



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 02:39 pm GMT

PDB ID : 5M94
Title : Crystal structure of Staphylococcus capitis divalent metal ion transporter (DMT) in complex with nanobody
Authors : Dutzler, R.; Ehrnstorfer, I.A.
Deposited on : 2016-10-31
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

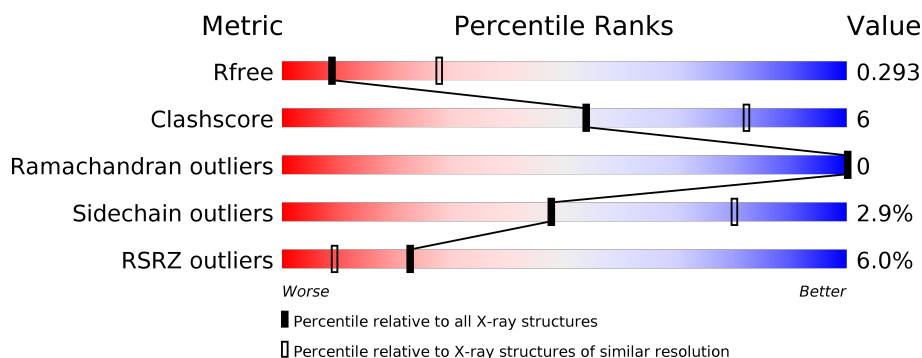
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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. 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	415	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>••</div> </div> </div>
1	C	415	<div> <div>9%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>••</div> </div> </div>
2	B	123	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>•</div> </div> </div>
2	D	123	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>•</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8048 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 Divalent metal cation transporter MntH.

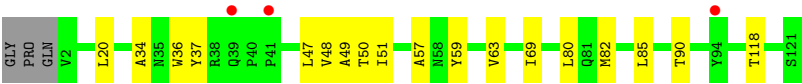
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3101	2060	492	537	12			
1	C	401	Total	C	N	O	S	0	0	0
			3101	2060	492	537	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	initiating methionine	UNP A0A0S4MEX1
A	42	ALA	-	expression tag	UNP A0A0S4MEX1
A	361	SER	ALA	engineered mutation	UNP A0A0S4MEX1
A	449	ALA	-	expression tag	UNP A0A0S4MEX1
A	450	LEU	-	expression tag	UNP A0A0S4MEX1
A	451	GLU	-	expression tag	UNP A0A0S4MEX1
A	452	VAL	-	expression tag	UNP A0A0S4MEX1
A	453	LEU	-	expression tag	UNP A0A0S4MEX1
A	454	PHE	-	expression tag	UNP A0A0S4MEX1
A	455	GLN	-	expression tag	UNP A0A0S4MEX1
C	41	MET	-	initiating methionine	UNP A0A0S4MEX1
C	42	ALA	-	expression tag	UNP A0A0S4MEX1
C	361	SER	ALA	engineered mutation	UNP A0A0S4MEX1
C	449	ALA	-	expression tag	UNP A0A0S4MEX1
C	450	LEU	-	expression tag	UNP A0A0S4MEX1
C	451	GLU	-	expression tag	UNP A0A0S4MEX1
C	452	VAL	-	expression tag	UNP A0A0S4MEX1
C	453	LEU	-	expression tag	UNP A0A0S4MEX1
C	454	PHE	-	expression tag	UNP A0A0S4MEX1
C	455	GLN	-	expression tag	UNP A0A0S4MEX1

- Molecule 2 is a protein called CAMELID ANTIBODY FRAGMENT, NANOBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total 923	C 564	N 172	O 183	S 4	0	0	0
2	D	120	Total 923	C 564	N 172	O 183	S 4	0	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	114.35Å 114.35Å 257.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.93 – 3.10 46.22 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.93-3.10) 99.4 (46.22-3.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.237 , 0.273 0.249 , 0.293	Depositor DCC
R_{free} test set	1785 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	118.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 89.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8048	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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 [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	A	0.26	0/3164	0.41	0/4306
1	C	0.26	0/3164	0.41	0/4306
2	B	0.25	0/937	0.46	0/1268
2	D	0.25	0/937	0.46	0/1268
All	All	0.26	0/8202	0.42	0/11148

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	A	3101	0	3279	43	0
1	C	3101	0	3279	38	0
2	B	923	0	897	12	0
2	D	923	0	897	10	0
All	All	8048	0	8352	100	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 6.

The worst 5 of 100 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:94:LYS:HD3	1:A:238:GLN:HE22	1.51	0.73
1:C:94:LYS:HD3	1:C:238:GLN:HE22	1.54	0.73
1:C:154:VAL:HG22	1:C:356:ARG:HE	1.57	0.69
2:D:20:LEU:HD12	2:D:80:LEU:HD23	1.78	0.66
1:A:154:VAL:HG22	1:A:356:ARG:HE	1.60	0.64

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	399/415 (96%)	389 (98%)	10 (2%)	0	100	100
1	C	399/415 (96%)	388 (97%)	11 (3%)	0	100	100
2	B	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
2	D	118/123 (96%)	118 (100%)	0	0	100	100
All	All	1034/1076 (96%)	1012 (98%)	22 (2%)	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	339/350 (97%)	326 (96%)	13 (4%)	38	74
1	C	339/350 (97%)	327 (96%)	12 (4%)	41	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	98/100 (98%)	98 (100%)	0	100	100
2	D	98/100 (98%)	98 (100%)	0	100	100
All	All	874/900 (97%)	849 (97%)	25 (3%)	48	80

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	420	THR
1	C	158	LEU
1	C	420	THR
1	A	440	LEU
1	C	165	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	C	238	GLN
2	D	13	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

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 [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	401/415 (96%)	-0.03	14 (3%) 44 22	63, 113, 166, 226	0
1	C	401/415 (96%)	0.17	36 (8%) 10 4	75, 147, 219, 277	0
2	B	120/123 (97%)	0.21	10 (8%) 12 4	83, 114, 157, 195	0
2	D	120/123 (97%)	-0.19	3 (2%) 58 35	88, 115, 156, 200	0
All	All	1042/1076 (96%)	0.06	63 (6%) 23 9	63, 121, 198, 277	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	415	PRO	7.3
1	C	414	GLY	6.2
1	C	259	ILE	5.9
1	C	168	ILE	5.1
1	A	421	TRP	4.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.