



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 11:29 PM UTC

PDB ID : 9F8W / pdb_00009f8w
Title : Crystal structure of the apo Pex5 peroxisomal cargo receptor from Trypanosoma brucei
Authors : Banasik, M.K.; Dubin, G.
Deposited on : 2024-05-07
Resolution : 2.35 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

<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

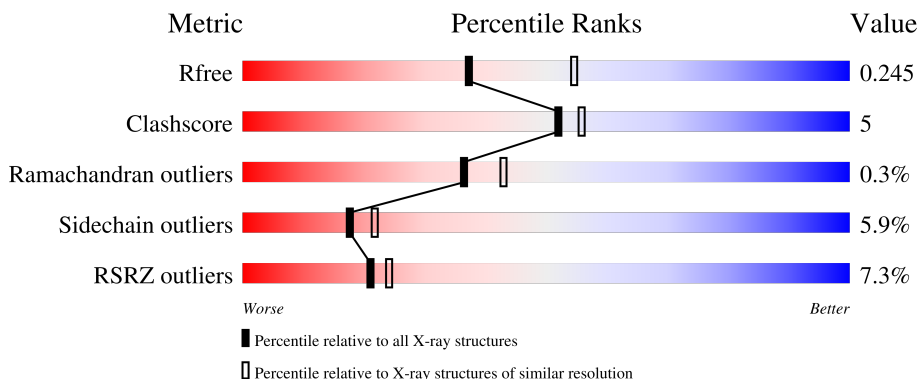
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	347	9% 78% 10% 10%
1	B	347	4% 78% 13% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4949 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 Peroxisome targeting signal 1 receptor PEX5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	1	0
			2377	1492	415	455	15			
1	B	319	Total	C	N	O	S	0	1	0
			2460	1538	429	475	18			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	315	MET	-	initiating methionine	UNP Q9U7C3
A	316	ALA	-	expression tag	UNP Q9U7C3
A	317	SER	-	expression tag	UNP Q9U7C3
A	318	MET	-	expression tag	UNP Q9U7C3
A	319	THR	-	expression tag	UNP Q9U7C3
A	320	GLY	-	expression tag	UNP Q9U7C3
A	321	GLY	-	expression tag	UNP Q9U7C3
A	322	GLN	-	expression tag	UNP Q9U7C3
A	323	GLN	-	expression tag	UNP Q9U7C3
A	324	MET	-	expression tag	UNP Q9U7C3
A	325	GLY	-	expression tag	UNP Q9U7C3
A	326	ARG	-	expression tag	UNP Q9U7C3
A	327	GLY	-	expression tag	UNP Q9U7C3
A	328	SER	-	expression tag	UNP Q9U7C3
A	329	GLU	-	expression tag	UNP Q9U7C3
A	330	PHE	-	expression tag	UNP Q9U7C3
A	331	MET	-	expression tag	UNP Q9U7C3
A	656	GLU	-	expression tag	UNP Q9U7C3
A	657	ASN	-	expression tag	UNP Q9U7C3
A	658	LEU	-	expression tag	UNP Q9U7C3
A	659	TYR	-	expression tag	UNP Q9U7C3
A	660	PHE	-	expression tag	UNP Q9U7C3
A	661	GLN	-	expression tag	UNP Q9U7C3
B	315	MET	-	initiating methionine	UNP Q9U7C3
B	316	ALA	-	expression tag	UNP Q9U7C3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	317	SER	-	expression tag	UNP Q9U7C3
B	318	MET	-	expression tag	UNP Q9U7C3
B	319	THR	-	expression tag	UNP Q9U7C3
B	320	GLY	-	expression tag	UNP Q9U7C3
B	321	GLY	-	expression tag	UNP Q9U7C3
B	322	GLN	-	expression tag	UNP Q9U7C3
B	323	GLN	-	expression tag	UNP Q9U7C3
B	324	MET	-	expression tag	UNP Q9U7C3
B	325	GLY	-	expression tag	UNP Q9U7C3
B	326	ARG	-	expression tag	UNP Q9U7C3
B	327	GLY	-	expression tag	UNP Q9U7C3
B	328	SER	-	expression tag	UNP Q9U7C3
B	329	GLU	-	expression tag	UNP Q9U7C3
B	330	PHE	-	expression tag	UNP Q9U7C3
B	331	MET	-	expression tag	UNP Q9U7C3
B	656	GLU	-	expression tag	UNP Q9U7C3
B	657	ASN	-	expression tag	UNP Q9U7C3
B	658	LEU	-	expression tag	UNP Q9U7C3
B	659	TYR	-	expression tag	UNP Q9U7C3
B	660	PHE	-	expression tag	UNP Q9U7C3
B	661	GLN	-	expression tag	UNP Q9U7C3

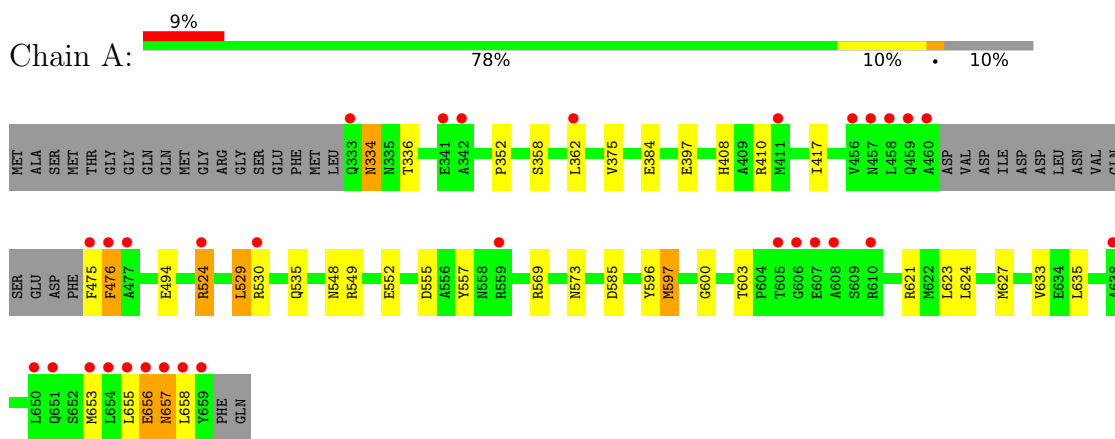
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	35	Total	O	0	0
			35	35		
2	B	77	Total	O	0	0
			77	77		

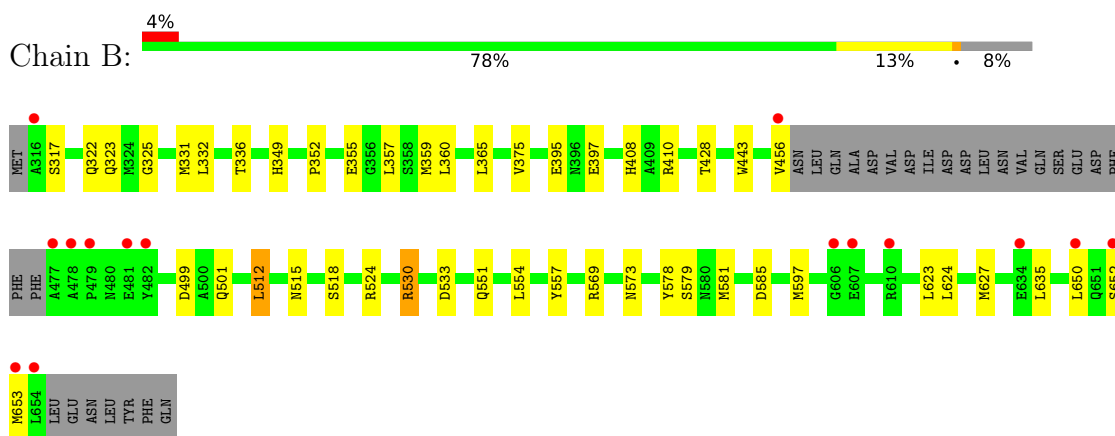
3 Residue-property plots [i](#)

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: Peroxisome targeting signal 1 receptor PEX5



- Molecule 1: Peroxisome targeting signal 1 receptor PEX5



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	206.54Å 206.54Å 67.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.89 – 2.35 47.89 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.89-2.35) 99.9 (47.89-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.246 0.204 , 0.245	Depositor DCC
R_{free} test set	2309 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4949	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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	1.11	1/2428 (0.0%)	1.48	4/3310 (0.1%)
1	B	1.07	0/2511	1.50	0/3409
All	All	1.09	1/4939 (0.0%)	1.49	4/6719 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	603	THR	N-CA	5.09	1.50	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ASN	CA-C-N	6.10	129.49	120.95
1	A	334	ASN	C-N-CA	6.10	129.49	120.95
1	A	529	LEU	CA-C-O	-5.17	116.58	122.01
1	A	555	ASP	CA-CB-CG	5.09	117.69	112.60

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	2377	0	2228	21	0
1	B	2460	0	2343	27	0
2	A	35	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	77	0	0	4	0
All	All	4949	0	4571	48	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.

The worst 5 of 48 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:596:TYR:HD2	1:A:655:LEU:HD12	1.34	0.92
1:B:349:HIS:NE2	1:B:355:GLU:HG3	1.97	0.79
1:A:596:TYR:CD2	1:A:655:LEU:HD12	2.23	0.71
1:A:623:LEU:HG	1:A:627:MET:HE2	1.74	0.69
1:B:349:HIS:CD2	1:B:355:GLU:HG3	2.28	0.67

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	310/347 (89%)	300 (97%)	8 (3%)	2 (1%)	21	24
1	B	316/347 (91%)	301 (95%)	15 (5%)	0	100	100
All	All	626/694 (90%)	601 (96%)	23 (4%)	2 (0%)	36	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	657	ASN
1	A	476	PHE

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	231/284 (81%)	216 (94%)	15 (6%)	15	18
1	B	248/284 (87%)	234 (94%)	14 (6%)	19	23
All	All	479/568 (84%)	450 (94%)	29 (6%)	18	20

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	657	ASN
1	B	635	LEU
1	B	336	THR
1	B	530	ARG
1	B	332	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	432	ASN
1	B	452	GLN
1	B	598	GLN
1	B	548	ASN
1	B	449	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 [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	313/347 (90%)	0.58	31 (9%) 13 14	25, 58, 92, 118	2 (0%)
1	B	319/347 (91%)	0.28	15 (4%) 36 42	29, 53, 88, 120	1 (0%)
All	All	632/694 (91%)	0.43	46 (7%) 21 24	25, 56, 90, 120	3 (0%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	475	PHE	7.6
1	B	316	ALA	7.4
1	A	460	ALA	6.3
1	A	559	ARG	5.8
1	A	459	GLN	5.5

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.