Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2017 – 07:31 PM EST

PDB ID	:	5HY2
Title	:	Structure-function analysis of functionally diverse members of the cyclic amide hydrolase family of Toblerone fold enzymes
Authors	:	Peat, T.S.; Balotra, S.; Wilding, M.; Newman, J.; Scott, C.
Deposited on	:	2016-02-01
Resolution	:	2.60 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:

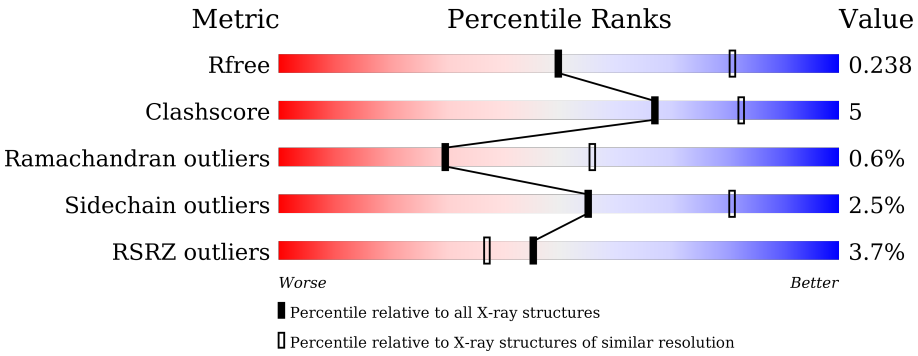
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	410	3% 72% 10% • 18%
1	B	410	3% 71% 10% 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4783 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 Ring-opening amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	1	0
			2395	1493	430	463	9			
1	B	330	Total	C	N	O	S	0	2	0
			2357	1467	429	452	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E3JD18
A	-18	GLY	-	expression tag	UNP E3JD18
A	-17	SER	-	expression tag	UNP E3JD18
A	-16	SER	-	expression tag	UNP E3JD18
A	-15	HIS	-	expression tag	UNP E3JD18
A	-14	HIS	-	expression tag	UNP E3JD18
A	-13	HIS	-	expression tag	UNP E3JD18
A	-12	HIS	-	expression tag	UNP E3JD18
A	-11	HIS	-	expression tag	UNP E3JD18
A	-10	HIS	-	expression tag	UNP E3JD18
A	-9	SER	-	expression tag	UNP E3JD18
A	-8	SER	-	expression tag	UNP E3JD18
A	-7	GLY	-	expression tag	UNP E3JD18
A	-6	LEU	-	expression tag	UNP E3JD18
A	-5	VAL	-	expression tag	UNP E3JD18
A	-4	PRO	-	expression tag	UNP E3JD18
A	-3	ARG	-	expression tag	UNP E3JD18
A	-2	GLY	-	expression tag	UNP E3JD18
A	-1	SER	-	expression tag	UNP E3JD18
A	0	HIS	-	expression tag	UNP E3JD18
B	-19	MET	-	initiating methionine	UNP E3JD18
B	-18	GLY	-	expression tag	UNP E3JD18
B	-17	SER	-	expression tag	UNP E3JD18
B	-16	SER	-	expression tag	UNP E3JD18
B	-15	HIS	-	expression tag	UNP E3JD18

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP E3JD18
B	-13	HIS	-	expression tag	UNP E3JD18
B	-12	HIS	-	expression tag	UNP E3JD18
B	-11	HIS	-	expression tag	UNP E3JD18
B	-10	HIS	-	expression tag	UNP E3JD18
B	-9	SER	-	expression tag	UNP E3JD18
B	-8	SER	-	expression tag	UNP E3JD18
B	-7	GLY	-	expression tag	UNP E3JD18
B	-6	LEU	-	expression tag	UNP E3JD18
B	-5	VAL	-	expression tag	UNP E3JD18
B	-4	PRO	-	expression tag	UNP E3JD18
B	-3	ARG	-	expression tag	UNP E3JD18
B	-2	GLY	-	expression tag	UNP E3JD18
B	-1	SER	-	expression tag	UNP E3JD18
B	0	HIS	-	expression tag	UNP E3JD18

- Molecule 2 is water.

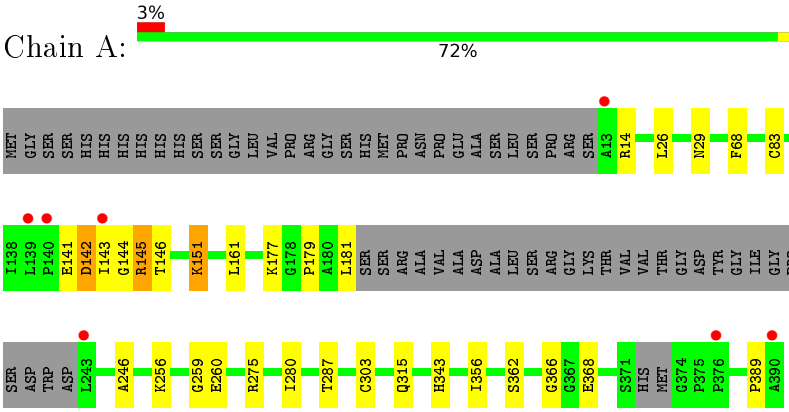
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	18	Total O 18 18	0	0
2	B	13	Total O 13 13	0	0

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 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.

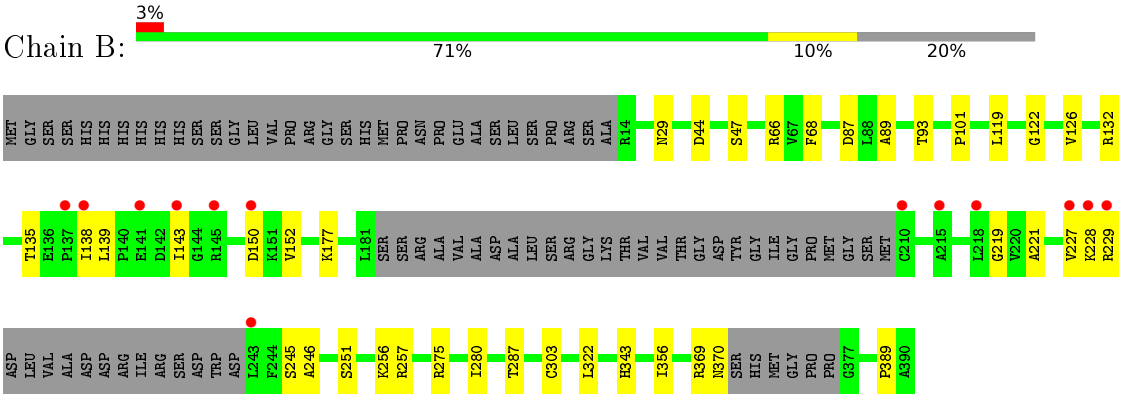
- Molecule 1: Ring-opening amidohydrolase

Chain A:



- Molecule 1: Ring-opening amidohydrolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.30Å 72.75Å 133.05Å 90.00° 92.22° 90.00°	Depositor
Resolution (Å)	41.50 – 2.60 40.64 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.50-2.60) 99.9 (40.64-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.202 , 0.241 0.205 , 0.238	Depositor DCC
R_{free} test set	1354 reflections (5.17%)	DCC
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4783	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0/2435	0.63	1/3321 (0.0%)
1	B	0.51	0/2395	0.62	2/3264 (0.1%)
All	All	0.52	0/4830	0.63	3/6585 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	LEU	CB-CG-CD1	5.72	120.73	111.00
1	B	66[A]	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	66[B]	ARG	NE-CZ-NH1	5.37	122.98	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	2395	0	2374	25	0
1	B	2357	0	2333	20	0
2	A	18	0	0	0	0
2	B	13	0	0	0	0
All	All	4783	0	4707	45	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 5.

All (45) 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:137:PRO:O	1:A:151:LYS:NZ	1.98	0.96
1:B:177:LYS:HD3	1:B:251:SER:HB2	1.53	0.90
1:B:93:THR:OG1	1:B:132:ARG:NH1	2.15	0.80
1:A:144:GLY:HA3	1:A:211:TRP:HD1	1.51	0.76
1:A:144:GLY:HA3	1:A:211:TRP:CD1	2.30	0.67
1:B:287:THR:HB	1:B:356:ILE:HD11	1.83	0.60
1:A:287:THR:HB	1:A:356:ILE:HD11	1.86	0.57
1:A:136:GLU:HB2	1:A:151:LYS:CD	2.34	0.57
1:A:179:PRO:HB3	1:A:256:LYS:O	2.08	0.53
1:A:126:VAL:O	1:A:275:ARG:HD3	2.10	0.52
1:B:138:ILE:HG22	1:B:257:ARG:O	2.11	0.51
1:B:228:LYS:O	1:B:229:ARG:C	2.47	0.50
1:A:142:ASP:N	1:A:142:ASP:OD1	2.42	0.50
1:B:177:LYS:HD3	1:B:251:SER:CB	2.33	0.50
1:A:101:PRO:HD2	1:A:104:ILE:HD12	1.95	0.49
1:A:366:GLY:HA2	1:A:368:GLU:OE1	2.12	0.48
1:A:94:VAL:O	1:A:177:LYS:NZ	2.39	0.48
1:B:152:VAL:HG23	1:B:219:GLY:HA3	1.96	0.47
1:A:246:ALA:HB1	1:A:280:ILE:HD11	1.97	0.46
1:A:122:GLY:O	1:A:389:PRO:HA	2.16	0.46
1:B:126:VAL:O	1:B:275:ARG:HD3	2.15	0.46
1:A:136:GLU:HB2	1:A:151:LYS:HD3	1.96	0.46
1:B:87:ASP:C	1:B:89:ALA:H	2.18	0.46
1:A:136:GLU:HB2	1:A:151:LYS:HD2	1.97	0.46
1:A:83:CYS:HB2	1:A:87:ASP:OD1	2.16	0.45
1:B:229:ARG:HD2	1:B:229:ARG:H	1.81	0.45
1:A:135:THR:OG1	1:A:259:GLY:N	2.47	0.45
1:A:141:GLU:OE1	1:A:141:GLU:N	2.47	0.45
1:A:145:ARG:CG	1:A:145:ARG:HH11	2.30	0.45
1:A:315:GLN:OE1	1:A:362:SER:HA	2.18	0.44
1:A:29:ASN:HB3	1:A:68:PHE:CZ	2.53	0.43
1:B:101:PRO:HB3	1:B:343:HIS:NE2	2.33	0.43
1:A:141:GLU:H	1:A:141:GLU:CD	2.22	0.43
1:B:246:ALA:HB1	1:B:280:ILE:HD11	2.00	0.43
1:B:221:ALA:HB2	1:B:245:SER:HB2	2.00	0.42
1:B:138:ILE:HD12	1:B:139:LEU:H	1.84	0.42
1:A:101:PRO:HG3	1:A:343:HIS:CE1	2.54	0.42
1:B:322:LEU:O	1:B:370:ASN:HB2	2.20	0.42
1:B:29:ASN:HB3	1:B:68:PHE:CZ	2.55	0.41
1:B:44:ASP:O	1:B:47:SER:OG	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.96	0.41
1:B:122:GLY:O	1:B:389:PRO:HA	2.21	0.41
1:B:135:THR:HG21	1:B:152:VAL:HG12	2.03	0.41
1:A:87:ASP:C	1:A:89:ALA:H	2.24	0.40
1:B:101:PRO:HB3	1:B:343:HIS:CE1	2.56	0.40

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	330/410 (80%)	318 (96%)	10 (3%)	2 (1%)	30	56
1	B	324/410 (79%)	312 (96%)	10 (3%)	2 (1%)	30	56
All	All	654/820 (80%)	630 (96%)	20 (3%)	4 (1%)	30	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	THR
1	B	256	LYS
1	A	143	ILE
1	B	143	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	246/310 (79%)	239 (97%)	7 (3%)	51 78
1	B	240/310 (77%)	235 (98%)	5 (2%)	61 85
All	All	486/620 (78%)	474 (98%)	12 (2%)	55 81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	142	ASP
1	A	145	ARG
1	A	151	LYS
1	A	161	LEU
1	A	260	GLU
1	A	303	CYS
1	B	119	LEU
1	B	150	ASP
1	B	227	VAL
1	B	303	CYS
1	B	369	ARG

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

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, 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	337/410 (82%)	-0.38	12 (3%)	46	38	26, 43, 101, 144	0
1	B	330/410 (80%)	-0.30	13 (3%)	43	35	28, 49, 114, 136	0
All	All	667/820 (81%)	-0.34	25 (3%)	45	37	26, 46, 110, 144	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	TRP	4.0
1	B	229	ARG	3.8
1	B	138	ILE	3.8
1	A	229	ARG	3.6
1	B	141	GLU	3.4
1	A	243	LEU	3.4
1	A	210	CYS	3.2
1	A	13	ALA	3.0
1	B	145	ARG	2.7
1	A	230	ASP	2.7
1	A	390	ALA	2.7
1	B	137	PRO	2.5
1	B	150	ASP	2.5
1	A	376	PRO	2.5
1	B	228	LYS	2.5
1	B	215	ALA	2.5
1	A	231	LEU	2.2
1	B	243	LEU	2.2
1	B	227	VAL	2.1
1	B	143	ILE	2.1
1	B	218	LEU	2.1
1	A	140	PRO	2.1
1	B	210	CYS	2.1
1	A	139	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	143	ILE	2.0

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.