



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:12 am BST

PDB ID : 3BCF
Title : Alpha-amylase B from Halothermothrix orenii
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Deposited on : 2007-11-12
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

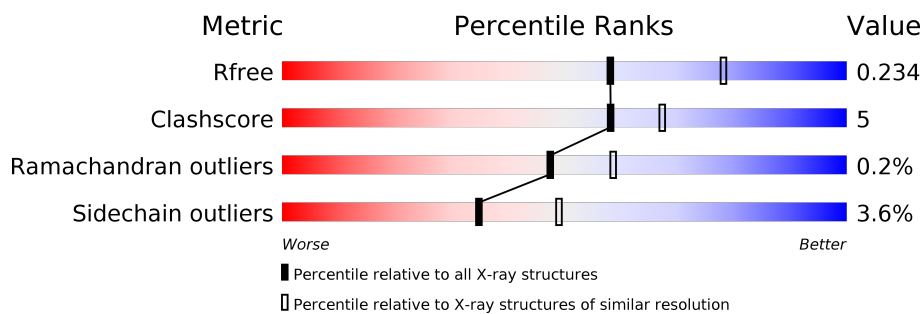
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	599	 83% 14% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5008 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 Alpha amylase, catalytic region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4747	3025	767	944	11			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

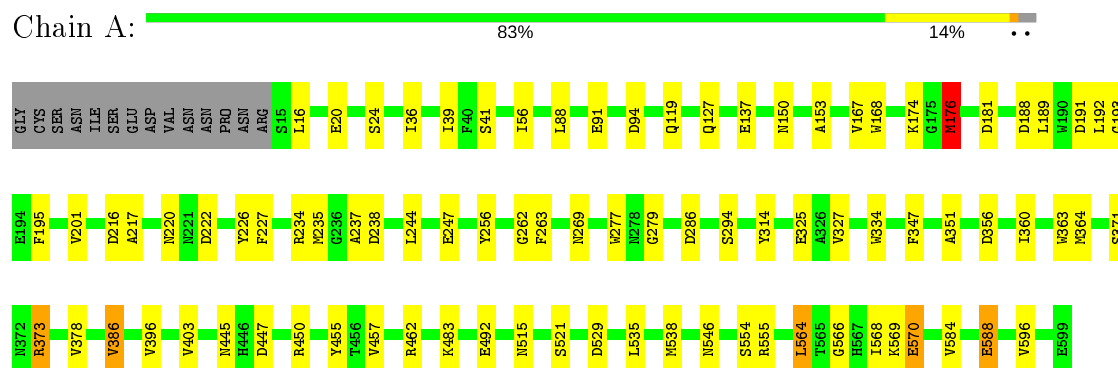
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total	O	0	0
			256	256		

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 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.

- Molecule 1: Alpha amylase, catalytic region



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.62Å 77.82Å 50.33Å 90.00° 99.38° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 40.16 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-2.30) 86.9 (40.16-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	16.14 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.229 0.200 , 0.234	Depositor DCC
R_{free} test set	2572 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5008	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: NA, CA

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	1.10	10/4878 (0.2%)	0.94	8/6645 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	GLU	CG-CD	8.06	1.64	1.51
1	A	378	VAL	CB-CG1	6.57	1.66	1.52
1	A	363	TRP	CB-CG	-6.03	1.39	1.50
1	A	351	ALA	CA-CB	5.91	1.64	1.52
1	A	396	VAL	CB-CG2	5.61	1.64	1.52
1	A	327	VAL	CB-CG2	5.51	1.64	1.52
1	A	492	GLU	CB-CG	5.50	1.62	1.52
1	A	226	TYR	CD1-CE1	5.49	1.47	1.39
1	A	588	GLU	CG-CD	5.42	1.60	1.51
1	A	137	GLU	CG-CD	5.12	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	MET	CG-SD-CE	8.31	113.50	100.20
1	A	188	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	A	181	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	234	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	356	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	447	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	462	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	529	ASP	CB-CG-OD1	5.01	122.81	118.30

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	4747	0	4383	44	0
2	A	4	0	0	0	0
3	A	1	0	0	0	0
4	A	256	0	0	5	0
All	All	5008	0	4383	44	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 5.

All (44) 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:A:237:ALA:HB2	1:A:263:PHE:CZ	2.29	0.67
1:A:237:ALA:HB2	1:A:263:PHE:CE1	2.29	0.67
1:A:247:GLU:HA	1:A:247:GLU:OE1	1.95	0.64
1:A:237:ALA:O	4:A:791:HOH:O	2.14	0.64
1:A:174:LYS:NZ	1:A:195:PHE:O	2.32	0.62
1:A:554:SER:O	1:A:555:ARG:HB2	1.99	0.62
1:A:546:ASN:OD1	1:A:546:ASN:N	2.32	0.62
1:A:176:MET:HG2	1:A:235:MET:HB3	1.88	0.56
1:A:566:GLY:O	1:A:569:LYS:NZ	2.43	0.52
1:A:193:GLY:HA2	1:A:201:VAL:O	2.09	0.52
1:A:20:GLU:HG3	1:A:39:ILE:HD12	1.91	0.52
1:A:568:ILE:HG22	1:A:570:GLU:HG3	1.92	0.52
1:A:515:ASN:HD21	1:A:521:SER:H	1.57	0.52
1:A:535:LEU:HD12	1:A:535:LEU:C	2.29	0.52
1:A:373:ARG:O	4:A:709:HOH:O	2.19	0.51
1:A:483:LYS:NZ	4:A:731:HOH:O	2.40	0.51
1:A:515:ASN:ND2	1:A:521:SER:H	2.11	0.49
1:A:16:LEU:HA	1:A:41:SER:OG	2.13	0.49
1:A:263:PHE:HB2	1:A:277:TRP:HB2	1.94	0.49
1:A:386:VAL:HG12	4:A:767:HOH:O	2.12	0.48
1:A:220:ASN:HA	4:A:722:HOH:O	2.13	0.48
1:A:216:ASP:O	1:A:217:ALA:C	2.52	0.48
1:A:237:ALA:HA	1:A:263:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:HG23	1:A:167:VAL:O	2.14	0.47
1:A:286:ASP:O	1:A:294:SER:HA	2.15	0.46
1:A:94:ASP:C	1:A:94:ASP:OD1	2.54	0.46
1:A:189:LEU:HB3	1:A:334:TRP:NE1	2.31	0.45
1:A:227:PHE:O	1:A:347:PHE:HA	2.17	0.44
1:A:36:ILE:HG21	1:A:88:LEU:HD22	1.99	0.44
1:A:56:ILE:HD13	1:A:56:ILE:N	2.31	0.44
1:A:238:ASP:N	1:A:262:GLY:O	2.51	0.44
1:A:564:LEU:HD23	1:A:596:VAL:HG11	2.00	0.43
1:A:360:ILE:HG23	1:A:360:ILE:HD12	1.70	0.43
1:A:127:GLN:HE22	1:A:445:ASN:HB2	1.82	0.43
1:A:286:ASP:HB3	1:A:314:TYR:OH	2.18	0.43
1:A:564:LEU:C	1:A:564:LEU:HD12	2.39	0.42
1:A:174:LYS:NZ	1:A:191:ASP:OD2	2.40	0.42
1:A:535:LEU:HD12	1:A:535:LEU:O	2.19	0.42
1:A:364:MET:HE2	1:A:364:MET:HB3	1.60	0.42
1:A:16:LEU:HD22	1:A:94:ASP:HB3	2.02	0.41
1:A:538:MET:HE2	1:A:584:VAL:HG12	2.03	0.41
1:A:244:LEU:HB2	1:A:256:TYR:CE2	2.56	0.41
1:A:192:LEU:N	1:A:192:LEU:HD23	2.34	0.41
1:A:150:ASN:O	1:A:153:ALA:HB3	2.22	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	583/599 (97%)	568 (97%)	14 (2%)	1 (0%)	47 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	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	504/517 (98%)	486 (96%)	18 (4%)	35 49

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	91	GLU
1	A	119	GLN
1	A	168	TRP
1	A	176	MET
1	A	222	ASP
1	A	269	ASN
1	A	325	GLU
1	A	371	SER
1	A	373	ARG
1	A	386	VAL
1	A	403	VAL
1	A	450	ARG
1	A	455	TYR
1	A	457	VAL
1	A	564	LEU
1	A	570	GLU
1	A	588	GLU

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	62	GLN
1	A	112	ASN
1	A	127	GLN

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Mol	Chain	Res	Type
1	A	173	ASN
1	A	221	ASN
1	A	248	ASN
1	A	515	ASN
1	A	581	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.