



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:40 PM UTC

PDB ID : 3XIS / pdb_00003xis
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 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

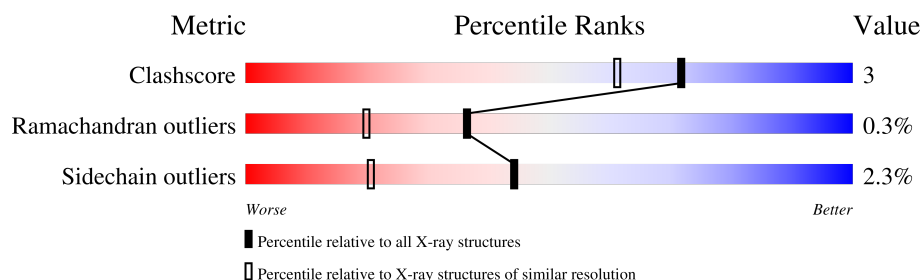
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (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 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](#)

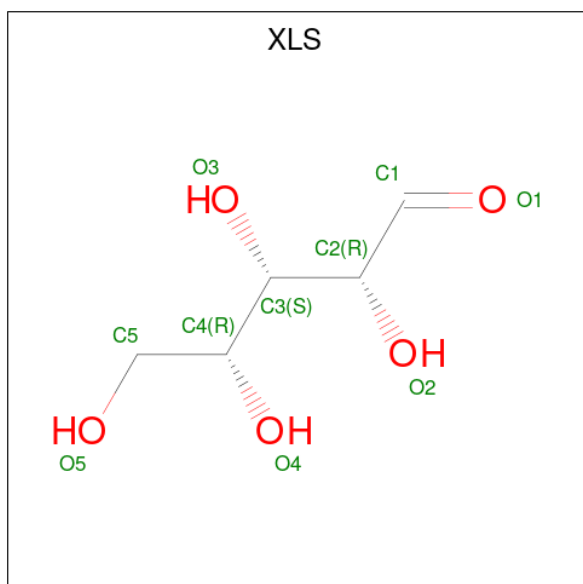
There are 5 unique types of molecules in this entry. The entry contains 3433 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

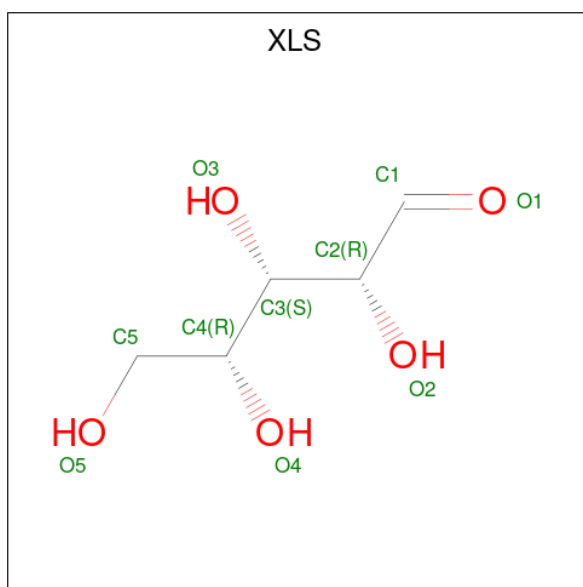
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	3049	1913	558	569	9	0	6	1

- Molecule 2 is alpha-D-xylopyranose (CCD ID: XLS) (formula: C₅H₁₀O₅).



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

- Molecule 3 is D-xylose (CCD ID: XLS) (formula: C₅H₁₀O₅).



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

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	362	Total	O	0	0
			362	362		

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 – 1.60	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}	0.151 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3433	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: XLS, MG, XYS

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	1.65	22/3158 (0.7%)	1.93	84/4270 (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	9

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	THR	CA-CB	7.92	1.65	1.54
1	A	295	ASP	N-CA	7.43	1.54	1.45
1	A	221	GLU	N-CA	7.33	1.55	1.46
1	A	230	HIS	ND1-CE1	7.15	1.39	1.32
1	A	340	ARG	CD-NE	-6.96	1.36	1.46
1	A	54	HIS	CA-C	6.83	1.61	1.52
1	A	140	ARG	N-CA	6.60	1.54	1.46
1	A	105	THR	CA-CB	6.38	1.61	1.53
1	A	188	ARG	N-CA	6.29	1.53	1.45
1	A	247	ASN	C-N	-6.26	1.25	1.33
1	A	249	GLN	N-CA	5.93	1.53	1.46
1	A	228	PHE	N-CA	5.78	1.51	1.46
1	A	17	THR	C-N	5.67	1.40	1.34
1	A	137	TRP	CA-C	5.64	1.59	1.52
1	A	23	ARG	CD-NE	-5.61	1.38	1.46
1	A	266	ARG	CD-NE	-5.59	1.38	1.46
1	A	247	ASN	CA-C	5.48	1.59	1.53
1	A	313	LEU	C-O	5.41	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	307	MET	C-N	-5.23	1.27	1.33
1	A	289	LYS	N-CA	5.18	1.53	1.46
1	A	293	THR	C-O	5.13	1.30	1.24
1	A	382	HIS	CD2-NE2	5.04	1.43	1.37

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	CD-NE-CZ	13.87	143.82	124.40
1	A	266	ARG	CD-NE-CZ	13.05	142.67	124.40
1	A	152	ARG	CD-NE-CZ	10.49	139.09	124.40
1	A	23	ARG	CD-NE-CZ	10.12	138.56	124.40
1	A	242	PHE	CA-CB-CG	10.00	123.80	113.80
1	A	294	GLU	O-C-N	8.99	133.44	123.10
1	A	24	ASP	CA-CB-CG	8.57	121.17	112.60
1	A	74	ARG	CD-NE-CZ	8.50	136.29	124.40
1	A	23	ARG	CG-CD-NE	8.48	130.66	112.00
1	A	331	ARG	NE-CZ-NH1	8.31	129.81	121.50
1	A	38	GLU	CB-CG-CD	8.25	126.63	112.60
1	A	4	GLN	CA-C-O	7.96	125.21	119.32
1	A	255	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	104	PHE	CA-CB-CG	7.43	121.23	113.80
1	A	348	GLN	N-CA-CB	7.31	120.61	110.01
1	A	247	ASN	CA-C-O	-7.18	113.47	120.94
1	A	247	ASN	O-C-N	7.15	131.05	122.75
1	A	340	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	A	358	GLU	CB-CG-CD	6.91	124.35	112.60
1	A	247	ASN	OD1-CG-ND2	-6.89	115.71	122.60
1	A	45	GLU	CA-CB-CG	6.85	127.80	114.10
1	A	188	ARG	NE-CZ-NH1	6.82	128.32	121.50
1	A	340	ARG	NE-CZ-NH2	-6.77	113.11	119.20
1	A	178	PHE	O-C-N	6.63	130.73	123.10
1	A	81	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	331	ARG	CD-NE-CZ	6.34	133.28	124.40
1	A	35	ASP	CA-CB-CG	6.33	118.93	112.60
1	A	139	GLY	O-C-N	6.30	128.92	122.24
1	A	368	ARG	CA-CB-CG	6.30	126.70	114.10
1	A	27	GLY	O-C-N	6.25	128.02	123.27
1	A	8	GLU	CA-CB-CG	6.24	126.58	114.10
1	A	174	TYR	CA-CB-CG	6.23	125.12	113.90
1	A	368	ARG	CD-NE-CZ	6.23	133.12	124.40
1	A	340	ARG	CG-CD-NE	6.20	125.63	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASN	CA-C-O	6.12	127.13	120.58
1	A	288	PHE	O-C-N	6.01	130.53	122.96
1	A	151	VAL	N-CA-C	5.99	116.73	110.62
1	A	290	PRO	N-CA-C	-5.94	103.46	110.70
1	A	288	PHE	CA-C-O	-5.83	114.98	121.51
1	A	10	ARG	CA-CB-CG	5.82	125.74	114.10
1	A	34	LEU	N-CA-CB	-5.64	101.22	110.52
1	A	178	PHE	CA-C-O	-5.62	114.65	121.28
1	A	345	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	354	ARG	CD-NE-CZ	5.61	132.25	124.40
1	A	107	ASN	O-C-N	5.58	128.04	122.12
1	A	24	ASP	CB-CA-C	5.51	121.03	110.17
1	A	157	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	312	ILE	N-CA-C	-5.49	105.14	110.42
1	A	113	ARG	CA-C-N	5.42	127.48	120.44
1	A	113	ARG	C-N-CA	5.42	127.48	120.44
1	A	57	ASP	O-C-N	5.41	129.26	122.23
1	A	347	LEU	O-C-N	5.39	127.62	122.07
1	A	189	GLY	CA-C-N	5.38	131.37	122.33
1	A	189	GLY	C-N-CA	5.38	131.37	122.33
1	A	275	LEU	O-C-N	5.31	127.75	122.12
1	A	348	GLN	CB-CG-CD	5.31	121.62	112.60
1	A	163	ASP	O-C-N	5.25	127.47	122.07
1	A	359	GLU	CB-CG-CD	5.18	121.40	112.60
1	A	226	LEU	O-C-N	5.17	128.72	122.94
1	A	156	ASP	O-C-N	5.16	127.59	122.12
1	A	82	THR	CA-CB-OG1	-5.16	101.86	109.60
1	A	188	ARG	NE-CZ-NH2	-5.16	114.56	119.20
1	A	380	MET	O-C-N	5.16	127.38	122.07
1	A	139	GLY	CA-C-N	-5.15	114.04	122.54
1	A	139	GLY	C-N-CA	-5.15	114.04	122.54
1	A	307	MET	CA-C-O	-5.14	115.42	120.82
1	A	364	ALA	O-C-N	5.14	128.01	122.15
1	A	370	MET	CA-C-N	5.11	129.81	122.40
1	A	370	MET	C-N-CA	5.11	129.81	122.40
1	A	122	ASN	CA-CB-CG	-5.11	107.49	112.60
1	A	312	ILE	N-CA-CB	5.11	116.53	110.55
1	A	54	HIS	N-CA-C	-5.10	102.22	110.32
1	A	110	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	255	ASP	CB-CA-C	5.08	118.39	110.67
1	A	170	THR	CA-CB-OG1	-5.07	102.00	109.60
1	A	266	ARG	O-C-N	-5.06	116.75	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	LEU	CA-C-N	5.04	126.99	120.44
1	A	313	LEU	C-N-CA	5.04	126.99	120.44
1	A	219	GLY	O-C-N	5.04	127.58	122.24
1	A	325	GLU	CA-CB-CG	5.04	124.17	114.10
1	A	370	MET	CA-C-O	-5.04	113.19	119.18
1	A	283	PRO	CA-C-N	5.03	130.21	122.77
1	A	283	PRO	C-N-CA	5.03	130.21	122.77
1	A	328	GLU	N-CA-CB	5.02	117.59	110.16

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	A	177	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 [i](#)

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	2914	19	0
2	A	10	0	0	0	0
3	A	10	0	19	1	0
4	A	2	0	0	0	0
5	A	362	0	0	6	0
All	All	3433	0	2933	19	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 (19) 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	1.30	0.80
1:A:92:ASN:HD21	1:A:95:THR:H	1.39	0.70
1:A:93:LEU:HD21	5:A:618:HOH:O	1.93	0.68
1:A:219:GLY:H	1:A:247:ASN:HD21	1.43	0.65
1:A:248:GLY:HA2	5:A:608:HOH:O	2.01	0.60
1:A:218:VAL:HG11	5:A:608:HOH:O	2.02	0.59
1:A:24:ASP:HB2	1:A:25:PRO:HD2	1.89	0.53
1:A:92:ASN:ND2	1:A:95:THR:H	2.07	0.51
1:A:266:ARG:HG3	5:A:454:HOH:O	2.11	0.51
1:A:119:THR:N	5:A:618:HOH:O	2.43	0.50
1:A:96:HIS:CD2	1:A:98:VAL:H	2.20	0.48
1:A:92:ASN:C	1:A:92:ASN:HD22	2.22	0.48
1:A:92:ASN:ND2	1:A:94:PHE:H	2.15	0.45
1:A:337:GLU:HG2	1:A:340:ARG:NH2	2.32	0.44
1:A:91:THR:HG21	5:A:618:HOH:O	2.18	0.43
1:A:137:TRP:HB3	3:A:393[A]:XYS:H51	2.02	0.42
1:A:323:ASP:HA	1:A:324:PRO:HD3	1.95	0.41
1:A:92:ASN:HD22	1:A:94:PHE:H	1.66	0.41
1:A:381:ASP:HB3	1:A:387[B]:ARG:HD2	2.02	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	390/387 (101%)	376 (96%)	13 (3%)	1 (0%)	36 20

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	306/303 (101%)	299 (98%)	7 (2%)	44 20

All (7) 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	247	ASN
1	A	347	LEU
1	A	348	GLN

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	77	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 [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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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
3	XYS	A	393[A]	-	10,10,10	1.99	2 (20%)	14,14,14	2.79	7 (50%)
3	XLS	A	393[B]	-	8,9,9	1.96	1 (12%)	10,11,11	1.49	1 (10%)

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	XYS	A	393[A]	-	-	-	0/1/1/1
3	XLS	A	393[B]	-	-	10/11/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	393[B]	XLS	O1-C1	5.38	1.40	1.20
3	A	393[A]	XYS	O5-C5	-4.54	1.36	1.43
3	A	393[A]	XYS	O5-C1	-3.16	1.38	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	393[A]	XYS	C5-O5-C1	7.58	128.21	112.46
3	A	393[B]	XLS	O2-C2-C1	3.33	118.05	110.48
3	A	393[A]	XYS	O5-C5-C4	3.05	118.06	110.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	393[A]	XYS	O1-C1-C2	2.95	117.55	108.98
3	A	393[A]	XYS	O4-C4-C3	2.81	115.98	110.15
3	A	393[A]	XYS	C1-C2-C3	-2.77	104.70	110.36
3	A	393[A]	XYS	O1-C1-O5	2.48	116.27	109.91
3	A	393[A]	XYS	O4-C4-C5	2.07	113.97	109.22

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	393[B]	XLS	O1-C1-C2-C3
3	A	393[B]	XLS	C1-C2-C3-C4
3	A	393[B]	XLS	C1-C2-C3-O3
3	A	393[B]	XLS	O2-C2-C3-O3
3	A	393[B]	XLS	C3-C4-C5-O5
3	A	393[B]	XLS	O4-C4-C5-O5
3	A	393[B]	XLS	O3-C3-C4-O4
3	A	393[B]	XLS	C2-C3-C4-O4
3	A	393[B]	XLS	O2-C2-C3-C4
3	A	393[B]	XLS	O3-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	393[A]	XYS	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

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.