



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:15 am BST

PDB ID : 4HQE  
Title : The crystal structure of QsrR-DNA complex  
Authors : He, C.; Ji, Q.; Zhang, L.  
Deposited on : 2012-10-25  
Resolution : 2.30 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.

---

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

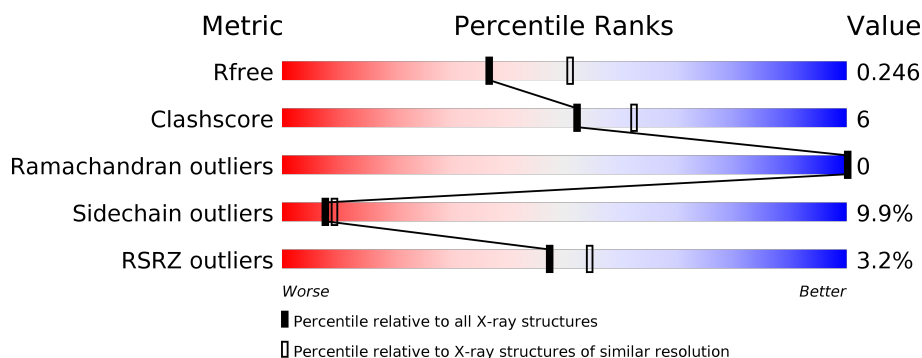
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	115	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>• 9%</div> </div> </div>
1	B	115	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div> </div>
2	C	17	<div> <div></div> <div> <div>76%</div> <div>24%</div> </div> </div>
3	D	17	<div> <div></div> <div> <div>47%</div> <div>47%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2498 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 QsrR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			842	542	138	156	6			
1	B	108	Total	C	N	O	S	0	0	0
			868	555	145	164	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q99SD5
A	-1	ASN	-	EXPRESSION TAG	UNP Q99SD5
A	0	ALA	-	EXPRESSION TAG	UNP Q99SD5
B	-2	SER	-	EXPRESSION TAG	UNP Q99SD5
B	-1	ASN	-	EXPRESSION TAG	UNP Q99SD5
B	0	ALA	-	EXPRESSION TAG	UNP Q99SD5

- Molecule 2 is a DNA chain called DNA (5'-D(\*GP\*GP\*TP\*AP\*TP\*AP\*AP\*TP\*AP\*AP\*TP\*TP\*AP\*TP\*AP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	17	Total	C	N	O	P	0	0	0
			347	169	62	100	16			

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

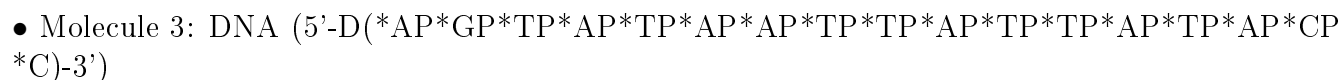
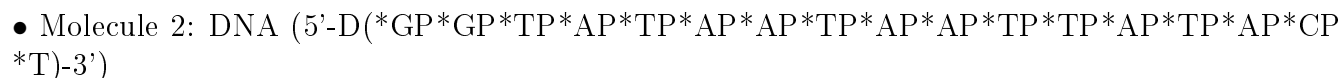
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	17	Total	C	N	O	P	0	0	0
			344	168	60	100	16			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total 31	O 31	0	0
4	B	45	Total 45	O 45	0	0
4	C	10	Total 10	O 10	0	0
4	D	11	Total 11	O 11	0	0

i

- Molecule 1: Transcriptional regulator QsrR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.19 Å 48.19 Å 156.81 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.82 – 2.30 23.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (23.82-2.30) 99.9 (23.81-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.31 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.205 , 0.260 0.197 , 0.246	Depositor DCC
$R_{free}$ test set	789 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2498	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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	0.47	0/859	0.61	0/1164
1	B	0.42	0/885	0.57	0/1201
2	C	0.73	0/389	1.42	4/599 (0.7%)
3	D	0.88	0/385	1.58	5/592 (0.8%)
All	All	0.58	0/2518	1.00	9/3556 (0.3%)

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	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	DG	O4'-C4'-C3'	-12.96	98.23	106.00
2	C	1	DG	O4'-C1'-N9	8.95	114.27	108.00
3	D	12	DT	O4'-C1'-N1	-7.46	102.78	108.00
3	D	2	DG	C4'-C3'-C2'	-6.15	97.56	103.10
2	C	10	DA	O4'-C1'-N9	-5.82	103.92	108.00
3	D	8	DT	O4'-C1'-C2'	-5.60	101.42	105.90
2	C	11	DT	O4'-C1'-N1	-5.54	104.12	108.00
3	D	9	DT	P-O5'-C5'	-5.11	112.72	120.90
2	C	12	DT	O4'-C1'-N1	-5.02	104.49	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	SER	Peptide

## 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	842	0	860	16	0
1	B	868	0	878	6	0
2	C	347	0	196	0	0
3	D	344	0	196	4	0
4	A	31	0	0	1	0
4	B	45	0	0	0	0
4	C	10	0	0	0	0
4	D	11	0	0	2	0
All	All	2498	0	2130	23	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 6.

All (23) 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)
3:D:14:DT:H2"	3:D:15:DA:H5"	1.59	0.84
3:D:13:DA:H2"	3:D:14:DT:H5"	1.72	0.70
3:D:4:DA:N7	4:D:104:HOH:O	2.29	0.64
1:A:3:GLU:O	1:B:29:ARG:NH2	2.33	0.61
1:A:38:SER:OG	4:A:230:HOH:O	2.17	0.60
1:A:81:LEU:HD22	1:A:85:GLY:HA3	1.88	0.56
1:A:94:PRO:HG2	1:B:94:PRO:HG3	1.92	0.51
1:A:27:LEU:HB3	1:A:81:LEU:HG	1.93	0.50
1:A:104:ASP:HA	1:A:105:LEU:C	2.33	0.49
1:A:27:LEU:O	1:A:33:CYS:HA	2.12	0.48
1:A:17:ARG:HD3	4:D:111:HOH:O	2.14	0.46
1:B:81:LEU:HB3	1:B:86:LYS:HG3	1.98	0.46
1:A:18:SER:HB3	1:B:17:ARG:HH22	1.82	0.45
1:A:33:CYS:HB3	1:A:81:LEU:HB2	1.99	0.45
1:A:67:LYS:HG3	1:A:79:TYR:CE2	2.53	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:MET:O	1:B:44:LEU:HB2	2.16	0.44
1:A:19:TRP:CD2	1:A:47:ILE:HD12	2.53	0.44
1:A:14:ILE:HG13	1:A:14:ILE:H	1.55	0.43
1:B:27:LEU:O	1:B:33:CYS:HA	2.18	0.43
1:A:15:LEU:HA	1:A:15:LEU:HD23	1.89	0.41
1:A:5:CYS:HA	1:A:6:PRO:HD3	1.89	0.41
3:D:9:DT:H1'	3:D:10:DA:H5'	2.03	0.41
1:A:71:SER:HA	1:A:75:VAL:HG22	2.02	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	103/115 (90%)	97 (94%)	6 (6%)	0	100	100
1	B	106/115 (92%)	103 (97%)	3 (3%)	0	100	100
All	All	209/230 (91%)	200 (96%)	9 (4%)	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	94/102 (92%)	84 (89%)	10 (11%)	6	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	97/102 (95%)	88 (91%)	9 (9%)	9	10
All	All	191/204 (94%)	172 (90%)	19 (10%)	8	9

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	3	GLU
1	A	14	ILE
1	A	17	ARG
1	A	27	LEU
1	A	45	LYS
1	A	54	LEU
1	A	71	SER
1	A	88	LEU
1	A	100	GLN
1	B	9	GLU
1	B	14	ILE
1	B	24	ILE
1	B	44	LEU
1	B	54	LEU
1	B	58	GLU
1	B	73	SER
1	B	88	LEU
1	B	110	THR

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	105/115 (91%)	0.12	4 (3%) 40 47	28, 40, 61, 76	0
1	B	108/115 (93%)	0.10	4 (3%) 41 48	29, 40, 56, 67	0
2	C	17/17 (100%)	-0.09	0 100 100	38, 52, 61, 62	0
3	D	17/17 (100%)	-0.24	0 100 100	42, 51, 63, 65	0
All	All	247/264 (93%)	0.07	8 (3%) 47 54	28, 41, 61, 76	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	LEU	4.9
1	B	110	THR	3.9
1	A	104	ASP	2.9
1	B	3	GLU	2.6
1	A	73	SER	2.4
1	B	7	TYR	2.2
1	B	24	ILE	2.2
1	A	1	MET	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.