



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:21 am BST

PDB ID : 3CO5  
Title : Crystal structure of sigma-54 interaction domain of putative transcriptional response regulator from *Neisseria gonorrhoeae*  
Authors : Osipiuk, J.; Hendricks, R.; Bigelow, L.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2008-03-27  
Resolution : 2.40 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 : 2.11  
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

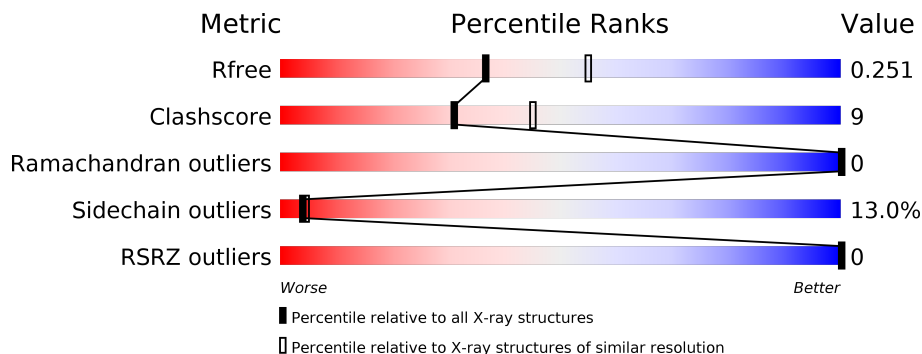
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	143	 73%      17%      • 6%
1	B	143	 72%      17%      • 8%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2064 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.

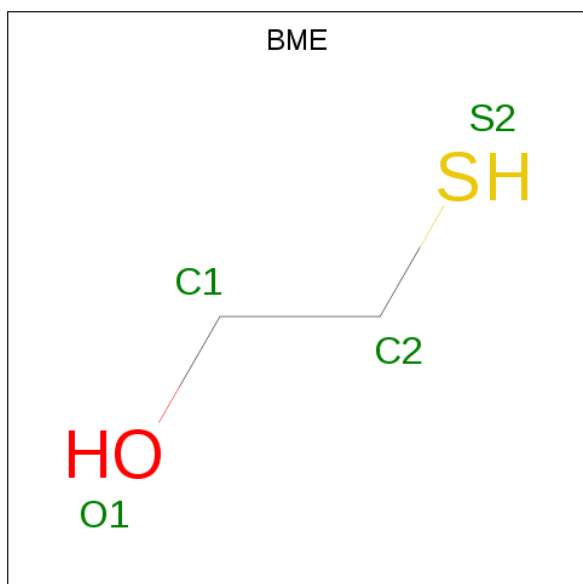
- Molecule 1 is a protein called Putative two-component system transcriptional response regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	134	1021	642	177	196	3	3	0	0	0
1	B	132	1010	637	175	192	3	3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	SER	-	EXPRESSION TAG	UNP Q5F5Q1
A	131	ASN	-	EXPRESSION TAG	UNP Q5F5Q1
A	132	ALA	-	EXPRESSION TAG	UNP Q5F5Q1
B	130	SER	-	EXPRESSION TAG	UNP Q5F5Q1
B	131	ASN	-	EXPRESSION TAG	UNP Q5F5Q1
B	132	ALA	-	EXPRESSION TAG	UNP Q5F5Q1

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

- Molecule 3 is water.

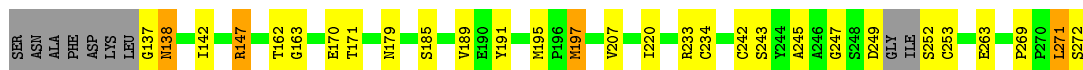
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	13	Total	O	0	0
			13	13		

### 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: Putative two-component system transcriptional response regulator

Chain A: 



- Molecule 1: Putative two-component system transcriptional response regulator

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.96 Å 67.96 Å 64.93 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.20 – 2.40 30.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.20-2.40) 99.7 (30.11-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.39 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.205 , 0.241 0.208 , 0.251	Depositor DCC
$R_{free}$ test set	644 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.6	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l 0.499 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% 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: BME

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	0.85	0/1036	0.84	1/1394 (0.1%)
1	B	0.86	0/1025	0.84	1/1381 (0.1%)
All	All	0.85	0/2061	0.84	2/2775 (0.1%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	247	GLY	N-CA-C	-5.42	99.55	113.10
1	B	267	ARG	NE-CZ-NH1	5.24	122.92	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	252	SER	Peptide
1	B	252	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	1021	0	1014	18	0
1	B	1010	0	1004	19	0
2	A	4	0	6	2	0
2	B	4	0	6	2	0
3	A	12	0	0	0	0
3	B	13	0	0	0	0
All	All	2064	0	2030	36	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 9.

All (36) 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:B:138:ASN:N	1:B:142:ILE:HG21	1.90	0.87
1:B:234:CYS:SG	2:B:301:BME:S2	2.46	0.76
1:A:242:CYS:HG	1:A:253:CYS:HG	0.74	0.74
1:A:197:MSE:HA	1:A:197:MSE:HE3	1.70	0.73
1:A:234:CYS:SG	2:A:301:BME:S2	2.63	0.72
1:A:189:VAL:CG2	1:A:220:ILE:HD13	2.21	0.71
1:A:189:VAL:HG22	1:A:220:ILE:HD13	1.73	0.70
1:B:233:ARG:HH21	1:B:233:ARG:CG	2.07	0.68
1:B:189:VAL:CG2	1:B:220:ILE:HD13	2.28	0.62
1:B:245:ALA:HB3	1:B:249:ASP:HB3	1.90	0.54
1:A:271:LEU:O	1:A:272:SER:CB	2.56	0.54
1:B:233:ARG:HH21	1:B:233:ARG:HG3	1.73	0.53
1:A:263:GLU:OE2	1:B:263:GLU:OE2	2.26	0.52
1:B:270:PRO:O	1:B:271:LEU:HD13	2.10	0.52
1:B:189:VAL:HG22	1:B:220:ILE:HD13	1.94	0.50
1:A:138:ASN:ND2	1:A:138:ASN:N	2.60	0.50
1:A:234:CYS:CB	2:A:301:BME:HS2	2.25	0.48
1:B:233:ARG:CG	1:B:233:ARG:NH2	2.71	0.47
1:B:201:GLN:HB2	2:B:301:BME:H11	1.96	0.47
1:B:189:VAL:HG21	1:B:220:ILE:HD13	1.95	0.46
1:B:138:ASN:N	1:B:142:ILE:HD13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:VAL:HG21	1:A:220:ILE:HD13	1.97	0.46
1:B:168:PRO:HB2	1:B:171:THR:HG23	1.96	0.46
1:A:189:VAL:HG22	1:A:220:ILE:CD1	2.44	0.45
1:B:245:ALA:N	1:B:249:ASP:OD2	2.47	0.45
1:A:147:ARG:HE	1:A:147:ARG:CA	2.28	0.44
1:A:147:ARG:HE	1:A:147:ARG:HA	1.83	0.44
1:A:245:ALA:HB3	1:A:249:ASP:OD2	2.18	0.44
1:A:137:GLY:HA3	1:A:138:ASN:HD22	1.83	0.43
1:B:195:MSE:N	1:B:196:PRO:CD	2.82	0.42
1:A:191:TYR:CD2	1:A:195:MSE:HE2	2.54	0.42
1:B:189:VAL:HG22	1:B:220:ILE:CD1	2.49	0.42
1:B:271:LEU:HD22	1:B:271:LEU:N	2.34	0.41
1:A:163:GLY:O	1:A:243:SER:HA	2.20	0.41
1:B:138:ASN:OD1	1:B:138:ASN:N	2.54	0.41
1:A:269:PRO:O	1:A:271:LEU:HD13	2.21	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	130/143 (91%)	124 (95%)	6 (5%)	0	100	100
1	B	128/143 (90%)	125 (98%)	3 (2%)	0	100	100
All	All	258/286 (90%)	249 (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	108/112 (96%)	96 (89%)	12 (11%)	6	8
1	B	107/112 (96%)	91 (85%)	16 (15%)	3	3
All	All	215/224 (96%)	187 (87%)	28 (13%)	4	4

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	142	ILE
1	A	147	ARG
1	A	162	THR
1	A	170	GLU
1	A	171	THR
1	A	179	ASN
1	A	185	SER
1	A	197	MSE
1	A	207	VAL
1	A	233	ARG
1	A	271	LEU
1	B	138	ASN
1	B	142	ILE
1	B	143	GLN
1	B	147	ARG
1	B	161	LEU
1	B	162	THR
1	B	170	GLU
1	B	171	THR
1	B	179	ASN
1	B	185	SER
1	B	193	ILE
1	B	197	MSE
1	B	232	GLU
1	B	233	ARG
1	B	254	GLU
1	B	271	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	146	ASN
1	A	179	ASN
1	A	201	GLN
1	B	179	ASN
1	B	201	GLN
1	B	221	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 carbohydrates 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	BME	A	301	-	3,3,3	0.30	0	1,2,2	0.04	0
2	BME	B	301	-	3,3,3	0.16	0	1,2,2	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BME	A	301	-	-	1/1/1/1	-
2	BME	B	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	BME	O1-C1-C2-S2
2	B	301	BME	O1-C1-C2-S2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	BME	2	0
2	B	301	BME	2	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	131/143 (91%)	-0.31	0	100, 100	33, 44, 64, 65	0
1	B	129/143 (90%)	-0.31	0	100, 100	33, 44, 69, 76	0
All	All	260/286 (90%)	-0.31	0	100, 100	33, 44, 65, 76	0

There are no RSRZ outliers to report.

### 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](#)

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	BME	B	301	4/4	0.90	0.20	89,90,90,91	0
2	BME	A	301	4/4	0.94	0.26	72,74,76,78	4

### 6.5 Other polymers [i](#)

There are no such residues in this entry.