



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:34 PM BST

PDB ID : 1XYB
Title : X-RAY CRYSTALLOGRAPHIC STRUCTURES OF D-XYLOSE ISOMERASE-SUBSTRATE COMPLEXES POSITION THE SUBSTRATE AND PROVIDE EVIDENCE FOR METAL MOVEMENT DURING CATALYSIS
Authors : Lavie, A.; Allen, K.N.; Petsko, G.A.; Ringe, D.
Deposited on : 1994-01-03
Resolution : 1.96 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 following versions of software and data (see [references ⓘ](#)) 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) : 2.13.1

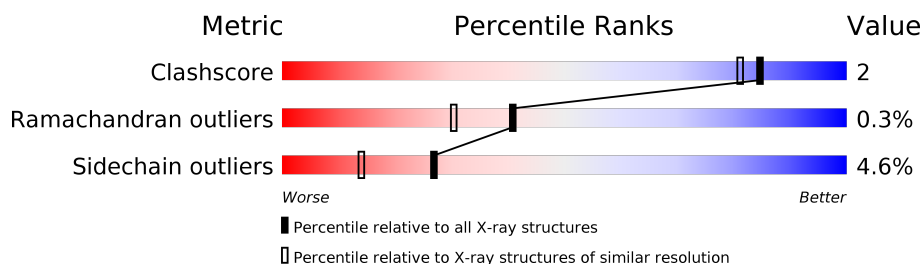
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)

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 on 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	386	
1	B	386	

2 Entry composition [i](#)

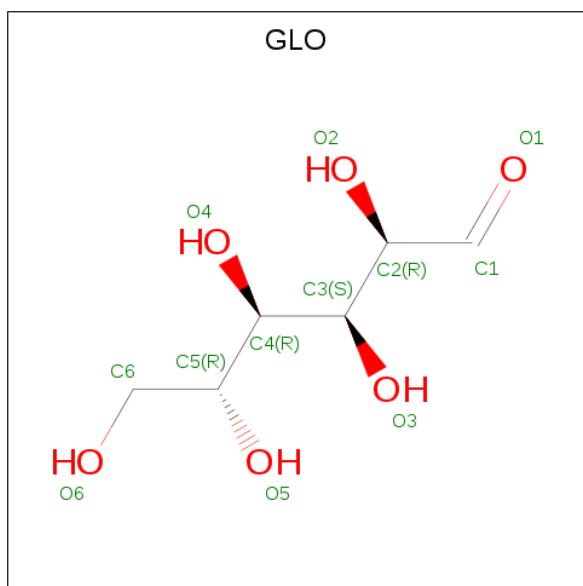
There are 4 unique types of molecules in this entry. The entry contains 6559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	386	Total	C	N	O	S	0	0	0
			3024	1904	540	572	8			
1	B	386	Total	C	N	O	S	0	0	0
			3024	1904	540	572	8			

- Molecule 2 is D-glucose (three-letter code: GLO) (formula: C₆H₁₂O₆).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 3	Mg 3	0	1
3	A	2	Total 3	Mg 3	0	1

- Molecule 4 is water.

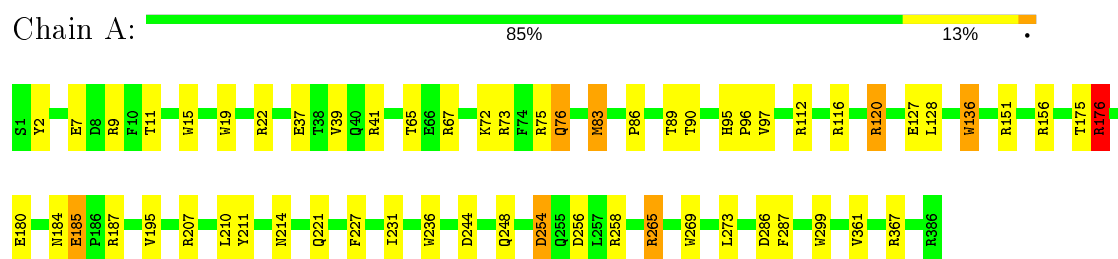
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total 248	O 248	0	0
4	B	233	Total 233	O 233	0	0

3 Residue-property plots

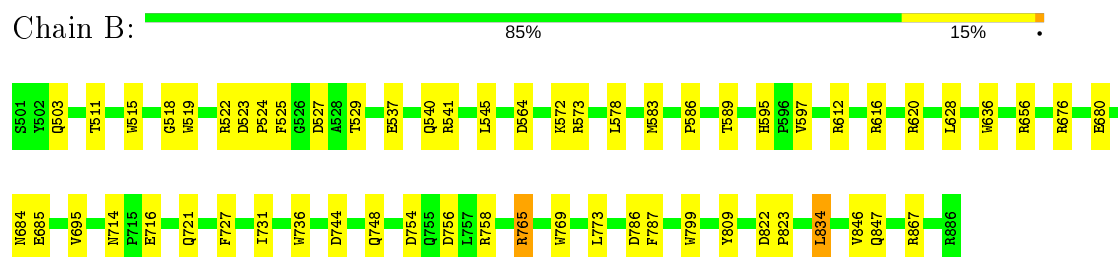
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• 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	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.70 Å 99.40 Å 94.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.96	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.96)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6559	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: MG, GLO

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	0.78	0/3096	1.39	51/4197 (1.2%)
1	B	0.80	1/3096 (0.0%)	1.37	38/4197 (0.9%)
All	All	0.79	1/6192 (0.0%)	1.38	89/8394 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	716	GLU	CD-OE1	-5.85	1.19	1.25

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH1	14.42	127.51	120.30
1	B	765	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	B	765	ARG	NE-CZ-NH2	-9.87	115.37	120.30
1	A	265	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	B	867	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	A	83	MET	CG-SD-CE	-8.13	87.19	100.20
1	B	612	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	519	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	B	799	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	B	583	MET	CG-SD-CE	-7.74	87.82	100.20
1	B	769	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	A	299	TRP	CD1-CG-CD2	7.68	112.44	106.30
1	A	73	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	616	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	A	156	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	A	19	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	A	116	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	136	TRP	CD1-CG-CD2	7.47	112.28	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	A	116	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	656	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	A	236	TRP	CD1-CG-CD2	7.29	112.13	106.30
1	A	269	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	A	367	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	176	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	515	TRP	CE2-CD2-CG	-7.07	101.64	107.30
1	A	15	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	B	846	VAL	CG1-CB-CG2	-7.05	99.62	110.90
1	B	799	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	A	136	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	B	758	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	515	TRP	CD1-CG-CD2	6.87	111.79	106.30
1	B	809	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	B	834	LEU	CA-CB-CG	-6.77	99.73	115.30
1	A	265	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	367	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	769	TRP	CE2-CD2-CG	-6.55	102.06	107.30
1	A	19	TRP	CE2-CD2-CG	-6.54	102.06	107.30
1	A	254	ASP	N-CA-CB	-6.54	98.83	110.60
1	A	187	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	41	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	B	754	ASP	N-CA-CB	-6.49	98.91	110.60
1	A	236	TRP	CE2-CD2-CG	-6.49	102.11	107.30
1	A	269	TRP	CE2-CD2-CG	-6.42	102.17	107.30
1	A	15	TRP	CD1-CG-CD2	6.42	111.43	106.30
1	B	519	TRP	CE2-CD2-CG	-6.36	102.21	107.30
1	A	299	TRP	CG-CD2-CE3	6.28	139.56	133.90
1	B	636	TRP	CD1-CG-CD2	6.27	111.32	106.30
1	B	522	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	75	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	736	TRP	CE2-CD2-CG	-6.20	102.34	107.30
1	A	112	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	112	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	299	TRP	CB-CG-CD1	-6.18	118.96	127.00
1	B	518	GLY	CA-C-N	6.15	130.73	117.20
1	B	636	TRP	CE2-CD2-CG	-6.15	102.38	107.30
1	B	616	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	195	VAL	CG1-CB-CG2	-6.06	101.21	110.90
1	A	22	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	67	ARG	NE-CZ-NH1	5.92	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	736	TRP	CD1-CG-CD2	5.91	111.03	106.30
1	A	258	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	695	VAL	CA-CB-CG2	-5.82	102.17	110.90
1	B	744	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	127	GLU	CA-CB-CG	5.80	126.16	113.40
1	A	73	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	527	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	176	ARG	CG-CD-NE	5.73	123.82	111.80
1	A	211	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	A	120	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	769	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	A	9	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	236	TRP	CG-CD2-CE3	5.47	138.82	133.90
1	A	286	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	151	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	75	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	786	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	515	TRP	CG-CD2-CE3	5.39	138.75	133.90
1	A	176	ARG	CD-NE-CZ	5.37	131.12	123.60
1	B	573	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	2	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	B	519	TRP	CG-CD1-NE1	-5.24	104.86	110.10
1	B	799	TRP	CB-CG-CD1	-5.24	120.18	127.00
1	A	2	TYR	N-CA-C	5.23	125.12	111.00
1	B	518	GLY	CA-C-O	-5.22	111.20	120.60
1	A	207	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	799	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	A	236	TRP	CG-CD1-NE1	-5.05	105.05	110.10
1	A	244	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3024	0	2909	15	0
1	B	3024	0	2906	13	0
2	A	12	0	12	3	0
2	B	12	0	12	1	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	248	0	0	1	0
4	B	233	0	0	1	0
All	All	6559	0	5839	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 2.

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:B:595:HIS:HD2	1:B:597:VAL:H	1.31	0.76
1:A:95:HIS:HD2	1:A:97:VAL:H	1.43	0.64
1:B:595:HIS:CD2	1:B:597:VAL:H	2.18	0.58
1:A:176:ARG:HB2	1:A:176:ARG:HH11	1.71	0.56
1:A:180:GLU:HG3	1:A:214:ASN:O	2.06	0.55
1:A:265:ARG:HG3	4:A:1097:HOH:O	2.08	0.53
1:B:680:GLU:HG3	1:B:714:ASN:O	2.09	0.53
1:A:185:GLU:OE1	1:A:254:ASP:HB3	2.09	0.51
1:A:89:THR:HG21	2:A:950:GLO:H62	1.93	0.50
1:A:72:LYS:O	1:A:76:GLN:HG2	2.11	0.50
1:A:95:HIS:CD2	1:A:97:VAL:H	2.28	0.48
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.80	0.47
1:B:589:THR:HG21	2:B:960:GLO:H61	1.98	0.46
1:B:765:ARG:HG3	4:B:1243:HOH:O	2.14	0.45
2:A:950:GLO:H1	1:B:525:PHE:CE1	2.54	0.43
1:A:256:ASP:HB3	1:A:287:PHE:HA	2.01	0.43
1:B:523:ASP:HB2	1:B:524:PRO:HD2	2.01	0.42
1:B:756:ASP:HB3	1:B:787:PHE:HA	2.02	0.42
1:A:136:TRP:CD2	2:A:950:GLO:H2	2.55	0.42
1:A:39:VAL:HG13	1:A:83:MET:HG3	2.02	0.41
1:A:227:PHE:CZ	1:A:231:ILE:HD11	2.55	0.41
1:B:721:GLN:HE21	1:B:748:GLN:HB3	1.85	0.41
1:B:727:PHE:CZ	1:B:731:ILE:HD11	2.56	0.41
1:A:96:PRO:HB3	1:B:529:THR:HG22	2.03	0.41
1:B:511:THR:HG21	1:B:586:PRO:HG2	2.02	0.40
1:A:11:THR:HG21	1:A:86:PRO:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:ASP:HA	1:B:823:PRO:HD3	1.94	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	384/386 (100%)	371 (97%)	12 (3%)	1 (0%)	41	30
1	B	384/386 (100%)	372 (97%)	11 (3%)	1 (0%)	41	30
All	All	768/772 (100%)	743 (97%)	23 (3%)	2 (0%)	41	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	685	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	302/302 (100%)	289 (96%)	13 (4%)	29	16
1	B	302/302 (100%)	287 (95%)	15 (5%)	24	11
All	All	604/604 (100%)	576 (95%)	28 (5%)	27	14

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	37	GLU
1	A	65	THR
1	A	76	GLN
1	A	90	THR
1	A	120	ARG
1	A	128	LEU
1	A	175	THR
1	A	176	ARG
1	A	184	ASN
1	A	210	LEU
1	A	273	LEU
1	A	361	VAL
1	B	503	GLN
1	B	537	GLU
1	B	540	GLN
1	B	541	ARG
1	B	545	LEU
1	B	564	ASP
1	B	572	LYS
1	B	578	LEU
1	B	620	ARG
1	B	628	LEU
1	B	676	ARG
1	B	684	ASN
1	B	773	LEU
1	B	834	LEU
1	B	847	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	184	ASN
1	A	221	GLN
1	A	308	ASN
1	B	595	HIS
1	B	684	ASN
1	B	721	GLN
1	B	808	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 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
2	GLO	B	960	3	10,11,11	1.09	1 (10%)	13,14,14	1.74	3 (23%)
2	GLO	A	950	3	10,11,11	1.03	1 (10%)	13,14,14	1.71	2 (15%)

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	GLO	B	960	3	-	2/14/16/16	-
2	GLO	A	950	3	-	1/14/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	950	GLO	C3-C2	2.36	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	960	GLO	C4-C3	2.14	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	950	GLO	C4-C3-C2	-4.81	105.15	113.54
2	B	960	GLO	C4-C3-C2	-4.39	105.88	113.54
2	A	950	GLO	O3-C3-C2	2.80	114.30	109.17
2	B	960	GLO	O3-C3-C2	2.46	113.68	109.17
2	B	960	GLO	C5-C4-C3	-2.07	109.23	112.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	960	GLO	C4-C5-C6-O6
2	B	960	GLO	O5-C5-C6-O6
2	A	950	GLO	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	960	GLO	1	0
2	A	950	GLO	3	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.