



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 06:13 PM UTC

PDB ID : 2D45 / pdb_00002d45
Title : Crystal structure of the MecI-mecA repressor-operator complex
Authors : Safo, M.K.; Ko, T.-P.; Musayev, F.N.; Zhao, Q.; Wang, A.H.-J.; Archer, G.L.
Deposited on : 2005-10-09
Resolution : 3.80 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

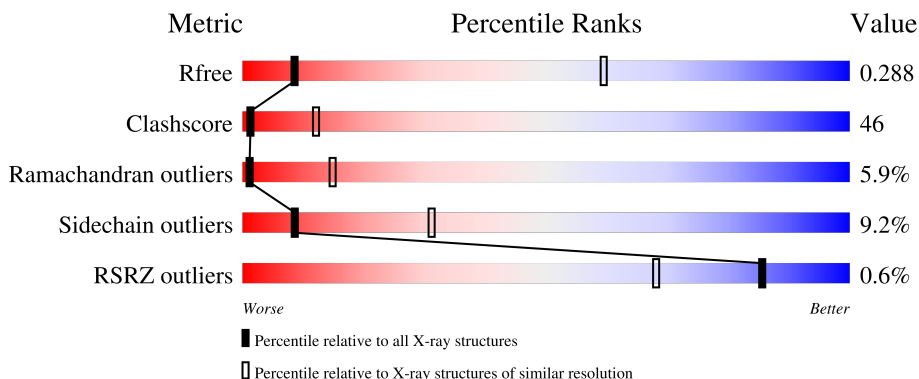
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



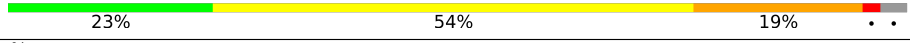

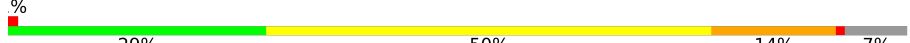
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	E	16	
1	F	16	
1	G	16	
1	H	16	
2	A	123	

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Mol	Chain	Length	Quality of chain
2	B	123	
2	C	123	
2	D	123	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5204 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 DNA chain called 5'-D(P*TP*AP*CP*TP*AP*CP*AP*TP*AP*TP*GP*TP*AP*GP*TP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	E	16	Total 328	C 158	N 58	O 96	P 16	0	0	0
1	F	16	Total 328	C 158	N 58	O 96	P 16	0	0	0
1	G	13	Total 265	C 128	N 46	O 78	P 13	0	0	0
1	H	12	Total 245	C 119	N 46	O 69	P 11	0	0	0

- Molecule 2 is a protein called Methicillin resistance regulatory protein mecI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	A	117	Total 990	C 638	N 161	O 188	Se 3	0	0	0
2	B	119	Total 1007	C 648	N 165	O 191	Se 3	0	0	0
2	C	117	Total 990	C 638	N 161	O 188	Se 3	0	0	0
2	D	115	Total 971	C 625	N 159	O 184	Se 3	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P68261
A	16	MSE	MET	modified residue	UNP P68261
A	21	MSE	MET	modified residue	UNP P68261
A	36	MSE	MET	modified residue	UNP P68261
B	1	MSE	MET	modified residue	UNP P68261
B	16	MSE	MET	modified residue	UNP P68261
B	21	MSE	MET	modified residue	UNP P68261

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Chain	Residue	Modelled	Actual	Comment	Reference
B	36	MSE	MET	modified residue	UNP P68261
C	1	MSE	MET	modified residue	UNP P68261
C	16	MSE	MET	modified residue	UNP P68261
C	21	MSE	MET	modified residue	UNP P68261
C	36	MSE	MET	modified residue	UNP P68261
D	1	MSE	MET	modified residue	UNP P68261
D	16	MSE	MET	modified residue	UNP P68261
D	21	MSE	MET	modified residue	UNP P68261
D	36	MSE	MET	modified residue	UNP P68261

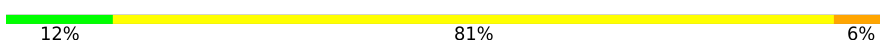
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0
3	G	4	Total O 4 4	0	0
3	H	5	Total O 5 5	0	0
3	A	16	Total O 16 16	0	0
3	B	14	Total O 14 14	0	0
3	C	11	Total O 11 11	0	0
3	D	28	Total O 28 28	0	0

3 Residue-property plots [i](#)

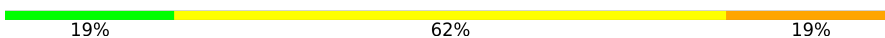
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 5'-D(P*TP*AP*CP*TP*AP*CP*AP*TP*AP*TP*GP*TP*AP*GP*TP*A)-3',

Chain E: 

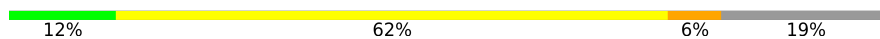


- Molecule 1: 5'-D(P*TP*AP*CP*TP*AP*CP*AP*TP*AP*TP*GP*TP*AP*GP*TP*A)-3',

Chain F: 

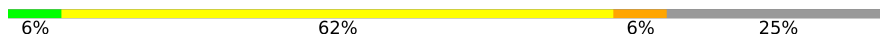


- Molecule 1: 5'-D(P*TP*AP*CP*TP*AP*CP*AP*TP*AP*TP*GP*TP*AP*GP*TP*A)-3',

Chain G: 



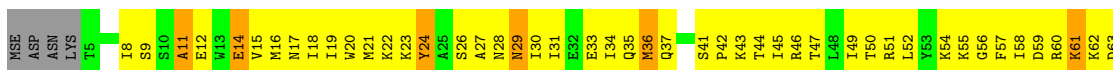
- Molecule 1: 5'-D(P*TP*AP*CP*TP*AP*CP*AP*TP*AP*TP*GP*TP*AP*GP*TP*A)-3',

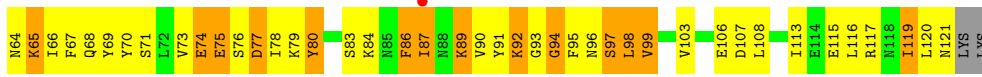
Chain H: 



- Molecule 2: Methicillin resistance regulatory protein mecI

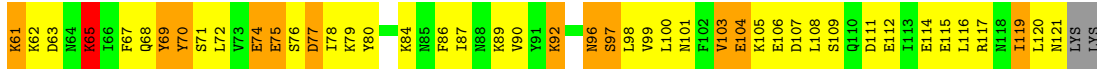
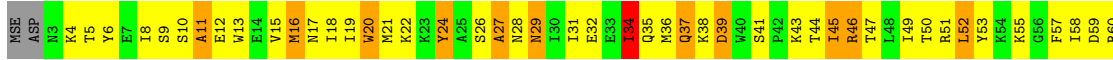
Chain A: 





- Molecule 2: Methicillin resistance regulatory protein mecI

Chain B: 23% 54% 19% ..



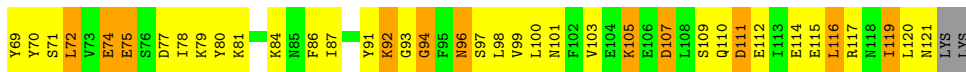
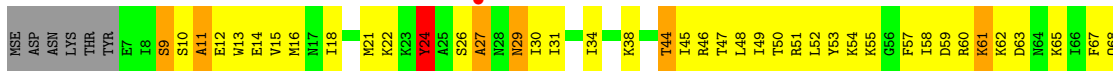
- Molecule 2: Methicillin resistance regulatory protein mecI

Chain C: % 35% 46% 13% • 5%



- Molecule 2: Methicillin resistance regulatory protein mecI

Chain D: % 29% 50% 14% • 7%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	61.46Å 61.46Å 419.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.80 40.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.00-3.80) 97.5 (40.00-3.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.264 , 0.297 0.253 , 0.288	Depositor DCC
R_{free} test set	493 reflections (5.37%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 109.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5204	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	E	0.61	0/367	0.85	0/564
1	F	0.50	0/367	0.85	1/564 (0.2%)
1	G	0.45	0/296	0.84	0/454
1	H	0.49	0/275	0.73	0/423
2	A	1.11	1/1005 (0.1%)	1.23	6/1344 (0.4%)
2	B	1.23	4/1022 (0.4%)	1.24	10/1366 (0.7%)
2	C	1.04	2/1005 (0.2%)	1.15	6/1344 (0.4%)
2	D	0.96	1/985 (0.1%)	1.13	9/1316 (0.7%)
All	All	0.98	8/5322 (0.2%)	1.10	32/7375 (0.4%)

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	E	0	1
1	F	0	2
1	G	0	1
1	H	0	1
2	A	0	1
All	All	0	6

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	45	ILE	CA-CB	-7.20	1.46	1.54
2	B	5	THR	N-CA	6.91	1.54	1.46
2	D	15	VAL	CA-CB	-6.79	1.46	1.54
2	B	4	LYS	CA-C	6.55	1.61	1.52
2	B	5	THR	CA-CB	5.97	1.64	1.53

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	65	LYS	N-CA-C	-9.16	98.71	113.19
1	F	216	DA	C2'-C3'-O3'	-7.91	99.64	111.50
2	A	55	LYS	N-CA-C	-7.89	102.64	111.71
2	B	57	PHE	N-CA-C	-7.72	104.36	114.31
2	A	119	ILE	N-CA-C	-7.04	105.19	113.42

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	212	DT	Sidechain
1	F	211	DG	Sidechain
1	F	212	DT	Sidechain
1	G	211	DG	Sidechain
1	H	212	DT	Sidechain

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	E	328	0	183	25	0
1	F	328	0	183	18	1
1	G	265	0	149	26	0
1	H	245	0	138	21	0
2	A	990	0	997	108	1
2	B	1007	0	1016	123	0
2	C	990	0	997	104	1
2	D	971	0	981	98	0
3	A	16	0	0	0	0
3	B	14	0	0	0	0
3	C	11	0	0	0	0
3	D	28	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	4	0	0	0	0
3	H	5	0	0	0	0
All	All	5204	0	4644	451	2

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 46.

The worst 5 of 451 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)
2:C:16:MSE:HE1	2:C:57:PHE:HB3	1.22	1.13
2:B:92:LYS:HE2	2:B:92:LYS:HA	1.31	1.09
1:H:211:DG:H2''	1:H:212:DT:H5''	1.33	1.07
2:C:16:MSE:HE1	2:C:57:PHE:CB	1.85	1.07
2:A:74:GLU:HB3	2:A:77:ASP:HB2	1.44	0.99

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:36:MSE:O	2:C:46:ARG:NH2[1_665]	2.16	0.04
1:F:201:DT:P	1:F:216:DA:O3'[4_765]	2.17	0.03

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	
2	A	115/123 (94%)	95 (83%)	11 (10%)	9 (8%)	1	11
2	B	117/123 (95%)	91 (78%)	20 (17%)	6 (5%)	1	17
2	C	115/123 (94%)	87 (76%)	22 (19%)	6 (5%)	1	17
2	D	113/123 (92%)	85 (75%)	22 (20%)	6 (5%)	1	16
All	All	460/492 (94%)	358 (78%)	75 (16%)	27 (6%)	1	15

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	75	GLU
2	C	75	GLU
2	C	94	GLY
2	D	75	GLU
2	A	35	GLN

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
2	A	111/113 (98%)	101 (91%)	10 (9%)	9 32
2	B	113/113 (100%)	96 (85%)	17 (15%)	3 16
2	C	111/113 (98%)	103 (93%)	8 (7%)	13 39
2	D	109/113 (96%)	103 (94%)	6 (6%)	19 45
All	All	444/452 (98%)	403 (91%)	41 (9%)	8 31

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	18	ILE
2	D	24	TYR
2	C	22	LYS
2	C	74	GLU
2	D	34	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	37	GLN
2	B	110	GLN
2	D	35	GLN
2	D	28	ASN
2	D	29	ASN

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 oligosaccharides 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 [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	E	16/16 (100%)	-0.23	0 100 100	97, 117, 141, 144	0
1	F	16/16 (100%)	-0.34	0 100 100	109, 124, 135, 141	0
1	G	13/16 (81%)	-0.20	0 100 100	127, 141, 162, 163	0
1	H	12/16 (75%)	0.03	0 100 100	122, 139, 182, 191	0
2	A	114/123 (92%)	-0.36	1 (0%) 81 60	71, 97, 173, 175	0
2	B	116/123 (94%)	-0.47	0 100 100	74, 102, 141, 146	0
2	C	114/123 (92%)	-0.33	1 (0%) 81 60	76, 124, 183, 186	0
2	D	112/123 (91%)	-0.23	1 (0%) 81 60	87, 123, 152, 154	0
All	All	513/556 (92%)	-0.33	3 (0%) 85 68	71, 114, 171, 191	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	111	ASP	2.3
2	D	27	ALA	2.2
2	A	87	ILE	2.0

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.