



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:32 pm GMT

PDB ID : 1CRL  
Title : INSIGHTS INTO INTERFACIAL ACTIVATION FROM AN 'OPEN'  
STRUCTURE OF CANDIDA RUGOSA LIPASE  
Authors : Grochulski, P.; Cygler, M.  
Deposited on : 1993-03-02  
Resolution : 2.06 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

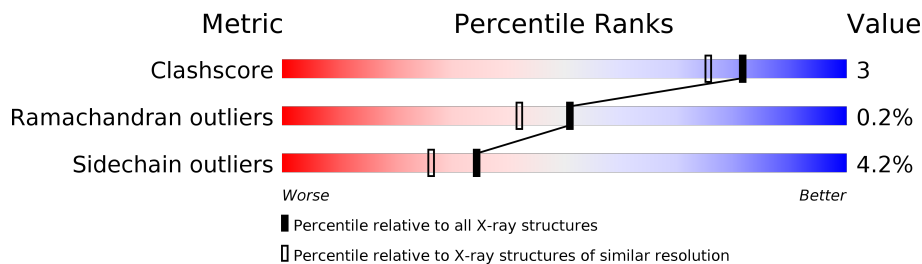
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.06 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	112137	2143 (2.08-2.04)
Ramachandran outliers	110173	2126 (2.08-2.04)
Sidechain outliers	110143	2126 (2.08-2.04)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	534	 87% 11%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4374 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 a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 4 is water.

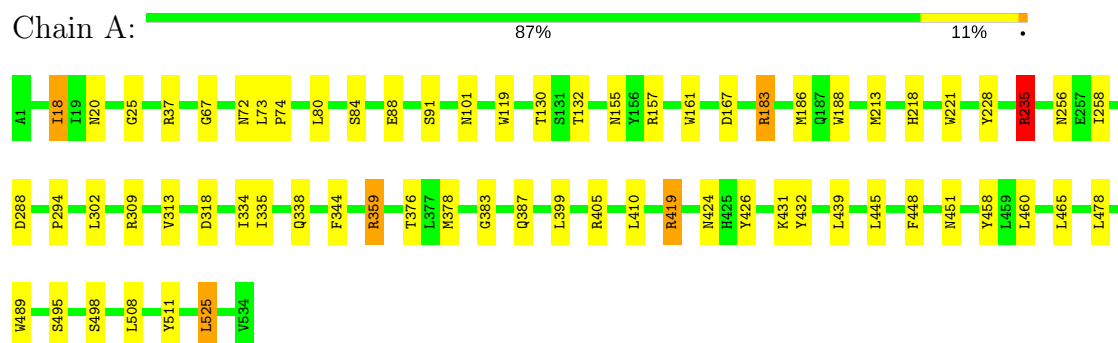
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total 310	O 310	0	0

### 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 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.

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 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.90Å 97.50Å 175.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.06	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.06)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.134 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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	0.71	0/4118	1.37	39/5601 (0.7%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	A	161	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	A	188	TRP	CD1-CG-CD2	7.78	112.52	106.30
1	A	119	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	A	188	TRP	CE2-CD2-CG	-7.32	101.45	107.30
1	A	221	TRP	CD1-CG-CD2	7.25	112.10	106.30
1	A	228	TYR	CB-CG-CD2	-7.24	116.66	121.00
1	A	489	TRP	CD1-CG-CD2	7.19	112.06	106.30
1	A	183	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	A	161	TRP	CE2-CD2-CG	-7.17	101.57	107.30
1	A	37	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	489	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	A	458	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	A	37	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	188	TRP	CB-CG-CD1	-6.34	118.75	127.00
1	A	188	TRP	CG-CD2-CE3	6.31	139.58	133.90
1	A	119	TRP	CE2-CD2-CG	-6.29	102.27	107.30
1	A	405	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	221	TRP	CE2-CD2-CG	-6.21	102.33	107.30
1	A	525	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	511	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	A	405	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	235	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	157	ARG	NE-CZ-NH1	5.80	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	MET	CG-SD-CE	-5.76	90.99	100.20
1	A	183	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	161	TRP	CG-CD2-CE3	5.53	138.87	133.90
1	A	80	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	460	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	213	MET	CG-SD-CE	-5.31	91.71	100.20
1	A	161	TRP	CG-CD1-NE1	-5.30	104.80	110.10
1	A	188	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	A	489	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	A	399	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	419	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	119	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	A	161	TRP	CB-CG-CD1	-5.02	120.48	127.00
1	A	318	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	309	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	4022	0	3893	23	0
2	A	28	0	25	1	0
3	A	14	0	13	0	0
4	A	310	0	0	4	0
All	All	4374	0	3931	24	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 3.

All (24) 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:338:GLN:HE21	1:A:451:ASN:HD21	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASN:HD21	1:A:495:SER:H	1.41	0.68
1:A:359:ARG:HE	1:A:378:MET:HE1	1.67	0.60
1:A:338:GLN:NE2	1:A:451:ASN:HD21	2.00	0.60
1:A:426:TYR:HD2	1:A:431:LYS:HD2	1.69	0.56
1:A:183:ARG:HH11	1:A:218:HIS:HD1	1.51	0.56
1:A:335:ILE:HG12	1:A:419:ARG:HG3	1.88	0.55
1:A:383:GLY:HA3	4:A:836:HOH:O	2.07	0.54
1:A:84:SER:O	1:A:88:GLU:HG2	2.08	0.54
1:A:167:ASP:H	1:A:256:ASN:HD21	1.58	0.50
1:A:235:ARG:HD3	1:A:478:LEU:HD21	1.94	0.49
2:A:990:NAG:H83	4:A:848:HOH:O	2.13	0.49
1:A:25:GLY:H	1:A:101:ASN:HD22	1.63	0.47
1:A:235:ARG:HD2	4:A:604:HOH:O	2.13	0.47
1:A:25:GLY:H	1:A:101:ASN:ND2	2.13	0.45
1:A:67:GLY:O	1:A:294:PRO:HA	2.17	0.45
1:A:445:LEU:HB3	1:A:448:PHE:HB3	1.99	0.44
1:A:73:LEU:HB3	1:A:74:PRO:HD3	1.98	0.44
1:A:338:GLN:HE21	1:A:451:ASN:ND2	2.08	0.44
1:A:334:ILE:HG12	1:A:432:TYR:HB2	1.98	0.43
1:A:424:ASN:ND2	1:A:495:SER:H	2.11	0.42
1:A:376:THR:HB	4:A:671:HOH:O	2.20	0.42
1:A:258:ILE:HD13	1:A:258:ILE:HA	1.80	0.41
1:A:130:THR:HG23	1:A:155:ASN:HD22	1.86	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%)	509 (96%)	22 (4%)	1 (0%)	51 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ILE

### 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	431/431 (100%)	413 (96%)	18 (4%)	34 26

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

Mol	Chain	Res	Type
1	A	18	ILE
1	A	20	ASN
1	A	72	ASN
1	A	91	SER
1	A	132	THR
1	A	235	ARG
1	A	288	ASP
1	A	302	LEU
1	A	313	VAL
1	A	344	PHE
1	A	359	ARG
1	A	387	GLN
1	A	410	LEU
1	A	439	LEU
1	A	465	LEU
1	A	498	SER
1	A	508	LEU
1	A	525	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	72	ASN
1	A	101	ASN

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Mol	Chain	Res	Type
1	A	155	ASN
1	A	182	GLN
1	A	240	GLN
1	A	256	ASN
1	A	330	ASN
1	A	338	GLN
1	A	424	ASN
1	A	456	GLN
1	A	500	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

2 carbohydrates 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	990	1,2	14,14,15	0.55	0	15,19,21	0.81	1 (6%)
2	NAG	A	991	2	14,14,15	0.37	0	15,19,21	1.10	1 (6%)

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	990	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	991	2	-	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	990	NAG	C1-C2-N2	-2.48	106.26	110.49
2	A	991	NAG	O3-C3-C2	2.38	114.48	109.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	990	NAG	1	0

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
3	NAG	A	994	1	14,14,15	0.60	0	15,19,21	1.53	4 (26%)

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
3	NAG	A	994	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	994	NAG	O7-C7-C8	-2.36	117.76	122.06
3	A	994	NAG	O3-C3-C4	-2.28	105.39	110.36
3	A	994	NAG	C1-O5-C5	2.67	115.84	112.17
3	A	994	NAG	C8-C7-N2	2.91	121.36	116.11

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.