wwPDB X-ray Structure Validation Summary Report (i)

Feb 3, 2024 – 10:01 PM EST

PDB ID	:	1N82
Title	:	The high-resolution crystal structure of IXT6, a thermophilic, intracellular xylanase from G. stearothermophilus
Authors	:	Solomon, V.; Teplitsky, A.; Golan, G.; Gilboa, R.; Reiland, V.; Shulami, S.; Moryles, S.; Zolotnitsky, G.; Shoham, Y.; Shoham, G.
Deposited on	:	2002-11-19
Resolution	:	1.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

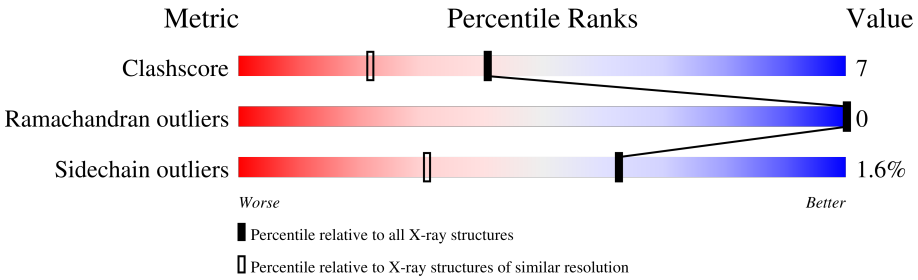
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 1.45 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	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)

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	331	86% 13%
1	B	331	81% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	473	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6096 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 intra-cellular xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	14	0
			2748	1766	480	489	13			
1	B	328	Total	C	N	O	S	0	12	0
			2731	1750	476	491	14			

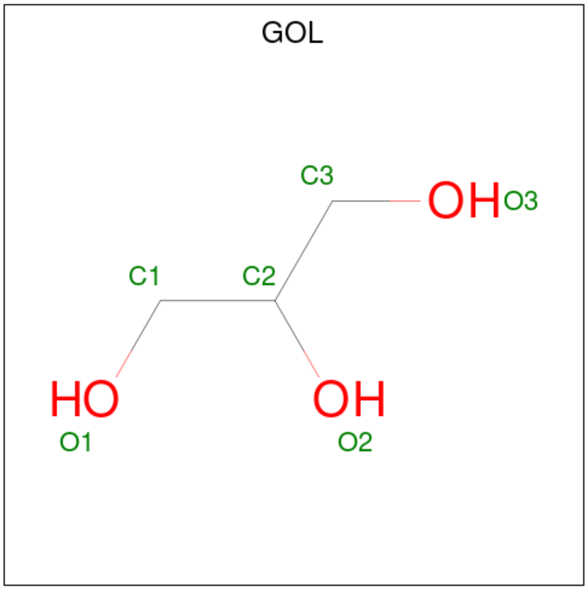
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ASP	ASN	conflict	UNP Q9ZFM8
B	1141	ASP	ASN	conflict	UNP Q9ZFM8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	295	Total O 295 295	0	0
4	B	236	Total O 236 236	0	0

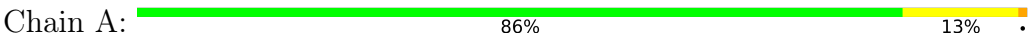
3 Residue-property plots (i)

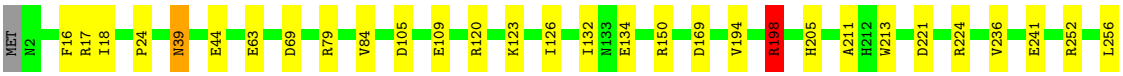
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

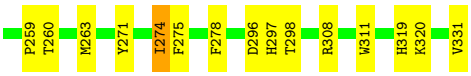
Note EDS was not executed.

• Molecule 1: intra-cellular xylanase

Chain A:







• Molecule 1: intra-cellular xylanase

Chain B:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	169.48Å 80.58Å 79.05Å 90.00° 91.89° 90.00°	Depositor
Resolution (Å)	15.00 – 1.45	Depositor
% Data completeness (in resolution range)	91.6 (15.00-1.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.159 , 0.194	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6096	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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: NA, GOL

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	0.68	1/2881 (0.0%)	1.24	15/3902 (0.4%)
1	B	0.60	0/2856	1.27	18/3868 (0.5%)
All	All	0.64	1/5737 (0.0%)	1.25	33/7770 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	VAL	C-OXT	16.77	1.55	1.23

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1120	ARG	NE-CZ-NH1	-15.71	112.44	120.30
1	A	198	ARG	NE-CZ-NH1	-12.42	114.09	120.30
1	B	1079	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	A	17	ARG	NE-CZ-NH2	-10.15	115.22	120.30
1	B	1308	ARG	NE-CZ-NH1	-9.46	115.57	120.30

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	2748	0	2652	30	0
1	B	2731	0	2625	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	54	0	72	8	0
3	B	30	0	40	4	0
4	A	295	0	0	5	0
4	B	236	0	0	9	0
All	All	6096	0	5389	78	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 7.

The worst 5 of 78 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:1174:LEU:H	1:B:1205:HIS:HD2	1.27	0.82
1:B:1259:PRO:HA	1:B:1263[A]:MET:HE3	1.69	0.74
1:B:1023:ASN:ND2	1:B:1026:THR:H	1.90	0.70
1:A:126:ILE:O	3:A:463:GOL:H12	1.92	0.69
1:B:1236:VAL:HG13	1:B:1286[A]:GLN:OE1	1.93	0.67

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	342/331 (103%)	334 (98%)	8 (2%)	0	100	100
1	B	338/331 (102%)	334 (99%)	4 (1%)	0	100	100
All	All	680/662 (103%)	668 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	297/291 (102%)	291 (98%)	6 (2%)	55 22
1	B	295/291 (101%)	291 (99%)	4 (1%)	67 37
All	All	592/582 (102%)	582 (98%)	10 (2%)	62 28

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1023	ASN
1	B	1143	LEU
1	B	1217	ARG
1	A	274[A]	ILE
1	A	274[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1046	HIS
1	B	1074	HIS
1	B	1319	HIS
1	B	1205	HIS
1	A	297	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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	GOL	B	473	-	5,5,5	0.90	0	5,5,5	1.31	1 (20%)
3	GOL	B	474	-	5,5,5	0.76	0	5,5,5	0.30	0
3	GOL	A	461	-	5,5,5	0.71	0	5,5,5	0.59	0
3	GOL	B	466	-	5,5,5	0.54	0	5,5,5	1.33	1 (20%)
3	GOL	B	455	-	5,5,5	0.54	0	5,5,5	1.25	0
3	GOL	B	464	-	5,5,5	0.62	0	5,5,5	0.45	0
3	GOL	A	476	-	5,5,5	0.70	0	5,5,5	0.88	0
3	GOL	A	469	-	5,5,5	0.61	0	5,5,5	0.34	0
3	GOL	A	463	-	5,5,5	0.60	0	5,5,5	1.52	1 (20%)
3	GOL	A	467	-	5,5,5	0.60	0	5,5,5	0.70	0
3	GOL	A	465	-	5,5,5	0.68	0	5,5,5	0.96	0
3	GOL	A	453	-	5,5,5	0.67	0	5,5,5	0.28	0
3	GOL	A	472	-	5,5,5	0.94	0	5,5,5	0.95	0
3	GOL	A	470	-	5,5,5	0.77	0	5,5,5	0.89	0

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	GOL	B	473	-	-	1/4/4/4	-
3	GOL	B	474	-	-	4/4/4/4	-
3	GOL	A	461	-	-	3/4/4/4	-
3	GOL	B	466	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	455	-	-	3/4/4/4	-
3	GOL	B	464	-	-	2/4/4/4	-
3	GOL	A	476	-	-	4/4/4/4	-
3	GOL	A	469	-	-	2/4/4/4	-
3	GOL	A	463	-	-	2/4/4/4	-
3	GOL	A	467	-	-	4/4/4/4	-
3	GOL	A	465	-	-	2/4/4/4	-
3	GOL	A	453	-	-	1/4/4/4	-
3	GOL	A	472	-	-	2/4/4/4	-
3	GOL	A	470	-	-	2/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	463	GOL	O2-C2-C1	2.77	121.34	109.12
3	B	473	GOL	O3-C3-C2	2.25	120.98	110.20
3	B	466	GOL	O2-C2-C3	2.10	118.35	109.12

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	461	GOL	O1-C1-C2-O2
3	A	461	GOL	O1-C1-C2-C3
3	A	463	GOL	C1-C2-C3-O3
3	A	465	GOL	C1-C2-C3-O3
3	A	465	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	473	GOL	4	0
3	A	463	GOL	1	0
3	A	465	GOL	1	0
3	A	472	GOL	3	0
3	A	470	GOL	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.