



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 02:02 PM GMT

PDB ID : 3NGM
Title : Crystal structure of lipase from *Gibberella zeae*
Authors : Lou, Z.Y.; Li, M.; Sun, Y.N.; Liu, Y.; Liu, Z.; Rao, Z.H.
Deposited on : 2010-06-12
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

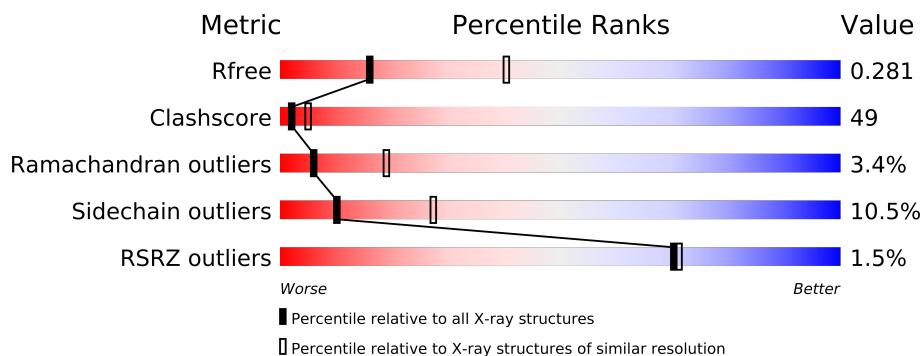
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	319	
1	B	319	
1	C	319	
1	D	319	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9010 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Extracellular lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2198	1369	384	435	10			
1	B	297	Total	C	N	O	S	0	0	0
			2198	1369	384	435	10			
1	C	297	Total	C	N	O	S	0	0	0
			2198	1369	384	435	10			
1	D	297	Total	C	N	O	S	0	0	0
			2198	1369	384	435	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	ILE	VAL	CONFLICT	UNP Q6WER3
A	316	SER	ARG	CONFLICT	UNP Q6WER3
A	317	ARG	PRO	CONFLICT	UNP Q6WER3
A	318	SER	LEU	CONFLICT	UNP Q6WER3
A	319	SER	ILE	CONFLICT	UNP Q6WER3
B	159	ILE	VAL	CONFLICT	UNP Q6WER3
B	316	SER	ARG	CONFLICT	UNP Q6WER3
B	317	ARG	PRO	CONFLICT	UNP Q6WER3
B	318	SER	LEU	CONFLICT	UNP Q6WER3
B	319	SER	ILE	CONFLICT	UNP Q6WER3
C	159	ILE	VAL	CONFLICT	UNP Q6WER3
C	316	SER	ARG	CONFLICT	UNP Q6WER3
C	317	ARG	PRO	CONFLICT	UNP Q6WER3
C	318	SER	LEU	CONFLICT	UNP Q6WER3
C	319	SER	ILE	CONFLICT	UNP Q6WER3
D	159	ILE	VAL	CONFLICT	UNP Q6WER3
D	316	SER	ARG	CONFLICT	UNP Q6WER3
D	317	ARG	PRO	CONFLICT	UNP Q6WER3
D	318	SER	LEU	CONFLICT	UNP Q6WER3
D	319	SER	ILE	CONFLICT	UNP Q6WER3

- Molecule 2 is water.

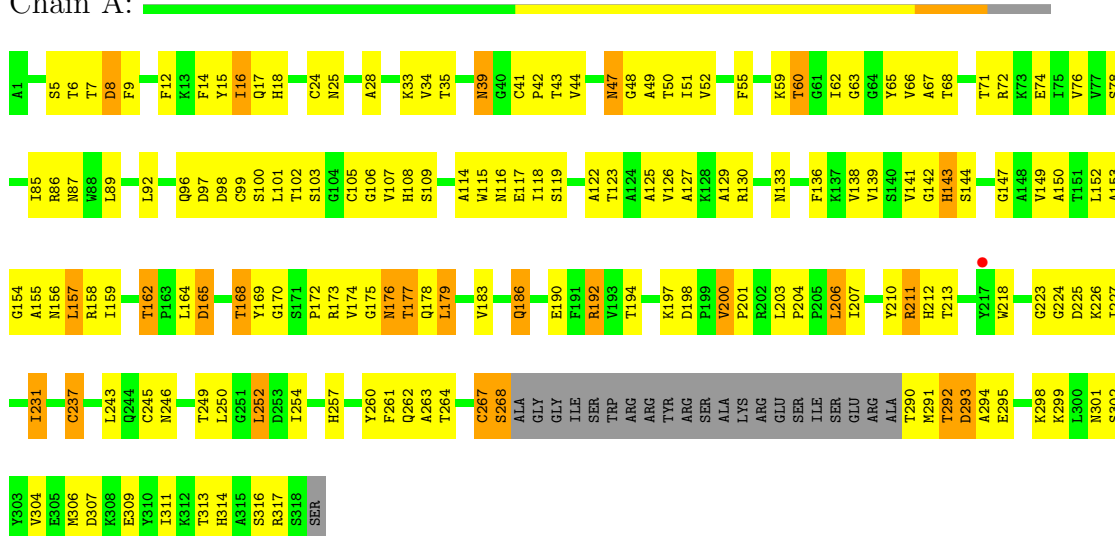
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	46	Total 46	O 46	0	0
2	B	53	Total 53	O 53	0	0
2	C	67	Total 67	O 67	0	0
2	D	52	Total 52	O 52	0	0

3 Residue-property plots

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 ($RSRZ > 2$). 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.

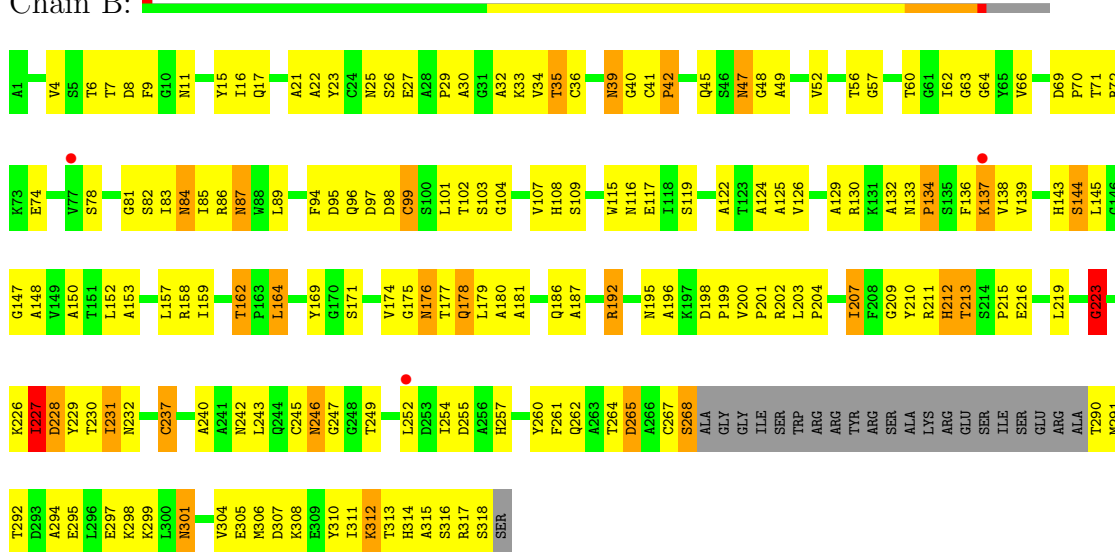
• Molecule 1: Extracellular lipase

Chain A:



• Molecule 1: Extracellular lipase

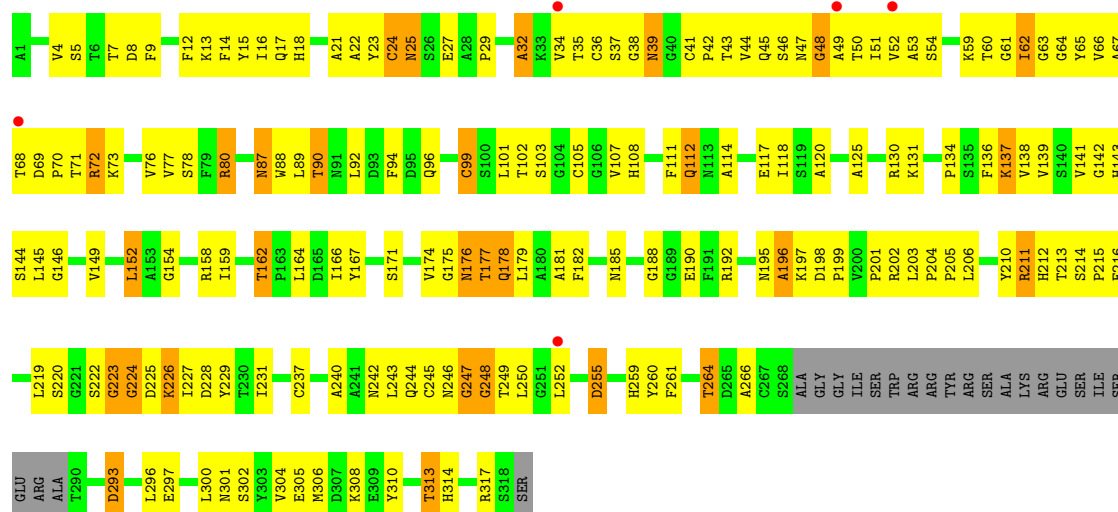
Chain B:



• Molecule 1: Extracellular lipase

V304	C237	A153	V76	A1
E305		G154	V77	V2
M306	Q244		I83	V4
	Q245	L157		S5
Y310	T249	R158	R86	T6
I311		I159	N87	T7
T312			W88	D8
H313	L252	T162	L89	
H314	D253	P163	T90	K13
S315	E254	G163		F14
S316	D255	L164		Y15
S317	A256	Y169	D85	I16
S318	H257		D97	Q17
SER	L258	R173	D98	
	H259	V174	C99	A21
	Y260	G175	S100	A22
	F261	N176	L101	V23
	Q262	T177	I102	C24
	A263	Q178	S103	N25
	T264	L179	G104	S26
	D265	A180	C105	E27
	A266		G106	A28
	C267	Q186	V107	P29
	S268		H108	
	ALA	E190	G110	T35
	GLY		S109	C36
	GLY	V193	F111	
	I1E		Q112	N39
	SER	A196	N113	G40
	TRP	K197	A114	C41
	ARG	D198	W115	P42
	ARG	P199	N116	T43
	TVR	V200	E117	V44
	ARG	P201	I118	O45
	SER	R202	S119	S46
	ALA	L203		N47
	LYS	P204	A122	G48
	ARG		T123	A49
	GLU	R211	A124	T50
	GLU	H212	A125	T51
	I1E			V52
	SER	T217	A129	
	GLU	W218	R130	F55
	ARG	L219	K131	
	ALA	S220	A132	K59
	T290	G221	N133	T60
	N291	G222		G61
	T292	G223	F136	162
	D293	G224	K137	
	A294	D225	V138	V65
	E295	K226	V139	
	L296	I227		V66
	E297	D228		
	K298	Y229	H143	D69
	K299	T230	S144	P70
	L300	I231	L145	T71
	N301	N232	G146	R72
	S302	D233	G147	K73
	S303	V234		E74
			A150	T75

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.42Å 91.00Å 195.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 45.50 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 82.7 (45.50-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.25 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.264 0.232 , 0.281	Depositor DCC
R_{free} test set	1422 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 15.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34055 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9010	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.41	1/2243 (0.0%)	0.73	4/3047 (0.1%)
1	B	0.47	1/2243 (0.0%)	0.74	3/3047 (0.1%)
1	C	0.39	0/2243	0.67	0/3047
1	D	0.37	0/2243	0.65	0/3047
All	All	0.41	2/8972 (0.0%)	0.70	7/12188 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	223	GLY	C-O	-6.07	1.14	1.23
1	A	268	SER	N-CA	-5.28	1.35	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	GLY	CA-C-O	-15.63	92.46	120.60
1	B	268	SER	CA-CB-OG	-8.38	88.56	111.20
1	A	224	GLY	N-CA-C	-6.55	96.72	113.10
1	A	267	CYS	C-N-CA	6.27	137.38	121.70
1	A	267	CYS	N-CA-C	6.14	127.58	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	CYS	Peptide
1	B	223	GLY	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2198	0	2113	178	0
1	B	2198	0	2111	238	0
1	C	2198	0	2111	216	0
1	D	2198	0	2111	230	0
2	A	46	0	0	33	0
2	B	53	0	0	47	0
2	C	67	0	0	55	0
2	D	52	0	0	43	0
All	All	9010	0	8446	844	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 49.

The worst 5 of 844 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:237:CYS:HB3	2:B:321:HOH:O	1.23	1.29
1:C:237:CYS:HB3	2:C:336:HOH:O	1.41	1.20
1:B:26:SER:HB3	2:B:320:HOH:O	1.41	1.15
1:C:70:PRO:HG2	2:C:330:HOH:O	1.43	1.15
1:C:102:THR:HA	2:C:332:HOH:O	1.48	1.09

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	293/319 (92%)	250 (85%)	39 (13%)	4 (1%)	16	49
1	B	293/319 (92%)	233 (80%)	50 (17%)	10 (3%)	6	19
1	C	293/319 (92%)	255 (87%)	29 (10%)	9 (3%)	7	21
1	D	293/319 (92%)	235 (80%)	41 (14%)	17 (6%)	3	7
All	All	1172/1276 (92%)	973 (83%)	159 (14%)	40 (3%)	6	19

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	84	ASN
1	B	228	ASP
1	C	224	GLY
1	D	25	ASN
1	D	62	ILE

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	231/248 (93%)	202 (87%)	29 (13%)	7	19
1	B	231/248 (93%)	206 (89%)	25 (11%)	9	26
1	C	231/248 (93%)	208 (90%)	23 (10%)	11	30
1	D	231/248 (93%)	211 (91%)	20 (9%)	15	39
All	All	924/992 (93%)	827 (90%)	97 (10%)	10	27

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	212	HIS
1	C	6	THR
1	D	178	GLN
1	B	215	PRO
1	B	267	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	178	GLN
1	C	25	ASN
1	D	112	GLN
1	B	186	GLN
1	B	262	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	297/319 (93%)	-0.12	1 (0%) 91 93	10, 34, 51, 68	0
1	B	297/319 (93%)	0.05	3 (1%) 79 79	19, 42, 62, 75	0
1	C	297/319 (93%)	0.08	9 (3%) 48 49	22, 38, 56, 65	0
1	D	297/319 (93%)	0.19	5 (1%) 67 68	18, 42, 66, 85	0
All	All	1188/1276 (93%)	0.05	18 (1%) 70 71	10, 39, 61, 85	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	52	VAL	3.1
1	C	217	TYR	2.7
1	D	34	VAL	2.5
1	B	77	VAL	2.4
1	C	66	VAL	2.4

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.