1.52	1.46

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	CD-NE-CZ	14.55	144.78	124.40
1	A	266	ARG	CD-NE-CZ	12.78	142.29	124.40
1	A	152	ARG	CD-NE-CZ	9.73	138.03	124.40
1	A	247	ASN	CA-CB-CG	9.22	121.82	112.60
1	A	113	ARG	NE-CZ-NH1	8.77	130.27	121.50
1	A	23	ARG	CD-NE-CZ	8.75	136.65	124.40
1	A	255[A]	ASP	CA-CB-CG	8.56	121.16	112.60
1	A	255[B]	ASP	CA-CB-CG	8.56	121.16	112.60
1	A	38	GLU	CB-CG-CD	8.14	126.43	112.60
1	A	23	ARG	CG-CD-NE	7.95	129.50	112.00
1	A	242	PHE	CA-CB-CG	7.87	121.67	113.80
1	A	24	ASP	CA-CB-CG	7.78	120.38	112.60
1	A	331	ARG	NE-CZ-NH1	7.53	129.03	121.50
1	A	276	GLU	CA-C-O	-7.03	112.96	120.42
1	A	266	ARG	NE-CZ-NH1	6.73	128.23	121.50
1	A	358	GLU	CB-CG-CD	6.66	123.92	112.60
1	A	55	ASP	CA-CB-CG	6.49	119.09	112.60
1	A	81	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	259	ARG	NE-CZ-NH2	6.47	125.02	119.20
1	A	296	PHE	N-CA-C	6.45	118.31	111.28
1	A	119	THR	O-C-N	6.32	128.91	122.09
1	A	342	THR	O-C-N	6.18	129.19	122.15
1	A	15	LEU	O-C-N	6.13	128.62	122.12
1	A	10	ARG	CA-CB-CG	6.10	126.31	114.10
1	A	74	ARG	CD-NE-CZ	6.10	132.94	124.40
1	A	203	ILE	O-C-N	6.09	127.86	121.89
1	A	340	ARG	CG-CD-NE	6.09	125.40	112.00
1	A	266	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	A	222	GLN	OE1-CD-NE2	-6.08	116.52	122.60
1	A	340	ARG	NE-CZ-NH2	-6.05	113.76	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255[A]	ASP	CB-CA-C	6.00	119.78	110.67
1	A	255[B]	ASP	CB-CA-C	6.00	119.78	110.67
1	A	24	ASP	CB-CA-C	5.97	121.94	110.17
1	A	222	GLN	CB-CG-CD	5.91	122.65	112.60
1	A	35	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	113	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	A	202	PHE	CA-C-O	-5.80	114.73	120.82
1	A	296	PHE	CA-C-N	5.79	128.04	120.28
1	A	296	PHE	C-N-CA	5.79	128.04	120.28
1	A	107	ASN	CA-C-O	-5.76	114.45	120.55
1	A	345	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	107	ASN	O-C-N	5.68	128.14	122.12
1	A	196	VAL	CA-C-O	-5.64	115.19	121.05
1	A	247	ASN	CB-CG-ND2	5.58	124.77	116.40
1	A	91	THR	CA-C-O	-5.57	114.81	120.71
1	A	231	GLY	O-C-N	5.55	127.52	122.19
1	A	45	GLU	CA-CB-CG	5.54	125.19	114.10
1	A	104	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	304	ALA	CA-C-N	5.47	126.05	119.98
1	A	304	ALA	C-N-CA	5.47	126.05	119.98
1	A	230	HIS	CA-C-N	5.47	126.05	119.98
1	A	230	HIS	C-N-CA	5.47	126.05	119.98
1	A	34	LEU	N-CA-CB	-5.46	101.50	110.52
1	A	310	TYR	CA-C-O	-5.41	115.14	120.82
1	A	348	GLN	N-CA-CB	5.40	117.99	109.94
1	A	76[A]	ARG	CA-CB-CG	5.40	124.89	114.10
1	A	76[B]	ARG	CA-CB-CG	5.40	124.89	114.10
1	A	221	GLU	O-C-N	5.38	128.88	122.27
1	A	110	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	305	GLY	CA-C-O	-5.36	115.23	120.75
1	A	112	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	A	340	ARG	NE-CZ-NH1	5.26	126.76	121.50
1	A	5	PRO	O-C-N	5.21	129.69	123.13
1	A	221	GLU	CG-CD-OE1	5.16	130.27	118.40
1	A	370	MET	CA-C-N	5.15	129.43	122.07
1	A	370	MET	C-N-CA	5.15	129.43	122.07
1	A	148	ALA	N-CA-C	5.14	117.78	111.82
1	A	207[A]	GLU	CB-CG-CD	5.14	121.34	112.60
1	A	207[B]	GLU	CB-CG-CD	5.14	121.34	112.60
1	A	183	LYS	O-C-N	-5.10	117.86	121.84
1	A	352	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	359	GLU	CB-CG-CD	5.09	121.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	ASP	CA-C-N	5.08	124.87	119.28
1	A	24	ASP	C-N-CA	5.08	124.87	119.28
1	A	76[A]	ARG	CB-CA-C	5.06	119.19	110.79
1	A	76[B]	ARG	CB-CA-C	5.06	119.19	110.79
1	A	199	ALA	CA-C-O	-5.05	115.06	120.42
1	A	247	ASN	N-CA-C	-5.03	100.09	110.80
1	A	167	GLU	CB-CG-CD	5.02	121.14	112.60
1	A	50	GLY	CA-C-O	-5.01	116.74	121.60
1	A	136	ALA	CA-C-N	-5.00	115.77	123.07
1	A	136	ALA	C-N-CA	-5.00	115.77	123.07

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
1	A	205[A]	ARG	Sidechain
1	A	205[B]	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	23	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	331	ARG	Sidechain
1	A	41	ARG	Sidechain
1	A	76[A]	ARG	Sidechain
1	A	76[B]	ARG	Sidechain

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	3049	0	2895	20	0
2	A	10	0	10	0	0
3	A	2	0	0	0	0
4	A	345	0	0	6	0
All	All	3406	0	2905	20	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 (20) 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:92:ASN:HD21	1:A:95:THR:H	1.24	0.86
1:A:96:HIS:HD2	1:A:98:VAL:H	1.30	0.80
1:A:93:LEU:HD21	4:A:618:HOH:O	1.96	0.65
1:A:219:GLY:H	1:A:247:ASN:HD21	1.43	0.64
1:A:248:GLY:HA2	4:A:608:HOH:O	2.01	0.60
1:A:92:ASN:ND2	1:A:94:PHE:H	2.00	0.59
1:A:218:VAL:HG11	4:A:608:HOH:O	2.03	0.58
1:A:92:ASN:ND2	1:A:95:THR:H	1.98	0.57
1:A:92:ASN:HD22	1:A:94:PHE:H	1.52	0.55
1:A:96:HIS:CD2	1:A:98:VAL:H	2.18	0.53
1:A:92:ASN:HD22	1:A:92:ASN:C	2.19	0.49
1:A:266:ARG:HG3	4:A:454:HOH:O	2.14	0.47
1:A:91:THR:HG21	4:A:618:HOH:O	2.15	0.46
1:A:223:MET:SD	1:A:255[B]:ASP:HB2	2.56	0.46
1:A:223:MET:SD	1:A:255[A]:ASP:HB3	2.57	0.44
1:A:337:GLU:HG2	1:A:340:ARG:NH2	2.32	0.44
1:A:23:ARG:HD3	1:A:24:ASP:N	2.33	0.44
1:A:119:THR:N	4:A:618:HOH:O	2.49	0.43
1:A:92:ASN:HD21	1:A:95:THR:N	2.05	0.41
1:A:381:ASP:HB3	1:A:387[B]:ARG:HD2	2.03	0.41

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	392/387 (101%)	377 (96%)	13 (3%)	2 (0%)	24 11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186[A]	GLU
1	A	186[B]	GLU

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	306/303 (101%)	296 (97%)	10 (3%)	33	10

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	91	THR
1	A	92	ASN
1	A	175	ASP
1	A	185	ASN
1	A	187	PRO
1	A	247	ASN
1	A	347	LEU
1	A	348	GLN
1	A	362	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	92	ASN
1	A	96	HIS
1	A	185	ASN
1	A	215	ASN
1	A	222	GLN
1	A	230	HIS
1	A	234	GLN
1	A	247	ASN

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 3 ligands modelled in this entry, 2 are 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	$\# Z > 2$
2	XYL	A	390	3	9,9,9	1.23	1 (11%)	11,11,11	1.37	1 (9%)

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
2	XYL	A	390	3	-	1/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	390	XYL	C1-C2	2.49	1.58	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	390	XYL	C1-C2-C3	-2.96	106.13	112.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	390	XYL	O4-C4-C5-O5

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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.