



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 1C7I / pdb_00001c7i
Title : THERMOPHYLIC PNB ESTERASE
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Deposited on : 2000-02-21
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

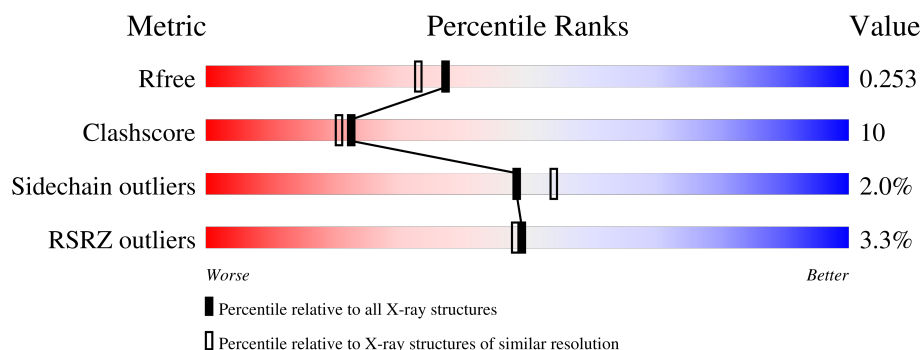
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	489	3% 76% 22% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3988 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 PROTEIN (PARA-NITROBENZYL ESTERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3784	2430	617	726	11			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	VAL	ALA	engineered mutation	UNP P37967
A	60	VAL	ILE	engineered mutation	UNP P37967
A	73	LYS	THR	engineered mutation	UNP P37967
A	144	MET	LEU	engineered mutation	UNP P37967
A	313	PHE	LEU	engineered mutation	UNP P37967
A	322	TYR	HIS	engineered mutation	UNP P37967
A	343	VAL	ALA	engineered mutation	UNP P37967
A	358	VAL	MET	engineered mutation	UNP P37967
A	370	PHE	TYR	engineered mutation	UNP P37967
A	400	THR	ALA	engineered mutation	UNP P37967
A	412	GLU	GLY	engineered mutation	UNP P37967
A	437	THR	ILE	engineered mutation	UNP P37967
A	459	SER	THR	engineered mutation	UNP P37967

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

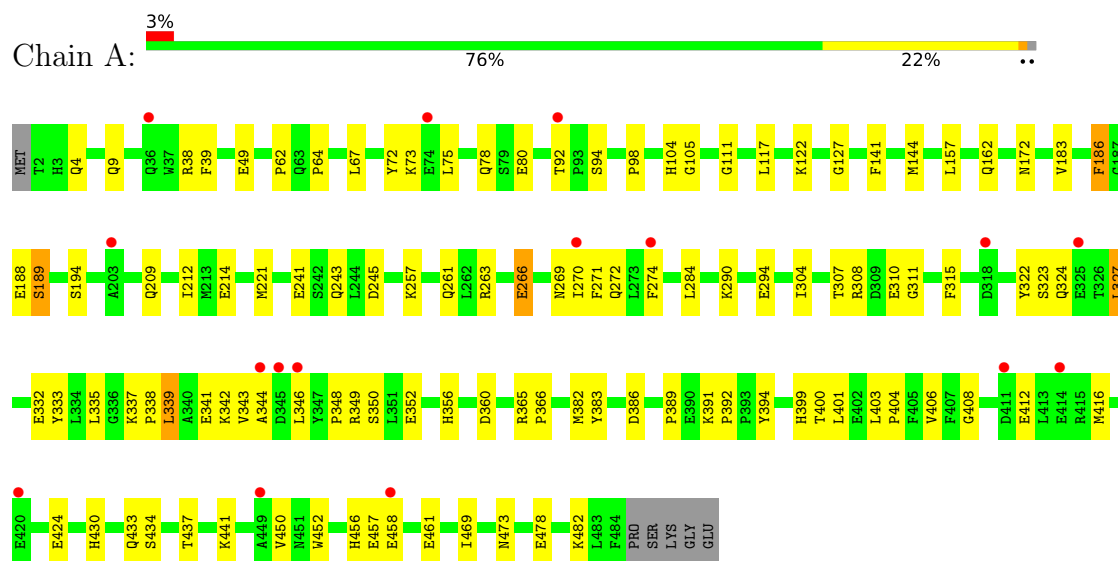
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total	O	0	0
			203	203		

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 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.

- Molecule 1: PROTEIN (PARA-NITROBENZYL ESTERASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.07Å 80.32Å 100.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.3 (25.00-2.00) 96.2 (25.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.245 0.212 , 0.253	Depositor DCC
R_{free} test set	3614 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.0	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	0.95	EDS
Total number of atoms	3988	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.42	1/3889 (0.0%)	0.91	17/5301 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	LYS	C-N	-10.12	1.19	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	TYR	O-C-N	6.88	131.83	123.16
1	A	4	GLN	N-CA-C	6.55	120.59	111.74
1	A	111	GLY	N-CA-C	6.19	119.82	112.33
1	A	360	ASP	N-CA-C	6.06	117.97	111.36
1	A	457	GLU	N-CA-C	5.94	119.63	112.38
1	A	401	LEU	N-CA-C	5.86	118.45	111.71
1	A	284	LEU	CA-C-N	5.74	125.86	119.32
1	A	284	LEU	C-N-CA	5.74	125.86	119.32
1	A	72	TYR	CA-C-N	-5.74	111.39	122.06
1	A	72	TYR	C-N-CA	-5.74	111.39	122.06
1	A	311	GLY	N-CA-C	5.59	120.70	113.27
1	A	144	MET	N-CA-C	-5.55	98.17	107.99
1	A	221	MET	N-CA-C	-5.27	101.53	109.85
1	A	80	GLU	N-CA-C	-5.22	106.01	112.38
1	A	64	PRO	N-CA-C	-5.18	103.63	111.41
1	A	189	SER	CB-CA-C	-5.02	110.80	116.63
1	A	73	LYS	N-CA-C	-5.02	107.15	113.28

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	3784	0	3670	78	0
2	A	1	0	0	0	0
3	A	203	0	0	2	0
All	All	3988	0	3670	78	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 10.

All (78) 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:343:VAL:HG13	1:A:346:LEU:HD12	1.57	0.85
1:A:323:SER:HA	1:A:349:ARG:HH12	1.43	0.83
1:A:183:VAL:H	1:A:209:GLN:NE2	1.80	0.79
1:A:412:GLU:HB3	1:A:416:MET:HE3	1.65	0.78
1:A:399:HIS:O	1:A:400:THR:HB	1.82	0.78
1:A:324:GLN:HE21	1:A:349:ARG:HB2	1.50	0.76
1:A:323:SER:CA	1:A:349:ARG:HH12	1.98	0.76
1:A:323:SER:C	1:A:349:ARG:HH12	2.00	0.70
1:A:324:GLN:NE2	1:A:349:ARG:HB2	2.07	0.70
1:A:337:LYS:HB2	1:A:338:PRO:HD3	1.74	0.69
1:A:183:VAL:H	1:A:209:GLN:HE21	1.40	0.69
1:A:9:GLN:HE21	1:A:172:ASN:HD21	1.40	0.68
1:A:391:LYS:HD3	1:A:392:PRO:N	2.09	0.67
1:A:266:GLU:HB3	1:A:274:PHE:CZ	2.29	0.67
1:A:257:LYS:O	1:A:261:GLN:HG3	1.96	0.66
1:A:461:GLU:HG2	1:A:473:ASN:OD1	1.97	0.64
1:A:269:ASN:HD22	1:A:271:PHE:H	1.45	0.64
1:A:450:VAL:HG22	1:A:469:ILE:HG21	1.86	0.58
1:A:323:SER:HA	1:A:349:ARG:NH1	2.15	0.57
1:A:391:LYS:HD3	1:A:392:PRO:O	2.08	0.53
1:A:266:GLU:CB	1:A:274:PHE:CZ	2.91	0.53
1:A:9:GLN:NE2	1:A:172:ASN:HD21	2.07	0.53
1:A:127:GLY:HA3	1:A:437:THR:HG21	1.92	0.52
1:A:322:TYR:HB2	1:A:327:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:HA	1:A:349:ARG:HH22	1.74	0.52
1:A:349:ARG:O	1:A:350:SER:HB3	2.10	0.51
1:A:365:ARG:HB3	1:A:366:PRO:HD3	1.91	0.51
1:A:456:HIS:CD2	1:A:458:GLU:HB2	2.46	0.51
1:A:404:PRO:HG3	1:A:416:MET:HE1	1.92	0.51
1:A:67:LEU:HD12	1:A:67:LEU:O	2.11	0.51
1:A:424:GLU:HB2	3:A:654:HOH:O	2.11	0.51
1:A:400:THR:HG23	1:A:403:LEU:HD12	1.93	0.51
1:A:406:VAL:O	1:A:433:GLN:HG2	2.11	0.51
1:A:98:PRO:HG2	1:A:441:LYS:HG2	1.92	0.50
1:A:186:PHE:CB	1:A:212:ILE:HB	2.42	0.50
1:A:117:LEU:HD13	1:A:416:MET:HE1	1.94	0.49
1:A:104:HIS:HE1	3:A:508:HOH:O	1.94	0.49
1:A:324:GLN:N	1:A:349:ARG:HH12	2.09	0.49
1:A:104:HIS:HD2	1:A:105:GLY:O	1.96	0.48
1:A:92:THR:HG22	1:A:94:SER:H	1.77	0.48
1:A:383:TYR:C	1:A:383:TYR:CD1	2.91	0.48
1:A:348:PRO:O	1:A:349:ARG:C	2.56	0.48
1:A:186:PHE:HB2	1:A:212:ILE:HB	1.96	0.48
1:A:337:LYS:O	1:A:341:GLU:HG3	2.14	0.47
1:A:335:LEU:HB3	1:A:339:LEU:HB3	1.96	0.47
1:A:38:ARG:HG2	1:A:39:PHE:CD2	2.50	0.47
1:A:343:VAL:O	1:A:344:ALA:C	2.58	0.47
1:A:383:TYR:HB3	1:A:452:TRP:CZ2	2.50	0.47
1:A:122:LYS:HD2	1:A:408:GLY:O	2.15	0.46
1:A:243:GLN:C	1:A:245:ASP:H	2.22	0.46
1:A:105:GLY:HA3	1:A:189:SER:HB3	1.96	0.46
1:A:450:VAL:CG2	1:A:469:ILE:HG21	2.45	0.46
1:A:404:PRO:HG3	1:A:416:MET:CE	2.45	0.46
1:A:307:THR:O	1:A:310:GLU:HG2	2.16	0.46
1:A:343:VAL:O	1:A:343:VAL:HG12	2.15	0.46
1:A:62:PRO:HA	1:A:78:GLN:OE1	2.16	0.46
1:A:478:GLU:O	1:A:482:LYS:HG3	2.15	0.45
1:A:290:LYS:O	1:A:294:GLU:HG2	2.16	0.45
1:A:412:GLU:HB3	1:A:416:MET:CE	2.43	0.45
1:A:304:ILE:O	1:A:382:MET:HA	2.17	0.45
1:A:162:GLN:OE1	1:A:194:SER:HB3	2.16	0.44
1:A:399:HIS:O	1:A:400:THR:CB	2.58	0.44
1:A:62:PRO:HG2	1:A:141:PHE:CE1	2.53	0.44
1:A:39:PHE:HA	1:A:157:LEU:HD11	2.00	0.44
1:A:389:PRO:HD2	1:A:394:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLN:N	1:A:349:ARG:NH1	2.66	0.43
1:A:272:GLN:HG2	1:A:333:TYR:CE2	2.53	0.43
1:A:391:LYS:HD3	1:A:391:LYS:C	2.43	0.43
1:A:270:ILE:HD12	1:A:315:PHE:CZ	2.54	0.42
1:A:308:ARG:HB2	1:A:386:ASP:OD1	2.19	0.42
1:A:383:TYR:HB3	1:A:452:TRP:HZ2	1.84	0.42
1:A:430:HIS:O	1:A:434:SER:HB2	2.20	0.41
1:A:188:GLU:HA	1:A:214:GLU:O	2.21	0.41
1:A:332:GLU:OE2	1:A:337:LYS:HG2	2.21	0.41
1:A:352:GLU:HG2	1:A:356:HIS:CD2	2.55	0.41
1:A:266:GLU:HG2	1:A:274:PHE:HZ	1.86	0.40
1:A:243:GLN:C	1:A:245:ASP:N	2.79	0.40
1:A:338:PRO:O	1:A:342:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	402/407 (99%)	394 (98%)	8 (2%)	48 54

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLU
1	A	75	LEU
1	A	186	PHE

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Mol	Chain	Res	Type
1	A	241	GLU
1	A	263	ARG
1	A	266	GLU
1	A	327	LEU
1	A	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	9	GLN
1	A	36	GLN
1	A	104	HIS
1	A	182	ASN
1	A	209	GLN
1	A	225	GLN
1	A	269	ASN
1	A	276	GLN
1	A	324	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	73:LYS	C	74:GLU	N	1.19

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	483/489 (98%)	0.21	16 (3%)	49 48	14, 30, 51, 62	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	PHE	4.3
1	A	420	GLU	3.8
1	A	36	GLN	2.9
1	A	325	GLU	2.9
1	A	414	GLU	2.9
1	A	458	GLU	2.9
1	A	449	ALA	2.6
1	A	92	THR	2.4
1	A	270	ILE	2.2
1	A	318	ASP	2.2
1	A	346	LEU	2.2
1	A	74	GLU	2.1
1	A	345	ASP	2.1
1	A	203	ALA	2.1
1	A	344	ALA	2.1
1	A	411	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	746	1/1	0.99	0.08	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.