



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 05:42 PM UTC

PDB ID : 3VIB / pdb_00003vib
Title : Structural basis for multidrug recognition and antimicrobial resistance by MTRR, an efflux pump regulator from *Neisseria Gonorrhoeae*
Authors : Kumaraswami, M.; Shafer, W.M.; Brennan, R.G.
Deposited on : 2011-09-27
Resolution : 2.40 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

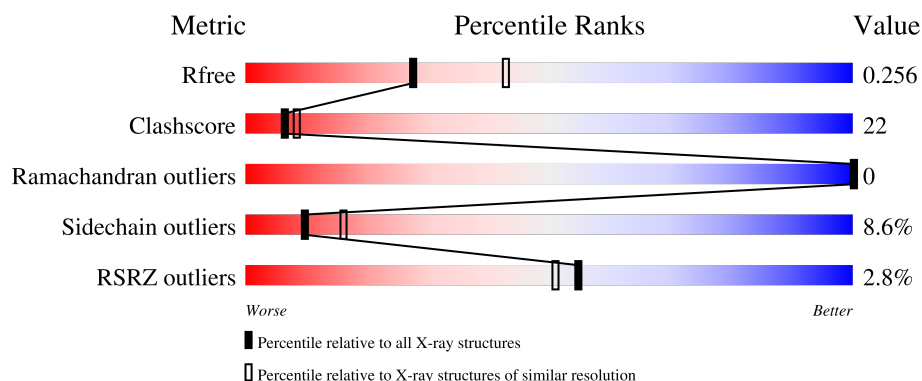
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	210	
1	B	210	
1	C	210	
1	D	210	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	C	212	-	-	X	-
3	CXS	A	212	-	-	X	-

2 Entry composition [i](#)

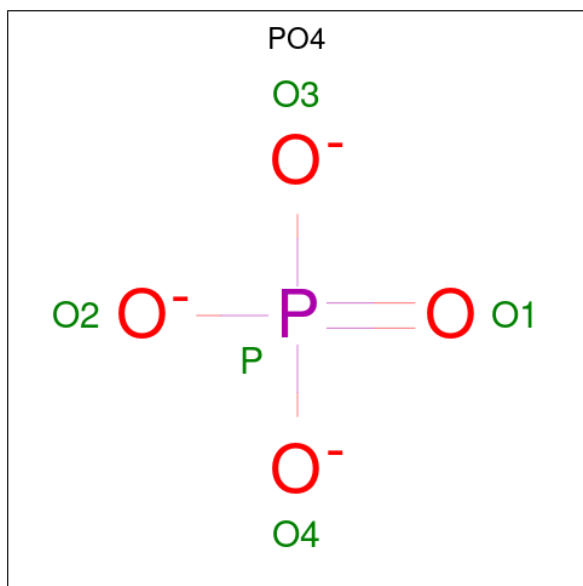
There are 4 unique types of molecules in this entry. The entry contains 6864 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MtrR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1570	1004	278	281	7			
1	B	194	Total	C	N	O	S	0	0	0
			1566	1001	279	279	7			
1	C	201	Total	C	N	O	S	0	0	0
			1601	1022	283	289	7			
1	D	194	Total	C	N	O	S	0	0	0
			1576	1007	279	283	7			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



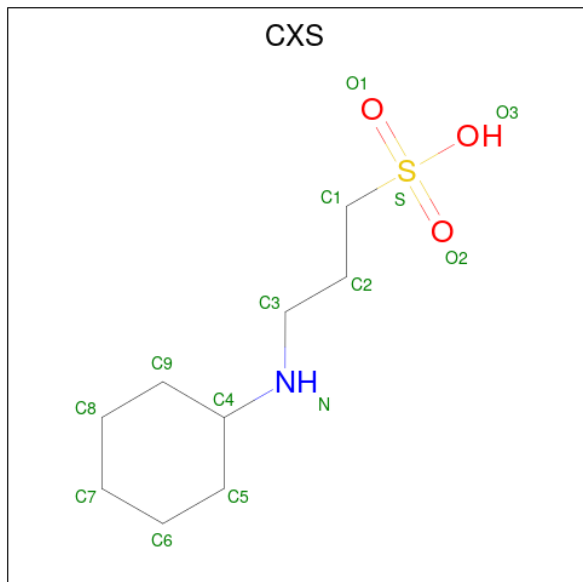
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

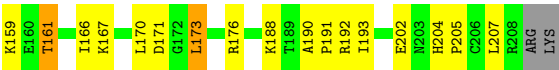
- Molecule 3 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (CCD ID: CXS) (formula: $C_9H_{19}NO_3S$).



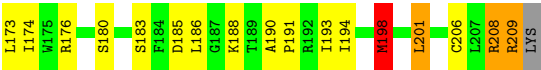
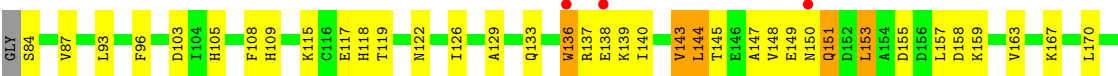
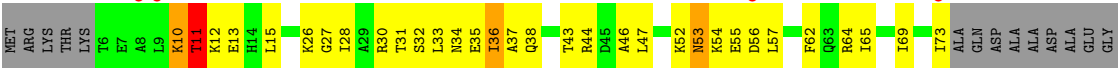
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	B	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	C	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	D	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total 124	O 124	0	0
4	B	125	Total 125	O 125	0	0
4	C	79	Total 79	O 79	0	0
4	D	132	Total 132	O 132	0	0



● Molecule 1: MtrR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.30Å 84.60Å 58.10Å 90.00° 103.90° 90.00°	Depositor
Resolution (Å)	45.46 – 2.40 45.46 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (45.46-2.40) 97.8 (45.46-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.256 0.212 , 0.256	Depositor DCC
R_{free} test set	6680 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6864	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CXS

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	0/1604	0.96	9/2165 (0.4%)
1	B	0.44	0/1600	0.95	9/2161 (0.4%)
1	C	0.44	0/1635	0.97	7/2211 (0.3%)
1	D	0.46	1/1610 (0.1%)	0.95	5/2175 (0.2%)
All	All	0.45	1/6449 (0.0%)	0.96	30/8712 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	198	MET	SD-CE	-6.00	1.64	1.79

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	THR	N-CA-C	-8.34	103.08	113.18
1	D	208	ARG	N-CA-C	8.12	122.49	112.59
1	A	72	CYS	N-CA-C	-7.98	100.58	113.19
1	B	54	LYS	N-CA-C	-7.64	102.96	111.82
1	C	114	LEU	N-CA-C	7.52	123.59	113.97

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	1570	0	1546	51	0
1	B	1566	0	1536	68	0
1	C	1601	0	1554	82	0
1	D	1576	0	1542	90	0
2	A	5	0	0	1	0
2	B	10	0	0	0	0
2	C	10	0	0	2	0
2	D	10	0	0	0	0
3	A	14	0	19	9	0
3	B	14	0	19	4	0
3	C	14	0	19	1	0
3	D	14	0	19	2	0
4	A	124	0	0	3	0
4	B	125	0	0	12	0
4	C	79	0	0	1	0
4	D	132	0	0	7	0
All	All	6864	0	6254	277	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 22.

The worst 5 of 277 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:136:TRP:CZ3	3:A:212:CXS:H62	1.23	1.62
1:A:136:TRP:CZ3	3:A:212:CXS:C6	2.17	1.26
1:D:137:ARG:HG2	1:D:167:LYS:HE3	1.36	1.07
1:D:34:ASN:OD1	1:D:44:ARG:HD3	1.62	1.00
1:D:10:LYS:HA	4:D:449:HOH:O	1.60	0.99

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	189/210 (90%)	184 (97%)	5 (3%)	0	100	100
1	B	190/210 (90%)	185 (97%)	5 (3%)	0	100	100
1	C	197/210 (94%)	190 (96%)	7 (4%)	0	100	100
1	D	190/210 (90%)	187 (98%)	3 (2%)	0	100	100
All	All	766/840 (91%)	746 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	164/179 (92%)	151 (92%)	13 (8%)	11	19
1	B	162/179 (90%)	148 (91%)	14 (9%)	10	16
1	C	163/179 (91%)	152 (93%)	11 (7%)	15	26
1	D	164/179 (92%)	146 (89%)	18 (11%)	6	9
All	All	653/716 (91%)	597 (91%)	56 (9%)	10	16

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	42	VAL
1	D	209	ARG
1	C	161	THR
1	D	201	LEU
1	D	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	122	ASN
1	C	200	ASN
1	D	151	GLN

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Mol	Chain	Res	Type
1	C	133	GLN
1	D	14	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	$\# Z > 2$
3	CXS	B	213	-	14,14,14	2.18	1 (7%)	18,18,18	1.27	2 (11%)
3	CXS	C	211	-	14,14,14	2.17	1 (7%)	18,18,18	1.26	2 (11%)
3	CXS	D	211	-	14,14,14	2.18	1 (7%)	18,18,18	1.26	2 (11%)
2	PO4	C	212	-	4,4,4	0.96	0	6,6,6	0.46	0
2	PO4	C	213	-	4,4,4	0.97	0	6,6,6	0.46	0
2	PO4	D	212	-	4,4,4	1.75	0	6,6,6	0.46	0
2	PO4	D	213	-	4,4,4	1.74	0	6,6,6	0.45	0
2	PO4	B	212	-	4,4,4	1.71	0	6,6,6	0.47	0
2	PO4	B	211	-	4,4,4	1.66	0	6,6,6	0.47	0
3	CXS	A	212	-	14,14,14	2.16	1 (7%)	18,18,18	1.26	2 (11%)
2	PO4	A	211	-	4,4,4	1.73	0	6,6,6	0.46	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
3	CXS	B	213	-	-	6/8/16/16	0/1/1/1
3	CXS	C	211	-	-	6/8/16/16	0/1/1/1
3	CXS	D	211	-	-	6/8/16/16	0/1/1/1
3	CXS	A	212	-	-	2/8/16/16	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	213	CXS	C1-S	-7.83	1.66	1.77
3	D	211	CXS	C1-S	-7.83	1.66	1.77
3	C	211	CXS	C1-S	-7.79	1.66	1.77
3	A	212	CXS	C1-S	-7.76	1.66	1.77

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	211	CXS	C3-N-C4	3.03	120.01	114.18
3	D	211	CXS	C3-N-C4	3.03	120.01	114.18
3	A	212	CXS	C3-N-C4	3.02	120.00	114.18
3	B	213	CXS	C3-N-C4	3.02	120.00	114.18
3	A	212	CXS	C2-C1-S	-2.46	109.47	113.25

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	213	CXS	C2-C1-S-O2
3	B	213	CXS	C5-C4-N-C3
3	C	211	CXS	C2-C1-S-O1
3	C	211	CXS	C2-C1-S-O2
3	C	211	CXS	S-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	213	CXS	4	0
3	C	211	CXS	1	0
3	D	211	CXS	2	0
2	C	212	PO4	2	0
3	A	212	CXS	9	0
2	A	211	PO4	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, 95th 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 ²)	Q<0.9
1	A	193/210 (91%)	0.10	4 (2%) 63 59	26, 45, 67, 81	0
1	B	194/210 (92%)	0.09	6 (3%) 51 47	27, 45, 64, 70	0
1	C	201/210 (95%)	0.24	5 (2%) 58 54	28, 47, 67, 96	0
1	D	194/210 (92%)	0.30	7 (3%) 46 42	28, 46, 70, 94	0
All	All	782/840 (93%)	0.18	22 (2%) 55 51	26, 46, 67, 96	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	ALA	4.9
1	A	73	ILE	3.9
1	D	56	ASP	3.7
1	A	136	TRP	3.4
1	D	150	ASN	3.3

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 oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
2	PO4	C	212	5/5	0.73	0.15	107,107,108,108	0
3	CXS	D	211	14/14	0.76	0.26	138,139,140,141	0
3	CXS	B	213	14/14	0.77	0.24	127,128,132,132	0
2	PO4	C	213	5/5	0.78	0.11	119,120,120,120	0
3	CXS	C	211	14/14	0.78	0.26	146,147,152,153	0
3	CXS	A	212	14/14	0.78	0.26	134,135,140,140	0
2	PO4	B	212	5/5	0.81	0.18	103,104,104,104	0
2	PO4	A	211	5/5	0.83	0.20	111,111,112,112	0
2	PO4	D	213	5/5	0.86	0.12	136,136,136,136	0
2	PO4	D	212	5/5	0.92	0.08	83,83,83,83	0
2	PO4	B	211	5/5	0.94	0.08	66,67,68,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.