



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:11 PM UTC

PDB ID : 1TRH / pdb_00001trh
Title : TWO CONFORMATIONAL STATES OF CANDIDA RUGOSA LIPASE
Authors : Grochulski, P.; Cygler, M.
Deposited on : 1993-11-18
Resolution : 2.10 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 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

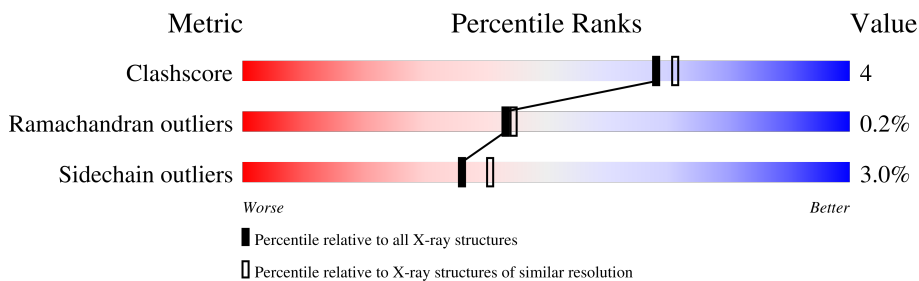
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	534	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4351 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 LIPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4022	2556	659	788	19			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is water.

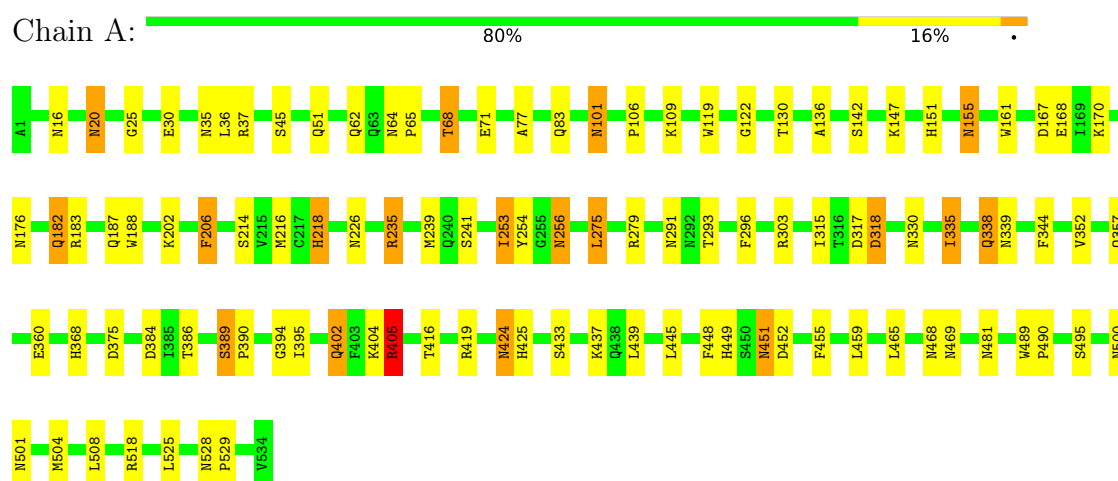
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	301	Total	O	0	0
			301	301		

3 Residue-property plots

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: LIPASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.00Å 106.70Å 59.80Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.148 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4351	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.90	7/4118 (0.2%)	1.66	74/5601 (1.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	449	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	425	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	335	ILE	CA-CB	5.48	1.61	1.54
1	A	151	HIS	CD2-NE2	-5.44	1.31	1.37
1	A	218	HIS	CD2-NE2	-5.41	1.31	1.37
1	A	395	ILE	CA-CB	5.23	1.61	1.54

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ASP	CA-CB-CG	12.89	125.50	112.60
1	A	182	GLN	OE1-CD-NE2	-10.32	112.28	122.60
1	A	452	ASP	CA-CB-CG	9.53	122.13	112.60
1	A	155	ASN	OD1-CG-ND2	-8.86	113.74	122.60
1	A	296	PHE	CA-CB-CG	8.55	122.35	113.80
1	A	330	ASN	OD1-CG-ND2	-8.17	114.43	122.60
1	A	528	ASN	CA-CB-CG	-8.03	104.57	112.60
1	A	357	GLN	OE1-CD-NE2	-7.96	114.64	122.60
1	A	206	PHE	CA-CB-CG	7.46	121.26	113.80
1	A	291	ASN	OD1-CG-ND2	-7.36	115.24	122.60
1	A	368	HIS	CB-CG-CD2	-7.20	121.84	131.20
1	A	101	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	A	339	ASN	OD1-CG-ND2	-6.93	115.67	122.60
1	A	187	GLN	OE1-CD-NE2	-6.92	115.68	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	GLN	OE1-CD-NE2	-6.67	115.93	122.60
1	A	330	ASN	CB-CG-ND2	6.65	126.37	116.40
1	A	303	ARG	N-CA-C	-6.54	97.17	108.56
1	A	500	ASN	OD1-CG-ND2	-6.43	116.17	122.60
1	A	344	PHE	CA-CB-CG	-6.30	107.50	113.80
1	A	357	GLN	CG-CD-NE2	6.23	125.74	116.40
1	A	384	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	45	SER	N-CA-C	-6.13	99.19	109.07
1	A	335	ILE	O-C-N	-6.05	116.53	123.07
1	A	161	TRP	CG-CD2-CE3	6.03	139.93	133.90
1	A	218	HIS	CA-CB-CG	-6.00	107.80	113.80
1	A	375	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	481	ASN	OD1-CG-ND2	-5.98	116.62	122.60
1	A	241	SER	CA-CB-OG	5.97	123.05	111.10
1	A	188	TRP	CB-CG-CD1	-5.96	117.97	126.90
1	A	170	LYS	CA-CB-CG	-5.94	102.22	114.10
1	A	235	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	A	256	ASN	CA-CB-CG	-5.92	106.68	112.60
1	A	235	ARG	NE-CZ-NH2	-5.89	113.89	119.20
1	A	136	ALA	N-CA-C	5.87	117.68	111.28
1	A	176	ASN	CA-CB-CG	5.82	118.42	112.60
1	A	16	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	A	451	ASN	OD1-CG-ND2	-5.77	116.83	122.60
1	A	315	ILE	N-CA-C	-5.76	97.56	106.72
1	A	151	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	62	GLN	OE1-CD-NE2	-5.56	117.04	122.60
1	A	500	ASN	CB-CG-ND2	5.50	124.64	116.40
1	A	317	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	469	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	A	404	LYS	CA-C-O	-5.40	114.69	120.42
1	A	235	ARG	CB-CG-CD	5.40	123.71	111.30
1	A	293	THR	N-CA-C	-5.38	102.70	110.40
1	A	368	HIS	CB-CG-ND1	5.38	130.78	122.70
1	A	405	ARG	CA-CB-CG	5.35	124.80	114.10
1	A	501	ASN	CA-CB-CG	5.34	117.94	112.60
1	A	187	GLN	CG-CD-NE2	5.34	124.41	116.40
1	A	352	VAL	O-C-N	-5.32	116.40	122.62
1	A	518	ARG	N-CA-C	5.31	118.76	111.54
1	A	468	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	424	ASN	OD1-CG-ND2	-5.28	117.33	122.60
1	A	338	GLN	N-CA-C	-5.25	101.97	110.32
1	A	318	ASP	CB-CA-C	5.25	116.25	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	LYS	CG-CD-CE	-5.24	99.25	111.30
1	A	389	SER	CA-C-O	-5.22	115.33	120.19
1	A	161	TRP	CE2-CD2-CG	-5.22	100.94	107.20
1	A	51	GLN	N-CA-C	5.21	118.20	110.48
1	A	188	TRP	CG-CD2-CE3	5.21	139.11	133.90
1	A	529	PRO	CA-C-N	5.20	125.50	119.47
1	A	529	PRO	C-N-CA	5.20	125.50	119.47
1	A	451	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	35	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	449	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	A	151	HIS	CB-CG-ND1	5.11	130.36	122.70
1	A	416	THR	N-CA-C	5.10	117.97	111.69
1	A	161	TRP	CB-CG-CD1	-5.05	119.32	126.90
1	A	402	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	A	226	ASN	OD1-CG-ND2	-5.03	117.58	122.60
1	A	119	TRP	CG-CD2-CE3	5.01	138.91	133.90
1	A	30	GLU	CA-C-N	5.00	125.53	120.38
1	A	30	GLU	C-N-CA	5.00	125.53	120.38

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	4022	0	3893	29	0
2	A	28	0	26	0	0
3	A	301	0	0	0	0
All	All	4351	0	3919	29	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 (29) 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:202:LYS:HA	1:A:235:ARG:HD2	1.64	0.79
1:A:338:GLN:HE21	1:A:451:ASN:HD21	1.32	0.76
1:A:183:ARG:HH11	1:A:218:HIS:HD1	1.41	0.68
1:A:167:ASP:H	1:A:256:ASN:HD21	1.45	0.65
1:A:182:GLN:HE22	1:A:214:SER:HB3	1.61	0.65
1:A:20:ASN:HA	1:A:106:PRO:HD3	1.83	0.60
1:A:424:ASN:HD21	1:A:495:SER:H	1.49	0.59
1:A:216:MET:HE2	1:A:239:MET:SD	2.49	0.53
1:A:168:GLU:HB3	1:A:275:LEU:HD22	1.91	0.51
1:A:37:ARG:HB2	1:A:279:ARG:HG2	1.93	0.51
1:A:130:THR:HG23	1:A:155:ASN:HD22	1.77	0.50
1:A:338:GLN:NE2	1:A:451:ASN:HD21	2.04	0.49
1:A:142:SER:HB2	1:A:147:LYS:O	2.14	0.48
1:A:338:GLN:HE21	1:A:451:ASN:ND2	2.08	0.47
1:A:389:SER:HA	1:A:390:PRO:C	2.41	0.46
1:A:77:ALA:HB1	1:A:445:LEU:HD12	1.98	0.45
1:A:25:GLY:H	1:A:101:ASN:HD22	1.65	0.45
1:A:402:GLN:OE1	1:A:405:ARG:HD2	2.17	0.44
1:A:437:LYS:HE3	1:A:504:MET:CE	2.46	0.44
1:A:253:ILE:HG13	1:A:254:TYR:N	2.32	0.44
1:A:68:THR:O	1:A:71:GLU:HG2	2.17	0.44
1:A:64:ASN:HA	1:A:65:PRO:HD3	1.85	0.43
1:A:36:LEU:HD23	1:A:36:LEU:HA	1.91	0.42
1:A:335:ILE:HG12	1:A:419:ARG:HG3	2.00	0.42
1:A:445:LEU:HB3	1:A:448:PHE:HB3	2.01	0.42
1:A:489:TRP:HA	1:A:490:PRO:HD2	1.81	0.41
1:A:386:THR:HA	1:A:394:GLY:O	2.20	0.41
1:A:335:ILE:O	1:A:433:SER:HA	2.21	0.40
1:A:455:PHE:HA	1:A:459:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	532/534 (100%)	506 (95%)	25 (5%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLY

5.3.2 Protein sidechains ⓘ

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	431/431 (100%)	418 (97%)	13 (3%)	36	41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	68	THR
1	A	109	LYS
1	A	206	PHE
1	A	253	ILE
1	A	275	LEU
1	A	318	ASP
1	A	360	GLU
1	A	405	ARG
1	A	439	LEU
1	A	465	LEU
1	A	508	LEU
1	A	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	35	ASN

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Mol	Chain	Res	Type
1	A	51	GLN
1	A	63	GLN
1	A	64	ASN
1	A	101	ASN
1	A	113	ASN
1	A	137	GLN
1	A	155	ASN
1	A	182	GLN
1	A	240	GLN
1	A	256	ASN
1	A	424	ASN
1	A	451	ASN
1	A	456	GLN
1	A	528	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 oligosaccharides 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	994	1	14,14,15	0.64	0	17,19,21	1.27	2 (11%)
2	NAG	A	990	1	14,14,15	0.67	0	17,19,21	1.08	0

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	NAG	A	994	1	-	0/6/23/26	0/1/1/1
2	NAG	A	990	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	994	NAG	C1-O5-C5	4.15	117.74	112.19
2	A	994	NAG	C6-C5-C4	-2.08	107.91	113.02

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.