



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 10:20 PM UTC

PDB ID : 5EUC / pdb_00005euc
Title : The role of the C-terminal region on the oligomeric state and enzymatic activity of Trypanosoma cruzi hypoxanthine phosphoribosyl transferase
Authors : Valsecchi, W.M.; Cousido-Siah, A.; Mitschler, A.; Podjarny, A.; Delfino, J.M.; Santos, J.
Deposited on : 2015-11-18
Resolution : 2.65 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

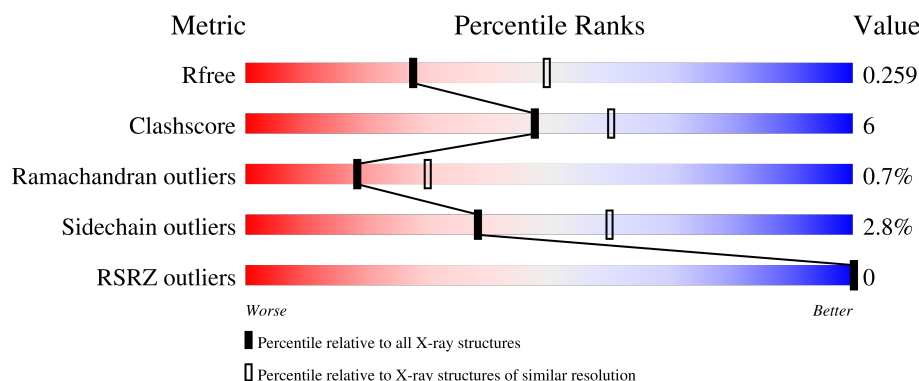
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	229	 75% 9% 14%
1	B	229	 74% 10% 15%
1	C	229	 67% 17% 16%
1	D	229	 68% 14% 17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6389 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 Hypoxanthine-guanine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1601	1024	277	293	7			
1	B	195	Total	C	N	O	S	0	0	0
			1581	1013	271	290	7			
1	C	193	Total	C	N	O	S	0	0	0
			1563	1002	266	288	7			
1	D	189	Total	C	N	O	S	0	0	0
			1533	985	259	282	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	LEU	-	expression tag	UNP Q4DRC4
A	223	GLU	-	expression tag	UNP Q4DRC4
A	224	HIS	-	expression tag	UNP Q4DRC4
A	225	HIS	-	expression tag	UNP Q4DRC4
A	226	HIS	-	expression tag	UNP Q4DRC4
A	227	HIS	-	expression tag	UNP Q4DRC4
A	228	HIS	-	expression tag	UNP Q4DRC4
A	229	HIS	-	expression tag	UNP Q4DRC4
B	222	LEU	-	expression tag	UNP Q4DRC4
B	223	GLU	-	expression tag	UNP Q4DRC4
B	224	HIS	-	expression tag	UNP Q4DRC4
B	225	HIS	-	expression tag	UNP Q4DRC4
B	226	HIS	-	expression tag	UNP Q4DRC4
B	227	HIS	-	expression tag	UNP Q4DRC4
B	228	HIS	-	expression tag	UNP Q4DRC4
B	229	HIS	-	expression tag	UNP Q4DRC4
C	222	LEU	-	expression tag	UNP Q4DRC4
C	223	GLU	-	expression tag	UNP Q4DRC4
C	224	HIS	-	expression tag	UNP Q4DRC4
C	225	HIS	-	expression tag	UNP Q4DRC4
C	226	HIS	-	expression tag	UNP Q4DRC4

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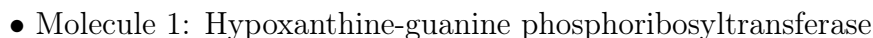
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Chain	Residue	Modelled	Actual	Comment	Reference
C	227	HIS	-	expression tag	UNP Q4DRC4
C	228	HIS	-	expression tag	UNP Q4DRC4
C	229	HIS	-	expression tag	UNP Q4DRC4
D	222	LEU	-	expression tag	UNP Q4DRC4
D	223	GLU	-	expression tag	UNP Q4DRC4
D	224	HIS	-	expression tag	UNP Q4DRC4
D	225	HIS	-	expression tag	UNP Q4DRC4
D	226	HIS	-	expression tag	UNP Q4DRC4
D	227	HIS	-	expression tag	UNP Q4DRC4
D	228	HIS	-	expression tag	UNP Q4DRC4
D	229	HIS	-	expression tag	UNP Q4DRC4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	40	Total O 40 40	0	0
2	C	19	Total O 19 19	0	0
2	D	23	Total O 23 23	0	0

- Molecule 1: Hypoxanthine-guanine phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	95.67Å 95.67Å 75.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.34 – 2.65 36.34 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.34-2.65) 99.9 (36.34-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.190 , 0.264 0.193 , 0.259	Depositor DCC
R_{free} test set	1150 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 17.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l 0.470 for h,-h-k,-l 0.033 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6389	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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	0.89	0/1633	1.00	2/2209 (0.1%)
1	B	0.88	0/1613	1.00	3/2183 (0.1%)
1	C	0.79	0/1594	0.94	2/2158 (0.1%)
1	D	0.80	0/1564	0.96	2/2118 (0.1%)
All	All	0.84	0/6404	0.98	9/8668 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	149	VAL	CA-C-N	-7.59	111.95	119.76
1	A	149	VAL	C-N-CA	-7.59	111.95	119.76
1	C	149	VAL	CA-C-N	-6.58	112.70	120.13
1	C	149	VAL	C-N-CA	-6.58	112.70	120.13
1	D	149	VAL	CA-C-N	-6.04	113.31	120.13
1	D	149	VAL	C-N-CA	-6.04	113.31	120.13
1	B	87	THR	N-CA-C	6.00	117.97	108.67
1	B	149	VAL	CA-C-N	-5.36	114.40	119.76
1	B	149	VAL	C-N-CA	-5.36	114.40	119.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	86	LEU	Peptide

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	1601	0	1611	19	0
1	B	1581	0	1590	17	0
1	C	1563	0	1569	25	0
1	D	1533	0	1540	20	0
2	A	29	0	0	3	0
2	B	40	0	0	4	0
2	C	19	0	0	1	0
2	D	23	0	0	1	0
All	All	6389	0	6310	70	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 6.

All (70) 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:B:147:ARG:NH1	1:B:151:PHE:O	2.14	0.79
1:A:16:GLU:OE1	1:A:19:ARG:NH1	2.17	0.77
1:A:85:GLY:C	1:A:86:LEU:HD22	2.12	0.72
1:A:147:ARG:NH1	1:A:151:PHE:O	2.22	0.72
1:A:87:THR:HB	1:D:103:GLU:OE1	1.95	0.67
1:D:149:VAL:HG22	1:D:150:PRO:HD2	1.75	0.66
1:C:149:VAL:HG22	1:C:150:PRO:HD2	1.77	0.65
1:A:195:ALA:O	1:A:198:GLN:HB2	1.98	0.64
1:C:126:MET:HE2	1:C:130:ARG:HH21	1.62	0.64
1:A:84:GLU:O	1:A:85:GLY:C	2.41	0.62
1:B:88:SER:OG	1:C:131:ARG:NH1	2.34	0.60
1:B:82:TYR:O	1:B:84:GLU:N	2.36	0.58
1:A:85:GLY:O	1:A:86:LEU:HD13	2.03	0.58
1:C:125:HIS:O	1:C:129:THR:HG23	2.05	0.57
1:A:148:ARG:NH2	2:A:302:HOH:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LEU:O	1:D:157:VAL:HB	2.07	0.55
1:C:112:ASP:HB2	1:C:170:LEU:HD21	1.89	0.54
1:D:73:ARG:HG3	1:D:73:ARG:HH11	1.72	0.54
1:A:88:SER:OG	1:D:131:ARG:NH1	2.41	0.53
1:B:148:ARG:NH2	2:B:303:HOH:O	2.42	0.53
1:B:156:VAL:HG22	2:B:301:HOH:O	2.08	0.53
1:D:147:ARG:NH1	1:D:151:PHE:O	2.42	0.53
1:A:63:ARG:HD3	1:C:56:MET:SD	2.49	0.52
1:B:85:GLY:C	2:B:316:HOH:O	2.53	0.52
1:D:125:HIS:O	1:D:129:THR:HG23	2.10	0.51
1:C:69:ASN:CG	2:C:302:HOH:O	2.54	0.51
1:B:156:VAL:CG2	2:B:301:HOH:O	2.59	0.50
1:D:112:ASP:O	1:D:140:LEU:HB3	2.12	0.50
1:A:103:GLU:OE1	1:D:87:THR:OG1	2.30	0.49
1:A:197:ARG:O	1:A:198:GLN:NE2	2.45	0.49
1:C:73:ARG:HH11	1:C:73:ARG:HG3	1.78	0.49
1:A:125:HIS:CD2	1:D:129:THR:HG21	2.47	0.48
1:A:142:ASP:OD1	1:A:147:ARG:NH2	2.46	0.48
1:B:164:PHE:HB2	1:B:185:LEU:HB3	1.95	0.48
1:B:125:HIS:CD2	1:C:129:THR:HG21	2.49	0.48
1:B:142:ASP:OD1	1:B:147:ARG:NH2	2.46	0.48
1:D:166:ILE:HG13	1:D:183:VAL:HG22	1.96	0.48
1:A:131:ARG:HD2	1:D:89:SER:HB3	1.96	0.47
1:C:127:TYR:O	1:C:130:ARG:HB2	2.15	0.46
1:D:50:VAL:O	1:D:54:SER:OG	2.30	0.46
1:D:127:TYR:O	1:D:130:ARG:HB2	2.15	0.46
1:B:131:ARG:HD2	1:C:89:SER:HB3	1.98	0.46
1:C:142:ASP:OD1	1:C:144:ARG:HG3	2.16	0.46
1:D:112:ASP:HB2	1:D:170:LEU:HD21	1.97	0.46
1:C:112:ASP:HB2	1:C:170:LEU:CD2	2.46	0.46
1:C:166:ILE:HG13	1:C:183:VAL:HG22	1.98	0.45
1:B:3:ARG:HD2	1:B:181:ASP:OD2	2.16	0.45
1:C:147:ARG:NH1	1:C:151:PHE:O	2.49	0.45
1:C:32:ASP:OD2	1:C:155:TYR:OH	2.18	0.44
1:C:112:ASP:O	1:C:140:LEU:HB3	2.18	0.44
1:D:113:ILE:HD11	1:D:143:LYS:HE3	2.00	0.44
1:A:51:LEU:HB3	1:A:52:LYS:HA	1.99	0.43
1:B:148:ARG:HA	1:B:148:ARG:HD2	1.95	0.43
1:D:144:ARG:HD3	2:D:301:HOH:O	2.18	0.43
1:D:128:PHE:C	1:D:130:ARG:H	2.27	0.42
1:D:140:LEU:HG	1:D:141:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HE	1:A:144:ARG:HB2	1.60	0.42
1:B:164:PHE:CB	1:B:185:LEU:HB3	2.49	0.42
1:C:113:ILE:HD11	1:C:143:LYS:HE3	2.02	0.42
1:C:12:LEU:HG	1:C:184:VAL:HG23	2.02	0.42
1:A:91:GLN:O	2:A:301:HOH:O	2.22	0.42
1:B:103:GLU:OE1	1:C:87:THR:OG1	2.34	0.42
1:C:138:VAL:HG23	1:C:155:TYR:HB2	2.03	0.41
1:B:125:HIS:HD2	1:C:129:THR:HG21	1.86	0.41
1:B:111:GLU:HG3	1:B:112:ASP:N	2.36	0.41
1:C:19:ARG:HH11	1:C:19:ARG:HB2	1.86	0.40
1:C:140:LEU:O	1:C:141:LEU:HD23	2.22	0.40
1:A:197:ARG:H	1:A:197:ARG:HG2	1.69	0.40
2:A:315:HOH:O	1:D:99:ARG:HB2	2.20	0.40
1:C:187:PRO:O	1:C:190:TYR:HB3	2.22	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	195/229 (85%)	188 (96%)	7 (4%)	0	100	100
1	B	193/229 (84%)	184 (95%)	7 (4%)	2 (1%)	12	20
1	C	191/229 (83%)	183 (96%)	7 (4%)	1 (0%)	24	39
1	D	187/229 (82%)	180 (96%)	5 (3%)	2 (1%)	11	19
All	All	766/916 (84%)	735 (96%)	26 (3%)	5 (1%)	18	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	83	GLY

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Mol	Chain	Res	Type
1	C	83	GLY
1	D	164	PHE
1	B	41	TYR
1	D	161	PRO

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	174/202 (86%)	168 (97%)	6 (3%)	32	53
1	B	172/202 (85%)	169 (98%)	3 (2%)	53	73
1	C	170/202 (84%)	165 (97%)	5 (3%)	37	58
1	D	168/202 (83%)	163 (97%)	5 (3%)	36	57
All	All	684/808 (85%)	665 (97%)	19 (3%)	38	60

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASP
1	A	86	LEU
1	A	115	ASP
1	A	148	ARG
1	A	197	ARG
1	A	198	GLN
1	B	2	PRO
1	B	31	ASP
1	B	148	ARG
1	C	4	GLU
1	C	31	ASP
1	C	86	LEU
1	C	115	ASP
1	C	148	ARG
1	D	4	GLU
1	D	31	ASP
1	D	86	LEU

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Mol	Chain	Res	Type
1	D	92	VAL
1	D	148	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	159	ASN
1	B	105	HIS
1	B	162	ASN
1	C	121	ASN
1	C	159	ASN
1	C	162	ASN
1	D	121	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 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	197/229 (86%)	-1.62	0 100 100	24, 37, 72, 115	0
1	B	195/229 (85%)	-1.63	0 100 100	23, 37, 61, 118	0
1	C	193/229 (84%)	-1.54	0 100 100	23, 42, 107, 135	0
1	D	189/229 (82%)	-1.55	0 100 100	24, 43, 92, 124	0
All	All	774/916 (84%)	-1.59	0 100 100	23, 39, 85, 135	0

There are no RSRZ outliers to report.

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.