

Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2020 – 02:47 PM BST

PDB ID : 1RED

Title : ENDO-1,4-BETA-XYLANASE II COMPLEX WITH 4,5-EPOXYPENTYL-

BETA-D-XYLOSIDE

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Deposited on : 1995-12-21

Resolution : 1.60 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 following versions of software and data (see references (1)) 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)

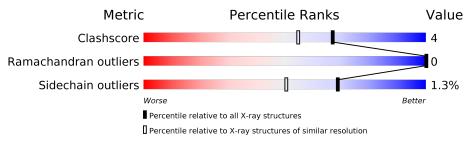
Validation Pipeline (wwPDB-VP) : 2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	Similar resolution		
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$		
Clashscore	141614	3665 (1.60-1.60)		
Ramachandran outliers	138981	3564 (1.60-1.60)		
Sidechain outliers	138945	3563 (1.60-1.60)		

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	A	190	87%	12%	•
1	В	190	91%	9%	•



2 Entry composition (i)

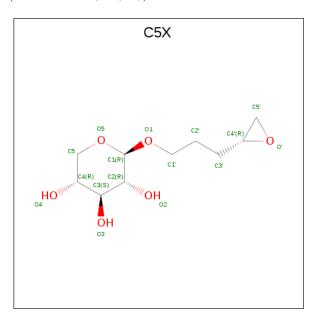
There are 4 unique types of molecules in this entry. The entry contains 3275 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENDO-1,4-BETA-XYLANASE II.

\mathbf{Mol}	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	190	Total	С	N	О	S	0	0	0
1	Λ	190	1480	934	253	292	1	U	U	0
1	В	190	Total	С	N	О	S	0	0	0
1	Ъ	190	1480	934	253	292	1	0	0	

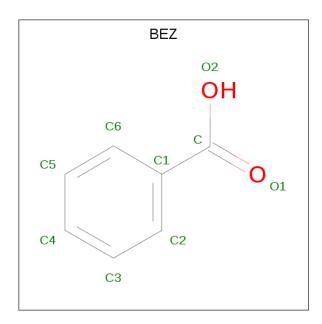
• Molecule 2 is 3-[(2R)-oxiran-2-yl]propyl beta-D-xylopyranoside (three-letter code: C5X) (formula: C₁₀H₁₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	В	1	Total 16	C 10	O 6	0	0

• Molecule 3 is BENZOIC ACID (three-letter code: BEZ) (formula: C₇H₆O₂).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	В	1	Total 9	C 7	O 2	0	0

• Molecule 4 is water.

Mol	Chain	Residues	${f Atoms}$	ZeroOcc	\mid AltConf \mid
4	A	150	Total O 150 150	0	0
4	В	140	Total O 140 140	0	0

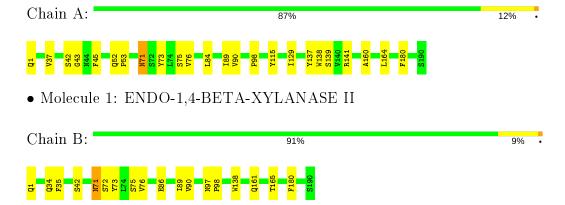


3 Residue-property plots (i)

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: ENDO-1,4-BETA-XYLANASE II





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 1 21 1	Depositor	
Cell constants	81.94Å 60.96Å 38.04Å	Depositor	
a, b, c, α , β , γ	90.00° 94.03° 90.00°	Depositor	
Resolution (Å)	8.00 - 1.60	Depositor	
% Data completeness	(Not available) (8.00-1.60)	Depositor	
(in resolution range)	(1101 available) (0.00 1.00)	Берозпот	
R_{merge}	0.07	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	X-PLOR	Depositor	
R, R_{free}	0.180 , 0.222	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3275	wwPDB-VP	
Average B, all atoms (Å ²)	20.0	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: BEZ, PCA, C5X

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		Boı	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.35	0/1519	0.64	$1/2073 \ (0.0\%)$	
1	В	0.49	1/1519 (0.1%)	0.64	0/2073	
All	All	0.43	1/3038 (0.0%)	0.64	1/4146 (0.0%)	

All (1) bond length outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
1	В	86	GLU	CD-OE2	13.76	1.40	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathbf{Ideal}(^{o})$
1	A	43	GLY	N-CA-C	-5.10	100.36	113.10

There are no chirality outliers.

There are no planarity outliers.

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	1480	0	1350	12	0
1	В	1480	0	1350	10	0
2	В	16	0	17	0	0
3	В	9	0	5	0	0

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Mol	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
4	A	150	0	0	0	0
4	В	140	0	0	0	0
All	All	3275	0	2722	22	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 4.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{array}$	Clash overlap (Å)
1:B:75:SER:HB3	1:B:90:VAL:HA	1.57	0.84
1:A:75:SER:HB3	1:A:90:VAL:HA	1.67	0.76
1:B:73:TYR:CZ	1:B:98:PRO:HB3	2.38	0.59
1:A:98:PRO:HB2	1:A:138:TRP:CZ3	2.38	0.59
1:A:73:TYR:CZ	1:A:98:PRO:HB3	2.43	0.53
1:B:73:TYR:CE1	1:B:98:PRO:HB3	2.44	0.52
1:A:160:ALA:HA	1:A:164:LEU:O	2.10	0.51
1:A:76:VAL:HB	1:A:89:ILE:HB	1.92	0.51
1:B:98:PRO:HB2	1:B:138:TRP:CZ3	2.47	0.49
1:B:42:SER:O	1:B:180:PHE:HA	2.13	0.48
1:B:76:VAL:HB	1:B:89:ILE:HB	1.96	0.48
1:B:34:GLN:HG2	1:B:35:PHE:N	2.28	0.47
1:B:165:THR:O	1:B:165:THR:HG23	2.16	0.45
1:A:71:ASN:C	1:A:71:ASN:HD22	2.21	0.43
1:A:84:LEU:HD22	1:A:129:ILE:HD11	2.01	0.43
1:A:115:TYR:CE2	1:A:141:ARG:HB2	2.54	0.42
1:A:52:GLN:HA	1:A:53:PRO:HA	1.92	0.42
1:A:37:VAL:HG11	1:A:45:PHE:CE1	2.54	0.41
1:A:137:TYR:CE1	1:A:164:LEU:HD13	2.55	0.41
1:B:97:ASN:HA	1:B:98:PRO:HD2	1.91	0.41
1:A:42:SER:O	1:A:180:PHE:HA	2.20	0.41
1:B:71:ASN:HD22	1:B:72:SER:N	2.19	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	sed Favoured Allowed		Outliers	Percentiles	
1	A	188/190 (99%)	180 (96%)	8 (4%)	0	100	100
1	В	188/190~(99%)	179 (95%)	9 (5%)	0	100	100
All	All	376/380 (99%)	359 (96%)	17 (4%)	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	155/155~(100%)	153 (99%)	2 (1%)	69 50
1	В	155/155~(100%)	153 (99%)	2 (1%)	69 50
All	All	310/310 (100%)	306 (99%)	4 (1%)	69 50

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	139	SER
1	В	71	ASN
1	В	161	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	41	ASN
1	A	67	ASN
1	A	71	ASN
1	A	143	ASN
1	A	157	ASN
1	A	161	GLN
1	В	71	ASN
1	В	121	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)

2 non-standard protein/DNA/RNA residues 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 C	Chain	Dec	T : 1-	B	ond leng	$_{ m gths}$	В	ond ang	gles	
MIOI	Type	Chain	m Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
1	PCA	В	1	1	7,8,9	2.64	3 (42%)	9,10,12	1.83	4 (44%)
1	PCA	A	1	1	7,8,9	2.50	3 (42%)	9,10,12	1.78	3 (33%)

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
1	PCA	В	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	_	0/0/11/13	0/1/1/1

All (6) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
1	В	1	PCA	CD-N	5.75	1.49	1.34
1	A	1	PCA	CD-N	5.39	1.48	1.34
1	В	1	PCA	CA-N	3.19	1.50	1.46
1	A	1	PCA	CA-N	3.03	1.50	1.46
1	A	1	PCA	CB-CG	-2.12	1.48	1.53
1	В	1	PCA	CB-CG	-2.11	1.48	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	В	1	PCA	OE-CD-CG	-2.56	122.30	126.76
1	A	1	PCA	OE-CD-CG	-2.52	122.37	126.76
1	В	1	PCA	CB-CA-C	-2.49	109.28	112.70
1	A	1	PCA	CB-CG-CD	2.23	108.00	104.40
1	A	1	PCA	CB-CA-C	-2.18	109.70	112.70
1	В	1	PCA	CA-N-CD	-2.10	106.40	113.58
1	В	1	PCA	CB-CG-CD	2.05	107.70	104.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	Iol Type Chain Res		Res Link		Bo	ond leng	ths	Bond angles		
MIOI	туре	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BEZ	В	402	_	7,9,9	2.88	1 (14%)	8,11,11	0.29	0
2	C5X	В	401	1	17,17,17	5.66	1 (5%)	21,23,23	5.17	4 (19%)

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	BEZ	В	402	_	-	0/0/4/4	0/1/1/1
2	C5X	В	401	1	-	1/7/26/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	${ m Observed}({ m \AA})$	$\mathbf{Ideal}(\mathbf{\AA})$
2	В	401	C5X	O'-C5'	23.11	2.38	1.43
3	В	402	BEZ	C1-C	-7.52	1.40	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	401	C5X	O'-C4'-C5'	19.10	108.96	60.04
2	В	401	C5X	O'-C5'-C4'	-10.27	34.33	59.62
2	В	401	C5X	C5'-O'-C4'	-8.64	36.71	60.34
2	В	401	C5X	O1-C1-C2	2.17	111.69	108.30

There are no chirality outliers.

All (1) torsion outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	${f Atoms}$
2	В	401	C5X	C2'-C3'-C4'-O'

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)

There are no chain breaks in this entry.



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.

