



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 19, 2023 – 04:09 am BST

PDB ID : 8PNL  
Title : Outward-open conformation of a Major Facilitator Superfamily (MFS) transporter MHAS2168, a homologue of Rv1410 from *M. tuberculosis*, in complex with an alpaca nanobody  
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Deposited on : 2023-06-30  
Resolution : 2.70 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](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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

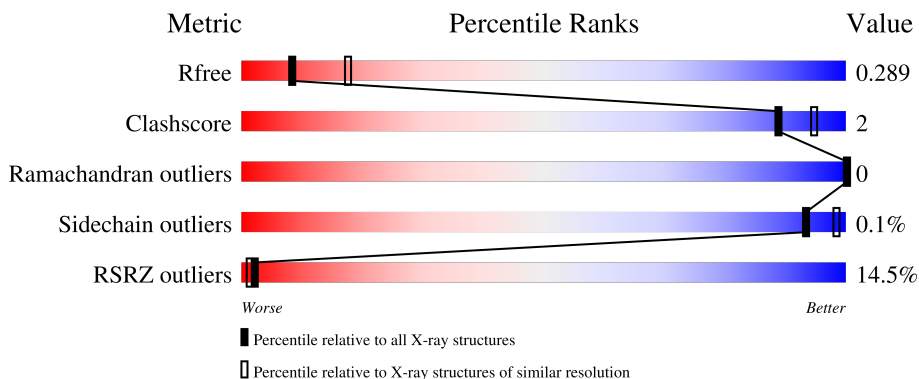
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	A	543	
1	C	543	
2	B	121	
2	D	121	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18026 atoms, of which 9202 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 Putative triacylglyceride transporter.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	483	7310	2341	3758	601	600	10	0	0	0
1	C	486	7358	2356	3781	605	606	10	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP K5B8L6
A	1	SER	-	expression tag	UNP K5B8L6
A	536	ALA	-	expression tag	UNP K5B8L6
A	537	LEU	-	expression tag	UNP K5B8L6
A	538	GLU	-	expression tag	UNP K5B8L6
A	539	VAL	-	expression tag	UNP K5B8L6
A	540	LEU	-	expression tag	UNP K5B8L6
A	541	PHE	-	expression tag	UNP K5B8L6
A	542	GLN	-	expression tag	UNP K5B8L6
C	0	MET	-	initiating methionine	UNP K5B8L6
C	1	SER	-	expression tag	UNP K5B8L6
C	536	ALA	-	expression tag	UNP K5B8L6
C	537	LEU	-	expression tag	UNP K5B8L6
C	538	GLU	-	expression tag	UNP K5B8L6
C	539	VAL	-	expression tag	UNP K5B8L6
C	540	LEU	-	expression tag	UNP K5B8L6
C	541	PHE	-	expression tag	UNP K5B8L6
C	542	GLN	-	expression tag	UNP K5B8L6

- Molecule 2 is a protein called Nb\_H2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	111	1688	533	836	153	161	5	0	0	0

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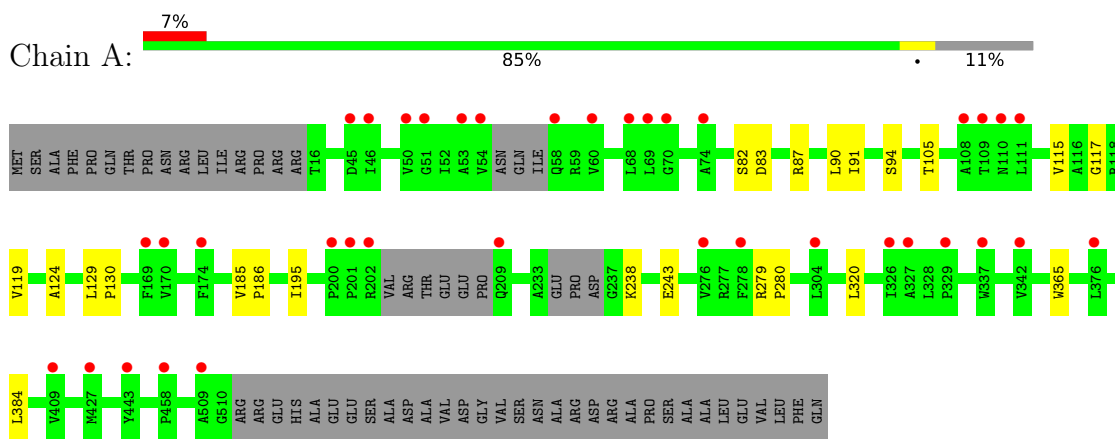
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	D	110	1670	528	827	151	159	5	0	0	0

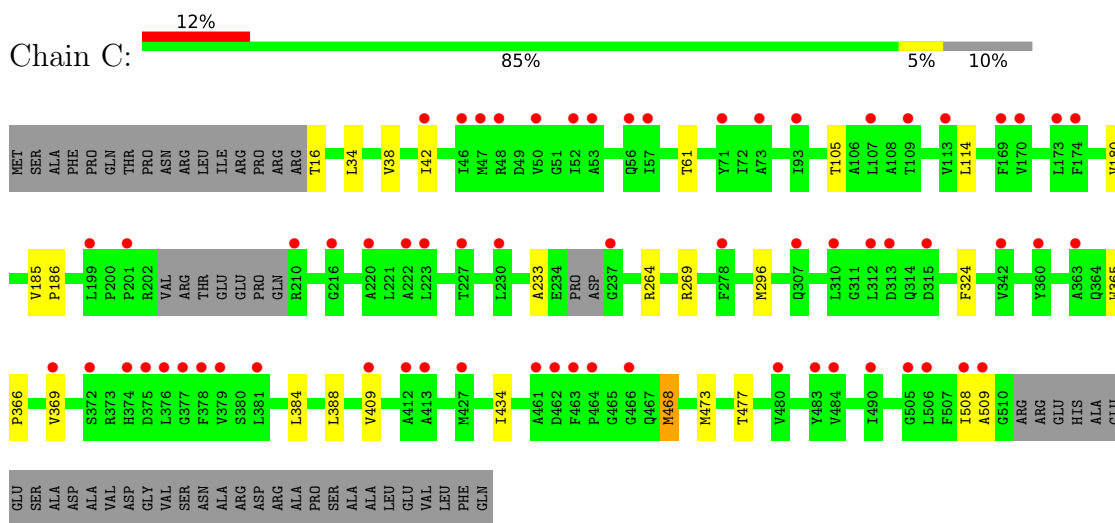
### 3 Residue-property plots

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.

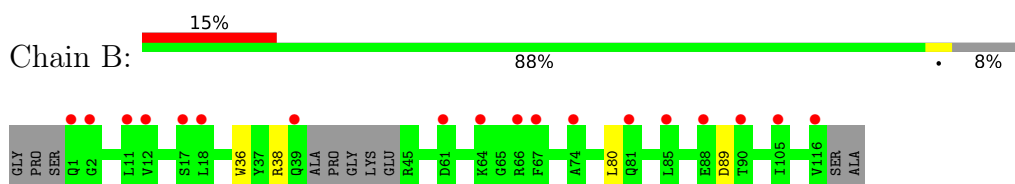
- Molecule 1: Putative triacylglyceride transporter



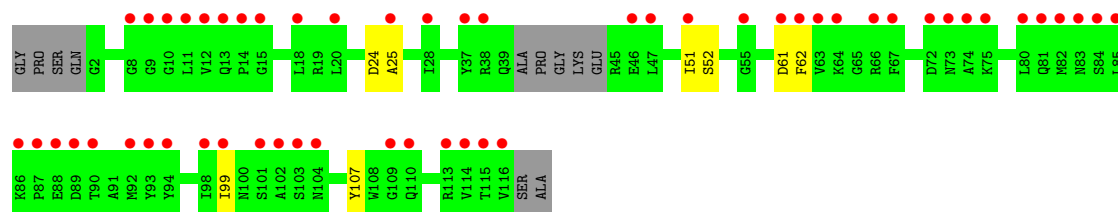

- Molecule 1: Putative triacylglyceride transporter



- Molecule 2: Nb\_H2



## ● Molecule 2: Nb\_H2

Chain D: 

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.78Å 160.70Å 82.96Å 90.00° 109.01° 90.00°	Depositor
Resolution (Å)	44.70 – 2.70 44.70 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.70-2.70) 99.5 (44.70-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.245 , 0.291 0.240 , 0.289	Depositor DCC
$R_{free}$ test set	1952 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.6	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 66.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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](#)

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	0/3622	0.53	0/4948
1	C	0.25	0/3648	0.52	0/4985
2	B	0.27	0/867	0.63	0/1168
2	D	0.26	0/858	0.63	0/1156
All	All	0.26	0/8995	0.55	0/12257

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	3552	3758	3755	12	2
1	C	3577	3781	3779	18	2
2	B	852	836	837	2	0
2	D	843	827	826	5	0
All	All	8824	9202	9197	35	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 2.

The worst 5 of 35 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:C:468:MET:SD	1:C:468:MET:N	2.59	0.75
1:A:365:TRP:CH2	1:A:384:LEU:HD12	2.40	0.57
1:C:365:TRP:CH2	1:C:384:LEU:HD12	2.39	0.57
1:C:473:MET:O	1:C:477:THR:HG23	2.06	0.56
1:C:508:ILE:HG22	1:C:509:ALA:H	1.71	0.55

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)
1:A:243:GLU:OE2	1:C:16:THR:OG1[1_556]	1.80	0.40
1:A:238:LYS:HZ1	1:C:468:MET:SD[2_555]	1.51	0.09

## 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	475/543 (88%)	471 (99%)	4 (1%)	0	100	100
1	C	480/543 (88%)	471 (98%)	9 (2%)	0	100	100
2	B	107/121 (88%)	105 (98%)	2 (2%)	0	100	100
2	D	106/121 (88%)	101 (95%)	5 (5%)	0	100	100
All	All	1168/1328 (88%)	1148 (98%)	20 (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	351/402 (87%)	351 (100%)	0	100	100
1	C	354/402 (88%)	353 (100%)	1 (0%)	92	98
2	B	89/95 (94%)	89 (100%)	0	100	100
2	D	88/95 (93%)	88 (100%)	0	100	100
All	All	882/994 (89%)	881 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	468	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides 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

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, 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	A	483/543 (88%)	0.70	37 (7%) 13 11	62, 82, 110, 134	0
1	C	486/543 (89%)	0.96	64 (13%) 3 2	66, 87, 116, 138	0
2	B	111/121 (91%)	0.91	18 (16%) 1 1	64, 93, 104, 115	0
2	D	110/121 (90%)	2.40	54 (49%) 0 0	106, 137, 151, 156	0
All	All	1190/1328 (89%)	0.98	173 (14%) 2 1	62, 87, 136, 156	0

The worst 5 of 173 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	10	GLY	10.5
2	D	11	LEU	10.4
2	D	114	VAL	7.6
2	B	2	GLY	6.8
1	C	509	ALA	6.8

### 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 monosaccharides 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.