Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 04:48 AM EST

PDB ID	:	1XIH
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:

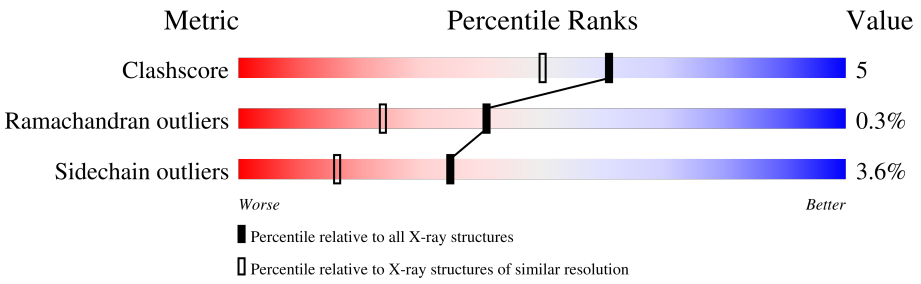
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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	66% 27% 6% ••

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3420 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.

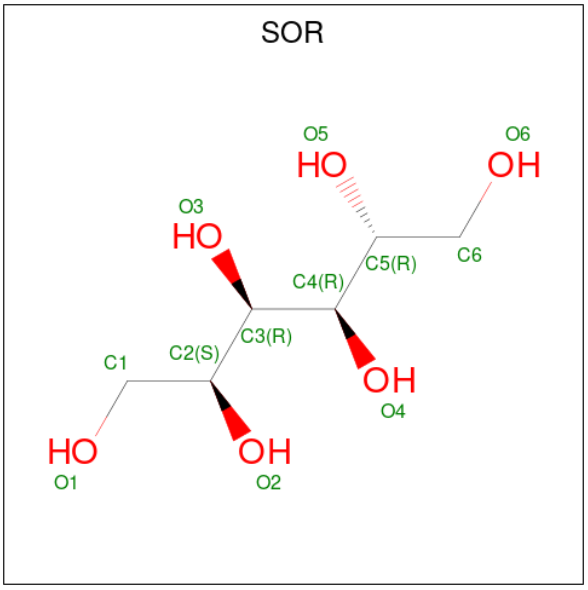
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	3032	1906	546	572	8	0	1	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 sorbitol (three-letter code: SOR) (formula: $C_6H_{14}O_6$).



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

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	375	375	375	0	0

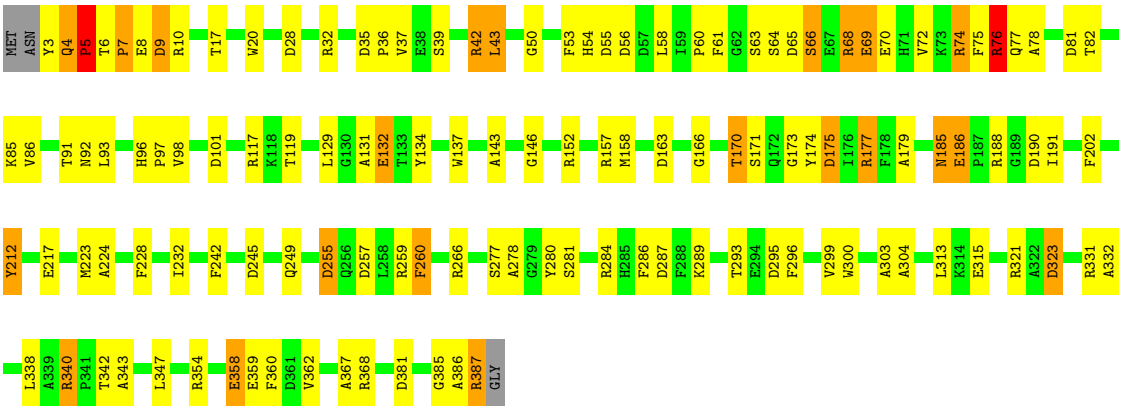
3 Residue-property plots (i)

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:



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	93.66Å 100.02Å 102.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3420	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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: SOR, 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	1.23	35/3112 (1.1%)	1.81	74/4212 (1.8%)

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	20

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	ASP	C-N	-12.23	1.05	1.34
1	A	7	PRO	C-N	9.58	1.56	1.34
1	A	36	PRO	C-N	9.24	1.55	1.34
1	A	278	ALA	C-N	8.52	1.48	1.33
1	A	98	VAL	C-N	8.43	1.53	1.34
1	A	255	ASP	C-N	8.12	1.52	1.34
1	A	119	THR	C-N	8.04	1.52	1.34
1	A	224	ALA	C-N	7.79	1.47	1.33
1	A	386	ALA	C-N	-7.64	1.16	1.34
1	A	35	ASP	C-N	7.61	1.48	1.34
1	A	63	SER	C-N	7.11	1.50	1.34
1	A	17	THR	C-N	6.78	1.49	1.34
1	A	61	PHE	C-N	-6.70	1.21	1.33
1	A	146	GLY	C-N	6.68	1.45	1.33
1	A	134	TYR	C-N	6.60	1.49	1.34
1	A	143	ALA	C-N	6.59	1.49	1.34
1	A	129	LEU	C-N	6.37	1.44	1.33
1	A	28	ASP	C-N	6.37	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	VAL	C-N	6.08	1.48	1.34
1	A	50	GLY	C-N	-6.07	1.20	1.34
1	A	281	SER	C-N	5.97	1.43	1.33
1	A	323	ASP	C-N	5.96	1.45	1.34
1	A	191	ILE	C-N	5.90	1.47	1.34
1	A	338	LEU	C-N	5.88	1.47	1.34
1	A	82	THR	C-N	5.59	1.43	1.33
1	A	202	PHE	C-N	5.58	1.46	1.34
1	A	152	ARG	C-N	5.52	1.46	1.34
1	A	304	ALA	C-N	5.37	1.42	1.33
1	A	3	TYR	C-N	-5.30	1.21	1.34
1	A	68	ARG	C-N	-5.20	1.22	1.34
1	A	93	LEU	C-N	5.17	1.46	1.34
1	A	190	ASP	C-N	5.11	1.45	1.34
1	A	92	ASN	C-N	5.10	1.45	1.34
1	A	332	ALA	C-N	-5.08	1.22	1.34
1	A	212	TYR	C-N	5.03	1.42	1.33

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	ARG	CD-NE-CZ	28.57	163.60	123.60
1	A	76	ARG	NE-CZ-NH2	-14.58	113.01	120.30
1	A	7	PRO	O-C-N	-13.52	101.07	122.70
1	A	117	ARG	NE-CZ-NH2	-13.05	113.78	120.30
1	A	387	ARG	CD-NE-CZ	12.56	141.18	123.60
1	A	387	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	A	259	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	A	331	ARG	NE-CZ-NH2	-11.09	114.75	120.30
1	A	266	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	A	368	ARG	NE-CZ-NH2	-10.39	115.11	120.30
1	A	266	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	A	387	ARG	CA-C-O	9.30	139.64	120.10
1	A	157	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	A	7	PRO	C-N-CA	8.26	142.34	121.70
1	A	188	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	173	GLY	O-C-N	-7.92	110.03	122.70
1	A	117	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	A	359	GLU	O-C-N	7.64	134.92	122.70
1	A	8	GLU	O-C-N	-7.37	110.91	122.70
1	A	381	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	177	ARG	NE-CZ-NH1	-6.72	116.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	163	ASP	CB-CG-OD1	6.65	124.29	118.30
1	A	340	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	315	GLU	O-C-N	-6.63	112.09	122.70
1	A	69	GLU	O-C-N	-6.62	112.10	122.70
1	A	340	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	266	ARG	CD-NE-CZ	6.54	132.76	123.60
1	A	174	TYR	CB-CG-CD1	6.30	124.78	121.00
1	A	284	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	295	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	74	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	245	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	163	ASP	O-C-N	-6.10	112.94	122.70
1	A	171	SER	O-C-N	-6.07	113.00	122.70
1	A	342	THR	C-N-CA	-6.03	106.63	121.70
1	A	5	PRO	CA-C-N	-6.02	103.95	117.20
1	A	56	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	177	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	A	217	GLU	OE1-CD-OE2	-5.98	116.13	123.30
1	A	66	SER	O-C-N	-5.96	113.16	122.70
1	A	190	ASP	O-C-N	5.95	132.21	122.70
1	A	9	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	A	321	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	173	GLY	CA-C-N	5.85	130.08	117.20
1	A	157	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	321	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	303	ALA	O-C-N	-5.69	113.60	122.70
1	A	242	PHE	CB-CG-CD2	-5.63	116.86	120.80
1	A	60	PRO	O-C-N	5.54	131.57	122.70
1	A	280	TYR	CB-CG-CD2	-5.51	117.69	121.00
1	A	152	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	260	PHE	C-N-CA	5.41	133.67	122.30
1	A	137	TRP	C-N-CA	-5.40	110.96	122.30
1	A	3	TYR	O-C-N	-5.36	114.12	122.70
1	A	354	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	381	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	354	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	179	ALA	CB-CA-C	5.27	118.01	110.10
1	A	300	TRP	O-C-N	-5.26	114.28	122.70
1	A	284	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	284	ARG	NH1-CZ-NH2	5.22	125.14	119.40
1	A	280	TYR	C-N-CA	-5.20	108.69	121.70
1	A	174	TYR	CB-CG-CD2	-5.17	117.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	343	ALA	C-N-CA	-5.15	108.82	121.70
1	A	101	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	146	GLY	O-C-N	-5.13	114.47	123.20
1	A	359	GLU	CA-C-N	-5.13	105.91	117.20
1	A	64	SER	CA-C-N	-5.08	106.03	117.20
1	A	74	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	245	ASP	O-C-N	5.07	130.81	122.70
1	A	293	THR	CA-CB-CG2	-5.05	105.33	112.40
1	A	358	GLU	O-C-N	-5.05	114.62	122.70
1	A	257	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	367	ALA	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	GLU	Mainchain
1	A	170	THR	Mainchain
1	A	177	ARG	Mainchain
1	A	223	MET	Mainchain
1	A	249	GLN	Mainchain
1	A	260	PHE	Mainchain
1	A	277	SER	Mainchain
1	A	286	PHE	Mainchain
1	A	287	ASP	Mainchain
1	A	299	VAL	Mainchain
1	A	358	GLU	Mainchain
1	A	385	GLY	Mainchain
1	A	5	PRO	Mainchain
1	A	53	PHE	Peptide
1	A	6	THR	Mainchain
1	A	65	ASP	Mainchain
1	A	68	ARG	Mainchain
1	A	69	GLU	Mainchain
1	A	7	PRO	Mainchain
1	A	85	LYS	Mainchain

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	3032	0	2891	27	0
2	A	12	0	11	0	0
3	A	1	0	0	0	0
4	A	375	0	0	8	0
All	All	3420	0	2902	27	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 5.

All (27) 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:42:ARG:HA	1:A:42:ARG:HE	1.62	0.64
1:A:340:ARG:HD2	4:A:637:HOH:O	2.00	0.61
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.22	0.55
1:A:289:LYS:HE2	4:A:727:HOH:O	2.07	0.54
1:A:58:LEU:HD11	1:A:75:PHE:CG	2.44	0.52
1:A:360:PHE:CD2	1:A:362:VAL:HG12	2.45	0.52
1:A:37:VAL:HB	1:A:78:ALA:HB2	1.93	0.50
1:A:185:ASN:HD22	1:A:186:GLU:HB2	1.79	0.48
1:A:4:GLN:HE21	1:A:5:PRO:HD2	1.81	0.46
1:A:212:TYR:HB3	4:A:739:HOH:O	2.13	0.46
1:A:20:TRP:CE3	1:A:289:LYS:HB3	2.51	0.46
1:A:76:ARG:HD3	4:A:770:HOH:O	2.17	0.45
1:A:10:ARG:NH1	4:A:741:HOH:O	2.49	0.44
1:A:186:GLU:OE1	1:A:255:ASP:OD1	2.36	0.44
1:A:387:ARG:HD2	4:A:684:HOH:O	2.18	0.44
1:A:70:GLU:O	1:A:74:ARG:HG3	2.17	0.43
1:A:323:ASP:OD2	1:A:387:ARG:NH2	2.50	0.43
1:A:289:LYS:HE2	4:A:695:HOH:O	2.18	0.43
1:A:228:PHE:CZ	1:A:232:ILE:HD11	2.53	0.43
1:A:32:ARG:HG2	1:A:296:PHE:HE2	1.84	0.43
1:A:54:HIS:O	1:A:55:ASP:C	2.57	0.43
1:A:77:GLN:NE2	1:A:81:ASP:OD1	2.52	0.43
1:A:86:VAL:O	1:A:131:ALA:HA	2.19	0.42
1:A:39:SER:O	1:A:43:LEU:HB2	2.20	0.41
1:A:9:ASP:O	1:A:10:ARG:HB2	2.20	0.40
1:A:158:MET:HE3	4:A:734:HOH:O	2.22	0.40
1:A:166:GLY:O	1:A:170:THR:HG23	2.22	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	384/388 (99%)	370 (96%)	13 (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	303/304 (100%)	292 (96%)	11 (4%)	35 16

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	42	ARG
1	A	43	LEU
1	A	66	SER
1	A	76	ARG
1	A	91	THR
1	A	132	GLU

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Mol	Chain	Res	Type
1	A	175	ASP
1	A	185	ASN
1	A	313	LEU
1	A	347	LEU

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	41	GLN
1	A	185	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 2 ligands modelled in this entry, 1 is 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	SOR	A	389	3	11,11,11	0.88	1 (9%)	14,14,14	1.80	2 (14%)

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	SOR	A	389	3	-	2/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	SOR	O1-C1	-2.38	1.32	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	389	SOR	O5-C5-C6	-4.41	98.79	109.14
2	A	389	SOR	O6-C6-C5	-3.66	103.10	111.07

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	389	SOR	C4-C5-C6-O6
2	A	389	SOR	O5-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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	50:GLY	C	51:VAL	N	1.20
1	A	386:ALA	C	387:ARG	N	1.16
1	A	175:ASP	C	176:ILE	N	1.05

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.