



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:03 AM UTC

PDB ID : 1XYB / pdb_00001xyb
Title : X-RAY CRYSTALLOGRAPHIC STRUCTURES OF D-XYLOSE ISOMERASE-SUBSTRATE COMPLEXES POSITION THE SUBSTRATE AND PROVIDE EVIDENCE FOR METAL MOVEMENT DURING CATALYSIS
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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 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

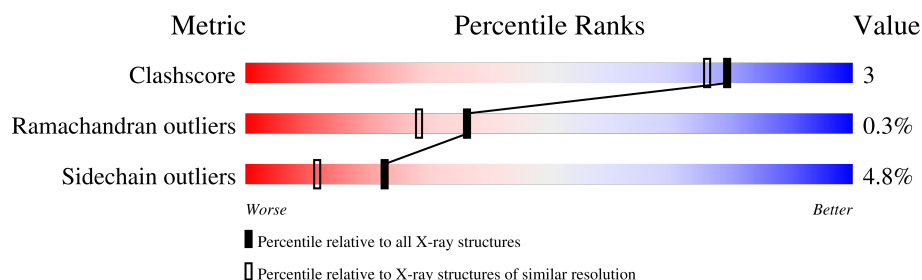
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (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 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	386	 84% 14% ..
1	B	386	 84% 14% .

2 Entry composition [i](#)

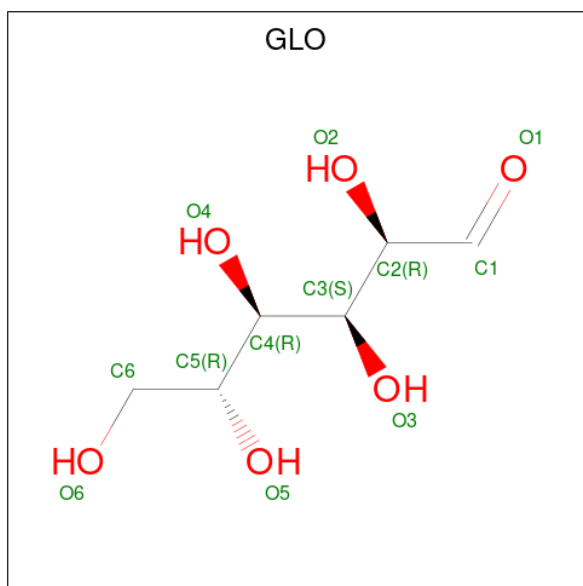
There are 4 unique types of molecules in this entry. The entry contains 6559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is water.

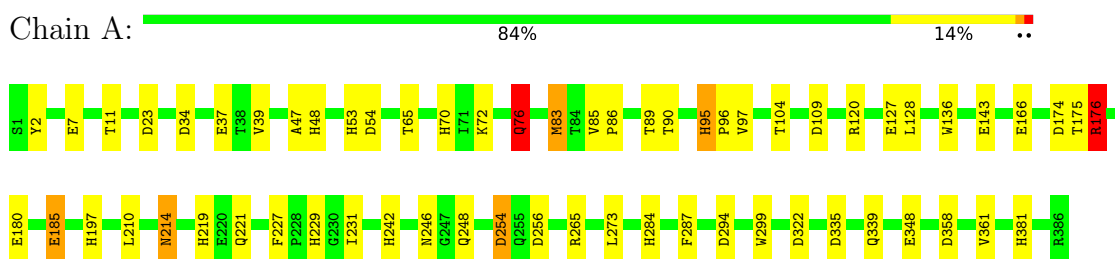
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	248	Total 248	O 248	0	0
4	B	233	Total 233	O 233	0	0

3 Residue-property plots

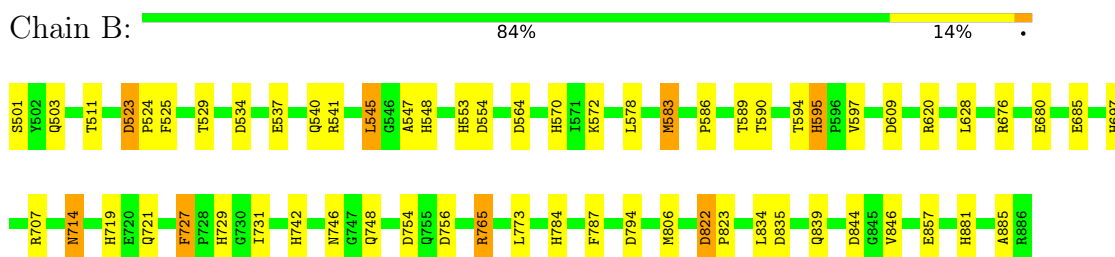
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	1.00	13/3096 (0.4%)	1.52	38/4197 (0.9%)
1	B	1.01	12/3096 (0.4%)	1.54	31/4197 (0.7%)
All	All	1.00	25/6192 (0.4%)	1.53	69/8394 (0.8%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	HIS	CD2-NE2	-6.70	1.30	1.37
1	B	570	HIS	CD2-NE2	-6.65	1.30	1.37
1	B	548	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	53	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	881	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	719	HIS	CG-ND1	-6.32	1.31	1.38
1	A	48	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	197	HIS	CD2-NE2	-6.26	1.30	1.37
1	B	553	HIS	CD2-NE2	-6.11	1.31	1.37
1	B	742	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	70	HIS	CD2-NE2	-6.01	1.31	1.37
1	A	381	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	219	HIS	CG-ND1	-5.95	1.31	1.38
1	B	697	HIS	CD2-NE2	-5.94	1.31	1.37
1	B	595	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	242	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	284	HIS	CD2-NE2	-5.67	1.31	1.37
1	A	104	THR	CA-CB	5.54	1.61	1.53
1	B	784	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	219	HIS	CD2-NE2	-5.31	1.32	1.37
1	A	284	HIS	CG-ND1	-5.21	1.32	1.38
1	A	229	HIS	CD2-NE2	-5.17	1.32	1.37
1	B	570	HIS	CG-ND1	-5.16	1.32	1.38
1	B	729	HIS	CD2-NE2	-5.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	719	HIS	CD2-NE2	-5.11	1.32	1.37

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASP	CA-CB-CG	10.57	123.17	112.60
1	A	2	TYR	N-CA-C	10.39	125.12	110.68
1	B	844	ASP	CA-CB-CG	8.21	120.81	112.60
1	B	523	ASP	CA-CB-CG	8.01	120.61	112.60
1	B	609	ASP	CA-CB-CG	7.88	120.48	112.60
1	B	534	ASP	CA-CB-CG	7.51	120.11	112.60
1	A	109	ASP	CA-CB-CG	7.23	119.83	112.60
1	A	381	HIS	CA-CB-CG	-7.15	106.65	113.80
1	A	294	ASP	CA-CB-CG	7.13	119.73	112.60
1	A	34	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	254	ASP	N-CA-CB	-6.57	98.83	109.60
1	A	53	HIS	CB-CG-CD2	-6.56	122.68	131.20
1	B	754	ASP	N-CA-CB	-6.52	98.91	109.60
1	B	534	ASP	CA-C-N	6.51	126.75	119.32
1	B	534	ASP	C-N-CA	6.51	126.75	119.32
1	A	322	ASP	CA-CB-CG	6.49	119.08	112.60
1	A	174	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	835	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	794	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	339	GLN	OE1-CD-NE2	-6.31	116.29	122.60
1	A	246	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	83	MET	CG-SD-CE	-6.23	87.19	100.90
1	B	822	ASP	CA-C-N	6.20	125.93	119.05
1	B	822	ASP	C-N-CA	6.20	125.93	119.05
1	B	881	HIS	CB-CG-CD2	-6.16	123.19	131.20
1	A	214	ASN	CA-C-N	6.14	126.05	119.85
1	A	214	ASN	C-N-CA	6.14	126.05	119.85
1	B	553	HIS	CB-CG-CD2	-6.04	123.35	131.20
1	A	127	GLU	CA-CB-CG	6.03	126.16	114.10
1	A	176	ARG	NE-CZ-NH1	6.01	127.51	121.50
1	B	583	MET	CG-SD-CE	-5.94	87.82	100.90
1	A	76	GLN	CB-CA-C	-5.87	100.87	110.85
1	A	335	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	846	VAL	N-CA-C	5.84	116.03	110.42
1	A	53	HIS	N-CA-C	-5.79	100.85	110.17
1	B	553	HIS	N-CA-C	-5.74	100.92	110.17
1	A	34	ASP	CA-C-N	5.70	126.08	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ASP	C-N-CA	5.70	126.08	119.47
1	A	299	TRP	CG-CD2-CE3	5.66	139.56	133.90
1	B	554	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	85	VAL	CA-C-N	5.63	125.24	119.56
1	A	85	VAL	C-N-CA	5.63	125.24	119.56
1	A	70	HIS	CB-CG-CD2	-5.62	123.89	131.20
1	A	54	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	570	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	B	714	ASN	CA-C-N	5.49	125.40	119.85
1	B	714	ASN	C-N-CA	5.49	125.40	119.85
1	A	48	HIS	CB-CG-CD2	-5.48	124.08	131.20
1	A	197	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	A	176	ARG	CG-CD-NE	5.38	123.82	112.00
1	A	322	ASP	CA-C-N	5.30	125.36	119.32
1	A	322	ASP	C-N-CA	5.30	125.36	119.32
1	A	299	TRP	CB-CG-CD1	-5.29	118.96	126.90
1	B	885	ALA	CA-C-N	5.27	131.19	121.70
1	B	885	ALA	C-N-CA	5.27	131.19	121.70
1	A	76	GLN	N-CA-CB	5.26	117.94	110.16
1	B	707	ARG	CA-C-N	5.26	125.57	119.47
1	B	707	ARG	C-N-CA	5.26	125.57	119.47
1	B	765	ARG	CA-CB-CG	-5.26	103.58	114.10
1	A	143	GLU	N-CA-C	-5.25	107.24	113.97
1	A	348	GLU	CB-CG-CD	5.25	121.52	112.60
1	B	594	THR	N-CA-C	5.21	116.77	111.14
1	B	839	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	174	ASP	O-C-N	-5.19	115.72	122.37
1	B	746	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	B	548	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	A	358	ASP	CA-CB-CG	5.11	117.71	112.60
1	B	846	VAL	CG1-CB-CG2	-5.08	99.62	110.80
1	B	727	PHE	CA-C-O	-5.01	113.98	118.79

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	17	0
1	B	3024	0	2906	16	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	32	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 3.

All (32) 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:547:ALA:O	1:B:583:MET:HE1	2.02	0.59
1:B:595:HIS:CD2	1:B:597:VAL:H	2.18	0.58
1:A:176:ARG:HH11	1:A:176:ARG:HB2	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:B:545:LEU:HB3	1:B:806:MET:HE1	1.91	0.52
1:B:583:MET:HA	1:B:583:MET:HE2	1.92	0.52
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:A:47:ALA:O	1:A:83:MET:HE1	2.16	0.46
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
1:A:83:MET:HA	1:A:83:MET:HE2	1.99	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	36	28
1	B	384/386 (100%)	372 (97%)	11 (3%)	1 (0%)	36	28
All	All	768/772 (100%)	743 (97%)	23 (3%)	2 (0%)	36	28

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%)	26	15
1	B	302/302 (100%)	286 (95%)	16 (5%)	20	9
All	All	604/604 (100%)	575 (95%)	29 (5%)	23	12

All (29) 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	166	GLU
1	A	175	THR
1	A	176	ARG
1	A	210	LEU
1	A	273	LEU
1	A	361	VAL
1	B	501	SER
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	590	THR
1	B	620	ARG
1	B	628	LEU
1	B	676	ARG
1	B	773	LEU
1	B	834	LEU
1	B	857	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN

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Mol	Chain	Res	Type
1	A	40	GLN
1	A	95	HIS
1	A	221	GLN
1	A	308	ASN
1	A	326	GLN
1	A	376	GLN
1	B	540	GLN
1	B	595	HIS
1	B	721	GLN
1	B	808	ASN
1	B	876	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	950	3	10,11,11	1.06	1 (10%)	13,14,14	1.69	2 (15%)
2	GLO	B	960	3	10,11,11	1.14	1 (10%)	13,14,14	1.76	4 (30%)

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	A	950	3	-	1/15/16/16	-
2	GLO	B	960	3	-	2/15/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	950	GLO	C3-C2	2.45	1.57	1.53
2	B	960	GLO	C4-C3	2.23	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	950	GLO	C4-C3-C2	-4.76	105.15	113.49
2	B	960	GLO	C4-C3-C2	-4.34	105.88	113.49
2	A	950	GLO	O3-C3-C2	2.78	114.30	109.13
2	B	960	GLO	O3-C3-C2	2.45	113.68	109.13
2	B	960	GLO	C5-C4-C3	-2.12	109.23	112.48
2	B	960	GLO	C6-C5-C4	2.09	116.42	112.17

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	A	950	GLO	3	0
2	B	960	GLO	1	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.