



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:11 AM UTC

PDB ID : 1XID / pdb_00001xid
Title : MODES OF BINDING SUBSTRATES AND THEIR ANALOGUES TO THE
ENZYME D-XYLOSE ISOMERASE
Authors : Carrell, H.L.; Glusker, J.P.
Deposited on : 1994-03-07
Resolution : 1.70 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

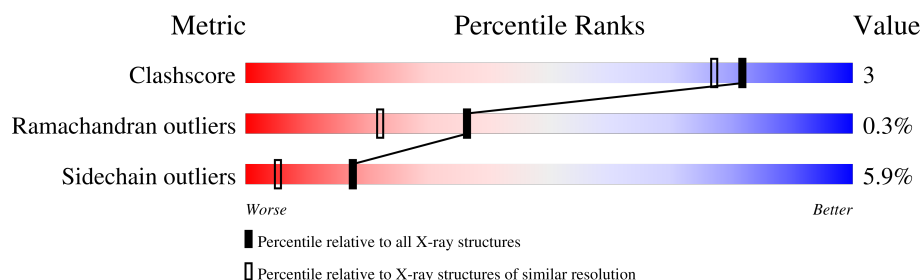
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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	 76% 19% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3359 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 D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3047	1915	548	575	9			

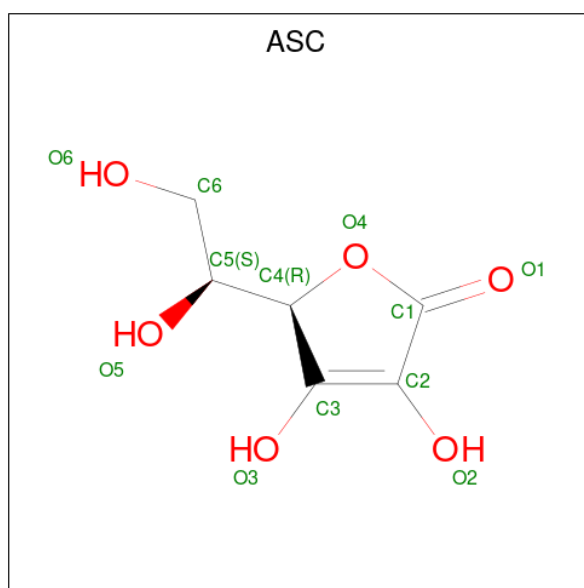
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is ASCORBIC ACID (CCD ID: ASC) (formula: C₆H₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	298	Total	O	0	0
			298	298		

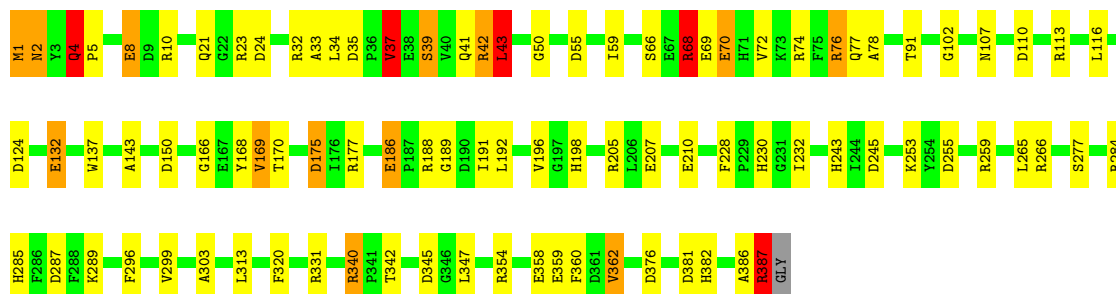
3 Residue-property plots

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: D-XYLOSE ISOMERASE

Chain A: 



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	93.80Å 99.74Å 103.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3359	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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: MN, ASC

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	1.27	7/3119 (0.2%)	2.12	95/4222 (2.3%)

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	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLY	C-O	7.32	1.32	1.23
1	A	196	VAL	CA-CB	6.53	1.61	1.54
1	A	340	ARG	CD-NE	-6.52	1.37	1.46
1	A	102	GLY	C-O	6.08	1.28	1.23
1	A	191	ILE	C-N	5.47	1.40	1.33
1	A	320	PHE	C-O	5.39	1.30	1.24
1	A	50	GLY	C-O	5.05	1.29	1.23

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	CD-NE-CZ	29.04	165.06	124.40
1	A	386	ALA	CA-C-N	22.68	162.52	121.70
1	A	386	ALA	C-N-CA	22.68	162.52	121.70
1	A	76	ARG	NE-CZ-NH2	-13.88	106.70	119.20
1	A	340	ARG	NE-CZ-NH1	13.36	134.86	121.50
1	A	10	ARG	CD-NE-CZ	13.21	142.89	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ASN	CA-CB-CG	-11.45	101.15	112.60
1	A	23	ARG	CD-NE-CZ	11.39	140.35	124.40
1	A	42	ARG	CD-NE-CZ	11.39	140.35	124.40
1	A	68	ARG	NE-CZ-NH2	10.46	128.62	119.20
1	A	340	ARG	NE-CZ-NH2	-10.42	109.82	119.20
1	A	177	ARG	NE-CZ-NH2	9.83	128.05	119.20
1	A	331	ARG	NH1-CZ-NH2	9.40	131.53	119.30
1	A	41	GLN	CB-CG-CD	9.37	128.53	112.60
1	A	266	ARG	NE-CZ-NH2	-8.96	111.14	119.20
1	A	331	ARG	NE-CZ-NH2	-8.95	111.14	119.20
1	A	386	ALA	CA-C-O	8.91	132.22	121.17
1	A	68	ARG	CA-CB-CG	8.90	131.91	114.10
1	A	76	ARG	NH1-CZ-NH2	8.28	130.06	119.30
1	A	177	ARG	NE-CZ-NH1	-8.10	113.40	121.50
1	A	386	ALA	O-C-N	-8.02	111.14	121.97
1	A	362	VAL	CA-C-O	-7.55	112.84	120.85
1	A	340	ARG	CA-C-O	-7.48	113.91	120.19
1	A	1	MET	O-C-N	7.38	134.80	123.00
1	A	110	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	169	VAL	N-CA-CB	-7.30	100.61	110.54
1	A	42	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	A	74	ARG	NE-CZ-NH2	-6.84	113.04	119.20
1	A	132	GLU	CA-CB-CG	6.77	127.65	114.10
1	A	253	LYS	CA-C-O	-6.67	114.00	120.94
1	A	299	VAL	O-C-N	6.66	128.44	121.91
1	A	265	LEU	CA-C-O	-6.62	113.53	120.55
1	A	198	HIS	CA-C-O	-6.55	113.60	120.55
1	A	37	VAL	CA-C-O	-6.53	113.20	120.25
1	A	50	GLY	CA-C-O	-6.46	115.33	121.60
1	A	175	ASP	CA-CB-CG	-6.34	106.26	112.60
1	A	358	GLU	CA-C-O	-6.32	113.80	120.63
1	A	69	GLU	CA-C-N	6.25	128.56	120.44
1	A	69	GLU	C-N-CA	6.25	128.56	120.44
1	A	4	GLN	CG-CD-NE2	6.24	125.77	116.40
1	A	24	ASP	CB-CA-C	6.21	122.41	110.17
1	A	188	ARG	NE-CZ-NH1	6.19	127.69	121.50
1	A	41	GLN	OE1-CD-NE2	-6.11	116.50	122.60
1	A	43	LEU	N-CA-CB	-6.08	101.16	110.16
1	A	76	ARG	CG-CD-NE	-6.07	98.66	112.00
1	A	68	ARG	NH1-CZ-NH2	-6.05	111.43	119.30
1	A	8	GLU	CA-CB-CG	6.04	126.17	114.10
1	A	331	ARG	CG-CD-NE	-6.03	98.73	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ARG	NE-CZ-NH1	6.01	127.51	121.50
1	A	168	TYR	CA-C-O	5.93	127.05	120.82
1	A	4	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	A	77	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	358	GLU	N-CA-C	-5.88	104.21	111.33
1	A	10	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	A	296	PHE	CA-C-O	-5.84	113.50	120.10
1	A	376	ASP	CA-CB-CG	-5.83	106.77	112.60
1	A	259	ARG	NE-CZ-NH1	5.80	127.30	121.50
1	A	192	LEU	CA-C-O	-5.78	115.43	121.55
1	A	35	ASP	CA-C-O	-5.71	114.09	119.80
1	A	345	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	137	TRP	CA-C-O	-5.65	114.42	120.46
1	A	196	VAL	CA-CB-CG2	-5.64	100.81	110.40
1	A	132	GLU	N-CA-CB	-5.60	102.30	110.53
1	A	277	SER	CB-CA-C	5.58	121.77	110.38
1	A	342	THR	O-C-N	5.58	128.51	122.15
1	A	113	ARG	CD-NE-CZ	5.57	132.19	124.40
1	A	287	ASP	CA-CB-CG	-5.56	107.04	112.60
1	A	284	ARG	NE-CZ-NH2	-5.54	114.21	119.20
1	A	72	VAL	CA-C-O	-5.54	114.90	121.05
1	A	303	ALA	O-C-N	-5.51	116.39	122.07
1	A	116	LEU	O-C-N	5.50	128.42	122.15
1	A	55	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	124	ASP	CA-C-O	-5.45	115.09	120.82
1	A	169	VAL	CB-CA-C	5.44	119.49	112.14
1	A	210	GLU	CB-CG-CD	5.42	121.81	112.60
1	A	168	TYR	O-C-N	-5.41	116.50	122.07
1	A	387	ARG	CB-CA-C	-5.41	99.82	110.10
1	A	207	GLU	CA-C-O	-5.39	114.70	120.42
1	A	68	ARG	N-CA-CB	5.37	117.95	109.94
1	A	382	HIS	CA-CB-CG	-5.37	108.43	113.80
1	A	362	VAL	O-C-N	5.37	127.36	121.83
1	A	205	ARG	CD-NE-CZ	5.34	131.87	124.40
1	A	21	GLN	OE1-CD-NE2	5.32	127.92	122.60
1	A	77	GLN	CG-CD-NE2	5.31	124.36	116.40
1	A	70	GLU	N-CA-C	5.25	116.69	111.07
1	A	107	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	150	ASP	CA-C-O	-5.23	114.69	120.60
1	A	143	ALA	O-C-N	5.16	128.94	123.42
1	A	303	ALA	CA-C-O	5.14	126.22	120.82
1	A	387	ARG	N-CA-CB	5.14	119.24	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	SER	CA-C-O	-5.13	115.11	120.55
1	A	362	VAL	N-CA-CB	5.11	118.24	110.58
1	A	230	HIS	CB-CG-ND1	-5.09	115.06	122.70
1	A	10	ARG	NH1-CZ-NH2	-5.05	112.74	119.30
1	A	243	HIS	CA-C-O	-5.04	115.84	121.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ASN	Peptide

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	3047	0	2917	15	0
2	A	2	0	0	0	0
3	A	12	0	6	0	0
4	A	298	0	0	2	1
All	All	3359	0	2923	15	1

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)
1:A:59:ILE:HG21	1:A:68:ARG:HG2	1.72	0.71
1:A:354:ARG:HB3	1:A:359:GLU:HG3	1.76	0.66
1:A:387:ARG:NH1	4:A:684:HOH:O	2.31	0.62
1:A:381:ASP:HB3	1:A:387:ARG:HG3	1.81	0.62
1:A:32:ARG:NH1	1:A:33:ALA:O	2.37	0.56
1:A:289:LYS:HE2	4:A:695:HOH:O	2.09	0.51
1:A:186:GLU:OE1	1:A:255:ASP:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HB	1:A:78:ALA:HB2	1.96	0.47
1:A:245:ASP:OD1	1:A:285:HIS:HD2	2.00	0.45
1:A:34:LEU:HD13	1:A:39:SER:OG	2.17	0.44
1:A:39:SER:O	1:A:43:LEU:HB2	2.18	0.44
1:A:228:PHE:CZ	1:A:232:ILE:HD11	2.54	0.42
1:A:4:GLN:HE21	1:A:5:PRO:HD2	1.85	0.41
1:A:166:GLY:O	1:A:170:THR:HG23	2.21	0.41
1:A:360:PHE:CD2	1:A:362:VAL:HG12	2.56	0.40

All (1) 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)
4:A:603:HOH:O	4:A:667:HOH:O[3_656]	2.19	0.01

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	22

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	304/304 (100%)	286 (94%)	18 (6%)	18 5

All (18) 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	42	ARG
1	A	43	LEU
1	A	66	SER
1	A	68	ARG
1	A	70	GLU
1	A	76	ARG
1	A	91	THR
1	A	132	GLU
1	A	169	VAL
1	A	175	ASP
1	A	313	LEU
1	A	340	ARG
1	A	347	LEU
1	A	387	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	71	HIS
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 [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 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$
3	ASC	A	389	2	12,12,12	1.19	2 (16%)	17,17,17	2.66	7 (41%)

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	ASC	A	389	2	-	5/6/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	389	ASC	O3-C3	-2.62	1.23	1.32
3	A	389	ASC	C2-C1	2.05	1.50	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	389	ASC	C6-C5-C4	7.40	124.32	111.86
3	A	389	ASC	O6-C6-C5	-4.59	101.52	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	389	ASC	O4-C1-C2	-3.06	107.15	109.86
3	A	389	ASC	O4-C4-C3	2.68	106.44	103.76
3	A	389	ASC	O5-C5-C4	-2.59	105.83	110.74
3	A	389	ASC	O4-C4-C5	-2.22	103.14	110.07
3	A	389	ASC	O2-C2-C1	2.09	127.32	122.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	389	ASC	O4-C4-C5-O5
3	A	389	ASC	C3-C4-C5-O5
3	A	389	ASC	O4-C4-C5-C6
3	A	389	ASC	C3-C4-C5-C6
3	A	389	ASC	C4-C5-C6-O6

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.