



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:31 AM UTC

PDB ID : 8XIA / pdb_00008xia
Title : X-RAY ANALYSIS OF D-XYLOSE ISOMERASE AT 1.9 ANGSTROMS:
NATIVE ENZYME IN COMPLEX WITH SUBSTRATE AND WITH A
MECHANISM-DESIGNED INACTIVATOR
Authors : Carrell, H.L.; Glusker, J.P.
Deposited on : 1990-10-11
Resolution : 1.90 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

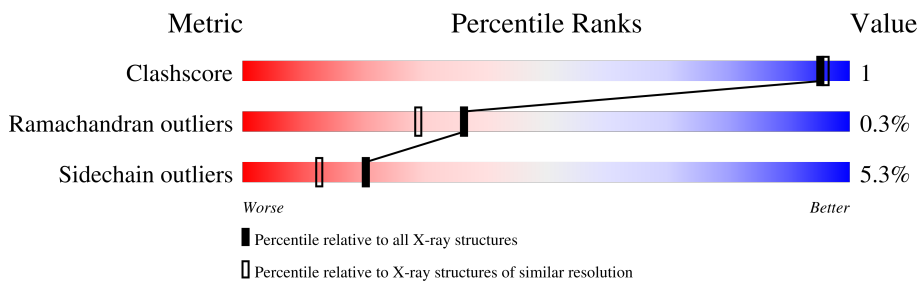
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	388	

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	389	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3347 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.

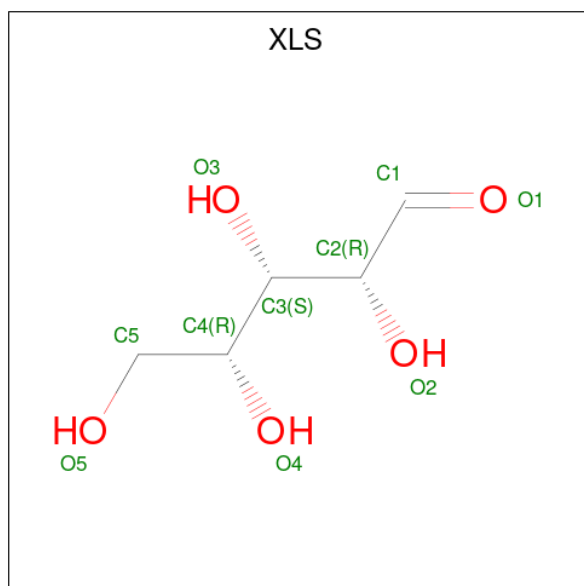
- Molecule 1 is a protein called XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	3044	1914	547	574	9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLN	ARG	conflict	UNP P24300

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



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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	291	Total 291	O 291	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	94.20Å 100.20Å 103.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.140 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3347	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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: MN, XLS

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	1.54	19/3116 (0.6%)	2.12	104/4218 (2.5%)

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	3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	ARG	CD-NE	-9.20	1.33	1.46
1	A	196	VAL	CA-CB	7.00	1.62	1.54
1	A	265	LEU	CB-CG	6.41	1.66	1.53
1	A	111	VAL	N-CA	6.21	1.53	1.46
1	A	54	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	274	LEU	C-O	5.90	1.30	1.24
1	A	218	VAL	CA-CB	5.88	1.60	1.54
1	A	243	HIS	N-CA	5.83	1.52	1.46
1	A	253	LYS	CA-CB	5.72	1.61	1.53
1	A	218	VAL	CB-CG1	5.55	1.70	1.52
1	A	90	THR	N-CA	5.55	1.52	1.45
1	A	82	THR	CA-CB	5.45	1.62	1.54
1	A	247	ASN	N-CA	5.44	1.53	1.46
1	A	293	THR	CB-OG1	5.43	1.52	1.43
1	A	276	GLU	C-O	5.32	1.30	1.24
1	A	342	THR	CA-CB	5.28	1.62	1.53
1	A	177	ARG	CD-NE	-5.16	1.39	1.46
1	A	302	SER	C-O	5.14	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	ARG	CD-NE	-5.00	1.39	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	CD-NE-CZ	25.22	159.70	124.40
1	A	340	ARG	NE-CZ-NH2	15.79	133.41	119.20
1	A	152	ARG	CD-NE-CZ	15.47	146.05	124.40
1	A	253	LYS	N-CA-CB	-12.80	91.77	111.35
1	A	340	ARG	NE-CZ-NH1	-10.81	110.69	121.50
1	A	76	ARG	NE-CZ-NH2	-10.27	109.96	119.20
1	A	68	ARG	NE-CZ-NH2	10.24	128.41	119.20
1	A	374	ARG	NE-CZ-NH2	10.10	128.29	119.20
1	A	266	ARG	NE-CZ-NH2	-10.03	110.17	119.20
1	A	386	ALA	CA-C-N	9.90	139.53	121.70
1	A	386	ALA	C-N-CA	9.90	139.53	121.70
1	A	328	GLU	CB-CG-CD	9.22	128.27	112.60
1	A	24	ASP	CB-CA-C	9.08	128.07	110.17
1	A	2	ASN	CB-CA-C	9.00	127.13	109.66
1	A	340	ARG	CD-NE-CZ	8.35	136.09	124.40
1	A	42	ARG	CD-NE-CZ	8.30	136.02	124.40
1	A	69	GLU	CB-CG-CD	8.05	126.28	112.60
1	A	21	GLN	OE1-CD-NE2	7.98	130.58	122.60
1	A	74	ARG	NE-CZ-NH2	-7.97	112.03	119.20
1	A	68	ARG	NH1-CZ-NH2	-7.86	109.09	119.30
1	A	306	CYS	O-C-N	7.84	130.24	122.09
1	A	68	ARG	CA-CB-CG	7.71	129.52	114.10
1	A	54	HIS	N-CA-C	-7.69	97.79	110.17
1	A	143	ALA	O-C-N	7.54	130.83	123.29
1	A	54	HIS	CB-CA-C	-7.51	96.81	109.50
1	A	274	LEU	CA-C-O	-7.21	113.28	120.70
1	A	336	ASP	CA-CB-CG	7.11	119.71	112.60
1	A	328	GLU	N-CA-CB	7.04	120.58	110.16
1	A	3	TYR	N-CA-CB	-7.04	97.81	110.82
1	A	55	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	386	ALA	N-CA-C	-6.90	103.15	112.26
1	A	52	THR	CA-CB-OG1	-6.90	99.25	109.60
1	A	266	ARG	NE-CZ-NH1	6.71	128.21	121.50
1	A	8	GLU	CA-CB-CG	6.56	127.23	114.10
1	A	144	GLU	N-CA-C	-6.53	105.61	113.97
1	A	185	ASN	OD1-CG-ND2	-6.46	116.14	122.60
1	A	290	PRO	N-CA-C	-6.44	102.85	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	VAL	O-C-N	6.42	128.89	121.96
1	A	294	GLU	N-CA-C	6.40	120.49	110.32
1	A	242	PHE	CA-CB-CG	6.39	120.19	113.80
1	A	277	SER	CB-CA-C	6.36	122.88	110.67
1	A	137	TRP	CA-C-O	-6.30	113.72	120.46
1	A	175	ASP	CA-CB-CG	-6.29	106.31	112.60
1	A	152	ARG	NE-CZ-NH2	-6.28	113.55	119.20
1	A	208	ARG	NE-CZ-NH2	-6.26	113.57	119.20
1	A	143	ALA	N-CA-CB	-6.22	101.12	111.57
1	A	17	THR	CA-C-O	-6.13	113.97	120.71
1	A	210	GLU	CB-CG-CD	6.11	122.98	112.60
1	A	150	ASP	N-CA-C	-6.10	99.27	108.96
1	A	7	PRO	CB-CA-C	6.00	122.28	112.26
1	A	309	ASN	OD1-CG-ND2	5.99	128.59	122.60
1	A	368	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	A	194	PRO	N-CA-C	5.97	121.33	113.86
1	A	176	ILE	CA-C-O	-5.95	114.54	120.90
1	A	357	PHE	CA-C-O	5.94	129.01	120.51
1	A	152	ARG	NE-CZ-NH1	5.89	127.39	121.50
1	A	359	GLU	CB-CG-CD	5.81	122.48	112.60
1	A	169	VAL	N-CA-CB	-5.79	102.67	110.54
1	A	222	GLN	CA-C-N	5.79	130.38	120.72
1	A	222	GLN	C-N-CA	5.79	130.38	120.72
1	A	104	PHE	CA-CB-CG	5.79	119.59	113.80
1	A	255	ASP	N-CA-CB	-5.76	100.15	109.60
1	A	169	VAL	CB-CA-C	5.72	119.86	112.14
1	A	266	ARG	CD-NE-CZ	5.71	132.39	124.40
1	A	253	LYS	CB-CA-C	-5.69	100.47	112.82
1	A	328	GLU	OE1-CD-OE2	-5.69	109.24	122.90
1	A	74	ARG	NE-CZ-NH1	5.68	127.18	121.50
1	A	68	ARG	CD-NE-CZ	-5.67	116.47	124.40
1	A	54	HIS	CA-CB-CG	-5.66	108.14	113.80
1	A	196	VAL	CA-CB-CG2	-5.62	100.84	110.40
1	A	57	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	256	GLN	CB-CG-CD	-5.56	103.14	112.60
1	A	107	ASN	CA-C-O	-5.54	114.55	120.42
1	A	285	HIS	CA-C-O	-5.52	114.30	120.54
1	A	345	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	373	GLU	CA-C-O	-5.51	114.58	120.42
1	A	37	VAL	N-CA-CB	5.48	118.00	110.54
1	A	132	GLU	N-CA-CB	-5.42	102.56	110.53
1	A	37	VAL	CA-CB-CG2	5.42	119.61	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	HIS	O-C-N	5.38	129.35	123.22
1	A	85	LYS	CG-CD-CE	5.37	123.65	111.30
1	A	67	GLU	CG-CD-OE2	-5.34	106.11	118.40
1	A	76	ARG	NH1-CZ-NH2	5.34	126.25	119.30
1	A	84	MET	CA-C-O	-5.34	115.33	121.47
1	A	263	GLY	CA-C-O	5.34	125.34	120.53
1	A	146	GLY	N-CA-C	5.33	119.13	112.73
1	A	170	THR	CB-CA-C	5.33	119.92	110.85
1	A	95	THR	N-CA-C	5.31	117.88	111.40
1	A	297	ASP	CA-C-N	5.27	125.80	120.00
1	A	297	ASP	C-N-CA	5.27	125.80	120.00
1	A	176	ILE	O-C-N	5.22	129.14	123.09
1	A	249	GLN	CA-C-N	-5.20	115.07	122.41
1	A	249	GLN	C-N-CA	-5.20	115.07	122.41
1	A	81	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	281	SER	CA-CB-OG	-5.19	100.71	111.10
1	A	296	PHE	N-CA-CB	5.15	117.69	110.12
1	A	262	ALA	N-CA-C	-5.12	103.93	110.53
1	A	342	THR	CA-CB-OG1	-5.10	101.96	109.60
1	A	251	GLY	N-CA-C	5.09	121.73	112.37
1	A	135	VAL	CA-CB-CG1	5.08	119.03	110.40
1	A	157	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	A	362	VAL	CA-C-O	-5.04	115.71	120.95
1	A	54	HIS	CE1-NE2-CD2	5.03	114.03	109.00
1	A	240	LYS	N-CA-C	5.01	119.34	112.88

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	374	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	3044	0	2914	7	2
2	A	10	0	7	0	0
3	A	2	0	0	0	0
4	A	291	0	0	1	2
All	All	3347	0	2921	7	2

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 1.

All (7) 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:59:ILE:HG21	1:A:68:ARG:HG2	1.87	0.57
1:A:152:ARG:HD3	4:A:635:HOH:O	2.09	0.51
1:A:4:GLN:HE21	1:A:5:PRO:HD2	1.84	0.43
1:A:228:PHE:CZ	1:A:232:ILE:HD11	2.55	0.42
1:A:186:GLU:HA	1:A:187:PRO:HA	1.90	0.41
1:A:245:ASP:OD2	1:A:285:HIS:HD2	2.02	0.41
1:A:34:LEU:HD13	1:A:39:SER:OG	2.21	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ARG:NH1	4:A:677:HOH:O[4_566]	1.18	1.02
1:A:387:ARG:NE	4:A:675:HOH:O[4_566]	2.02	0.18

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	385/388 (99%)	373 (97%)	11 (3%)	1 (0%)	36 29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLU

5.3.2 Protein sidechains ⓘ

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	303/304 (100%)	287 (95%)	16 (5%)	20	12

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	GLN
1	A	8	GLU
1	A	37	VAL
1	A	68	ARG
1	A	76	ARG
1	A	85	LYS
1	A	91	THR
1	A	132	GLU
1	A	169	VAL
1	A	175	ASP
1	A	313	LEU
1	A	328	GLU
1	A	347	LEU
1	A	359	GLU
1	A	374	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	GLN
1	A	285	HIS
1	A	348	GLN

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	XLS	A	389	3	8,9,9	3.44	4 (50%)	10,11,11	5.21	7 (70%)

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	389	3	-	6/11/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	XLS	O2-C2	-6.00	1.32	1.43
2	A	389	XLS	O1-C1	5.87	1.42	1.20
2	A	389	XLS	C3-C2	-3.56	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	XLS	C4-C3	2.83	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	XLS	O4-C4-C5	9.28	130.12	109.03
2	A	389	XLS	O3-C3-C4	8.09	127.31	108.93
2	A	389	XLS	C5-C4-C3	-7.92	96.03	112.17
2	A	389	XLS	C4-C3-C2	-4.20	102.69	112.70
2	A	389	XLS	O5-C5-C4	3.75	119.03	111.16
2	A	389	XLS	O3-C3-C2	3.37	115.39	109.13
2	A	389	XLS	O2-C2-C1	3.14	117.63	110.48

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	389	XLS	C1-C2-C3-C4
2	A	389	XLS	C1-C2-C3-O3
2	A	389	XLS	O2-C2-C3-C4
2	A	389	XLS	C2-C3-C4-C5
2	A	389	XLS	O3-C3-C4-C5
2	A	389	XLS	C2-C3-C4-O4

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.