



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:32 PM UTC

PDB ID : 4O2X / pdb_00004o2x
Title : Structure of a malarial protein
Authors : AhYoung, A.P.; Koehl, A.; Cascio, D.; Egea, P.F.
Deposited on : 2013-12-17
Resolution : 2.70 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (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

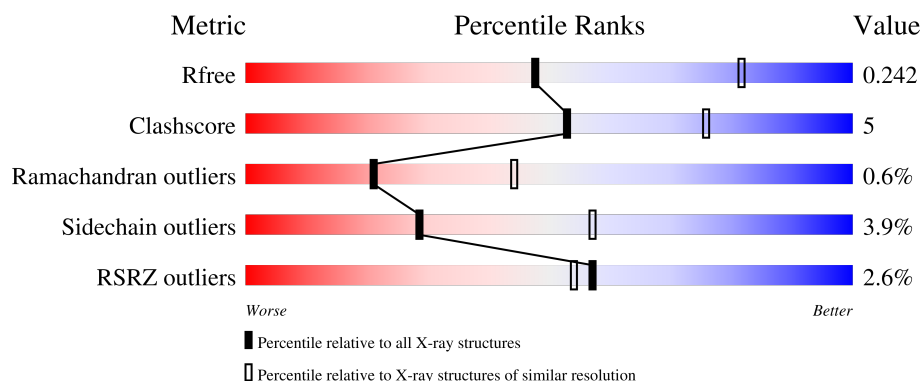
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

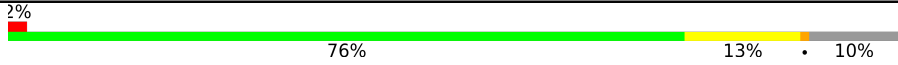
The reported resolution of this entry is 2.70 Å.

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	507	
1	B	507	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6833 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 Maltose-binding periplasmic protein, ATP-dependent Clp protease adaptor protein ClpS containing protein chimeric construct.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3422	2202	555	658	7			
1	B	454	Total	C	N	O	S	0	1	0
			3411	2187	555	662	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ASP	ALA	engineered mutation	UNP P0AEX9
A	84	LYS	ALA	engineered mutation	UNP P0AEX9
A	173	GLU	ALA	engineered mutation	UNP P0AEX9
A	174	ASN	ALA	engineered mutation	UNP P0AEX9
A	240	LYS	ALA	engineered mutation	UNP P0AEX9
A	360	GLU	ALA	engineered mutation	UNP P0AEX9
A	492	LEU	-	expression tag	UNP P0AEX9
A	493	VAL	-	expression tag	UNP P0AEX9
A	494	PRO	-	expression tag	UNP P0AEX9
A	495	ARG	-	expression tag	UNP P0AEX9
A	496	GLY	-	expression tag	UNP P0AEX9
A	497	SER	-	expression tag	UNP P0AEX9
A	498	HIS	-	expression tag	UNP P0AEX9
A	499	HIS	-	expression tag	UNP P0AEX9
A	500	HIS	-	expression tag	UNP P0AEX9
A	501	HIS	-	expression tag	UNP P0AEX9
A	502	HIS	-	expression tag	UNP P0AEX9
A	503	HIS	-	expression tag	UNP P0AEX9
A	504	HIS	-	expression tag	UNP P0AEX9
A	505	HIS	-	expression tag	UNP P0AEX9
A	506	HIS	-	expression tag	UNP P0AEX9
A	507	HIS	-	expression tag	UNP P0AEX9
B	83	ASP	ALA	engineered mutation	UNP P0AEX9
B	84	LYS	ALA	engineered mutation	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	173	GLU	ALA	engineered mutation	UNP P0AEX9
B	174	ASN	ALA	engineered mutation	UNP P0AEX9
B	240	LYS	ALA	engineered mutation	UNP P0AEX9
B	360	GLU	ALA	engineered mutation	UNP P0AEX9
B	492	LEU	-	expression tag	UNP Q8IEB2
B	493	VAL	-	expression tag	UNP Q8IEB2
B	494	PRO	-	expression tag	UNP Q8IEB2
B	495	ARG	-	expression tag	UNP Q8IEB2
B	496	GLY	-	expression tag	UNP Q8IEB2
B	497	SER	-	expression tag	UNP Q8IEB2
B	498	HIS	-	expression tag	UNP Q8IEB2
B	499	HIS	-	expression tag	UNP Q8IEB2
B	500	HIS	-	expression tag	UNP Q8IEB2
B	501	HIS	-	expression tag	UNP Q8IEB2
B	502	HIS	-	expression tag	UNP Q8IEB2
B	503	HIS	-	expression tag	UNP Q8IEB2
B	504	HIS	-	expression tag	UNP Q8IEB2
B	505	HIS	-	expression tag	UNP Q8IEB2
B	506	HIS	-	expression tag	UNP Q8IEB2
B	507	HIS	-	expression tag	UNP Q8IEB2

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	97.85Å 97.85Å 298.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	73.67 – 2.70 73.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (73.67-2.70) 97.4 (73.67-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1555)	Depositor
R, R_{free}	0.185 , 0.239 0.197 , 0.242	Depositor DCC
R_{free} test set	3226 reflections (7.50%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6833	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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

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	0.61	0/3502	0.92	9/4784 (0.2%)
1	B	0.58	0/3494	0.95	13/4776 (0.3%)
All	All	0.60	0/6996	0.94	22/9560 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	THR	CA-C-N	-6.84	113.26	120.03
1	B	81	THR	C-N-CA	-6.84	113.26	120.03
1	B	91	TYR	CA-C-N	5.77	125.89	119.32
1	B	91	TYR	C-N-CA	5.77	125.89	119.32
1	B	298	LYS	CA-C-N	5.65	126.90	119.84
1	B	298	LYS	C-N-CA	5.65	126.90	119.84
1	B	27	LYS	CB-CG-CD	-5.64	98.33	111.30
1	A	45	GLU	N-CA-C	-5.54	106.03	112.89
1	B	48	PHE	CA-C-N	-5.52	114.12	119.87
1	B	48	PHE	C-N-CA	-5.52	114.12	119.87
1	A	126	PRO	O-C-N	5.44	123.81	121.31
1	B	123	LEU	CA-C-N	5.44	125.09	119.05
1	B	123	LEU	C-N-CA	5.44	125.09	119.05
1	A	123	LEU	CA-C-N	5.43	125.26	119.28
1	A	123	LEU	C-N-CA	5.43	125.26	119.28
1	A	61	ILE	N-CA-C	5.40	115.67	108.11
1	A	298	LYS	CA-C-N	5.34	126.52	119.84
1	A	298	LYS	C-N-CA	5.34	126.52	119.84
1	A	48	PHE	CA-C-N	-5.08	114.59	119.87
1	A	48	PHE	C-N-CA	-5.08	114.59	119.87
1	B	154	GLU	CA-C-N	5.03	124.81	119.28
1	B	154	GLU	C-N-CA	5.03	124.81	119.28

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	3422	0	3268	36	0
1	B	3411	0	3232	31	0
All	All	6833	0	6500	67	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 5.

All (67) 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:116:LEU:HD11	1:A:225:MET:HE2	1.46	0.95
1:B:77:LEU:HB3	1:B:105:ILE:HD11	1.63	0.81
1:A:413:LEU:HB2	1:A:455:ILE:HD11	1.75	0.68
1:A:458:THR:HG21	1:A:462:LYS:HD3	1.79	0.63
1:A:412:ILE:HD12	1:A:480:ILE:HD12	1.80	0.63
1:B:100:TYR:HA	1:B:102:GLY:H	1.63	0.62
1:A:271:SER:O	1:A:274:LYS:NZ	2.32	0.61
1:B:458:THR:HG21	1:B:462:LYS:HD3	1.81	0.61
1:B:5:GLU:OE2	1:B:6:GLY:N	2.34	0.60
1:A:77:LEU:HB3	1:A:105:ILE:HD11	1.84	0.60
1:B:49:PRO:HG3	1:B:71:TYR:HE1	1.68	0.58
1:A:372:ASN:HB3	1:A:375:LYS:HE2	1.85	0.58
1:B:413:LEU:HB2	1:B:455:ILE:HD11	1.84	0.58
1:B:174:ASN:O	1:B:174:ASN:ND2	2.40	0.55
1:B:439:LYS:HE2	1:B:443:ILE:HD11	1.89	0.54
1:B:246:THR:OG1	1:B:247:VAL:N	2.40	0.53
1:A:127:PRO:HD2	1:A:225:MET:HE3	1.92	0.52
1:A:190:LYS:HD3	1:A:359:ASP:OD2	2.11	0.51
1:A:409:TRP:CZ2	1:A:460:LYS:HD2	2.46	0.51
1:A:279:GLU:O	1:A:283:ASN:HB2	2.12	0.50
1:B:342:TYR:O	1:B:346:THR:HG23	2.11	0.50
1:B:174:ASN:C	1:B:176:LYS:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:PRO:HA	1:A:233:TRP:CE2	2.47	0.49
1:A:77:LEU:HD23	1:A:105:ILE:HG13	1.94	0.49
1:A:469:GLU:O	1:A:473:ASN:ND2	2.46	0.49
1:B:62:PHE:CE1	1:B:265:ALA:HB2	2.47	0.48
1:B:63:TRP:HB3	1:B:68:PHE:HE1	1.79	0.48
1:A:127:PRO:HD2	1:A:225:MET:CE	2.44	0.48
1:A:213:ILE:HG12	1:A:412:ILE:CD1	2.43	0.48
1:A:371:ALA:HB3	1:A:376:ILE:HD11	1.96	0.47
1:A:179:ILE:HD13	1:A:179:ILE:H	1.79	0.47
1:A:62:PHE:HA	1:A:264:SER:O	2.14	0.47
1:B:69:GLY:O	1:B:73:GLN:HG3	2.15	0.47
1:A:116:LEU:HD21	1:A:225:MET:CE	2.45	0.47
1:A:41:PRO:HG2	1:A:44:LEU:HB3	1.96	0.46
1:B:417:ASP:HB2	1:B:424:VAL:HG21	1.98	0.46
1:B:49:PRO:HG3	1:B:71:TYR:CE1	2.50	0.45
1:B:77:LEU:HD11	1:B:266:GLY:HA3	1.98	0.45
1:A:48:PHE:HB3	1:A:49:PRO:HD3	1.99	0.45
1:B:63:TRP:HB3	1:B:68:PHE:CE1	2.51	0.44
1:A:65:HIS:CD2	1:A:97:ALA:HB1	2.52	0.44
1:B:43:LYS:O	1:B:47:LYS:HB2	2.19	0.43
1:A:5:GLU:HA	1:A:6:GLY:HA3	1.67	0.43
1:A:49:PRO:HG3	1:A:71:TYR:HE1	1.84	0.43
1:A:171:LYS:HG3	1:A:181:ASP:OD2	2.19	0.43
1:B:137:ASP:OD2	1:B:204:HIS:ND1	2.48	0.43
1:B:77:LEU:HD13	1:B:267:ILE:O	2.19	0.42
1:A:90:LEU:HD22	1:A:305:LEU:HA	2.01	0.42
1:B:373:LEU:HD23	1:B:373:LEU:O	2.19	0.42
1:A:372:ASN:O	1:A:376:ILE:HG12	2.19	0.42
1:A:168:TYR:CE1	1:A:171:LYS:HG2	2.54	0.42
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.87	0.42
1:B:338:SER:OG	1:B:380:ARG:NH1	2.53	0.42
1:A:159:TRP:CE2	1:A:163:ALA:HB2	2.55	0.42
1:B:169:ALA:HA	1:B:340:PHE:CE2	2.55	0.42
1:A:52:ALA:HB1	1:A:76:LEU:HD11	2.02	0.41
1:A:171:LYS:HB2	1:A:181:ASP:HB3	2.01	0.41
1:B:230:PRO:HA	1:B:233:TRP:CE2	2.56	0.41
1:B:80:ILE:HG22	1:B:267:ILE:HD12	2.02	0.41
1:A:41:PRO:HB2	1:A:47:LYS:HD3	2.01	0.41
1:A:212:SER:OG	1:A:482:GLU:HG2	2.21	0.41
1:A:62:PHE:CE1	1:A:265:ALA:HB2	2.55	0.41
1:B:243:TYR:OH	1:B:317:ARG:NH1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD23	1:B:140:LEU:HA	1.95	0.40
1:B:409:TRP:CZ2	1:B:460:LYS:HD2	2.56	0.40
1:B:161:LEU:HD23	1:B:196:LEU:HB2	2.04	0.40

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	453/507 (89%)	425 (94%)	27 (6%)	1 (0%)	43	68
1	B	451/507 (89%)	423 (94%)	24 (5%)	4 (1%)	14	35
All	All	904/1014 (89%)	848 (94%)	51 (6%)	5 (1%)	21	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	174	ASN
1	B	415	ASN
1	B	418	ILE
1	A	63	TRP
1	B	99	ARG

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	337/418 (81%)	323 (96%)	14 (4%)	26	55
1	B	337/418 (81%)	324 (96%)	13 (4%)	28	57
All	All	674/836 (81%)	647 (96%)	27 (4%)	28	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	36	VAL
1	A	42	ASP
1	A	61	ILE
1	A	77	LEU
1	A	98	VAL
1	A	101	ASN
1	A	179	ILE
1	A	326	GLN
1	A	333	ASN
1	A	406	THR
1	A	456	LEU
1	A	457	SER
1	A	464	GLU
1	B	19	ASN
1	B	23	GLU
1	B	42[A]	ASP
1	B	42[B]	ASP
1	B	61	ILE
1	B	77	LEU
1	B	99	ARG
1	B	171	LYS
1	B	326	GLN
1	B	333	ASN
1	B	381	ASN
1	B	434	GLN
1	B	472	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	GLN
1	B	153	GLN
1	B	381	ASN

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Mol	Chain	Res	Type
1	B	434	GLN

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](#)

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 [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	457/507 (90%)	-0.07	9 (1%) 65 62	51, 74, 124, 182	0
1	B	454/507 (89%)	0.04	15 (3%) 49 45	53, 79, 128, 183	1 (0%)
All	All	911/1014 (89%)	-0.02	24 (2%) 57 54	51, 76, 127, 183	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	GLU	5.2
1	B	418	ILE	4.8
1	A	383	ILE	4.4
1	A	406	THR	4.1
1	A	46	GLU	4.0
1	A	50	GLN	3.5
1	B	100	TYR	3.3
1	B	382	VAL	3.2
1	B	375	LYS	2.8
1	B	50	GLN	2.7
1	B	46	GLU	2.7
1	B	27	LYS	2.6
1	B	6	GLY	2.5
1	A	382	VAL	2.4
1	B	81	THR	2.3
1	A	175	GLY	2.3
1	B	419	HIS	2.2
1	B	381	ASN	2.2
1	B	407	SER	2.2
1	B	75	GLY	2.2
1	A	75	GLY	2.1
1	A	68	PHE	2.1
1	B	275	GLU	2.1
1	B	104	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.