



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:26 am BST

PDB ID : 5ZKO  
Title : Crystal structure of the CRT2-CREB-CRE complex  
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Deposited on : 2018-03-24  
Resolution : 3.05 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](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	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

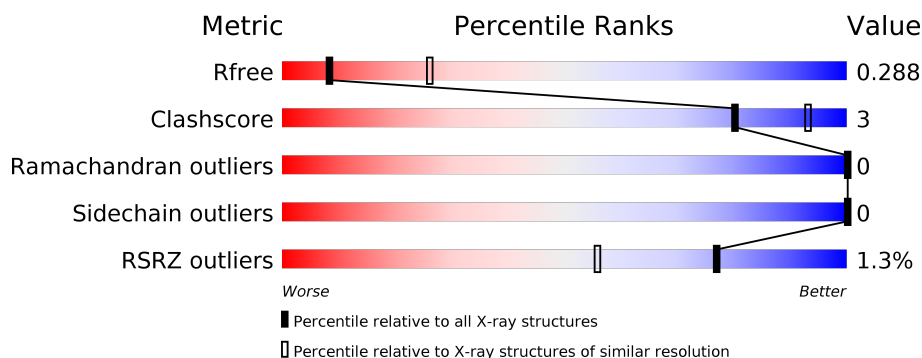
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.05 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))
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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 respectively. 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	59	<div> <div></div> <div>86%</div> <div>10%</div> </div>
1	C	59	<div> <div>2%</div> <div></div> <div>86%</div> <div>10%</div> </div>
2	B	20	<div> <div>70%</div> <div>30%</div> </div>
2	D	20	<div> <div>70%</div> <div>30%</div> </div>
3	G	80	<div> <div>49%</div> <div>5%</div> <div>46%</div> </div>
3	H	80	<div> <div>3%</div> <div></div> <div>50%</div> <div>5%</div> <div>45%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2404 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 Cyclic AMP-responsive element-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	0	0	0
			448	277	88	79	4			
1	C	53	Total	C	N	O	S	0	0	0
			448	277	88	79	4			

- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*TP\*TP\*GP\*GP\*CP\*TP\*GP\*AP\*CP\*GP\*TP\*CP\*AP\*GP\*CP\*CP\*AP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	P	0	0	0
			407	194	76	118	19			
2	D	20	Total	C	N	O	P	0	0	0
			407	194	76	118	19			


- Molecule 3 is a protein called CREB-regulated transcription coactivator 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	43	Total	C	N	O	S	0	0	0
			344	211	65	66	2			
3	H	44	Total	C	N	O	S	0	0	0
			350	214	66	68	2			

### 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: Cyclic AMP-responsive element-binding protein 1

Chain A: 



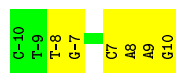
- Molecule 1: Cyclic AMP-responsive element-binding protein 1

Chain C: 



- Molecule 2: DNA (5'-D(\*CP\*TP\*TP\*GP\*GP\*CP\*TP\*GP\*AP\*CP\*GP\*TP\*CP\*AP\*GP\*CP\*CP\*AP\*AP\*G)-3')

Chain B: 



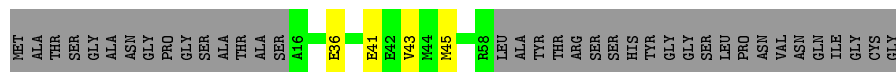
- Molecule 2: DNA (5'-D(\*CP\*TP\*TP\*GP\*GP\*CP\*TP\*GP\*AP\*CP\*GP\*TP\*CP\*AP\*GP\*CP\*CP\*AP\*AP\*G)-3')

Chain D: 



- Molecule 3: CREB-regulated transcription coactivator 2

Chain G: 



- Molecule 3: CREB-regulated transcription coactivator 2



MET	ALA	THR	SER	GLY	ALA	ASN	GLY	PRO	GLY	SER	ALA	THR	ALA	S15	A16	S17	N18	E36	V43	I47	R51	R58	LEU	ALA	TYR	THR	ARG	SER	SER	HIS	TVR	GLY	GLY	SER	LEU	PRO	ASN	VAL	ASN	GLN	ILE	GLY	CYS	GLY
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.30 Å 41.32 Å 122.58 Å 90.00° 90.61° 90.00°	Depositor
Resolution (Å)	46.71 – 3.05 46.71 – 3.05	Depositor EDS
% Data completeness (in resolution range)	93.8 (46.71-3.05) 95.0 (46.71-3.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 3.06 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.242 , 0.285 0.244 , 0.288	Depositor DCC
$R_{free}$ test set	469 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	1.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2404	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.82% 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

### 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	0.19	0/449	0.30	0/593
1	C	0.19	0/449	0.31	0/593
2	B	0.48	0/456	0.84	0/702
2	D	0.48	0/456	0.85	0/702
3	G	0.21	0/346	0.33	0/459
3	H	0.20	0/352	0.31	0/467
All	All	0.33	0/2508	0.59	0/3516

There are no bond length outliers.

There are no bond angle outliers.

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	448	0	484	2	0
1	C	448	0	484	2	0
2	B	407	0	226	3	0
2	D	407	0	226	3	0
3	G	344	0	352	3	0
3	H	350	0	357	3	0
All	All	2404	0	2129	12	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 3.

All (12) 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:314:ARG:NH2	3:G:36:GLU:OE2	2.23	0.71
1:A:326:ILE:HG23	3:H:43:VAL:HG21	1.84	0.58
2:D:-8:DT:H2"	2:D:-7:DG:C8	2.40	0.57
2:B:-8:DT:H2"	2:B:-7:DG:C8	2.40	0.56
2:B:9:DA:H2"	2:B:10:DG:H5"	1.94	0.50
3:G:41:GLU:O	3:G:45:MET:HB2	2.16	0.46
2:B:7:DC:H2"	2:B:8:DA:N7	2.31	0.46
1:C:326:ILE:HG23	3:G:43:VAL:HG21	1.98	0.45
2:D:-6:DG:H2"	2:D:-5:DC:H5"	1.99	0.44
3:H:47:ILE:O	3:H:51:ARG:HG3	2.20	0.41
2:D:-1:DC:H2'	2:D:1:DG:C8	2.56	0.41
1:C:314:ARG:NH2	3:H:36:GLU:OE2	2.41	0.41

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	51/59 (86%)	51 (100%)	0	0	100	100
1	C	51/59 (86%)	51 (100%)	0	0	100	100
3	G	41/80 (51%)	41 (100%)	0	0	100	100
3	H	42/80 (52%)	40 (95%)	2 (5%)	0	100	100
All	All	185/278 (66%)	183 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.



### 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	49/54 (91%)	49 (100%)	0	100	100
1	C	49/54 (91%)	49 (100%)	0	100	100
3	G	36/61 (59%)	36 (100%)	0	100	100
3	H	37/61 (61%)	37 (100%)	0	100	100
All	All	171/230 (74%)	171 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 ⓘ

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	53/59 (89%)	0.38	0 <span>100</span> <span>100</span>	48, 77, 104, 121	0
1	C	53/59 (89%)	0.52	1 (1%) <span>66</span> <span>43</span>	57, 81, 116, 142	0
2	B	20/20 (100%)	0.32	0 <span>100</span> <span>100</span>	74, 82, 116, 118	0
2	D	20/20 (100%)	0.27	0 <span>100</span> <span>100</span>	71, 79, 112, 113	0
3	G	43/80 (53%)	0.24	0 <span>100</span> <span>100</span>	68, 96, 128, 130	0
3	H	44/80 (55%)	0.51	2 (4%) <span>33</span> <span>15</span>	63, 99, 134, 142	0
All	All	233/318 (73%)	0.40	3 (1%) <span>77</span> <span>56</span>	48, 85, 128, 142	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	292	LYS	3.5
3	H	17	SER	3.2
3	H	18	ASN	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.