



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:32 AM BST

PDB ID : 4XIS
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 : 1.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.13.1

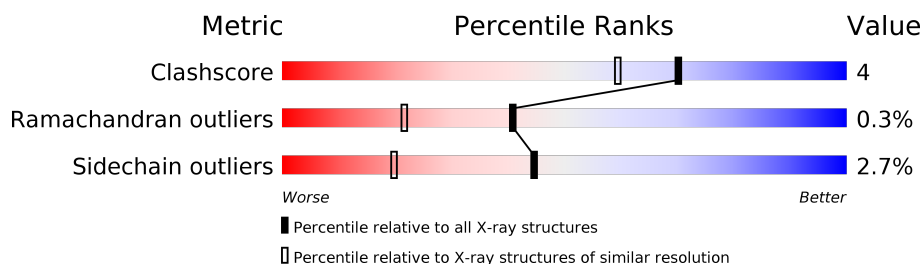
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	387	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XLS	A	393[A]	X	-	-	-

2 Entry composition [i](#)

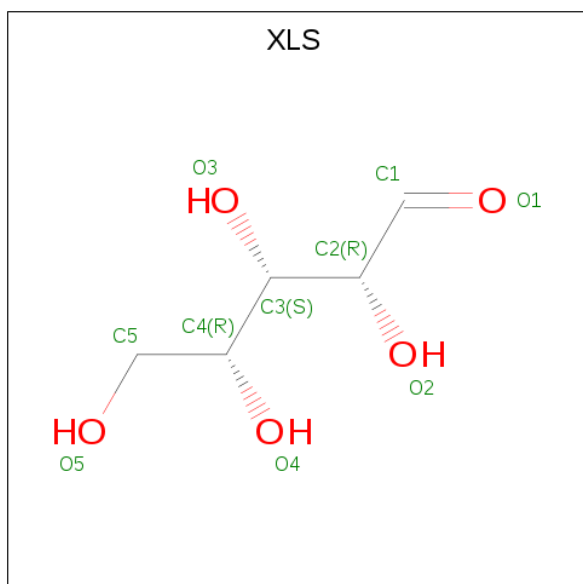
There are 5 unique types of molecules in this entry. The entry contains 3527 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

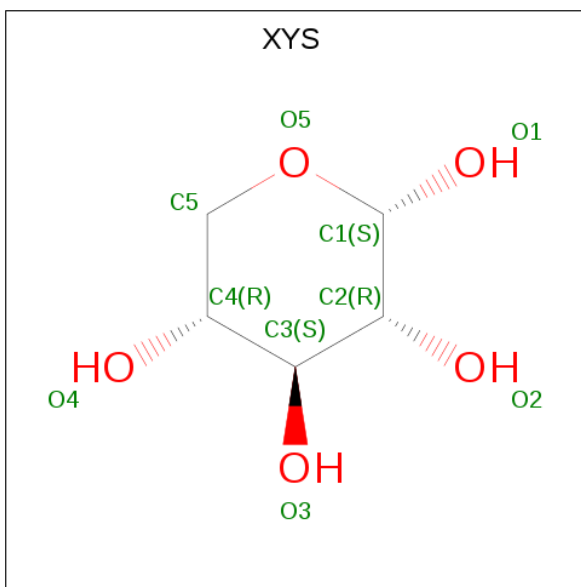
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	3100	1940	575	576	9	0	17	1

- Molecule 2 is D-xylose (three-letter code: XLS) (formula: C₅H₁₀O₅).



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

- Molecule 3 is alpha-D-xylopyranose (three-letter code: XYS) (formula: C₅H₁₀O₅).



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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

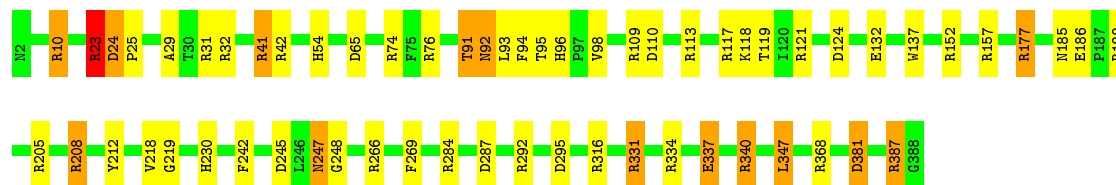
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	1
			3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	400	Total	O	0	4
			404	404		

Note EDS was not executed.

Chain A: 84% 12% .



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 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.135 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3527	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

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: YYS, XLS, MN

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	1.20	5/3265 (0.2%)	1.72	88/4413 (2.0%)

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	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132[A]	GLU	CG-CD	-7.63	1.40	1.51
1	A	132[B]	GLU	CG-CD	-7.63	1.40	1.51
1	A	113	ARG	CZ-NH2	5.92	1.40	1.33
1	A	132[A]	GLU	CD-OE2	5.71	1.31	1.25
1	A	132[B]	GLU	CD-OE2	5.71	1.31	1.25

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132[A]	GLU	CB-CG-CD	15.23	155.32	114.20
1	A	132[B]	GLU	CB-CG-CD	15.23	155.32	114.20
1	A	113	ARG	NE-CZ-NH1	14.21	127.41	120.30
1	A	331	ARG	NE-CZ-NH1	13.59	127.10	120.30
1	A	331	ARG	NE-CZ-NH2	-12.31	114.15	120.30
1	A	74	ARG	CD-NE-CZ	11.87	140.22	123.60
1	A	74	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	A	157	ARG	NE-CZ-NH2	11.34	125.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266[A]	ARG	CD-NE-CZ	10.27	137.98	123.60
1	A	266[B]	ARG	CD-NE-CZ	10.27	137.98	123.60
1	A	188	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	A	188	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	381	ASP	CB-CG-OD1	9.17	126.55	118.30
1	A	74	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	A	124	ASP	CB-CG-OD1	8.82	126.24	118.30
1	A	10	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	A	368	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	31	ARG	NE-CZ-NH2	-8.63	115.99	120.30
1	A	23[A]	ARG	CD-NE-CZ	8.61	135.66	123.60
1	A	23[B]	ARG	CD-NE-CZ	8.61	135.66	123.60
1	A	10	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	A	292	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	A	177	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	A	266[A]	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	A	266[B]	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	A	113	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	340[A]	ARG	CD-NE-CZ	7.98	134.78	123.60
1	A	340[B]	ARG	CD-NE-CZ	7.98	134.78	123.60
1	A	121	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	284	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	31	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	23[A]	ARG	CG-CD-NE	7.64	127.85	111.80
1	A	23[B]	ARG	CG-CD-NE	7.64	127.85	111.80
1	A	316	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	205[A]	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	205[B]	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	295	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	340[A]	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	340[B]	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	177	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	208	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	A	387[A]	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	387[B]	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	284	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	76[A]	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	A	76[B]	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	A	266[A]	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	266[B]	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	340[A]	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	A	340[B]	ARG	NE-CZ-NH1	6.61	123.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132[A]	GLU	OE1-CD-OE2	-6.56	115.42	123.30
1	A	132[B]	GLU	OE1-CD-OE2	-6.56	115.42	123.30
1	A	42	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	121	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	109	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	334	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	24	ASP	CB-CA-C	6.24	122.88	110.40
1	A	109	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	32	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	76[A]	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	76[B]	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	124	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	245	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	152	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	41	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	205[A]	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	205[B]	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	152	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	347	LEU	CB-CG-CD2	5.80	120.86	111.00
1	A	132[A]	GLU	CG-CD-OE1	5.78	129.86	118.30
1	A	132[B]	GLU	CG-CD-OE1	5.78	129.86	118.30
1	A	117	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	287	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	212	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	A	42	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	242	PHE	CB-CG-CD2	-5.54	116.92	120.80
1	A	269	PHE	CB-CG-CD1	-5.50	116.95	120.80
1	A	76[A]	ARG	CA-CB-CG	5.48	125.46	113.40
1	A	76[B]	ARG	CA-CB-CG	5.48	125.46	113.40
1	A	208	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	242	PHE	CB-CG-CD1	5.45	124.61	120.80
1	A	205[A]	ARG	CD-NE-CZ	5.42	131.19	123.60
1	A	205[B]	ARG	CD-NE-CZ	5.42	131.19	123.60
1	A	65	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	337	GLU	CG-CD-OE1	5.30	128.91	118.30
1	A	110	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	287	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	157	ARG	NH1-CZ-NH2	-5.03	113.87	119.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	ARG	Sidechain
1	A	208	ARG	Sidechain
1	A	331	ARG	Sidechain
1	A	41	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	3100	0	2952	22	0
2	A	10	0	7	0	0
3	A	10	0	9	2	0
4	A	3	0	0	0	0
5	A	404	0	0	8	0
All	All	3527	0	2968	22	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 4.

All (22) 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:96:HIS:HD2	1:A:98:VAL:H	1.32	0.76
1:A:92:ASN:HD21	1:A:95:THR:H	1.36	0.73
1:A:340[B]:ARG:NH2	5:A:528:HOH:O	1.68	0.67
1:A:93:LEU:HD21	5:A:618:HOH:O	1.97	0.63
1:A:248:GLY:HA2	5:A:608:HOH:O	2.00	0.61
1:A:218:VAL:HG11	5:A:608:HOH:O	2.00	0.61
1:A:219:GLY:H	1:A:247:ASN:HD21	1.54	0.56
1:A:24:ASP:HB2	1:A:25:PRO:HD2	1.87	0.56
1:A:96:HIS:CD2	1:A:98:VAL:H	2.19	0.54
1:A:92:ASN:C	1:A:92:ASN:HD22	2.14	0.50
1:A:92:ASN:ND2	1:A:94:PHE:H	2.10	0.50
1:A:340[B]:ARG:NE	5:A:528:HOH:O	2.40	0.49
1:A:337:GLU:HG2	1:A:340[A]:ARG:NH2	2.27	0.49
1:A:137:TRP:CE3	3:A:394[B]:XYS:H51	2.47	0.49
1:A:91:THR:HG21	5:A:618:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:HIS:NE2	3:A:394[B]:XYS:H52	2.29	0.46
1:A:92:ASN:HD22	1:A:94:PHE:H	1.64	0.46
1:A:381:ASP:HB3	1:A:387[B]:ARG:HD2	1.98	0.45
1:A:119:THR:N	5:A:618:HOH:O	2.49	0.45
1:A:92:ASN:ND2	1:A:95:THR:H	2.07	0.45
1:A:118:LYS:HB3	5:A:618:HOH:O	2.19	0.42
1:A:23[B]:ARG:HG2	1:A:29:ALA:N	2.36	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	402/387 (104%)	387 (96%)	14 (4%)	1 (0%)	47 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	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	317/303 (105%)	308 (97%)	9 (3%)	43 18

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	23[A]	ARG
1	A	23[B]	ARG
1	A	91	THR
1	A	92	ASN
1	A	185	ASN
1	A	230	HIS
1	A	247	ASN
1	A	347	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	92	ASN
1	A	96	HIS
1	A	215	ASN
1	A	222	GLN
1	A	230	HIS
1	A	247	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	XLS	A	393[A]	-	8,9,9	2.91	2 (25%)	10,11,11	2.51	2 (20%)
3	XYS	A	394[B]	-	10,10,10	2.06	2 (20%)	14,14,14	3.70	7 (50%)

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	XLS	A	393[A]	-	1/1/3/4	4/10/12/12	-
3	XYS	A	394[B]	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	393[A]	XLS	O1-C1	6.19	1.44	1.19
3	A	394[B]	XYS	O5-C1	-5.32	1.35	1.43
2	A	393[A]	XLS	O2-C2	-4.60	1.34	1.43
3	A	394[B]	XYS	C1-C2	2.45	1.58	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	394[B]	XYS	O5-C5-C4	9.84	125.96	110.77
2	A	393[A]	XLS	O2-C2-C1	5.86	123.89	110.08
3	A	394[B]	XYS	O1-C1-O5	5.30	123.52	109.72
3	A	394[B]	XYS	O1-C1-C2	4.32	121.19	109.03
2	A	393[A]	XLS	C3-C2-C1	3.89	123.35	111.10
3	A	394[B]	XYS	O4-C4-C5	3.78	116.89	109.15
3	A	394[B]	XYS	C5-O5-C1	3.50	118.60	112.71
3	A	394[B]	XYS	O2-C2-C3	3.01	117.30	110.35
3	A	394[B]	XYS	C1-C2-C3	-2.22	105.70	110.31

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	393[A]	XLS	C2

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	393[A]	XLS	C1-C2-C3-C4
2	A	393[A]	XLS	C1-C2-C3-O3
2	A	393[A]	XLS	O2-C2-C3-O3
2	A	393[A]	XLS	O4-C4-C5-O5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	394[B]	XYS	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 ⓘ

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.