



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 06:51 PM GMT

PDB ID : 2FW2
Title : Catalytic domain of CDY
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Deposited on : 2006-01-31
Resolution : 2.20 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>

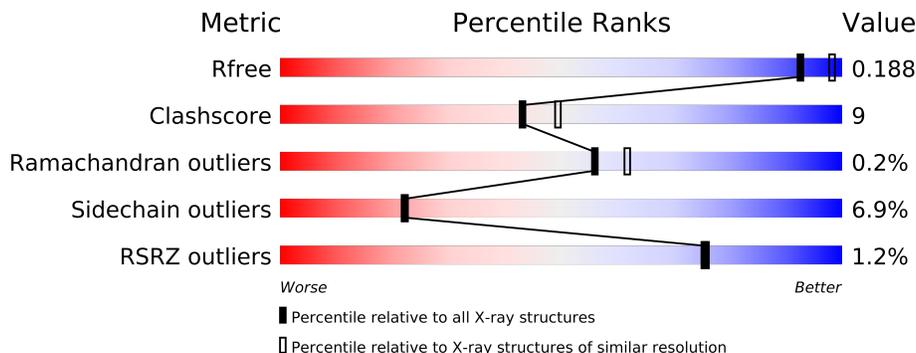
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	260	
1	B	260	
1	C	260	
1	D	260	
1	E	260	
1	F	260	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12641 atoms, of which 0 are hydrogen and 0 are deuterium.

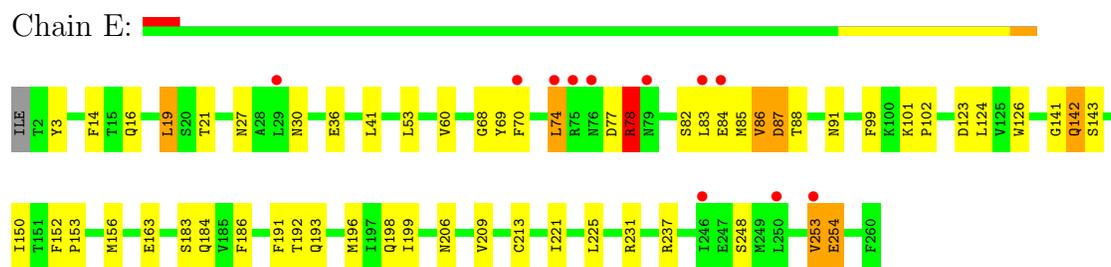
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Testis-specific chromodomain protein Y 2.

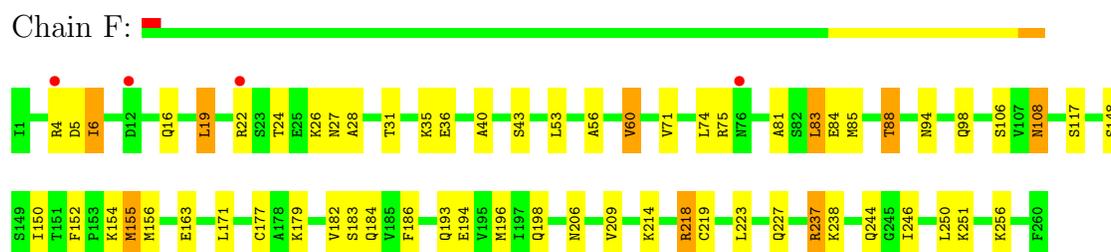
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	258	2018	1281	338	384	15	0	2	0
1	B	255	1975	1254	332	374	15	0	0	0
1	C	256	1993	1265	335	378	15	0	1	0
1	D	257	1989	1263	335	376	15	0	0	0
1	E	259	1993	1266	335	377	15	0	0	0
1	F	260	2009	1275	338	381	15	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	152	Total 152	O 152	0	0
2	B	123	Total 123	O 123	0	0
2	C	134	Total 134	O 134	0	0
2	D	101	Total 101	O 101	0	0
2	E	70	Total 70	O 70	0	0
2	F	84	Total 84	O 84	0	0



- Molecule 1: Testis-specific chromodomain protein Y 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.45Å 133.58Å 82.33Å 90.00° 117.56° 90.00°	Depositor
Resolution (Å)	72.93 – 2.20 48.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (72.93-2.20) 99.3 (48.75-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.253 0.187 , 0.188	Depositor DCC
R_{free} test set	3925 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.7	EDS
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 77766 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12641	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.68	1/2049 (0.0%)	0.75	2/2765 (0.1%)
1	B	0.59	1/2005 (0.0%)	0.72	1/2708 (0.0%)
1	C	0.67	1/2023 (0.0%)	0.69	0/2731
1	D	0.64	2/2019 (0.1%)	0.66	0/2726
1	E	0.68	3/2024 (0.1%)	0.72	2/2733 (0.1%)
1	F	0.56	0/2040	0.65	0/2754
All	All	0.64	8/12160 (0.1%)	0.70	5/16417 (0.0%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	78	ARG	CZ-NH2	14.43	1.51	1.33
1	E	78	ARG	CZ-NH1	7.91	1.43	1.33
1	C	219	CYS	CB-SG	-7.59	1.69	1.82
1	A	219	CYS	CB-SG	-6.61	1.71	1.82
1	D	213	CYS	CB-SG	-6.07	1.72	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	78	ARG	NE-CZ-NH1	-15.78	112.41	120.30
1	B	51	LEU	CA-CB-CG	6.37	129.95	115.30
1	E	78	ARG	NH1-CZ-NH2	5.37	125.31	119.40
1	A	171	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	74	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2018	0	2037	51	0
1	B	1975	0	2010	37	0
1	C	1993	0	2028	31	0
1	D	1989	0	2022	38	0
1	E	1993	0	2007	38	0
1	F	2009	0	2030	48	0
2	A	152	0	0	3	0
2	B	123	0	0	3	0
2	C	134	0	0	4	0
2	D	101	0	0	3	0
2	E	70	0	0	0	0
2	F	84	0	0	5	0
All	All	12641	0	12134	212	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 9.

The worst 5 of 212 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:91:ASN:HB3	2:C:382:HOH:O	1.54	1.04
1:A:257:ILE:HG23	1:A:258:ASP:H	1.18	1.03
1:F:223:LEU:O	1:F:227:GLN:HG3	1.66	0.95
1:A:257:ILE:CG2	1:A:258:ASP:H	1.89	0.84
1:A:108:ASN:H	1:A:108:ASN:HD22	1.25	0.84

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	258/260 (99%)	251 (97%)	6 (2%)	1 (0%)	43	45
1	B	253/260 (97%)	248 (98%)	5 (2%)	0	100	100
1	C	255/260 (98%)	250 (98%)	5 (2%)	0	100	100
1	D	255/260 (98%)	250 (98%)	5 (2%)	0	100	100
1	E	257/260 (99%)	247 (96%)	8 (3%)	2 (1%)	27	24
1	F	258/260 (99%)	253 (98%)	5 (2%)	0	100	100
All	All	1536/1560 (98%)	1499 (98%)	34 (2%)	3 (0%)	56	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	LYS
1	E	254	GLU
1	E	78	ARG

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	222/223 (100%)	206 (93%)	16 (7%)	21	20
1	B	218/223 (98%)	198 (91%)	20 (9%)	13	12
1	C	220/223 (99%)	205 (93%)	15 (7%)	22	23
1	D	219/223 (98%)	205 (94%)	14 (6%)	25	26
1	E	217/223 (97%)	205 (94%)	12 (6%)	30	34
1	F	220/223 (99%)	206 (94%)	14 (6%)	25	26
All	All	1316/1338 (98%)	1225 (93%)	91 (7%)	22	22

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	80	THR

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Mol	Chain	Res	Type
1	C	238	LYS
1	F	155	MET
1	C	84[A]	GLU
1	C	193	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	220	ASN
1	D	42	ASN
1	F	184	GLN
1	C	244	GLN
1	D	27	ASN

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 (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	258/260 (99%)	-0.37	1 (0%) 90 92	15, 22, 35, 50	0
1	B	255/260 (98%)	-0.45	0 100 100	20, 27, 40, 47	0
1	C	256/260 (98%)	-0.52	0 100 100	18, 26, 34, 41	0
1	D	257/260 (98%)	-0.29	3 (1%) 75 76	19, 29, 41, 50	0
1	E	259/260 (99%)	-0.07	11 (4%) 35 35	24, 37, 56, 61	0
1	F	260/260 (100%)	-0.20	4 (1%) 70 71	21, 33, 45, 49	0
All	All	1545/1560 (99%)	-0.32	19 (1%) 75 76	15, 28, 45, 61	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	THR	3.7
1	E	246	ILE	3.4
1	E	250	LEU	3.2
1	E	74	LEU	3.2
1	E	70	PHE	2.7

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

There are no such residues in this entry.