

wwPDB X-ray Structure Validation Summary Report (i)

Oct 18, 2023 – 10:58 AM EDT

PDB ID : 2DBT

Title: Crystal structure of chitinase C from Streptomyces griseus HUT6037

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Deposited on : 2005-12-16

Resolution : 3.14 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)

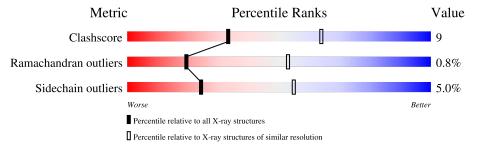
Validation Pipeline (wwPDB-VP) : 2.36

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 3.14 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	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)

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	265	63%	13% •	23%			
1	В	265	55%	20% •	23%			
1	С	265	63%	14%	23%			



2 Entry composition (i)

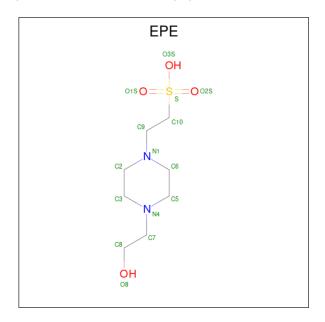
There are 3 unique types of molecules in this entry. The entry contains 4794 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 chitinase C.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Λ	205	Total	С	N	О	S	0	0	0
1	A	205	1576	999	269	302	6	0	U	
1	D	205	Total	С	N	О	S	0	0	0
1	Ъ	200	1576	999	269	302	6	0	U	U
1	С	205	Total	С	N	О	S	0	0	0
1		205	1576	999	269	302	6		U	U

• Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
9	Λ	1	Total	С	N	О	S	0	0	
	Λ	1	15	8	2	4	1	0		
9	D	1	Total	С	N	О	S	0	0	
	Б	1	15	8	2	4	1	0	U	
2	С	1	Total	С	N	О	S	0	0	
	$\frac{2}{2}$	1	15	8	2	4	1	0		



• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	В	6	Total O 6 6	0	0
3	С	7	Total O 7 7	0	0

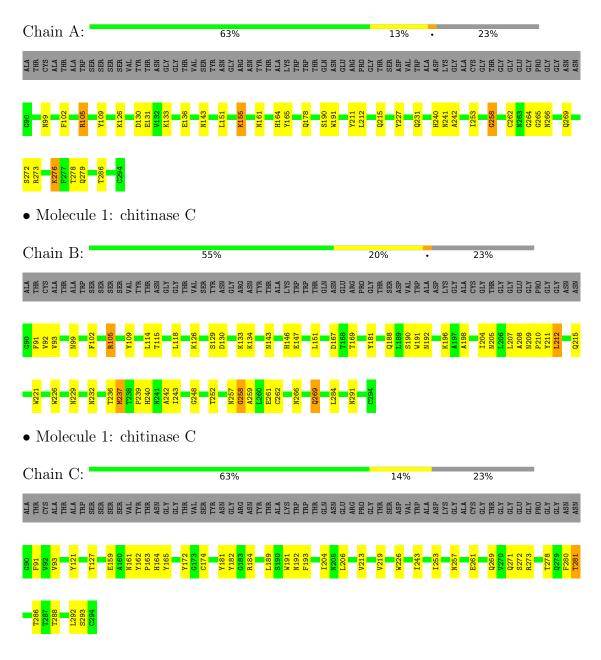


3 Residue-property plots (i)

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: chitinase C





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	153.12Å 153.12Å 90.03Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.32 - 3.14	Depositor
% Data completeness	100.0 (58.32-3.14)	Depositor
(in resolution range)	100.0 (00.02 0.14)	Берозног
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.174 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4794	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: EPE

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	\mathbf{angles}
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.58	0/1620	0.65	0/2207
1	В	0.58	0/1620	0.64	0/2207
1	С	0.52	0/1620	0.61	0/2207
All	All	0.56	0/4860	0.64	0/6621

There are no bond length outliers.

There are no bond angle outliers.

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	1576	0	1479	24	0
1	В	1576	0	1479	33	0
1	С	1576	0	1479	27	0
2	A	15	0	17	0	0
2	В	15	0	17	2	0
2	С	15	0	17	0	0
3	A	8	0	0	0	0
3	В	6	0	0	0	0
3	С	7	0	0	0	0
All	All	4794	0	4488	80	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 9.

The worst 5 of 80 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:B:232:ASN:HB3	1:B:237:MET:O	1.72	0.90
1:A:164:HIS:ND1	1:C:164:HIS:HB3	1.95	0.81
1:A:126:LYS:HA	1:A:133:LYS:HD3	1.63	0.79
1:B:102:PHE:O	1:B:105:ARG:HG2	1.92	0.69
1:A:99:ASN:OD1	1:A:105:ARG:NH1	2.26	0.68

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	P	erce	ntiles
1	A	203/265~(77%)	185 (91%)	17 (8%)	1 (0%)		29	63
1	В	203/265 (77%)	182 (90%)	18 (9%)	3 (2%)		10	37
1	С	203/265 (77%)	188 (93%)	14 (7%)	1 (0%)		29	63
All	All	609/795 (77%)	555 (91%)	49 (8%)	5 (1%)		19	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLY
1	В	258	GLY
1	В	129	SER
1	В	169	THR
1	С	191	TRP



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	Perce	entiles
1	A	160/203~(79%)	151 (94%)	9 (6%)	21	50
1	В	160/203 (79%)	153 (96%)	7 (4%)	28	59
1	С	160/203 (79%)	152 (95%)	8 (5%)	24	55
All	All	480/609 (79%)	456 (95%)	24 (5%)	24	55

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	237	MET
1	С	243	ILE
1	С	127	THR
1	С	269	GLN
1	A	276	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	209	ASN
1	С	279	GLN
1	В	215	GLN
1	С	282	GLN
1	В	246	ASN

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)

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	Tuno	Chain	Res Linl		Во	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EPE	С	295	-	15,15,15	0.87	1 (6%)	18,20,20	2.12	7 (38%)
2	EPE	A	295	-	15,15,15	0.91	1 (6%)	18,20,20	1.92	6 (33%)
2	EPE	В	295	-	15,15,15	0.85	1 (6%)	18,20,20	2.28	7 (38%)

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	EPE	С	295	-	-	3/9/19/19	0/1/1/1
2	EPE	A	295	-	-	4/9/19/19	0/1/1/1
2	EPE	В	295	-	-	6/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
2	С	295	EPE	C10-S	3.05	1.81	1.77
2	A	295	EPE	C10-S	3.00	1.81	1.77
2	В	295	EPE	C10-S	2.87	1.81	1.77

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	295	EPE	C5-N4-C3	5.93	122.18	108.83

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
2	С	295	EPE	O2S-S-C10	4.13	111.89	106.92
2	С	295	EPE	C5-N4-C3	3.91	117.62	108.83
2	С	295	EPE	O3S-S-C10	3.80	111.91	105.77
2	В	295	EPE	O3S-S-C10	3.47	111.39	105.77

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	295	EPE	C10-C9-N1-C2
2	A	295	EPE	C10-C9-N1-C6
2	В	295	EPE	C10-C9-N1-C2
2	В	295	EPE	S-C10-C9-N1
2	В	295	EPE	C9-C10-S-O1S

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	295	EPE	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 (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.

