Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:16 PM GMT

PDB ID	:	4C1B
Title	:	Esterase domain of the ZfL2-1 ORF1 protein from the zebrafish ZfL2-1 retrotransposon
Authors	:	Schneider, A.M.; Weichenrieder, O.
Deposited on	:	2013-08-11
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

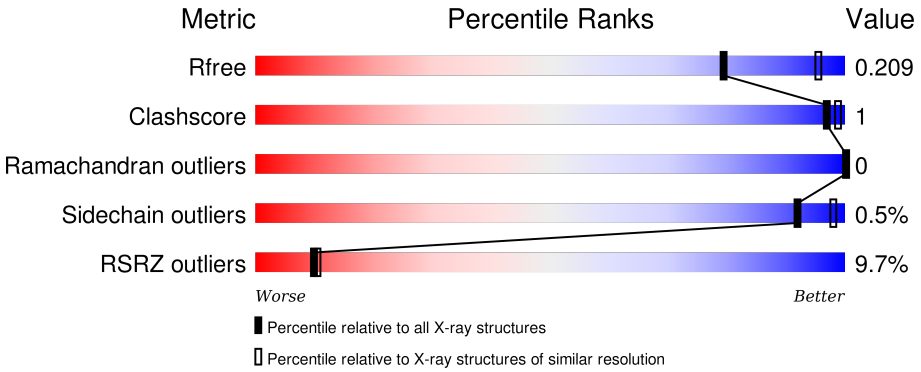
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

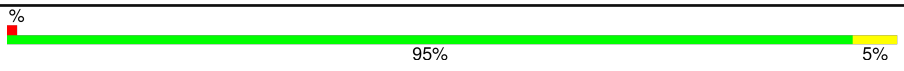
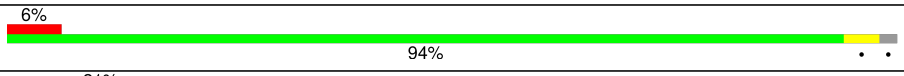
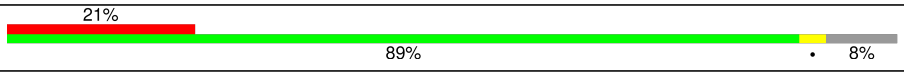
The reported resolution of this entry is 2.50 Å.

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	171	
1	B	171	
1	C	171	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8108 atoms, of which 4083 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 ORF1-ENCODED PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	171	Total	C	H	N	O	S	0	0	0
			2740	853	1392	255	237	3			
1	B	168	Total	C	H	N	O	S	0	0	0
			2709	843	1377	252	234	3			
1	C	158	Total	C	H	N	O	S	0	0	0
			2585	807	1314	241	220	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	GLY	-	EXPRESSION TAG	UNP Q3LG57
A	133	PRO	-	EXPRESSION TAG	UNP Q3LG57
A	134	ALA	-	EXPRESSION TAG	UNP Q3LG57
A	135	MET	-	EXPRESSION TAG	UNP Q3LG57
B	132	GLY	-	EXPRESSION TAG	UNP Q3LG57
B	133	PRO	-	EXPRESSION TAG	UNP Q3LG57
B	134	ALA	-	EXPRESSION TAG	UNP Q3LG57
B	135	MET	-	EXPRESSION TAG	UNP Q3LG57
C	132	GLY	-	EXPRESSION TAG	UNP Q3LG57
C	133	PRO	-	EXPRESSION TAG	UNP Q3LG57
C	134	ALA	-	EXPRESSION TAG	UNP Q3LG57
C	135	MET	-	EXPRESSION TAG	UNP Q3LG57

- Molecule 2 is water.

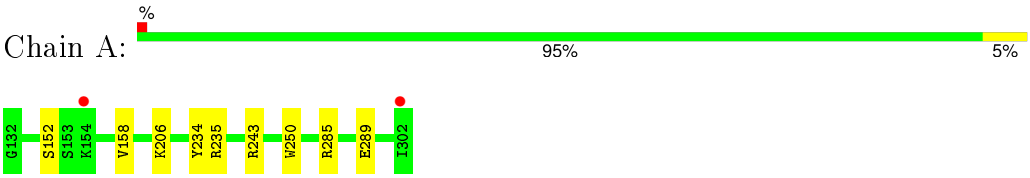
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	25	Total	O	0	0
			25	25		
2	C	11	Total	O	0	0
			11	11		

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 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.

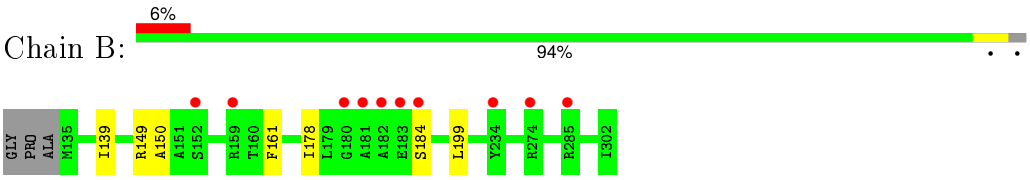
- Molecule 1: ORF1-ENCODED PROTEIN

Chain A:



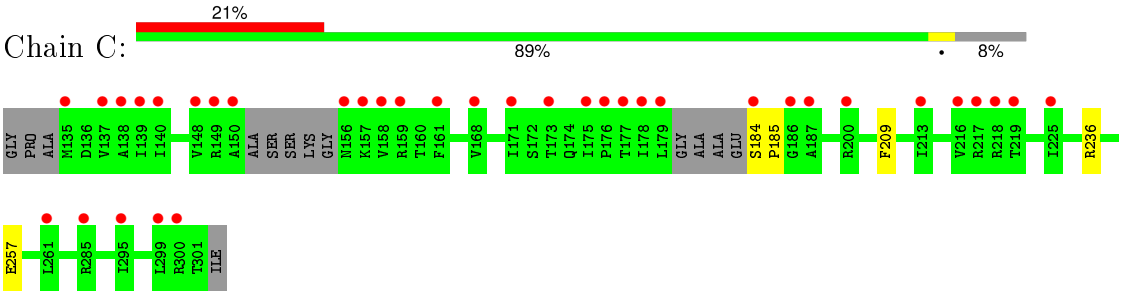
- Molecule 1: ORF1-ENCODED PROTEIN

Chain B:



- Molecule 1: ORF1-ENCODED PROTEIN

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	111.26Å 111.26Å 115.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.71 – 2.50 45.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.71-2.50) 100.0 (45.71-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.167 , 0.210 0.162 , 0.209	Depositor DCC
R_{free} test set	1243 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 46.8	EDS
Estimated twinning fraction	0.006 for l,-k,h 0.016 for -l,-k,-h 0.013 for -h,-l,-k 0.004 for -h,l,k 0.034 for -h,k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 24350 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8108	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.53	0/1376	0.65	0/1865
1	B	0.55	0/1359	0.64	0/1841
1	C	0.49	0/1296	0.63	1/1754 (0.1%)
All	All	0.53	0/4031	0.64	1/5460 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	236	ARG	NE-CZ-NH2	-6.62	116.99	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	1348	1392	1389	7	0
1	B	1332	1377	1374	3	1
1	C	1271	1314	1311	1	1
2	A	38	0	0	0	0
2	B	25	0	0	0	0
2	C	11	0	0	0	0
All	All	4025	4083	4074	10	1

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 1.

All (10) 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:206:LYS:HG2	1:A:250:TRP:CE2	2.40	0.57
1:A:206:LYS:HG2	1:A:250:TRP:CZ2	2.41	0.55
1:C:184:SER:N	1:C:185:PRO:CD	2.71	0.54
1:B:139:ILE:HD11	1:B:150:ALA:HB2	1.91	0.52
1:A:243:ARG:NH2	1:B:199:LEU:O	2.47	0.47
1:A:152:SER:HB3	1:A:158:VAL:HG23	1.98	0.45
1:B:161:PHE:CD2	1:B:178:ILE:HD12	2.54	0.42
1:A:234:TYR:CE2	1:A:235:ARG:HG3	2.54	0.42
1:A:285:ARG:O	1:A:289:GLU:HG3	2.21	0.41
1:A:285:ARG:HD3	1:A:285:ARG:HA	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ARG:NH2	1:C:257:GLU:O[8_555]	2.08	0.12

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	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
1	B	166/171 (97%)	160 (96%)	6 (4%)	0	100	100
1	C	152/171 (89%)	145 (95%)	7 (5%)	0	100	100
All	All	487/513 (95%)	468 (96%)	19 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	146/146 (100%)	146 (100%)	0	100	100
1	B	145/146 (99%)	144 (99%)	1 (1%)	88	97
1	C	140/146 (96%)	139 (99%)	1 (1%)	88	97
All	All	431/438 (98%)	429 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	184	SER
1	C	209	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

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, 95^{th} 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	171/171 (100%)	0.38	2 (1%) 81 83	26, 41, 72, 110	0
1	B	168/171 (98%)	0.51	10 (5%) 25 28	23, 41, 97, 132	0
1	C	158/171 (92%)	1.20	36 (22%) 1 1	30, 62, 98, 133	0
All	All	497/513 (96%)	0.69	48 (9%) 10 10	23, 46, 95, 133	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	MET	11.4
1	C	158	VAL	6.4
1	C	157	LYS	6.3
1	C	137	VAL	6.2
1	C	156	ASN	6.1
1	B	182	ALA	5.9
1	C	159	ARG	5.4
1	B	183	GLU	5.1
1	C	178	ILE	4.7
1	A	154	LYS	4.3
1	C	175	ILE	3.8
1	C	187	ALA	3.7
1	C	285	ARG	3.7
1	C	179	LEU	3.6
1	B	180	GLY	3.6
1	C	219	THR	3.5
1	C	176	PRO	3.4
1	C	177	THR	3.3
1	B	152	SER	3.3
1	C	161	PHE	3.3
1	C	138	ALA	3.2
1	C	225	ILE	3.1
1	C	216	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	218	ARG	3.0
1	C	300	ARG	2.9
1	C	295	ILE	2.9
1	B	181	ALA	2.8
1	C	184	SER	2.8
1	C	139	ILE	2.7
1	C	140	ILE	2.7
1	B	274	ARG	2.5
1	C	213	ILE	2.5
1	B	184	SER	2.4
1	B	234	TYR	2.3
1	B	285	ARG	2.3
1	C	150	ALA	2.3
1	A	302	ILE	2.3
1	C	261	LEU	2.3
1	C	186	GLY	2.2
1	C	149	ARG	2.2
1	B	159	ARG	2.2
1	C	299	LEU	2.1
1	C	200	ARG	2.1
1	C	148	VAL	2.1
1	C	168	VAL	2.1
1	C	171	ILE	2.1
1	C	217	ARG	2.1
1	C	173	THR	2.1

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 carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.