



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 31, 2018 – 06:35 PM EDT

PDB ID : 6C2S  
Title : Transcriptional repressor, CouR, bound to a 23-mer DNA duplex  
Authors : Cogan, D.P.; Nair, S.K.  
Deposited on : 2018-01-08  
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031172
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031172

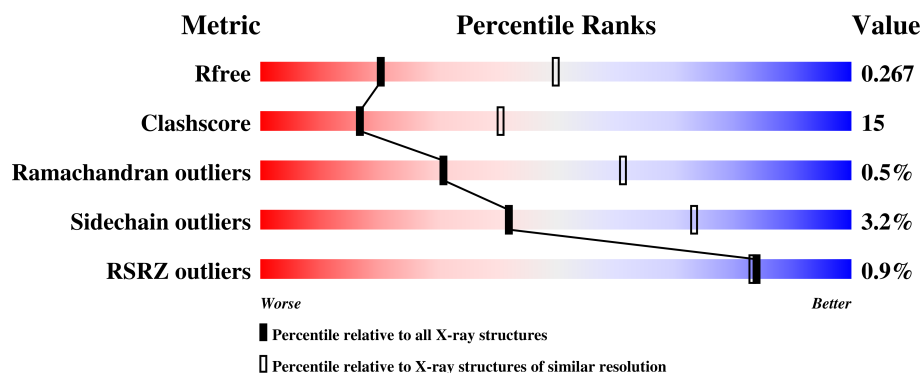
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	111664	2715 (2.90-2.82)
Clashscore	122126	2976 (2.90-2.82)
Ramachandran outliers	120053	2913 (2.90-2.82)
Sidechain outliers	120020	2916 (2.90-2.82)
RSRZ outliers	108989	2654 (2.90-2.82)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	186	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>15%</div> <div>•</div> <div>24%</div> </div> </div>
1	B	186	<div> <div></div> <div> <div>57%</div> <div>18%</div> <div>•</div> <div>24%</div> </div> </div>
1	C	186	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>18%</div> <div>•</div> <div>24%</div> </div> </div>
1	D	186	<div> <div>%</div> <div> <div></div> <div>51%</div> <div>26%</div> <div></div> <div>24%</div> </div> </div>
2	U	23	<div> <div></div> <div> <div>65%</div> <div>30%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	X	23	<div><div></div><div>61%</div><div>35%</div><div></div></div>
3	V	23	<div><div></div><div>52%</div><div>39%</div><div>9%</div></div>
3	Y	23	<div><div></div><div>70%</div><div>22%</div><div>9%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6293 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 Transcriptional regulator, MarR family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1101	689	209	197	6			
1	B	142	Total	C	N	O	S	0	0	0
			1095	686	206	197	6			
1	C	142	Total	C	N	O	S	0	0	0
			1101	689	209	197	6			
1	D	142	Total	C	N	O	S	0	0	0
			1095	686	206	197	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q6N8V9
A	-1	GLY	-	expression tag	UNP Q6N8V9
A	0	SER	-	expression tag	UNP Q6N8V9
B	-2	SER	-	expression tag	UNP Q6N8V9
B	-1	GLY	-	expression tag	UNP Q6N8V9
B	0	SER	-	expression tag	UNP Q6N8V9
C	-2	SER	-	expression tag	UNP Q6N8V9
C	-1	GLY	-	expression tag	UNP Q6N8V9
C	0	SER	-	expression tag	UNP Q6N8V9
D	-2	SER	-	expression tag	UNP Q6N8V9
D	-1	GLY	-	expression tag	UNP Q6N8V9
D	0	SER	-	expression tag	UNP Q6N8V9

- Molecule 2 is a DNA chain called 23-mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	U	23	Total	C	N	O	P	0	0	0
			464	227	76	139	22			
2	X	23	Total	C	N	O	P	0	0	0
			464	227	76	139	22			

- Molecule 3 is a DNA chain called 23-mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	23	Total 473	C 229	N 89	O 133	P 22	0	0	0
3	Y	23	Total 473	C 229	N 89	O 133	P 22	0	0	0

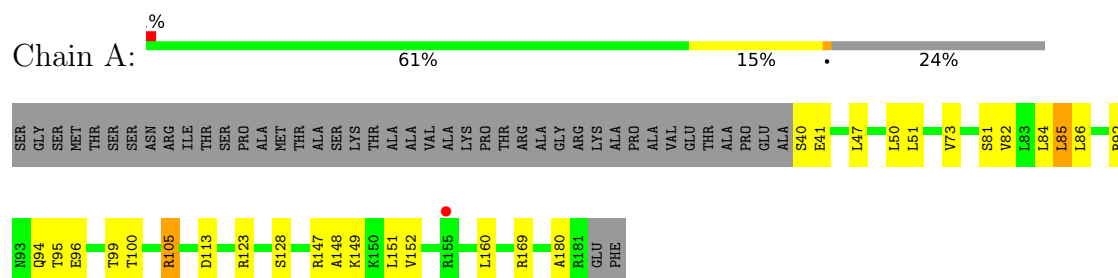
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	U	4	Total 4	O 4	0	0
4	B	5	Total 5	O 5	0	0
4	V	1	Total 1	O 1	0	0
4	C	1	Total 1	O 1	0	0
4	D	4	Total 4	O 4	0	0
4	Y	2	Total 2	O 2	0	0

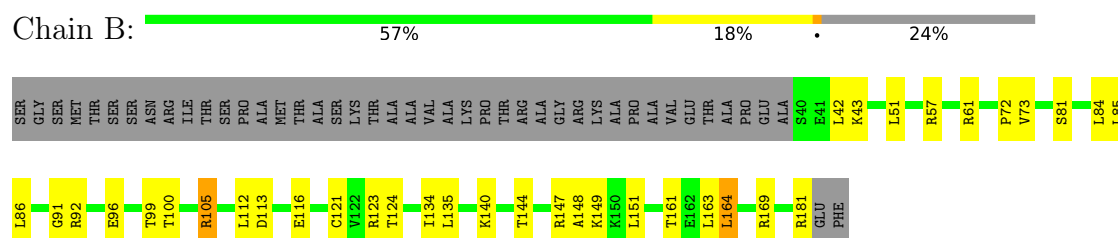
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

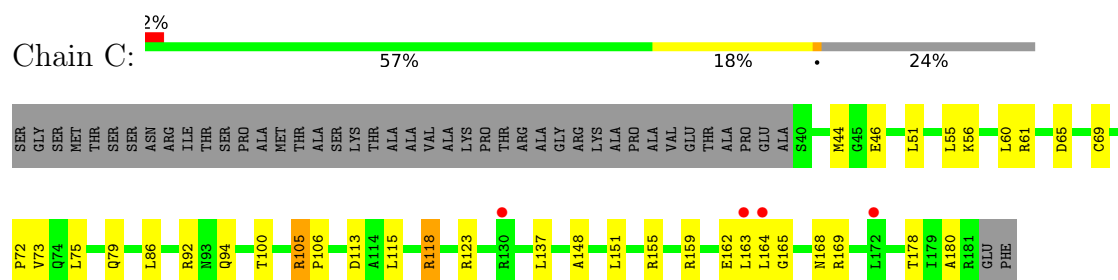
- Molecule 1: Transcriptional regulator, MarR family



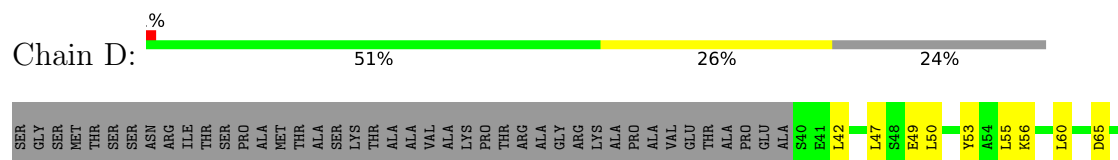
- Molecule 1: Transcriptional regulator, MarR family



- Molecule 1: Transcriptional regulator, MarR family

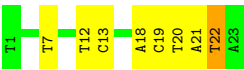


- Molecule 1: Transcriptional regulator, MarR family

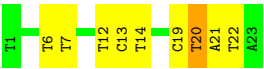




• Molecule 2: 23-mer



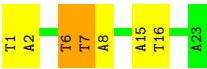
• Molecule 2: 23-mer



• Molecule 3: 23-mer



• Molecule 3: 23-mer



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.58Å 58.75Å 168.09Å 90.00° 105.02° 90.00°	Depositor
Resolution (Å)	32.74 – 2.85 36.21 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.8 (32.74-2.85) 99.7 (36.21-2.85)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.85Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.215 , 0.267 0.218 , 0.267	Depositor DCC
$R_{free}$ test set	1510 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.0	Xtriage
Anisotropy	0.942	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 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	0.45	0/1113	0.77	0/1501
1	B	0.44	0/1107	0.76	0/1494
1	C	0.48	0/1113	0.76	0/1501
1	D	0.47	0/1107	0.73	0/1494
2	U	1.26	2/518 (0.4%)	1.16	0/797
2	X	1.11	2/518 (0.4%)	1.13	0/797
3	V	1.26	3/532 (0.6%)	1.06	0/820
3	Y	1.03	1/532 (0.2%)	1.09	1/820 (0.1%)
All	All	0.76	8/6540 (0.1%)	0.89	1/9224 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	19	DC	O3'-P	-8.20	1.51	1.61
2	U	22	DT	O3'-P	-7.66	1.51	1.61
3	V	2	DA	O3'-P	-6.52	1.53	1.61
3	V	1	DT	O3'-P	-5.97	1.53	1.61
2	X	20	DT	O3'-P	-5.48	1.54	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	7	DT	O4'-C4'-C3'	-5.11	102.46	104.50

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1101	0	1156	27	0
1	B	1095	0	1145	39	0
1	C	1101	0	1155	50	0
1	D	1095	0	1145	39	0
2	U	464	0	265	19	0
2	X	464	0	266	8	0
3	V	473	0	263	19	0
3	Y	473	0	263	9	0
4	A	10	0	0	2	0
4	B	5	0	0	1	0
4	C	1	0	0	0	0
4	D	4	0	0	1	0
4	U	4	0	0	0	0
4	V	1	0	0	0	0
4	Y	2	0	0	0	0
All	All	6293	0	5658	178	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 15.

The worst 5 of 178 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)
2:U:13:DC:N4	3:V:11:DG:O6	1.58	1.36
2:U:13:DC:N3	3:V:11:DG:N1	1.77	1.30
2:U:12:DT:H2''	2:U:13:DC:C5'	1.74	1.18
1:C:164:LEU:HD23	1:C:165:GLY:N	1.58	1.17
3:V:1:DT:H2''	3:V:2:DA:O5'	1.43	1.10

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	140/186 (75%)	136 (97%)	3 (2%)	1 (1%)	24	54
1	B	140/186 (75%)	137 (98%)	3 (2%)	0	100	100
1	C	140/186 (75%)	136 (97%)	3 (2%)	1 (1%)	24	54
1	D	140/186 (75%)	137 (98%)	2 (1%)	1 (1%)	24	54
All	All	560/744 (75%)	546 (98%)	11 (2%)	3 (0%)	31	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	180	ALA
1	A	180	ALA
1	C	180	ALA

### 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	117/151 (78%)	112 (96%)	5 (4%)	32	63
1	B	116/151 (77%)	110 (95%)	6 (5%)	25	55
1	C	117/151 (78%)	115 (98%)	2 (2%)	63	86
1	D	116/151 (77%)	114 (98%)	2 (2%)	63	86
All	All	466/604 (77%)	451 (97%)	15 (3%)	42	73

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	51	LEU
1	B	86	LEU
1	C	118	ARG
1	B	43	LYS
1	C	105	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	142/186 (76%)	-0.20	1 (0%) 87 87	36, 57, 71, 88	0
1	B	142/186 (76%)	-0.13	0 100 100	40, 59, 103, 119	0
1	C	142/186 (76%)	0.05	4 (2%) 53 48	50, 70, 105, 118	0
1	D	142/186 (76%)	-0.30	1 (0%) 87 87	44, 63, 79, 94	0
2	U	23/23 (100%)	-0.27	0 100 100	34, 49, 59, 62	0
2	X	23/23 (100%)	-0.42	0 100 100	38, 58, 76, 82	0
3	V	23/23 (100%)	-0.35	0 100 100	40, 46, 55, 57	0
3	Y	23/23 (100%)	-0.21	0 100 100	44, 61, 74, 77	0
All	All	660/836 (78%)	-0.17	6 (0%) 84 83	34, 61, 92, 119	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	163	LEU	3.1
1	D	163	LEU	2.5
1	A	155	ARG	2.4
1	C	130	ARG	2.3
1	C	164	LEU	2.2

### 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.