Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 07:53 PM EST

PDB ID	:	1XID
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 (i) 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 (i)) were used in the production of this report:

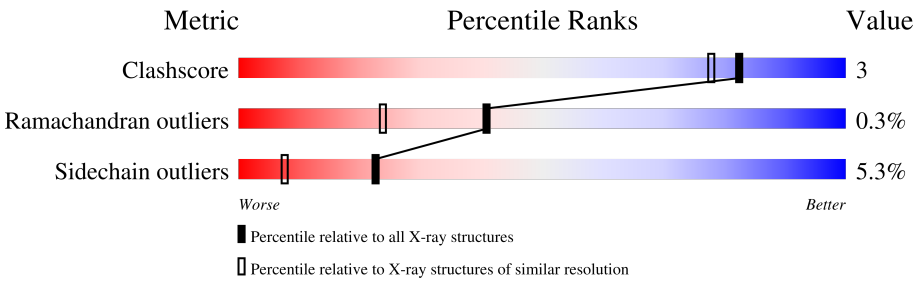
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	74% 21% • •

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
			Total	C	N	O	S			
1	A	387	3047	1915	548	575	9	0	0	0

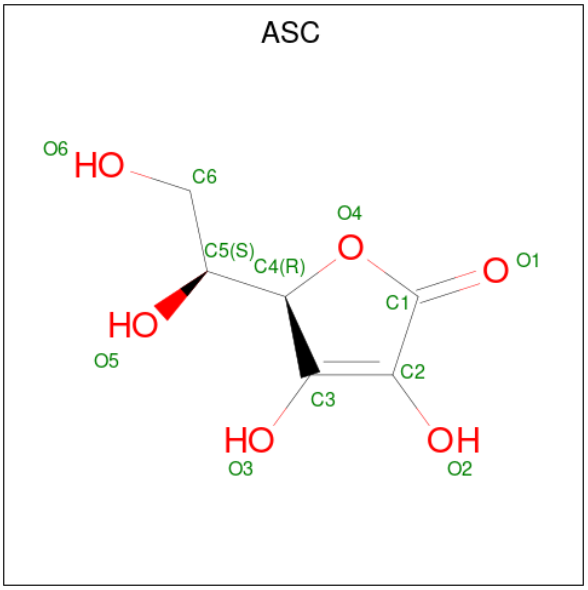
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is ASCORBIC ACID (three-letter code: ASC) (formula: $C_6H_8O_6$).



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

- Molecule 4 is water.

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

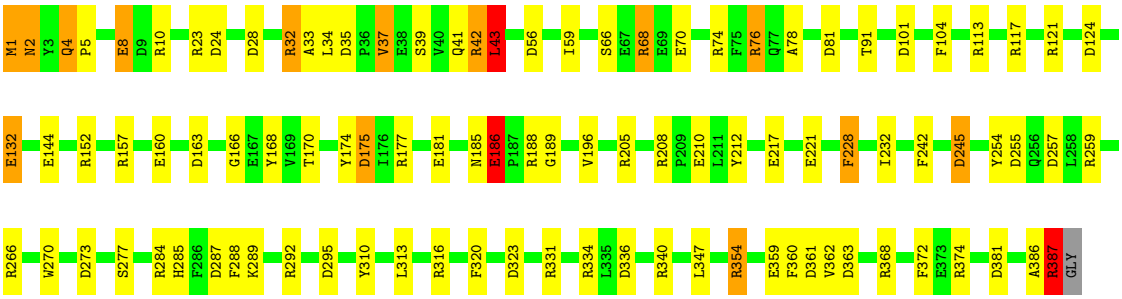
3 Residue-property plots (i)

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: 74% 21%



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ASC, 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	1.00	4/3119 (0.1%)	2.15	113/4222 (2.7%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	GLU	CD-OE1	-6.12	1.19	1.25
1	A	189	GLY	C-O	5.58	1.32	1.23
1	A	340	ARG	CD-NE	-5.49	1.37	1.46
1	A	160	GLU	CD-OE2	5.05	1.31	1.25

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	ARG	CD-NE-CZ	29.61	165.06	123.60
1	A	340	ARG	NE-CZ-NH1	29.12	134.86	120.30
1	A	76	ARG	NE-CZ-NH2	-27.19	106.70	120.30
1	A	340	ARG	NE-CZ-NH2	-20.96	109.82	120.30
1	A	266	ARG	NE-CZ-NH2	-18.32	111.14	120.30
1	A	331	ARG	NE-CZ-NH2	-18.32	111.14	120.30
1	A	68	ARG	NE-CZ-NH2	16.64	128.62	120.30
1	A	386	ALA	C-N-CA	16.33	162.52	121.70
1	A	177	ARG	NE-CZ-NH2	15.49	128.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	188	ARG	NE-CZ-NH1	14.79	127.69	120.30
1	A	74	ARG	NE-CZ-NH2	-14.52	113.04	120.30
1	A	74	ARG	NE-CZ-NH1	14.42	127.51	120.30
1	A	10	ARG	NE-CZ-NH1	14.13	127.37	120.30
1	A	259	ARG	NE-CZ-NH1	14.01	127.30	120.30
1	A	177	ARG	NE-CZ-NH1	-13.80	113.40	120.30
1	A	10	ARG	CD-NE-CZ	13.78	142.89	123.60
1	A	284	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	A	368	ARG	NE-CZ-NH1	12.10	126.35	120.30
1	A	23	ARG	CD-NE-CZ	11.96	140.35	123.60
1	A	42	ARG	CD-NE-CZ	11.96	140.35	123.60
1	A	331	ARG	NH1-CZ-NH2	11.02	131.53	119.40
1	A	266	ARG	NE-CZ-NH1	10.73	125.66	120.30
1	A	292	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	A	368	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	A	208	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	42	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	A	117	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	A	188	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	A	76	ARG	NH1-CZ-NH2	9.69	130.06	119.40
1	A	35	ASP	CB-CG-OD1	9.53	126.87	118.30
1	A	28	ASP	CB-CG-OD1	9.40	126.76	118.30
1	A	32	ARG	NE-CZ-NH1	9.21	124.90	120.30
1	A	374	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	354	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	A	316	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	A	254	TYR	CB-CG-CD2	-8.76	115.74	121.00
1	A	68	ARG	CA-CB-CG	8.41	131.91	113.40
1	A	152	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	157	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	121	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	A	287	ASP	CB-CG-OD1	7.88	125.39	118.30
1	A	361	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	A	117	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	1	MET	O-C-N	7.56	134.80	122.70
1	A	363	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	295	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	163	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	68	ARG	NH1-CZ-NH2	-7.24	111.43	119.40
1	A	386	ALA	O-C-N	-7.22	111.14	122.70
1	A	175	ASP	CB-CG-OD1	-7.20	111.82	118.30
1	A	217	GLU	OE1-CD-OE2	-7.14	114.73	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	GLU	OE1-CD-OE2	7.13	131.86	123.30
1	A	124	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	168	TYR	CB-CG-CD1	-7.05	116.77	121.00
1	A	56	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	245	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	273	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	196	VAL	CA-CB-CG2	-6.73	100.81	110.90
1	A	41	GLN	CB-CG-CD	6.51	128.53	111.60
1	A	132	GLU	CA-CB-CG	6.48	127.65	113.40
1	A	387	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	35	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	334	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	A	76	ARG	CG-CD-NE	-6.26	98.66	111.80
1	A	23	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	331	ARG	CG-CD-NE	-6.22	98.73	111.80
1	A	186	GLU	OE1-CD-OE2	-6.17	115.89	123.30
1	A	277	SER	CB-CA-C	6.14	121.77	110.10
1	A	113	ARG	CD-NE-CZ	6.14	132.19	123.60
1	A	10	ARG	NH1-CZ-NH2	-6.06	112.74	119.40
1	A	310	TYR	CB-CG-CD2	-6.04	117.37	121.00
1	A	24	ASP	CB-CA-C	6.01	122.41	110.40
1	A	101	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	175	ASP	OD1-CG-OD2	5.96	134.62	123.30
1	A	331	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	A	374	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	205	ARG	CD-NE-CZ	5.91	131.87	123.60
1	A	144	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	A	76	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	A	323	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	8	GLU	CA-CB-CG	5.81	126.17	113.40
1	A	386	ALA	CA-C-O	5.77	132.22	120.10
1	A	174	TYR	CB-CG-CD1	5.77	124.46	121.00
1	A	336	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	81	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	259	ARG	NH1-CZ-NH2	-5.62	113.22	119.40
1	A	242	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	A	212	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	A	2	ASN	CA-CB-CG	-5.57	101.15	113.40
1	A	168	TYR	CB-CG-CD2	5.56	124.33	121.00
1	A	181	GLU	CG-CD-OE2	-5.55	107.20	118.30
1	A	310	TYR	CB-CG-CD1	5.45	124.27	121.00
1	A	254	TYR	CB-CG-CD1	5.42	124.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	104	PHE	CB-CG-CD2	-5.37	117.05	120.80
1	A	372	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	A	228	PHE	CB-CG-CD2	-5.32	117.08	120.80
1	A	257	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	387	ARG	CB-CA-C	-5.29	99.82	110.40
1	A	221	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	A	175	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	A	210	GLU	OE1-CD-OE2	5.23	129.57	123.30
1	A	124	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	43	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	160	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	A	208	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	42	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
1	A	266	ARG	CD-NE-CZ	5.05	130.67	123.60
1	A	113	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	113	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	270	TRP	CE3-CZ3-CH2	5.02	126.73	121.20
1	A	372	PHE	CB-CG-CD1	5.02	124.31	120.80
1	A	288	PHE	CB-CG-CD1	-5.01	117.29	120.80
1	A	320	PHE	CB-CG-CD1	-5.01	117.29	120.80

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 (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	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
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%)	41 24

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%)	288 (95%)	16 (5%)	22 7

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	42	ARG
1	A	43	LEU
1	A	66	SER
1	A	70	GLU
1	A	76	ARG
1	A	91	THR
1	A	132	GLU
1	A	175	ASP
1	A	185	ASN
1	A	313	LEU
1	A	347	LEU
1	A	387	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	4	GLN
1	A	250	ASN
1	A	285	HIS

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 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	1.28	2 (16%)	17,17,17	2.59	6 (35%)

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	-3.01	1.23	1.33
3	A	389	ASC	C2-C1	2.22	1.50	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	389	ASC	C6-C5-C4	7.24	124.32	111.86
3	A	389	ASC	O6-C6-C5	-4.39	101.52	111.07
3	A	389	ASC	O4-C1-C2	-3.05	107.15	109.86
3	A	389	ASC	O4-C4-C3	2.65	106.44	103.71
3	A	389	ASC	O5-C5-C4	-2.51	105.83	110.77
3	A	389	ASC	O4-C4-C5	-2.11	103.14	110.04

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 (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.