



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:43 PM GMT

PDB ID : 1LPP
Title : ANALOGS OF REACTION INTERMEDIATES IDENTIFY A UNIQUE
SUBSTRATE BINDING SITE IN CANDIDA RUGOSA LIPASE
Authors : Grochulski, P.G.; Cygler, M.C.
Deposited on : 1995-01-17
Resolution : 2.18 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

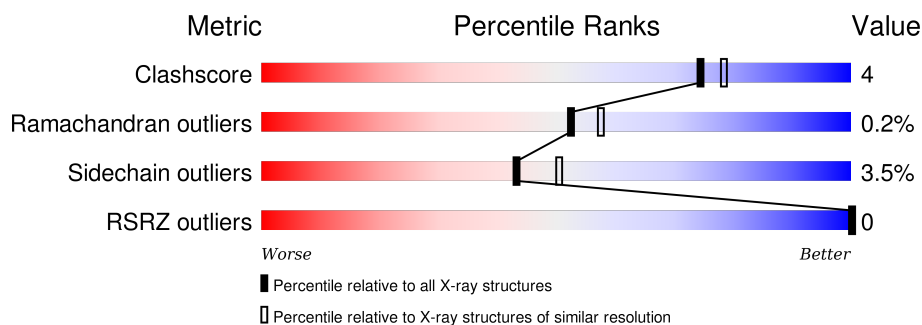
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

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	549	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	991	-	-	-	X
5	HDS	A	561	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4400 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 SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: 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		

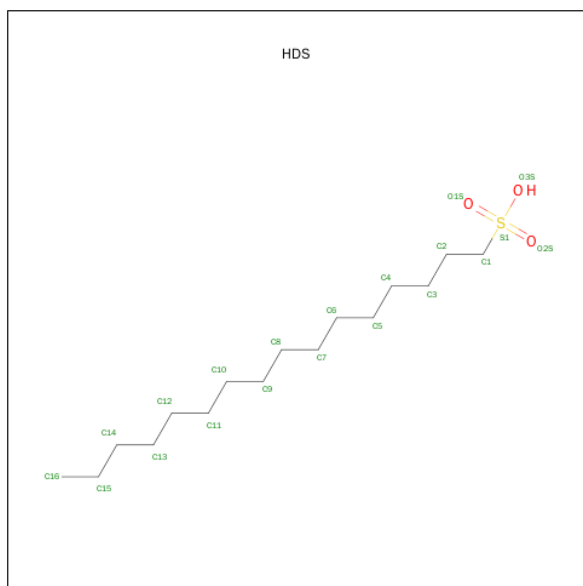
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is 1-HEXADECANOSULFONIC ACID (three-letter code: HDS) (formula: C₁₆H₃₄O₃S).




Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			19	16	2	1		
5	A	1	Total	C	O	S	0	0
			19	16	2	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	296	Total	O	0	0
			296	296		

- Molecule 1: LIPASE

Chain A:  86% 11% ••

Residue	State
RET	Gray
GLU	Gray
LEU	Gray
ALA	Gray
LEU	Gray
ALA	Gray
LEU	Gray
SER	Gray
LEU	Gray
ILE	Gray
ALA	Gray
SER	Gray
VAL	Gray
ALA	Gray
ALA	Gray
A1	Green
T13	Yellow
I20	Yellow
Q25	Yellow
F38	Yellow
K52	Yellow
S55	Yellow
S59	Yellow
L73	Yellow
P74	Yellow
K85	Yellow
B88	Yellow
S93	Yellow
M101	Yellow
T130	Yellow
M155	Yellow
S174	Yellow
Q182	Yellow
R183	Yellow
K202	Yellow
I205	Yellow
F206	Yellow
S209	Yellow
S214	Yellow
H218	Yellow
I219	Green
L220	Yellow
K231	Yellow
R235	Red
A236	Green
G237	Yellow
I238	Yellow
S241	Yellow
I253	Yellow
Y254	Yellow
D268	Yellow
D318	Red
K327	Yellow
Y328	Yellow
I334	Yellow
Q338	Yellow
R359	Yellow
K363	Yellow
D371	Yellow
G383	Yellow
D384	Yellow
S389	Yellow
P390	Yellow
L410	Yellow
M424	Yellow
Y432	Yellow
K437	Yellow
D438	Green
L439	Yellow
H449	Yellow
S450	Yellow
M451	Yellow
S462	Yellow
L465	Red
I466	Yellow
M469	Yellow
L486	Green
S495	Yellow
M504	Yellow
I505	Yellow
L508	Yellow
L525	Yellow
Y534	Green

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	65.10Å 97.40Å 176.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.18 54.12 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.18) 86.3 (54.12-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.05Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.137 , (Not available) 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 101.3	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 30888 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4400	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: CA, HDS, 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	0.46	0/4118	0.71	1/5601 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	318	ASP	CB-CG-OD1	5.29	123.07	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3892	32	0
2	A	14	0	13	0	0
3	A	28	0	25	0	0
4	A	2	0	0	0	0
5	A	38	0	66	0	0
6	A	296	0	0	2	0
All	All	4400	0	3996	32	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.

The worst 5 of 32 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:424:ASN:HD21	1:A:495:SER:H	1.23	0.84
1:A:338:GLN:HE21	1:A:451:ASN:HD21	1.38	0.70
1:A:183:ARG:HH11	1:A:218:HIS:HD1	1.39	0.66
1:A:182:GLN:HE22	1:A:214:SER:HB3	1.63	0.62
1:A:383:GLY:HA3	6:A:889:HOH:O	2.01	0.60

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	532/549 (97%)	510 (96%)	21 (4%)	1 (0%)	52 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	ASP

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	431/441 (98%)	416 (96%)	15 (4%)	43 50

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	ASP
1	A	318	ASP
1	A	465	LEU
1	A	235	ARG
1	A	439	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	240	GLN
1	A	330	ASN
1	A	456	GLN
1	A	187	GLN
1	A	424	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	$\# Z > 2$
3	NAG	A	992	1,3	14,14,15	0.89	0	15,19,21	1.02	0
3	NAG	A	994	3	14,14,15	0.84	0	15,19,21	1.34	3 (20%)

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	992	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	994	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	994	NAG	C3-C4-C5	-2.21	106.35	110.20
3	A	994	NAG	O3-C3-C4	-2.19	105.40	110.34
3	A	994	NAG	C4-C3-C2	2.23	114.70	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
5	HDS	A	560	-	16,18,19	0.27	0	16,18,21	0.74	0
5	HDS	A	561	-	16,18,19	0.37	0	16,18,21	0.91	1 (6%)
2	NAG	A	991	1	14,14,15	1.19	2 (14%)	15,19,21	1.87	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
5	HDS	A	560	-	-	0/15/16/17	0/0/0/0
5	HDS	A	561	-	-	0/15/16/17	0/0/0/0
2	NAG	A	991	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	991	NAG	C6-C5	2.06	1.59	1.51
2	A	991	NAG	C3-C2	2.54	1.58	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	991	NAG	O3-C3-C4	-2.36	105.02	110.34
2	A	991	NAG	O7-C7-C8	-2.29	117.86	122.06
2	A	991	NAG	O3-C3-C2	2.59	114.25	109.11
5	A	561	HDS	O1S-S1-C1	3.01	111.97	105.54
2	A	991	NAG	C1-O5-C5	4.97	118.55	112.25

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 [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	534/549 (97%)	-0.62	0 100 100	9, 17, 35, 52	0

There are no RSRZ outliers to report.

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](#)

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(Å ²)	Q<0.9
3	NAG	A	994	14/15	0.93	0.13	-	16,23,32,38	14
3	NAG	A	992	14/15	0.96	0.08	-	21,24,33,36	0

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
5	HDS	A	561	19/20	0.97	0.19	5.63	17,43,48,48	10
2	NAG	A	991	14/15	0.91	0.10	2.06	26,31,38,44	0
5	HDS	A	560	19/20	0.99	0.09	0.43	13,19,26,28	0
4	CA	A	589	1/1	0.97	0.08	-0.47	38,38,38,38	0
4	CA	A	590	1/1	0.99	0.29	-	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.