W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:38 AM GMT

PDB ID	:	4K3V
Title	:	Structure of Staphylococcus aureus MntC
Authors	:	Parris, K.D.; Mosyak, L.
Deposited on	:	2013-04-11
Resolution	:	2.20 Å(reported)

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1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.20 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		3
Ramachandran outliers		0.8%
Sidechain outliers		1.5%
RSRZ outliers		9.6%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
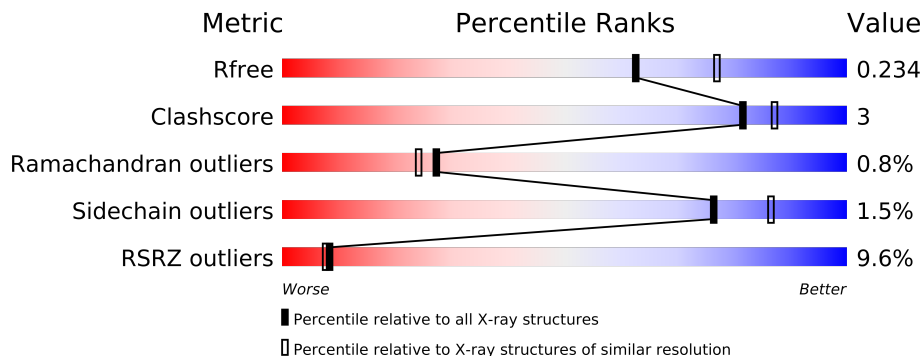
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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 >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	309	
1	B	309	

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4404 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ABC superfamily ATP binding cassette transporter, binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total 2027	C 1288	N 340	O 393	S 6	0	0	0
1	B	278	Total 2221	C 1406	N 371	O 437	S 7	0	0	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mn 1	0	0
2	A	1	Total 1	Mn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total 62	O 62	0	0
3	B	92	Total 92	O 92	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
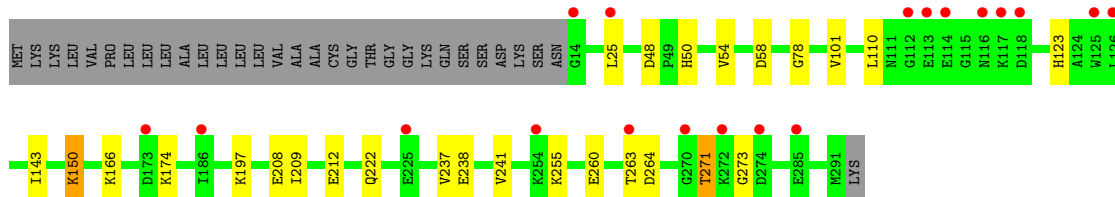
• Molecule 1: ABC superfamily ATP binding cassette transporter, binding protein

Chain A:
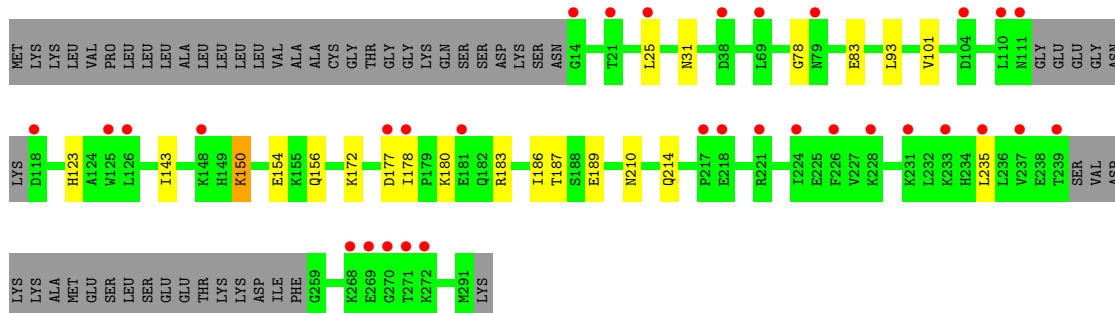
• Molecule 1: ABC superfamily ATP binding cassette transporter, binding protein

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.48Å 68.36Å 107.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.00 – 2.20 22.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	79.0 (23.00-2.20) 79.0 (22.30-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.19 (at 2.19Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.198 , 0.219 0.205 , 0.234	Depositor DCC
R_{free} test set	1039 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 60.2	EDS
Estimated twinning fraction	0.096 for k,h,-l	Xtriage
L-test for twinning	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Outliers	0 of 20528 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4404	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	0/2064	0.71	2/2772 (0.1%)
1	B	0.46	0/2261	0.67	0/3035
All	All	0.47	0/4325	0.69	2/5807 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	ILE	N-CA-C	-7.39	91.04	111.00
1	A	177	ASP	C-N-CA	5.04	134.31	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2   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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2027	0	2031	10	0
1	B	2221	0	2224	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	62	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	92	0	0	3	0
All	All	4404	0	4255	27	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (27) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:263:THR:HG23	1:B:264:ASP:H	1.39	0.87
1:A:186:ILE:HG21	1:A:235:LEU:HD23	1.65	0.79
1:A:186:ILE:CG2	1:A:235:LEU:HD23	2.20	0.71
1:B:263:THR:HG21	3:B:419:HOH:O	1.96	0.64
1:A:25:LEU:HD22	1:A:101:VAL:HG21	1.78	0.64
1:A:187:THR:HG23	1:A:189:GLU:O	1.97	0.64
1:B:25:LEU:CD2	1:B:101:VAL:HG21	2.28	0.63
1:A:180:LYS:HA	1:A:183:ARG:HD3	1.84	0.59
1:B:25:LEU:HD22	1:B:101:VAL:HG21	1.86	0.57
1:B:263:THR:HG23	1:B:264:ASP:N	2.16	0.54
1:A:25:LEU:CD2	1:A:101:VAL:HG21	2.37	0.54
1:B:54:VAL:HG13	1:B:58:ASP:HB2	1.88	0.53
1:B:166:LYS:HG3	3:B:488:HOH:O	2.09	0.52
1:B:25:LEU:HD21	1:B:101:VAL:HG21	1.92	0.52
1:B:238:GLU:HG2	1:B:241:VAL:HG22	1.92	0.51
1:A:31:ASN:O	1:A:156:GLN:HG3	2.15	0.47
1:B:209:ILE:O	1:B:212:GLU:HG2	2.15	0.47
1:B:143:ILE:HG23	1:B:150:LYS:HB2	1.97	0.47
1:B:222:GLN:NE2	3:B:417:HOH:O	2.48	0.46
1:A:83:GLU:HG3	1:A:93:LEU:HD11	1.99	0.45
1:A:210:ASN:HA	1:A:214:GLN:HE21	1.82	0.44
1:A:143:ILE:HG23	1:A:150:LYS:HB2	1.99	0.44
1:B:255:LYS:HD3	1:B:255:LYS:HA	1.89	0.43
1:B:110:LEU:HD22	1:B:208:GLU:HG2	2.01	0.42
1:B:48:ASP:OD1	1:B:50:HIS:HD2	2.03	0.41
1:B:271:THR:HG23	1:B:273:GLY:H	1.85	0.41
1:B:237:VAL:O	1:B:260:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	247/309 (80%)	236 (96%)	9 (4%)	2 (1%)	27	24
1	B	276/309 (89%)	267 (97%)	7 (2%)	2 (1%)	30	28
All	All	523/618 (85%)	503 (96%)	16 (3%)	4 (1%)	27	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	B	123	HIS
1	A	78	GLY
1	B	78	GLY

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	223/270 (83%)	220 (99%)	3 (1%)	80	89
1	B	245/270 (91%)	241 (98%)	4 (2%)	75	85
All	All	468/540 (87%)	461 (98%)	7 (2%)	76	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	LYS
1	A	154	GLU
1	A	172	LYS
1	B	150	LYS
1	B	174	LYS

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Mol	Chain	Res	Type
1	B	197	LYS
1	B	271	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	214	GLN
1	A	234	HIS
1	B	79	ASN
1	B	111	ASN
1	B	222	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

5.7 Other polymers (i)

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	253/309 (81%)	0.70	32 (12%)	4	4	18, 40, 71, 89	0
1	B	278/309 (89%)	0.32	19 (6%)	17	16	16, 35, 60, 73	0
All	All	531/618 (85%)	0.50	51 (9%)	8	8	16, 37, 66, 89	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	LYS	6.0
1	A	270	GLY	4.7
1	A	217	PRO	4.2
1	A	235	LEU	4.0
1	A	79	ASN	3.9
1	B	114	GLU	3.8
1	B	225	GLU	3.7
1	B	117	LYS	3.6
1	A	118	ASP	3.5
1	A	178	ILE	3.3
1	B	14	GLY	3.2
1	A	228	LYS	3.1
1	A	181	GLU	3.0
1	A	239	THR	3.0
1	A	177	ASP	3.0
1	B	272	LYS	2.9
1	B	173	ASP	2.9
1	B	125	TRP	2.7
1	A	126	LEU	2.7
1	B	118	ASP	2.7
1	A	111	ASN	2.7
1	A	269	GLU	2.6
1	A	271	THR	2.6
1	A	104	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	110	LEU	2.6
1	A	125	TRP	2.6
1	A	268	LYS	2.6
1	A	272	LYS	2.6
1	B	254	LYS	2.6
1	A	226	PHE	2.5
1	B	113	GLU	2.5
1	B	285	GLU	2.5
1	A	231	LYS	2.5
1	A	237	VAL	2.4
1	B	25	LEU	2.4
1	A	25	LEU	2.4
1	A	14	GLY	2.4
1	A	218	GLU	2.4
1	B	116	ASN	2.3
1	B	126	LEU	2.3
1	A	148	LYS	2.3
1	A	224	ILE	2.2
1	A	38	ASP	2.2
1	A	221	ARG	2.2
1	A	69	LEU	2.2
1	B	112	GLY	2.1
1	B	274	ASP	2.1
1	A	21	THR	2.1
1	B	263	THR	2.1
1	B	186	ILE	2.1
1	B	270	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MN	B	301	1/1	0.11	-0.96	20,20,20,20	0
2	MN	A	301	1/1	0.08	-2.63	30,30,30,30	0

6.5 Other polymers ⓘ

There are no such residues in this entry.