



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 07:04 am GMT

PDB ID : 4HQN
Title : Crystal structure of manganese-loaded Plasmodium vivax TRAP protein
Authors : Song, G.; Koksai, A.C.; Lu, C.; Springer, T.A.
Deposited on : 2012-10-25
Resolution : 2.20 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

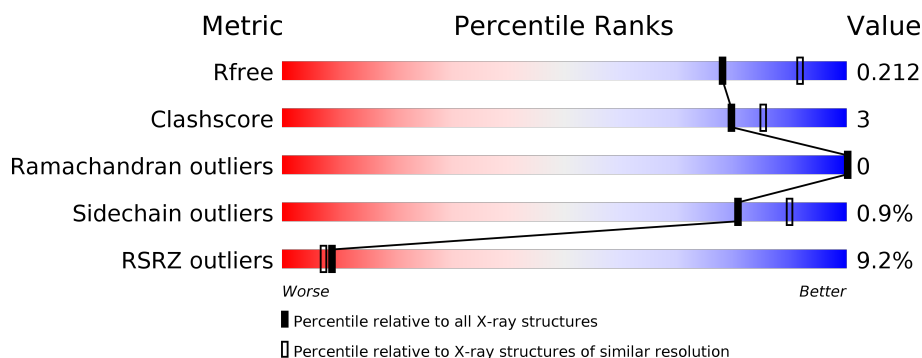
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (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. 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	266	<div> <div>15%</div> <div>89%</div> <div>6%</div> <div>5%</div> </div>
1	B	266	<div> <div>2%</div> <div>87%</div> <div>9%</div> <div>.</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4589 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 Sporozoite surface protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	2	0
			2003	1251	355	382	15			
1	B	256	Total	C	N	O	S	0	2	0
			2023	1265	362	381	15			

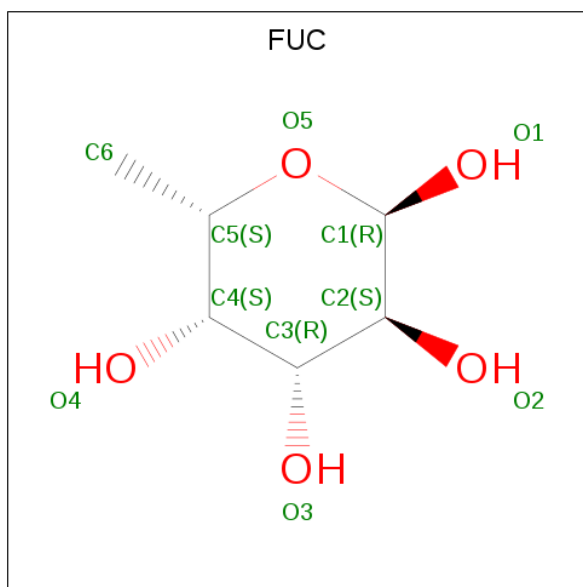
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLN	SER	ENGINEERED MUTATION	UNP Q9TVF0
A	91	SER	ASN	ENGINEERED MUTATION	UNP Q9TVF0
A	128	SER	ASN	ENGINEERED MUTATION	UNP Q9TVF0
A	180	ARG	SER	ENGINEERED MUTATION	UNP Q9TVF0
A	284	HIS	-	EXPRESSION TAG	UNP Q9TVF0
A	285	HIS	-	EXPRESSION TAG	UNP Q9TVF0
A	286	HIS	-	EXPRESSION TAG	UNP Q9TVF0
A	287	HIS	-	EXPRESSION TAG	UNP Q9TVF0
A	288	HIS	-	EXPRESSION TAG	UNP Q9TVF0
A	289	HIS	-	EXPRESSION TAG	UNP Q9TVF0
A	290	ALA	-	EXPRESSION TAG	UNP Q9TVF0
B	42	GLN	SER	ENGINEERED MUTATION	UNP Q9TVF0
B	91	SER	ASN	ENGINEERED MUTATION	UNP Q9TVF0
B	128	SER	ASN	ENGINEERED MUTATION	UNP Q9TVF0
B	180	ARG	SER	ENGINEERED MUTATION	UNP Q9TVF0
B	284	HIS	-	EXPRESSION TAG	UNP Q9TVF0
B	285	HIS	-	EXPRESSION TAG	UNP Q9TVF0
B	286	HIS	-	EXPRESSION TAG	UNP Q9TVF0
B	287	HIS	-	EXPRESSION TAG	UNP Q9TVF0
B	288	HIS	-	EXPRESSION TAG	UNP Q9TVF0
B	289	HIS	-	EXPRESSION TAG	UNP Q9TVF0
B	290	ALA	-	EXPRESSION TAG	UNP Q9TVF0

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

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

- Molecule 3 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	283	Total	O	0	0
			283	283		
6	B	234	Total	O	0	0
			234	234		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.59Å 96.57Å 159.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 2.20 39.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.88-2.20) 87.8 (39.88-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.172 , 0.212 0.174 , 0.212	Depositor DCC
R_{free} test set	2403 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4589	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, MN, FUC, 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	A	0.37	0/2046	0.53	0/2773
1	B	0.37	0/2066	0.51	0/2799
All	All	0.37	0/4112	0.52	0/5572

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

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	2003	0	1985	10	0
1	B	2023	0	2019	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	9	0	0
3	B	10	0	9	0	0
4	A	11	0	10	0	0
4	B	11	0	10	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	283	0	0	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	234	0	0	1	2
All	All	4589	0	4042	24	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 3.

All (24) 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:103:GLN:NE2	6:A:452:HOH:O	2.30	0.65
1:B:196[B]:ARG:HH21	1:B:205:GLU:H	1.43	0.64
1:B:47:LEU:HD11	1:B:156:MET:HE3	1.85	0.58
1:A:45:LEU:HD21	1:A:154:ILE:HD12	1.93	0.50
1:B:115:THR:HG23	1:B:118:ARG:HH21	1.77	0.49
1:B:196[B]:ARG:NH2	1:B:205:GLU:H	2.11	0.48
1:A:156:MET:HG2	1:A:186:ILE:HD13	1.97	0.46
1:B:77:LEU:HD12	1:B:107:LYS:HA	1.98	0.45
1:B:150:ILE:HD11	1:B:230:VAL:HG23	1.98	0.45
1:A:219:ALA:O	1:A:223:ILE:HG12	2.16	0.45
1:B:246:TRP:CD2	1:B:260[B]:ARG:HG3	2.53	0.44
1:B:164:LYS:NZ	6:B:577:HOH:O	2.50	0.43
1:A:224:LYS:HB3	1:A:225:PRO:HD3	1.99	0.43
1:B:106:ASP:OD2	1:B:109:GLN:HG3	2.19	0.43
1:B:215:ASP:OD2	1:B:217:ASN:HB2	2.18	0.43
1:A:205:GLU:HA	1:A:206:PRO:HD3	1.76	0.42
1:B:45:LEU:HD21	1:B:154:ILE:HD12	2.02	0.42
1:A:103:GLN:HG2	1:A:109:GLN:HB3	2.00	0.42
1:B:246:TRP:CD2	1:B:260[A]:ARG:HG3	2.55	0.42
1:A:47:LEU:HD11	1:A:156:MET:HE3	2.02	0.41
1:A:224:LYS:HD2	6:A:582:HOH:O	2.19	0.41
1:B:210:PHE:CD1	1:B:226:PHE:HZ	2.38	0.41
1:A:232:THR:HA	1:B:39:CYS:O	2.21	0.41
1:B:145:ASN:H	1:B:145:ASN:HD22	1.69	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)
6:A:530:HOH:O	6:B:556:HOH:O[1_655]	2.11	0.09
6:A:446:HOH:O	6:B:495:HOH:O[4_545]	2.14	0.06

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	254/266 (96%)	245 (96%)	9 (4%)	0	100	100
1	B	256/266 (96%)	247 (96%)	9 (4%)	0	100	100
All	All	510/532 (96%)	492 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	225/234 (96%)	223 (99%)	2 (1%)	81	90
1	B	227/234 (97%)	225 (99%)	2 (1%)	81	90
All	All	452/468 (97%)	448 (99%)	4 (1%)	81	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	HIS
1	A	282	CYS
1	B	145	ASN
1	B	258	HIS

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

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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	FUC	A	302	1,4	9,10,11	1.38	2 (22%)	13,14,16	1.54	2 (15%)
4	BGC	A	303	3	11,11,12	0.65	0	15,15,17	0.89	2 (13%)
3	FUC	B	302	1,4	9,10,11	1.34	1 (11%)	13,14,16	1.10	0
4	BGC	B	303	3	11,11,12	0.67	0	15,15,17	1.02	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	A	302	1,4	-	0/0/17/20	0/1/1/1
4	BGC	A	303	3	-	0/2/19/22	0/1/1/1
3	FUC	B	302	1,4	-	0/0/17/20	0/1/1/1
4	BGC	B	303	3	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	FUC	O5-C1	-2.50	1.39	1.43
3	A	302	FUC	C1-C2	2.09	1.57	1.52
3	A	302	FUC	C2-C3	2.78	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	BGC	O5-C5-C6	2.06	110.40	107.15
4	B	303	BGC	O5-C5-C6	2.18	110.60	107.15
4	A	303	BGC	C1-C2-C3	2.21	112.45	109.66
3	A	302	FUC	O5-C1-C2	2.81	115.16	110.78
3	A	302	FUC	C1-C2-C3	3.42	113.99	109.66

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, 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	254/266 (95%)	0.56	41 (16%) 1 1	26, 46, 125, 156	0
1	B	256/266 (96%)	-0.08	6 (2%) 60 58	31, 60, 90, 130	0
All	All	510/532 (95%)	0.24	47 (9%) 9 7	26, 53, 119, 156	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	GLU	6.8
1	A	265	LEU	6.8
1	A	274	VAL	6.7
1	A	255	ARG	5.3
1	A	243	TRP	5.1
1	B	204	ARG	4.8
1	A	242	PRO	4.6
1	A	277	CYS	4.4
1	A	263	PRO	4.3
1	B	28	VAL	4.3
1	A	271	THR	4.3
1	A	253	CYS	4.3
1	A	239	ASN	4.3
1	A	273	MET	4.3
1	A	275	SER	4.1
1	A	241	GLY	4.0
1	A	276	GLU	3.9
1	B	29	VAL	3.7
1	A	250	SER	3.7
1	A	206	PRO	3.5
1	A	256	GLY	3.4
1	A	264	SER	3.4
1	A	204	ARG	3.2
1	A	254	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	261	SER	3.1
1	A	257	THR	3.0
1	A	270	THR	3.0
1	A	258	HIS	2.9
1	A	281	GLU	2.9
1	A	246	TRP	2.8
1	B	92	TYR	2.6
1	A	260	ARG	2.6
1	A	248	ALA	2.6
1	A	244	ASP	2.6
1	B	108	ARG	2.5
1	A	266	HIS	2.5
1	A	251	VAL	2.4
1	A	207	ASN	2.4
1	A	238	ALA	2.4
1	A	240	CYS	2.3
1	B	119	LYS	2.3
1	A	252	THR	2.2
1	A	205	GLU	2.1
1	A	259	SER	2.0
1	A	283	PRO	2.0
1	A	272	HIS	2.0
1	A	262	ARG	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 carbohydrates 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, 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FUC	A	302	10/11	0.80	0.19	68,100,108,110	0
4	BGC	A	303	11/12	0.87	0.20	117,121,122,123	0
4	BGC	B	303	11/12	0.95	0.10	40,44,49,49	0
5	CL	A	304	1/1	0.98	0.12	32,32,32,32	0
3	FUC	B	302	10/11	0.98	0.10	37,42,45,45	0
2	MN	B	301	1/1	0.99	0.11	46,46,46,46	0
5	CL	B	304	1/1	0.99	0.08	46,46,46,46	0
2	MN	A	301	1/1	1.00	0.13	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.