



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:34 AM GMT

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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

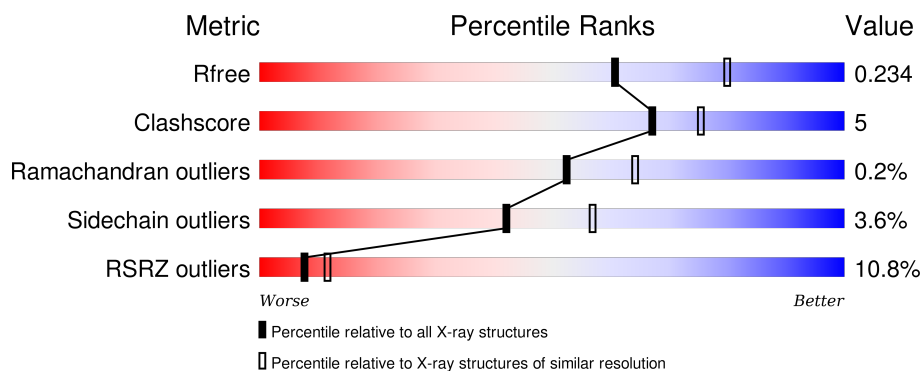
1 Overall quality at a glance

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	599	<div> <div>11%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>

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		

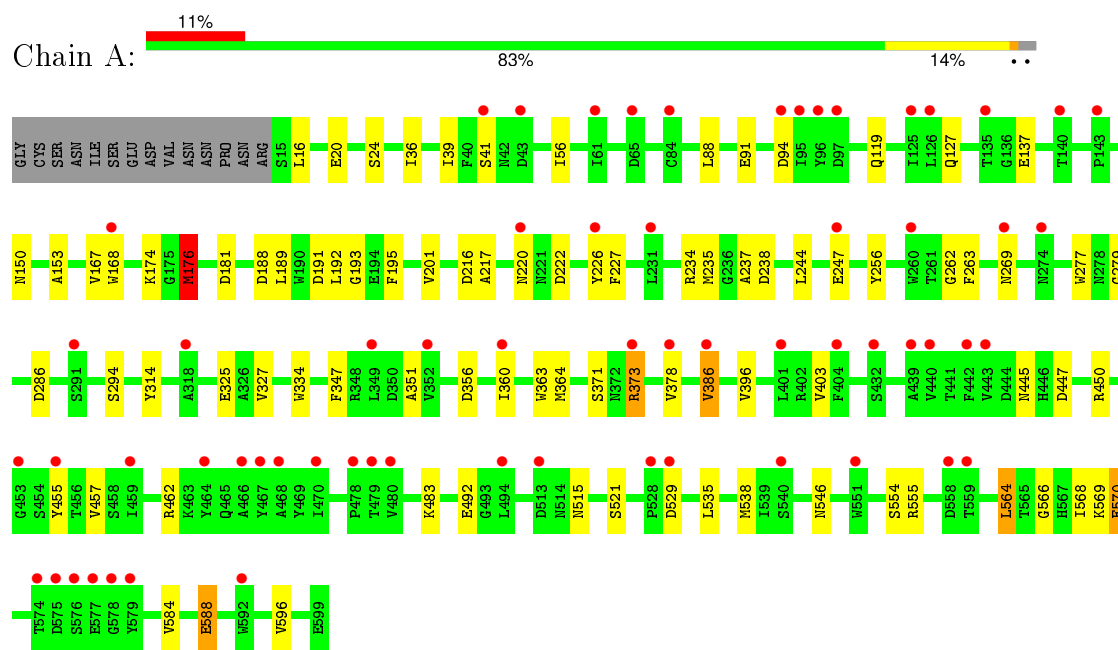
- Molecule 4 is water.

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 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 ($\text{RSRZ} > 2$). 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.

- 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	1902 reflections (5.34%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 51305 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:20:GLU:HG3	1:A:39:ILE:HD12	1.91	0.52
1:A:193:GLY:HA2	1:A:201:VAL:O	2.09	0.52
1:A:568:ILE:HG22	1:A:570:GLU:HG3	1.92	0.52
1:A:535:LEU:HD12	1:A:535:LEU:C	2.29	0.52
1:A:515:ASN:HD21	1:A:521:SER:H	1.57	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:263:PHE:HB2	1:A:277:TRP:HB2	1.94	0.49
1:A:16:LEU:HA	1:A:41:SER:OG	2.13	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:127:GLN:HE22	1:A:445:ASN:HB2	1.82	0.43
1:A:360:ILE:HG23	1:A:360:ILE:HD12	1.70	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%)	52 64

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%)	42 57

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	585/599 (97%)	0.87	63 (10%) 8 11	28, 45, 60, 72	9 (1%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	592	TRP	8.9
1	A	540	SER	6.4
1	A	386	VAL	5.7
1	A	61	ILE	5.3
1	A	577	GLU	5.1
1	A	455	TYR	4.6
1	A	95	ILE	4.3
1	A	274	ASN	4.2
1	A	558	ASP	4.0
1	A	84	CYS	3.9
1	A	125	ILE	3.9
1	A	453	GLY	3.7
1	A	432	SER	3.7
1	A	96	TYR	3.7
1	A	65	ASP	3.6
1	A	97	ASP	3.5
1	A	378	VAL	3.5
1	A	528	PRO	3.4
1	A	140	THR	3.2
1	A	291	SER	3.1
1	A	440	VAL	3.1
1	A	373	ARG	3.0
1	A	43	ASP	3.0
1	A	480	VAL	2.9
1	A	467	TYR	2.8
1	A	470	ILE	2.8
1	A	41	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	575	ASP	2.7
1	A	513	ASP	2.7
1	A	247	GLU	2.7
1	A	126	LEU	2.7
1	A	220	ASN	2.7
1	A	231	LEU	2.7
1	A	442	PHE	2.6
1	A	404	PHE	2.5
1	A	478	PRO	2.5
1	A	143	PRO	2.5
1	A	352	VAL	2.4
1	A	576	SER	2.4
1	A	94	ASP	2.4
1	A	401	LEU	2.4
1	A	168	TRP	2.4
1	A	559	THR	2.4
1	A	269	ASN	2.4
1	A	578	GLY	2.4
1	A	494	LEU	2.3
1	A	479	THR	2.3
1	A	551	TRP	2.3
1	A	443	VAL	2.2
1	A	579	TYR	2.2
1	A	574	THR	2.2
1	A	466	ALA	2.2
1	A	529	ASP	2.2
1	A	260	TRP	2.2
1	A	360	ILE	2.2
1	A	226	TYR	2.2
1	A	135	THR	2.2
1	A	464	TYR	2.1
1	A	349	LEU	2.1
1	A	459	ILE	2.1
1	A	439	ALA	2.0
1	A	318	ALA	2.0
1	A	468	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	A	705	1/1	0.93	0.28	1.49	58,58,58,58	0
3	NA	A	704	1/1	0.97	0.09	-2.51	29,29,29,29	0
2	CA	A	701	1/1	0.93	0.08	-2.72	34,34,34,34	0
2	CA	A	703	1/1	0.97	0.09	-2.74	43,43,43,43	0
2	CA	A	702	1/1	0.96	0.06	-3.73	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.