wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 08:01 PM GMT

PDB ID	:	1IEV
Title	:	CRYSTAL STRUCTURE OF BARLEY BETA-D-GLUCAN GLUCOHYDROLASE ISOENZYME EXO1 IN COMPLEX WITH CYCLOHEXITOL
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Deposited on	:	2001-04-11
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

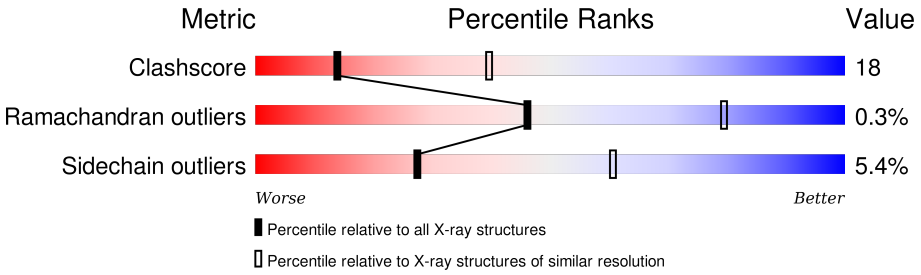
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	605	67% 30% •

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
2	NAG	A	616	X	-	X	-
3	MAN	A	615	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4878 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.

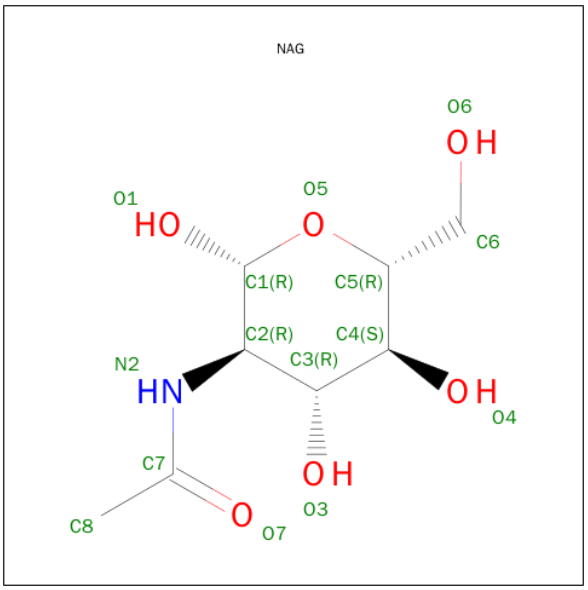
- Molecule 1 is a protein called BETA-D-GLUCAN GLUCOHYDROLASE ISOENZYME EXO1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4566	2891	787	862	26			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	LYS	ASN	SEE REMARK 999	GB 4566505

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

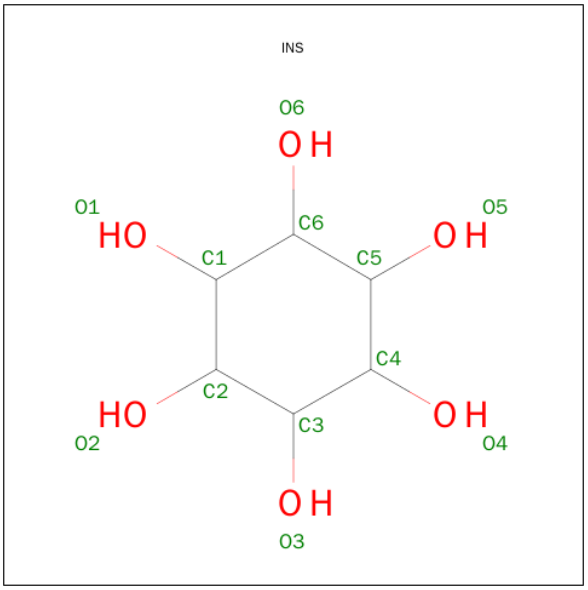


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			60	34	2	24		

- Molecule 4 is 1,2,3,4,5,6-HEXAHYDROXY-CYCLOHEXANE (three-letter code: INS) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	213	Total	O	0	0
			213	213		

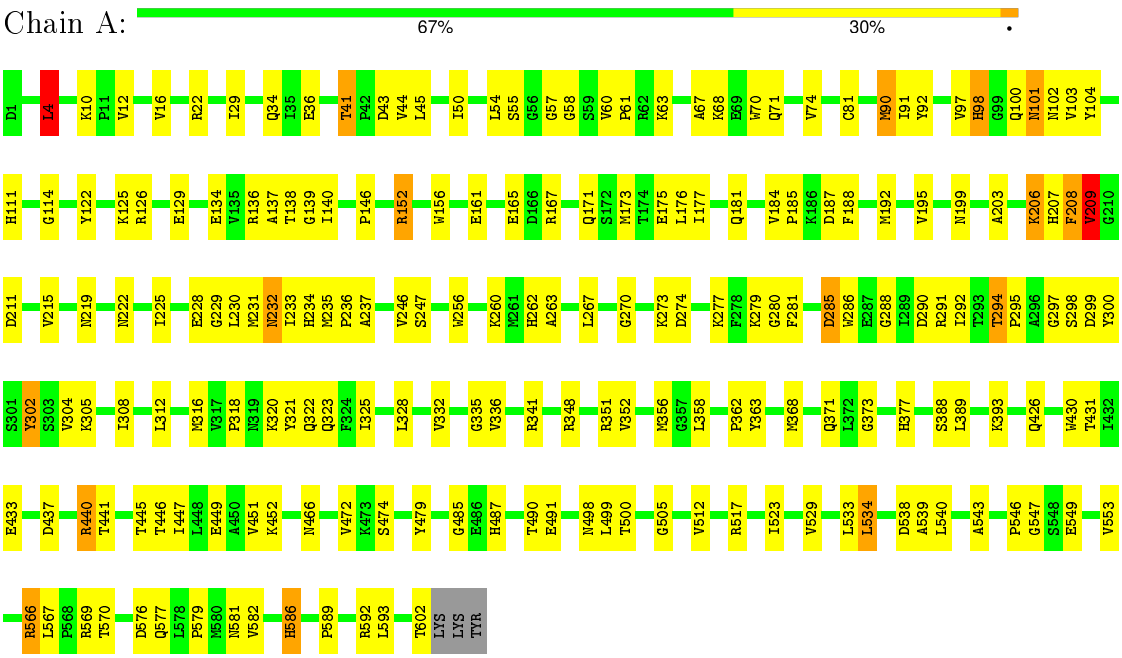
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: BETA-D-GLUCAN GLUCOHYDROLASE ISOENZYME EXO1

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.01Å 101.01Å 181.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.80)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4878	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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: FUC, MAN, BMA, NAG, INS

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	0.90	1/4663 (0.0%)	1.01	10/6334 (0.2%)

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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ASP	CG-OD1	7.09	1.41	1.25

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	208	PHE	CA-C-N	-7.60	100.47	117.20
1	A	4	LEU	CA-CB-CG	6.70	130.71	115.30
1	A	208	PHE	C-N-CA	6.27	137.38	121.70
1	A	43	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	206	LYS	C-N-CA	5.77	136.12	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	A	208	PHE	Mainchain
1	A	302	TYR	Sidechain

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	4566	0	4551	153	0
2	A	28	0	25	16	0
3	A	60	0	52	16	0
4	A	11	0	10	2	0
5	A	213	0	0	20	0
All	All	4878	0	4638	170	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 18.

The worst 5 of 170 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)
3:A:615:MAN:C4	3:A:615:MAN:C5	1.92	1.45
2:A:616:NAG:C5	2:A:616:NAG:O5	1.70	1.37
3:A:615:MAN:C3	3:A:615:MAN:C5	2.05	1.35
3:A:615:MAN:H3	3:A:615:MAN:C5	1.75	1.09
3:A:615:MAN:H3	3:A:615:MAN:H5	1.30	1.07

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	600/605 (99%)	564 (94%)	34 (6%)	2 (0%)	46 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	VAL
1	A	505	GLY

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	485/488 (99%)	459 (95%)	26 (5%)	27 60

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	LEU
1	A	294	THR
1	A	586	HIS
1	A	232	ASN
1	A	290	ASP

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

Mol	Chain	Res	Type
1	A	219	ASN
1	A	232	ASN
1	A	377	HIS
1	A	199	ASN
1	A	262	HIS

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

5 carbohydrates are modelled in this entry.

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	NAG	A	611	1,3	14,14,15	2.22	4 (28%)	15,19,21	1.73	4 (26%)
3	NAG	A	612	3	14,14,15	1.87	5 (35%)	15,19,21	1.83	4 (26%)
3	BMA	A	613	3	11,11,12	3.18	7 (63%)	14,15,17	2.00	5 (35%)
3	FUC	A	614	3	10,10,11	1.81	4 (40%)	14,14,16	1.46	2 (14%)
3	MAN	A	615	3,2	11,11,12	6.68	8 (72%)	14,15,17	10.65	13 (92%)

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	NAG	A	611	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	612	3	-	0/6/23/26	0/1/1/1
3	BMA	A	613	3	-	0/2/19/22	0/1/1/1
3	FUC	A	614	3	-	0/0/17/20	0/1/1/1
3	MAN	A	615	3,2	-	0/2/19/22	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	613	BMA	C6-C5	-2.76	1.42	1.51
3	A	613	BMA	O5-C5	-2.61	1.37	1.43
3	A	611	NAG	O4-C4	-2.43	1.37	1.43
3	A	614	FUC	O4-C4	2.01	1.47	1.43
3	A	613	BMA	O3-C3	2.02	1.47	1.43

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	615	MAN	C3-C4-C5	-22.86	70.34	110.20
3	A	615	MAN	C1-C2-C3	-14.39	92.52	109.54
3	A	615	MAN	C2-C3-C4	-14.20	86.92	111.04
3	A	615	MAN	O2-C2-C1	-12.30	84.55	109.21
3	A	615	MAN	O4-C4-C3	-9.96	87.91	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	615	MAN	16	0

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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	NAG	A	610	1	14,14,15	2.46	4 (28%)	15,19,21	3.32	9 (60%)
2	NAG	A	616	3	14,14,15	5.98	7 (50%)	15,19,21	6.11	10 (66%)
4	INS	A	617	1	11,11,12	3.01	5 (45%)	15,16,18	4.04	10 (66%)

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	NAG	A	610	1	-	0/6/23/26	0/1/1/1
2	NAG	A	616	3	1/1/5/7	0/6/23/26	0/1/1/1
4	INS	A	617	1	-	0/0/20/24	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	610	NAG	O5-C1	-6.10	1.33	1.43
2	A	610	NAG	C1-C2	-2.11	1.49	1.52
4	A	617	INS	O3-C3	2.39	1.48	1.43
2	A	616	NAG	O4-C4	2.47	1.48	1.43
4	A	617	INS	O5-C5	3.11	1.50	1.43

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	616	NAG	C2-N2-C7	-10.34	109.75	123.04
2	A	616	NAG	C3-C2-N2	-8.65	89.84	110.56
4	A	617	INS	O2-C2-C1	-6.86	93.25	110.06
2	A	610	NAG	O5-C5-C6	-5.94	94.48	107.35
2	A	610	NAG	C3-C4-C5	-5.36	100.86	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	616	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	610	NAG	2	0
2	A	616	NAG	14	0
4	A	617	INS	2	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 will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.