



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 05:59 AM GMT

PDB ID : 2B0L
Title : C-terminal DNA binding domain of transcriptional pleiotropic repressor CodY.
Authors : Levnikov, V.M.; Blagova, E.; Joseph, P.; Sonenshein, A.L.; Wilkinson, A.J.
Deposited on : 2005-09-14
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

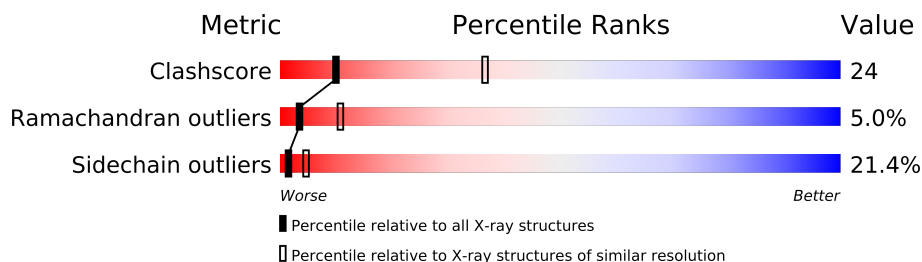
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
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 2.90 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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)

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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	102	
1	B	102	
1	C	102	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2300 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 GTP-sensing transcriptional pleiotropic repressor codY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	2	0
			783	493	141	145	4			
1	B	95	Total	C	N	O	S	4	4	0
			768	485	135	143	5			
1	C	94	Total	C	N	O	S	107	0	0
			730	461	128	138	3			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	158	GLY	-	CLONING ARTIFACT	UNP P39779
A	159	SER	-	CLONING ARTIFACT	UNP P39779
A	160	SER	-	CLONING ARTIFACT	UNP P39779
A	161	HIS	-	EXPRESSION TAG	UNP P39779
A	162	HIS	-	EXPRESSION TAG	UNP P39779
A	163	HIS	-	EXPRESSION TAG	UNP P39779
A	164	HIS	-	EXPRESSION TAG	UNP P39779
A	165	HIS	-	EXPRESSION TAG	UNP P39779
A	166	HIS	-	EXPRESSION TAG	UNP P39779
A	167	MET	-	INITIATING METHIONINE	UNP P39779
B	158	GLY	-	CLONING ARTIFACT	UNP P39779
B	159	SER	-	CLONING ARTIFACT	UNP P39779
B	160	SER	-	CLONING ARTIFACT	UNP P39779
B	161	HIS	-	EXPRESSION TAG	UNP P39779
B	162	HIS	-	EXPRESSION TAG	UNP P39779
B	163	HIS	-	EXPRESSION TAG	UNP P39779
B	164	HIS	-	EXPRESSION TAG	UNP P39779
B	165	HIS	-	EXPRESSION TAG	UNP P39779
B	166	HIS	-	EXPRESSION TAG	UNP P39779
B	167	MET	-	INITIATING METHIONINE	UNP P39779
C	158	GLY	-	CLONING ARTIFACT	UNP P39779
C	159	SER	-	CLONING ARTIFACT	UNP P39779
C	160	SER	-	CLONING ARTIFACT	UNP P39779

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Chain	Residue	Modelled	Actual	Comment	Reference
C	161	HIS	-	EXPRESSION TAG	UNP P39779
C	162	HIS	-	EXPRESSION TAG	UNP P39779
C	163	HIS	-	EXPRESSION TAG	UNP P39779
C	164	HIS	-	EXPRESSION TAG	UNP P39779
C	165	HIS	-	EXPRESSION TAG	UNP P39779
C	166	HIS	-	EXPRESSION TAG	UNP P39779
C	167	MET	-	INITIATING METHIONINE	UNP P39779

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	18	Total O 18 18	0	0
2	B	1	Total O 1 1	0	0

4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	68.13Å 68.13Å 164.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	100.0 (10.00-2.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.202 , 0.250	Depositor
Wilson B-factor (Å ²)	77.5	Xtriage
Anisotropy	0.152	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 8411 reflections (0.012%)	Xtriage
Total number of atoms	2300	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.57% 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	0.55	0/794	0.70	0/1065
1	B	0.47	0/780	0.70	0/1045
1	C	0.24	0/738	0.43	1/991 (0.1%)
All	All	0.44	0/2312	0.63	1/3101 (0.0%)

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	3
1	B	0	1
1	C	0	2
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	HIS	Peptide
1	A	233	ARG	Peptide
1	A	234	SER	Peptide
1	B	193	GLU	Peptide
1	C	210	VAL	Peptide
1	C	236	GLY	Peptide

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	783	0	799	48	0
1	B	768	0	795	44	0
1	C	730	0	753	23	0
2	A	18	0	0	0	0
2	B	1	0	0	0	0
All	All	2300	0	2347	103	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 24.

All (103) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174[B]:MET:HE1	1:B:174[B]:MET:CA	1.62	1.28
1:A:174[B]:MET:CE	1:B:174[B]:MET:HA	1.70	1.19
1:A:174[B]:MET:CE	1:B:174[B]:MET:CA	2.28	1.07
1:A:174[B]:MET:HE1	1:B:174[B]:MET:CB	1.86	1.04
1:A:170:ALA:O	1:A:174[A]:MET:HG3	1.59	1.01
1:C:206:ILE:HD13	1:C:206:ILE:N	1.74	1.00
1:A:174[B]:MET:CE	1:B:174[B]:MET:CB	2.44	0.96
1:A:256:LEU:C	1:A:256:LEU:HD23	1.85	0.94
1:A:190:ILE:HG23	1:A:201:LEU:HD13	1.47	0.94
1:A:174[B]:MET:HE1	1:B:174[B]:MET:HB3	1.50	0.94
1:A:174[B]:MET:CE	1:B:174[B]:MET:HB3	2.02	0.89
1:A:237:MET:CG	1:A:238:LYS:H	1.88	0.85
1:A:174[B]:MET:HE2	1:B:174[B]:MET:HA	1.61	0.83
1:A:247:ASN:HD22	1:A:247:ASN:H	1.22	0.83
1:A:235:LEU:O	1:A:237:MET:HG2	1.80	0.81
1:A:237:MET:HG3	1:A:238:LYS:H	1.46	0.79
1:A:247:ASN:HD22	1:A:247:ASN:N	1.81	0.79
1:A:237:MET:HG3	1:A:238:LYS:HG2	1.68	0.75
1:B:172:VAL:O	1:B:176:ILE:HG22	1.85	0.75
1:C:247:ASN:H	1:C:247:ASN:HD22	1.34	0.74
1:B:170:ALA:O	1:B:174[B]:MET:HG3	1.92	0.69
1:B:186:ALA:O	1:B:190:ILE:HD12	1.92	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:188:GLU:O	1:C:192:GLU:HG2	1.94	0.67
1:C:206:ILE:HD13	1:C:206:ILE:H	1.57	0.66
1:B:190:ILE:HD11	1:B:217:ILE:HG23	1.79	0.64
1:B:214:ARG:HG2	1:B:214:ARG:O	1.97	0.63
1:C:167:MET:O	1:C:171:VAL:HG23	1.98	0.63
1:A:237:MET:HG3	1:A:238:LYS:CG	2.28	0.63
1:C:187:ILE:HG13	1:C:224:LEU:HD11	1.79	0.63
1:A:164[B]:HIS:CE1	1:A:167:MET:HB2	2.35	0.61
1:A:247:ASN:H	1:A:247:ASN:ND2	1.96	0.61
1:C:200:LEU:HA	1:C:241:TYR:HA	1.82	0.60
1:A:174[B]:MET:HE2	1:B:174[B]:MET:CB	2.31	0.60
1:A:235:LEU:O	1:A:236:GLY:C	2.41	0.59
1:C:172:VAL:O	1:C:176:ILE:HG13	2.03	0.59
1:A:164[B]:HIS:CG	1:A:164[B]:HIS:O	2.57	0.58
1:B:232:SER:HB3	1:B:242:ILE:HD13	1.85	0.57
1:B:185:GLU:O	1:B:188:GLU:HB3	2.04	0.57
1:A:190:ILE:HG23	1:A:201:LEU:CD1	2.30	0.57
1:A:237:MET:CG	1:A:238:LYS:N	2.62	0.57
1:C:206:ILE:N	1:C:206:ILE:CD1	2.48	0.57
1:C:247:ASN:N	1:C:247:ASN:HD22	2.02	0.57
1:B:230:ILE:HG22	1:B:244:VAL:HA	1.86	0.56
1:A:256:LEU:C	1:A:256:LEU:CD2	2.60	0.56
1:B:253:LEU:O	1:B:256:LEU:HG	2.05	0.56
1:B:253:LEU:HD12	1:B:256:LEU:CD1	2.37	0.55
1:B:201:LEU:HD12	1:B:202:VAL:H	1.72	0.55
1:C:193:GLU:O	1:C:194:LEU:C	2.46	0.54
1:A:256:LEU:O	1:A:256:LEU:HD23	2.07	0.54
1:A:165:HIS:O	1:A:166:HIS:C	2.46	0.54
1:A:180:SER:N	1:A:183:GLU:OE2	2.31	0.54
1:C:209:ARG:HG2	1:C:209:ARG:O	2.07	0.54
1:A:165:HIS:O	1:A:167:MET:N	2.42	0.53
1:A:165:HIS:O	1:A:168:SER:N	2.41	0.53
1:B:183:GLU:OE1	1:B:223:LYS:NZ	2.39	0.53
1:B:253:LEU:O	1:B:255:ASN:N	2.42	0.52
1:B:172:VAL:HG11	1:B:252:GLU:HB3	1.91	0.52
1:A:246:ASN:OD1	1:A:246:ASN:C	2.49	0.51
1:B:170:ALA:O	1:B:174[A]:MET:HG3	2.12	0.50
1:B:167[A]:MET:O	1:B:170:ALA:HB3	2.11	0.49
1:A:165:HIS:HB3	1:A:248:LYS:HD3	1.95	0.49
1:A:252:GLU:O	1:A:255:ASN:HB3	2.13	0.48
1:A:174[B]:MET:SD	1:B:174[B]:MET:HB3	2.54	0.48
1:B:198:GLU:HA	1:B:242:ILE:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:206:ILE:CD1	1:C:206:ILE:H	2.21	0.47
1:B:171:VAL:HA	1:B:174[A]:MET:SD	2.54	0.47
1:B:194:LEU:HG	1:B:195:ASP:H	1.79	0.47
1:C:232:SER:HA	1:C:241:TYR:O	2.15	0.47
1:C:168:SER:O	1:C:172:VAL:HG23	2.15	0.47
1:B:179:LEU:HD23	1:B:223:LYS:HD3	1.98	0.46
1:B:184:LEU:HD23	1:B:184:LEU:HA	1.82	0.46
1:B:253:LEU:HD12	1:B:256:LEU:HD11	1.98	0.46
1:B:194:LEU:HG	1:B:195:ASP:N	2.31	0.46
1:A:256:LEU:HD23	1:A:257:LYS:N	2.31	0.46
1:C:203:ALA:HB3	1:C:214:ARG:NE	2.31	0.45
1:B:214:ARG:CG	1:B:214:ARG:O	2.65	0.45
1:A:187:ILE:HD13	1:A:190:ILE:HD12	1.98	0.45
1:A:194:LEU:HD23	1:A:196:GLY:O	2.17	0.45
1:A:174[B]:MET:HE2	1:B:174[B]:MET:CG	2.47	0.44
1:B:253:LEU:HD12	1:B:256:LEU:HD12	1.99	0.44
1:A:174[B]:MET:HE2	1:B:174[B]:MET:CA	2.27	0.44
1:C:241:TYR:C	1:C:241:TYR:CD2	2.91	0.44
1:B:184:LEU:HD22	1:B:256:LEU:HD13	2.00	0.44
1:A:206:ILE:O	1:A:210:VAL:HG23	2.18	0.43
1:B:184:LEU:CD2	1:B:256:LEU:HD13	2.49	0.43
1:C:234:SER:O	1:C:235:LEU:C	2.57	0.42
1:C:199:GLY:O	1:C:242:ILE:N	2.51	0.42
1:C:234:SER:O	1:C:235:LEU:O	2.38	0.42
1:B:253:LEU:O	1:B:254:GLU:C	2.58	0.42
1:A:183:GLU:OE2	1:A:223:LYS:NZ	2.53	0.42
1:A:246:ASN:OD1	1:A:248:LYS:N	2.53	0.42
1:B:233:ARG:C	1:B:235:LEU:H	2.23	0.41
1:B:211:GLY:C	1:B:212:ILE:HG13	2.34	0.41
1:A:171:VAL:HA	1:A:174[A]:MET:SD	2.60	0.41
1:C:202:VAL:HG22	1:C:239:GLY:CA	2.51	0.41
1:A:233:ARG:O	1:A:234:SER:C	2.59	0.41
1:C:180:SER:H	1:C:183:GLU:HB2	1.85	0.41
1:B:232:SER:HA	1:B:241:TYR:O	2.20	0.40
1:A:247:ASN:N	1:A:247:ASN:ND2	2.53	0.40
1:B:176:ILE:HD13	1:B:176:ILE:C	2.42	0.40
1:C:221:LEU:O	1:C:225:GLU:HB2	2.21	0.40

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	98/102 (96%)	79 (81%)	13 (13%)	6 (6%)	2	7
1	B	97/102 (95%)	81 (84%)	12 (12%)	4 (4%)	4	17
1	C	92/102 (90%)	73 (79%)	15 (16%)	4 (4%)	4	15
All	All	287/306 (94%)	233 (81%)	40 (14%)	14 (5%)	3	12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	237	MET
1	B	254	GLU
1	A	234	SER
1	A	236	GLY
1	A	255	ASN
1	B	194	LEU
1	B	247	ASN
1	C	194	LEU
1	C	235	LEU
1	A	238	LYS
1	B	197	ASN
1	C	193	GLU
1	C	180	SER

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	87/88 (99%)	71 (82%)	16 (18%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	86/88 (98%)	71 (83%)	15 (17%)	3	8
1	C	81/88 (92%)	58 (72%)	23 (28%)	0	2
All	All	254/264 (96%)	200 (79%)	54 (21%)	1	5

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	HIS
1	A	167	MET
1	A	182	SER
1	A	184	LEU
1	A	193	GLU
1	A	195	ASP
1	A	212	ILE
1	A	219	ASN
1	A	221	LEU
1	A	234	SER
1	A	238	LYS
1	A	240	THR
1	A	247	ASN
1	A	248	LYS
1	A	253	LEU
1	A	256	LEU
1	B	163	HIS
1	B	167[A]	MET
1	B	167[B]	MET
1	B	173	GLN
1	B	176	ILE
1	B	184	LEU
1	B	193	GLU
1	B	201	LEU
1	B	209	ARG
1	B	212	ILE
1	B	213	THR
1	B	219	ASN
1	B	222	ARG
1	B	247	ASN
1	B	255	ASN
1	C	165	HIS
1	C	166	HIS
1	C	169	LYS

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Mol	Chain	Res	Type
1	C	182	SER
1	C	187	ILE
1	C	194	LEU
1	C	198	GLU
1	C	201	LEU
1	C	204	SER
1	C	206	ILE
1	C	212	ILE
1	C	213	THR
1	C	214	ARG
1	C	216	VAL
1	C	217	ILE
1	C	221	LEU
1	C	238	LYS
1	C	240	THR
1	C	241	TYR
1	C	242	ILE
1	C	247	ASN
1	C	248	LYS
1	C	254	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	B	247	ASN
1	C	247	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.