



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 04:36 AM EDT

PDB ID : 6ZYV
Title : Structure of a Plasmodium PIR protein ectodomain
Authors : Harrison, T.E.; Higgins, M.K.
Deposited on : 2020-08-03
Resolution : 2.15 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

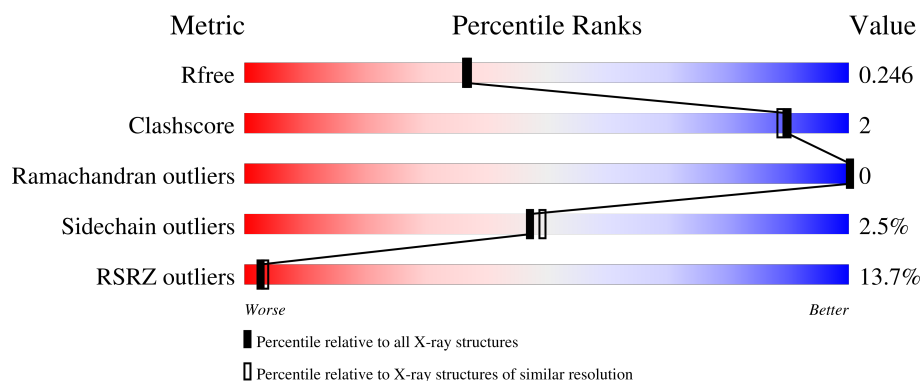
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	304	<div> <div>8%</div> <div>76%</div> <div>22%</div> </div>
1	B	304	<div> <div>5%</div> <div>73%</div> <div>22%</div> </div>
1	C	304	<div> <div>18%</div> <div>66%</div> <div>7%</div> <div>28%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5719 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 CIR protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1913	1201	310	386	16			
1	B	236	Total	C	N	O	S	0	0	0
			1896	1190	305	385	16			
1	C	220	Total	C	N	O	S	0	0	0
			1778	1123	291	349	15			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	SER	engineered mutation	UNP A0A077TLQ4
A	125	ALA	THR	engineered mutation	UNP A0A077TLQ4
A	152	ALA	SER	engineered mutation	UNP A0A077TLQ4
A	176	ALA	SER	engineered mutation	UNP A0A077TLQ4
A	179	ALA	THR	engineered mutation	UNP A0A077TLQ4
B	5	ALA	SER	engineered mutation	UNP A0A077TLQ4
B	125	ALA	THR	engineered mutation	UNP A0A077TLQ4
B	152	ALA	SER	engineered mutation	UNP A0A077TLQ4
B	176	ALA	SER	engineered mutation	UNP A0A077TLQ4
B	179	ALA	THR	engineered mutation	UNP A0A077TLQ4
C	5	ALA	SER	engineered mutation	UNP A0A077TLQ4
C	125	ALA	THR	engineered mutation	UNP A0A077TLQ4
C	152	ALA	SER	engineered mutation	UNP A0A077TLQ4
C	176	ALA	SER	engineered mutation	UNP A0A077TLQ4
C	179	ALA	THR	engineered mutation	UNP A0A077TLQ4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	56	Total	O	0	0
			56	56		
2	B	55	Total	O	0	0
			55	55		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	21	Total	O	0	0
			21	21		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.17Å 63.61Å 199.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 2.15 49.84 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.84-2.15) 98.1 (49.84-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, R_{free}	0.212 , 0.237 0.216 , 0.246	Depositor DCC
R_{free} test set	2184 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5719	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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	0.44	0/1952	0.56	0/2642
1	B	0.42	0/1934	0.55	0/2619
1	C	0.37	0/1814	0.55	0/2450
All	All	0.41	0/5700	0.56	0/7711

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	1913	0	1812	5	0
1	B	1896	0	1788	9	0
1	C	1778	0	1701	10	0
2	A	56	0	0	0	0
2	B	55	0	0	0	0
2	C	21	0	0	0	0
All	All	5719	0	5301	20	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 2.

All (20) 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:212:LEU:HD23	1:B:28:TYR:CD2	2.28	0.68
1:A:212:LEU:HD23	1:B:28:TYR:CG	2.37	0.59
1:C:146:LEU:HD22	1:C:210:GLN:HB3	1.87	0.57
1:C:95:LEU:HA	1:C:98:ILE:HG22	1.92	0.52
1:C:205:ASP:HA	1:C:209:LYS:HB2	1.91	0.51
1:C:228:ASN:H	1:C:232:SER:HB3	1.77	0.49
1:A:216:SER:HG	1:B:28:TYR:HD1	1.61	0.48
1:C:182:LEU:O	1:C:186:GLN:HG3	2.15	0.47
1:C:146:LEU:HD22	1:C:210:GLN:CB	2.46	0.46
1:A:212:LEU:CD2	1:B:28:TYR:CD2	2.99	0.45
1:C:205:ASP:HA	1:C:209:LYS:CB	2.47	0.45
1:C:111:LYS:HG3	1:C:144:ILE:HG21	2.00	0.44
1:B:226:CYS:O	1:B:230:GLN:HG2	2.18	0.43
1:B:182:LEU:O	1:B:186:GLN:HG3	2.18	0.43
1:A:22:LEU:HD12	1:A:22:LEU:HA	1.91	0.42
1:C:146:LEU:CD2	1:C:210:GLN:HB3	2.47	0.42
1:B:242:THR:CG2	1:B:243:THR:N	2.83	0.42
1:C:93:LEU:HD22	1:C:214:ILE:HD13	2.02	0.42
1:B:242:THR:HG22	1:B:243:THR:HG23	2.03	0.41
1:B:72:HIS:ND1	1:B:77:ASP:OD2	2.53	0.41

There are no symmetry-related clashes.

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	236/304 (78%)	230 (98%)	6 (2%)	0	100	100
1	B	232/304 (76%)	224 (97%)	8 (3%)	0	100	100
1	C	214/304 (70%)	202 (94%)	12 (6%)	0	100	100
All	All	682/912 (75%)	656 (96%)	26 (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	219/279 (78%)	214 (98%)	5 (2%)	50	53
1	B	218/279 (78%)	213 (98%)	5 (2%)	50	53
1	C	203/279 (73%)	197 (97%)	6 (3%)	41	40
All	All	640/837 (76%)	624 (98%)	16 (2%)	47	49

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASP
1	A	77	ASP
1	A	120	THR
1	A	130	SER
1	A	135	ASN
1	B	31	VAL
1	B	36	THR
1	B	77	ASP
1	B	137	LYS
1	B	174	ASN
1	C	37	LEU
1	C	40	ASP
1	C	134	SER
1	C	151	LYS
1	C	181	CYS
1	C	224	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	116	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 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 [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	238/304 (78%)	0.67	25 (10%) 6 9	39, 56, 97, 113	0
1	B	236/304 (77%)	0.59	14 (5%) 22 30	37, 59, 100, 120	0
1	C	220/304 (72%)	1.33	56 (25%) 0 0	45, 84, 133, 161	0
All	All	694/912 (76%)	0.85	95 (13%) 3 3	37, 65, 120, 161	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	THR	11.4
1	C	205	ASP	10.9
1	C	174	ASN	8.3
1	B	130	SER	7.0
1	B	131	ALA	6.1
1	C	204	ASP	5.7
1	C	211	ILE	5.7
1	A	176	ALA	5.4
1	B	28	TYR	5.2
1	C	79	CYS	5.1
1	C	201	VAL	5.0
1	B	132	SER	4.8
1	C	231	HIS	4.2
1	C	169	ASN	4.2
1	B	134	SER	4.2
1	C	8	LEU	4.0
1	C	152	ALA	4.0
1	A	28	TYR	3.9
1	A	31	VAL	3.9
1	C	173	LYS	3.9
1	C	107	ILE	3.8
1	C	149	MET	3.8
1	C	190	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	80	SER	3.6
1	C	202	ASP	3.6
1	C	175	GLU	3.6
1	C	200	ASN	3.5
1	C	148	ASN	3.4
1	C	207	SER	3.4
1	A	30	GLY	3.4
1	A	24	ILE	3.4
1	C	24	ILE	3.4
1	C	197	ASN	3.3
1	C	209	LYS	3.2
1	B	133	ASP	3.2
1	B	176	ALA	3.2
1	A	45	LYS	3.1
1	C	138	GLY	3.1
1	C	171	LEU	3.1
1	C	81	GLN	3.1
1	C	208	TYR	3.1
1	C	154	ILE	3.0
1	C	112	ASN	3.0
1	C	170	GLU	3.0
1	C	73	ILE	3.0
1	A	130	SER	2.9
1	C	131	ALA	2.9
1	C	87	TYR	2.9
1	C	203	THR	2.9
1	C	239	THR	2.9
1	A	132	SER	2.8
1	C	230	GLN	2.8
1	C	188	PHE	2.8
1	A	25	ASP	2.7
1	A	169	ASN	2.7
1	A	27	ILE	2.7
1	C	172	ASP	2.7
1	C	193	GLN	2.7
1	C	144	ILE	2.6
1	C	88	ALA	2.6
1	C	215	LEU	2.6
1	B	128	VAL	2.6
1	C	178	TYR	2.6
1	C	223	ILE	2.6
1	C	206	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	135	ASN	2.5
1	C	238	PRO	2.5
1	A	131	ALA	2.5
1	A	177	ASN	2.5
1	B	177	ASN	2.5
1	A	46	ASN	2.4
1	C	235	PRO	2.4
1	A	174	ASN	2.4
1	C	168	TYR	2.4
1	A	20	ASP	2.4
1	C	196	LEU	2.3
1	C	92	ILE	2.3
1	A	175	GLU	2.3
1	C	135	ASN	2.3
1	A	201	VAL	2.3
1	C	153	ILE	2.2
1	A	97	TYR	2.2
1	B	29	THR	2.2
1	C	210	GLN	2.2
1	A	22	LEU	2.1
1	A	81	GLN	2.1
1	C	184	ASP	2.1
1	C	181	CYS	2.1
1	B	25	ASP	2.1
1	B	53	GLU	2.1
1	A	172	ASP	2.0
1	B	44	MET	2.0
1	C	189	VAL	2.0
1	A	55	ASN	2.0
1	A	221	ASN	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 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.