



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5FCD / pdb\_00005fcd  
Title : Crystal structure of MccD protein  
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Deposited on : 2015-12-15  
Resolution : 2.10 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.

The types of validation reports are described at

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

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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)  
Xtrriage (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

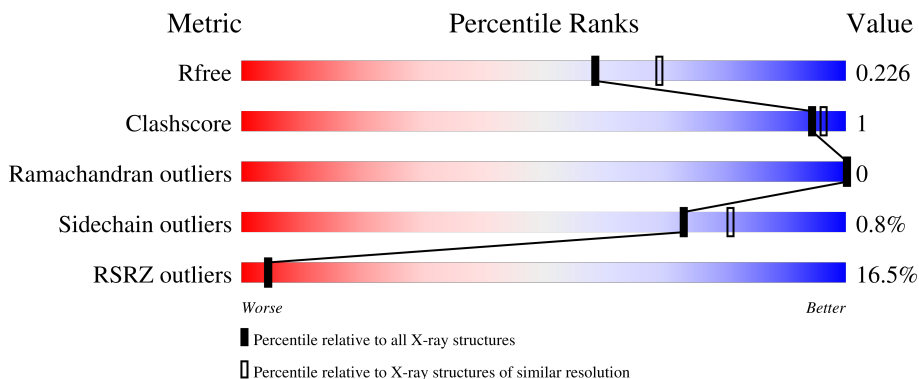
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	D	5	100%
2	E	6	100%
3	A	267	12% (red), 80% (green), 5% (yellow), 15% (grey)
3	B	267	15% (red), 83% (green), 5% (yellow), 15% (grey)

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7451 atoms, of which 3478 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 UNK-UNK-UNK-MSE-UNK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	Se			
1	D	5	59	17	31	5	5	1	0	0	0

- Molecule 2 is a protein called UNK-UNK-UNK-UNK-MSE-UNK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	Se			
2	E	6	69	20	36	6	6	1	0	0	0

- Molecule 3 is a protein called MccD.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
3	A	228	3600	1177	1752	315	344	8	4	0	3	0
3	B	228	3457	1141	1659	309	336	7	5	0	1	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total	O	0	0
			137	137		
5	B	128	Total	O	0	0
			128	128		

### 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: UNK-UNK-UNK-MSE-UNK

Chain D:  100%


There are no outlier residues recorded for this chain.

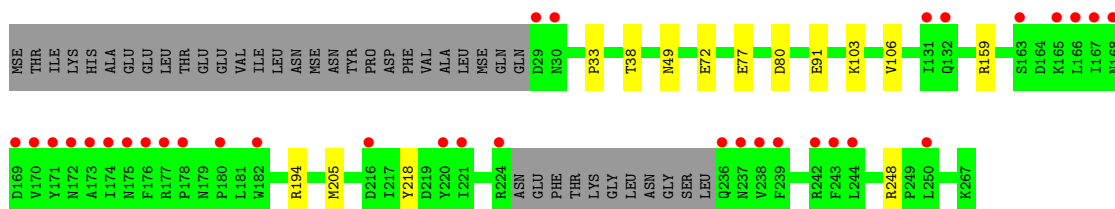
- Molecule 2: UNK-UNK-UNK-UNK-MSE-UNK

Chain E:  100%


There are no outlier residues recorded for this chain.

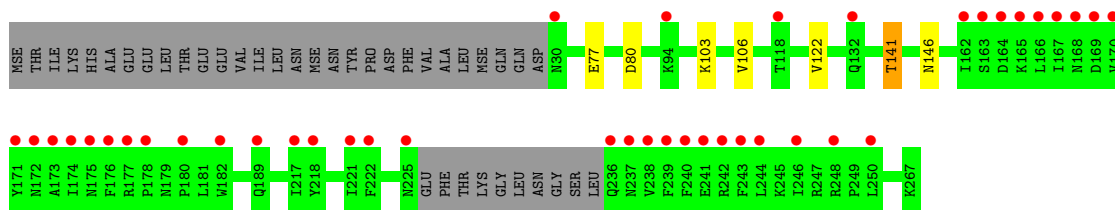
- Molecule 3: MccD

Chain A:  12% 80% 5% 15%



- Molecule 3: MccD

Chain B:  15% 83% 15%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.10Å 95.10Å 128.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.22 – 2.10 39.22 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.22-2.10) 97.1 (39.22-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.10Å)	Xtrriage
Refinement program	PHENIX dev_1888	Depositor
R, $R_{free}$	0.199 , 0.223 0.199 , 0.226	Depositor DCC
$R_{free}$ test set	1875 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 68.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: CL

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	D	0.06	0/7	0.33	0/7
2	E	0.22	0/7	0.61	0/7
3	A	0.28	0/1900	0.60	0/2562
3	B	0.28	0/1836	0.62	0/2482
All	All	0.28	0/3750	0.61	0/5058

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	D	28	31	15	0	0
2	E	33	36	16	0	0
3	A	1848	1752	1741	6	1
3	B	1798	1659	1657	3	0
4	A	1	0	0	0	0
5	A	137	0	0	1	1
5	B	128	0	0	0	1
All	All	3973	3478	3429	9	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 1.

All (9) 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)
3:A:159:ARG:NH2	3:A:205:MSE:O	2.27	0.68
3:A:194:ARG:N	5:A:402:HOH:O	2.40	0.53
3:A:49:ASN:HA	3:A:72:GLU:CG	2.49	0.43
3:B:80:ASP:O	3:B:106:VAL:HA	2.19	0.42
3:A:77:GLU:HA	3:A:103:LYS:O	2.19	0.42
3:A:33:PRO:O	3:A:38:THR:OG1	2.34	0.41
3:A:80:ASP:O	3:A:106:VAL:HA	2.20	0.41
3:B:122:VAL:HG21	3:B:141:THR:HG23	2.03	0.41
3:B:77:GLU:HA	3:B:103:LYS:O	2.21	0.41

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)
5:A:535:HOH:O	5:B:416:HOH:O[5_555]	2.14	0.06
3:A:91:GLU:OE1	3:A:218:TYR:HH[2_545]	1.56	0.04

## 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	D	1/5 (20%)	1 (100%)	0	0	100	100
2	E	1/6 (17%)	0	1 (100%)	0	100	100
3	A	227/267 (85%)	219 (96%)	8 (4%)	0	100	100
3	B	225/267 (84%)	218 (97%)	7 (3%)	0	100	100
All	All	454/545 (83%)	438 (96%)	16 (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	D	-	1 (100%)	0	100	100
2	E	-	1 (100%)	0	100	100
3	A	197/233 (84%)	196 (100%)	1 (0%)	81	88
3	B	184/233 (79%)	182 (99%)	2 (1%)	65	74
All	All	383/466 (82%)	380 (99%)	3 (1%)	73	81

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	248	ARG
3	B	141	THR
3	B	146	ASN

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

Mol	Chain	Res	Type
3	A	45	HIS
3	A	142	HIS
3	A	188	HIS
3	A	257	GLN
3	B	117	ASN
3	B	127	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](#)

Of 1 ligands modelled in this entry, 1 is 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.

No monomer is involved in short contacts.

## 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

### 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, 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	D	0/5	-	-	-	-
2	E	0/6	-	-	-	-
3	A	224/267 (83%)	0.61	33 (14%) <b>6</b> <b>6</b>	16, 37, 96, 136	2 (0%)
3	B	224/267 (83%)	0.71	41 (18%) <b>3</b> <b>3</b>	19, 36, 117, 208	1 (0%)
All	All	448/545 (82%)	0.66	74 (16%) <b>4</b> <b>4</b>	16, 37, 109, 208	3 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	167	ILE	8.3
3	B	173	ALA	7.2
3	B	174	ILE	6.8
3	A	167	ILE	6.5
3	B	170	VAL	6.3
3	B	175	ASN	6.0
3	A	176	PHE	5.9
3	B	168	ASN	5.7
3	A	224	ARG	5.5
3	A	175	ASN	5.2
3	A	173	ALA	5.1
3	B	176	PHE	5.0
3	A	174	ILE	4.6
3	B	166	LEU	4.6
3	B	169	ASP	4.6
3	B	172	ASN	4.4
3	A	220	TYR	4.2
3	B	171	TYR	4.2
3	B	237	ASN	4.0
3	A	170	VAL	4.0
3	A	169	ASP	4.0
3	A	172	ASN	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	B	178	PRO	3.8
3	B	225	ASN	3.7
3	B	238	VAL	3.6
3	A	171	TYR	3.6
3	A	238	VAL	3.6
3	B	243	PHE	3.5
3	A	168	ASN	3.4
3	A	237	ASN	3.4
3	B	177	ARG	3.4
3	A	165	LYS	3.4
3	B	240	PHE	3.4
3	A	239	PHE	3.3
3	A	29	ASP	3.3
3	B	162	ILE	3.2
3	A	243	PHE	3.2
3	B	246	ILE	3.1
3	B	222	PHE	3.1
3	B	163	SER	3.1
3	A	166	LEU	3.1
3	A	177	ARG	3.0
3	B	30	ASN	2.9
3	B	221	ILE	2.8
3	B	242	ARG	2.7
3	B	132	GLN	2.7
3	A	250	LEU	2.7
3	A	182	TRP	2.7
3	B	239	PHE	2.7
3	A	221	ILE	2.5
3	A	163	SER	2.5
3	B	182	TRP	2.5
3	A	131	ILE	2.5
3	A	244	LEU	2.4
3	B	94	LYS	2.4
3	B	164	ASP	2.4
3	B	180	PRO	2.4
3	B	165	LYS	2.3
3	B	250	LEU	2.3
3	B	217	ILE	2.3
3	B	248	ARG	2.2
3	A	132	GLN	2.2
3	A	30	ASN	2.2
3	B	118	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	A	236	GLN	2.2
3	B	218	TYR	2.2
3	A	242	ARG	2.2
3	B	236	GLN	2.2
3	A	216	ASP	2.2
3	B	241	GLU	2.1
3	B	244	LEU	2.0
3	A	178	PRO	2.0
3	A	180	PRO	2.0
3	B	189	GLN	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 [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
4	CL	A	301	1/1	0.98	0.03	19,19,19,19	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.