



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3H5O  
Title : The crystal structure of transcription regulator GntR from *Chromobacterium violaceum*  
Authors : Zhang, Z.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2009-04-22  
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.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.16  
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) : 2.16

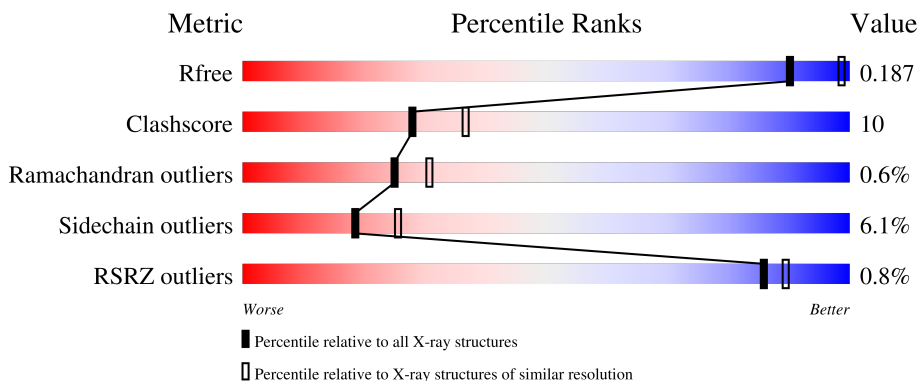
# 1 Overall quality at a glance

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 of 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	339	 63% 14% • 20%
1	B	339	 65% 13% • 20%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4334 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 GntR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	271	2059	1283	377	384	7	8	0	0	0
1	B	271	2067	1287	377	388	7	8	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MSE	-	expression tag	UNP Q7NTU7
A	10	SER	-	expression tag	UNP Q7NTU7
A	11	LEU	-	expression tag	UNP Q7NTU7
A	340	GLU	-	expression tag	UNP Q7NTU7
A	341	GLY	-	expression tag	UNP Q7NTU7
A	342	HIS	-	expression tag	UNP Q7NTU7
A	343	HIS	-	expression tag	UNP Q7NTU7
A	344	HIS	-	expression tag	UNP Q7NTU7
A	345	HIS	-	expression tag	UNP Q7NTU7
A	346	HIS	-	expression tag	UNP Q7NTU7
A	347	HIS	-	expression tag	UNP Q7NTU7
B	9	MSE	-	expression tag	UNP Q7NTU7
B	10	SER	-	expression tag	UNP Q7NTU7
B	11	LEU	-	expression tag	UNP Q7NTU7
B	340	GLU	-	expression tag	UNP Q7NTU7
B	341	GLY	-	expression tag	UNP Q7NTU7
B	342	HIS	-	expression tag	UNP Q7NTU7
B	343	HIS	-	expression tag	UNP Q7NTU7
B	344	HIS	-	expression tag	UNP Q7NTU7
B	345	HIS	-	expression tag	UNP Q7NTU7
B	346	HIS	-	expression tag	UNP Q7NTU7
B	347	HIS	-	expression tag	UNP Q7NTU7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	91	Total	O	0	0
			91	91		



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.37Å 67.88Å 90.36Å 90.00° 92.43° 90.00°	Depositor
Resolution (Å)	90.17 – 2.30 90.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (90.17-2.30) 99.9 (90.28-2.30)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.189 , 0.231 0.188 , 0.187	Depositor DCC
$R_{free}$ test set	1514 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtrriage
Anisotropy	0.394	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4334	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.35	0/2085	0.53	0/2813
1	B	0.37	0/2093	0.52	0/2823
All	All	0.36	0/4178	0.52	0/5636

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 [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	2059	0	2055	46	0
1	B	2067	0	2063	38	0
2	A	5	0	0	1	0
2	B	5	0	0	1	0
3	A	107	0	0	0	0
3	B	91	0	0	0	0
All	All	4334	0	4118	82	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 10.

All (82) 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:229:SER:HA	1:A:233:MSE:CE	1.80	1.10
1:A:229:SER:HA	1:A:233:MSE:HE1	1.38	1.04
1:A:233:MSE:HE3	1:A:258:LEU:HD21	1.45	0.99
1:A:337:ARG:HH11	1:A:337:ARG:HG2	1.43	0.84
1:A:72:THR:HG22	1:A:102:GLN:HB2	1.61	0.81
1:A:71:ARG:N	1:A:71:ARG:HD3	1.98	0.77
1:B:333:LEU:O	1:B:334:MSE:HE2	1.85	0.76
1:A:337:ARG:HG2	1:A:337:ARG:NH1	2.04	0.70
1:A:325:ARG:HG2	1:A:325:ARG:HH21	1.58	0.68
1:A:229:SER:HA	1:A:233:MSE:HE2	1.72	0.67
1:A:145:LEU:HD13	1:A:152:VAL:HG11	1.74	0.67
1:B:81:ALA:HB3	2:B:2:SO4:O2	1.95	0.66
1:A:120:ARG:HA	1:A:123:LEU:HD22	1.78	0.65
1:B:282:PHE:O	1:B:283:ASN:HB2	1.98	0.62
1:A:325:ARG:CG	1:A:325:ARG:HH21	2.12	0.62
1:A:282:PHE:O	1:A:283:ASN:HB2	1.99	0.62
1:B:332:ARG:HG2	1:B:334:MSE:CE	2.32	0.59
1:B:225:ASP:OD1	1:B:227:GLN:HG3	2.03	0.58
1:A:286:GLN:NE2	1:B:231:MSE:H	2.03	0.57
1:B:196:LEU:HB3	1:B:201:MSE:HE2	1.86	0.56
1:A:71:ARG:O	1:A:101:TYR:HA	2.05	0.56
1:A:103:MSE:HE3	1:A:105:ILE:HD11	1.88	0.56
1:B:71:ARG:HB2	1:B:128:ASP:OD2	2.06	0.56
1:A:180:HIS:HE1	1:A:339:SER:OG	1.90	0.55
1:A:225:ASP:OD1	1:A:227:GLN:HG2	2.06	0.55
1:A:71:ARG:O	1:A:102:GLN:N	2.36	0.54
1:B:180:HIS:CE1	1:B:340:GLU:OE2	2.60	0.54
1:B:196:LEU:HG	1:B:201:MSE:HE1	1.89	0.54
1:B:141:PHE:O	1:B:145:LEU:HD13	2.08	0.54
1:A:143:ARG:H	1:A:143:ARG:HH11	1.57	0.52
1:B:84:VAL:O	1:B:302:ARG:HD2	2.10	0.52
1:B:196:LEU:HG	1:B:201:MSE:CE	2.41	0.51
1:A:229:SER:CA	1:A:233:MSE:HE1	2.27	0.51
1:A:120:ARG:O	1:A:123:LEU:HB2	2.11	0.51
1:A:71:ARG:HG2	1:A:72:THR:HG23	1.92	0.50
1:A:233:MSE:HE3	1:A:258:LEU:CD2	2.31	0.50
1:B:76:LEU:HD12	1:B:132:ILE:CD1	2.42	0.50
1:B:333:LEU:C	1:B:334:MSE:HE2	2.32	0.49
1:A:325:ARG:CG	1:A:325:ARG:NH2	2.74	0.49
1:B:196:LEU:HD22	1:B:226:PRO:HA	1.95	0.49
1:A:284:ASP:HA	1:A:297:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:HIS:HE1	1:B:340:GLU:OE2	1.96	0.48
1:B:248:CYS:O	1:B:276:ARG:NH2	2.48	0.47
1:A:155:MSE:O	1:A:156:MSE:HB2	2.15	0.47
1:B:280:ALA:HA	1:B:296:THR:O	2.16	0.46
1:B:119:LEU:HD21	1:B:145:LEU:HD12	1.98	0.46
1:B:332:ARG:HG2	1:B:334:MSE:HE1	1.96	0.46
1:A:227:GLN:HB2	1:A:228:PRO:HD2	1.98	0.46
1:B:332:ARG:CD	1:B:334:MSE:HE1	2.46	0.46
1:B:313:LEU:O	1:B:317:ILE:HG23	2.16	0.45
1:B:123:LEU:HD12	1:B:123:LEU:HA	1.80	0.45
1:A:113:GLY:O	1:A:117:GLN:HG3	2.17	0.45
1:B:128:ASP:HB3	1:B:317:ILE:HD13	2.00	0.44
1:A:101:TYR:CE1	1:A:314:LEU:HD11	2.53	0.44
1:A:81:ALA:HB3	2:A:1:SO4:O2	2.18	0.44
1:B:72:THR:HG22	1:B:102:GLN:HB3	2.00	0.44
1:B:336:ARG:O	1:B:340:GLU:HG2	2.18	0.44
1:B:125:HIS:O	1:B:126:ARG:C	2.56	0.43
1:B:187:ARG:HA	1:B:187:ARG:HD3	1.84	0.43
1:B:212:ASP:OD1	1:B:217:ARG:HD3	2.19	0.43
1:B:194:ALA:HA	1:B:225:ASP:O	2.18	0.43
1:B:332:ARG:CG	1:B:334:MSE:HE1	2.49	0.43
1:B:253:CYS:HB2	1:B:259:ALA:HB2	2.01	0.42
1:A:194:ALA:HA	1:A:225:ASP:O	2.19	0.42
1:A:227:GLN:HB2	1:A:228:PRO:CD	2.49	0.42
1:A:286:GLN:HE22	1:B:231:MSE:H	1.67	0.42
1:A:116:LEU:HD11	1:A:140:PRO:HG2	2.02	0.41
1:A:126:ARG:N	1:A:127:PRO:CD	2.83	0.41
1:B:317:ILE:O	1:B:317:ILE:HG13	2.11	0.41
1:B:233:MSE:O	1:B:237:MSE:HG3	2.20	0.41
1:B:78:PRO:HD2	1:B:85:PHE:CE2	2.55	0.41
1:A:271:ILE:HG23	1:A:276:ARG:HD3	2.03	0.41
1:A:190:GLY:HA2	1:A:221:LEU:O	2.20	0.41
1:A:337:ARG:HH11	1:A:337:ARG:CG	2.21	0.41
1:A:260:ILE:HG12	1:A:291:CYS:SG	2.61	0.40
1:A:128:ASP:N	1:A:128:ASP:OD1	2.55	0.40
1:A:140:PRO:HA	1:A:143:ARG:HD2	2.03	0.40
1:A:139:GLU:O	1:A:143:ARG:NH1	2.55	0.40
1:A:92:ILE:HG22	1:A:96:LEU:HD22	2.03	0.40
1:B:119:LEU:HD21	1:B:145:LEU:CD1	2.52	0.40
1:A:119:LEU:O	1:A:123:LEU:HD13	2.21	0.40
1:A:124:GLN:HB2	1:A:124:GLN:HE21	1.59	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	269/339 (79%)	256 (95%)	12 (4%)	1 (0%)	34	42
1	B	269/339 (79%)	255 (95%)	12 (4%)	2 (1%)	22	26
All	All	538/678 (79%)	511 (95%)	24 (4%)	3 (1%)	25	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	B	283	ASN
1	B	126	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	212/259 (82%)	196 (92%)	16 (8%)	13	17
1	B	214/259 (83%)	204 (95%)	10 (5%)	26	37
All	All	426/518 (82%)	400 (94%)	26 (6%)	18	25

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	A	116	LEU
1	A	123	LEU
1	A	124	GLN
1	A	128	ASP
1	A	143	ARG
1	A	157	ASP
1	A	192	LEU
1	A	196	LEU
1	A	207	TYR
1	A	227	GLN
1	A	315	GLN
1	A	325	ARG
1	A	333	LEU
1	A	335	LEU
1	A	337	ARG
1	B	116	LEU
1	B	124	GLN
1	B	126	ARG
1	B	192	LEU
1	B	196	LEU
1	B	276	ARG
1	B	317	ILE
1	B	325	ARG
1	B	333	LEU
1	B	335	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	124	GLN
1	A	147	GLN
1	A	180	HIS
1	A	255	ASN
1	A	267	GLN
1	A	268	GLN
1	A	283	ASN
1	A	286	GLN
1	B	102	GLN
1	B	109	HIS
1	B	180	HIS
1	B	268	GLN

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Mol	Chain	Res	Type
1	B	286	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	B	2	-	4,4,4	1.01	0	6,6,6	0.71	0
2	SO4	A	1	-	4,4,4	0.94	0	6,6,6	0.72	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	SO4	1	0
2	A	1	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	263/339 (77%)	-0.01	3 (1%) 80 85	19, 33, 64, 72	0
1	B	263/339 (77%)	-0.06	1 (0%) 92 95	20, 33, 55, 73	0
All	All	526/678 (77%)	-0.04	4 (0%) 86 89	19, 33, 60, 73	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	ALA	3.6
1	A	143	ARG	2.9
1	A	139	GLU	2.8
1	A	319	GLY	2.5

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	2	5/5	0.94	0.25	40,47,48,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1	5/5	0.95	0.17	43,44,51,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.