



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 8J8P / pdb_00008j8p
Title : Structure of the four-component Paf1 complex from *Saccharomyces eubayanus*
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Deposited on : 2023-05-02
Resolution : 2.70 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

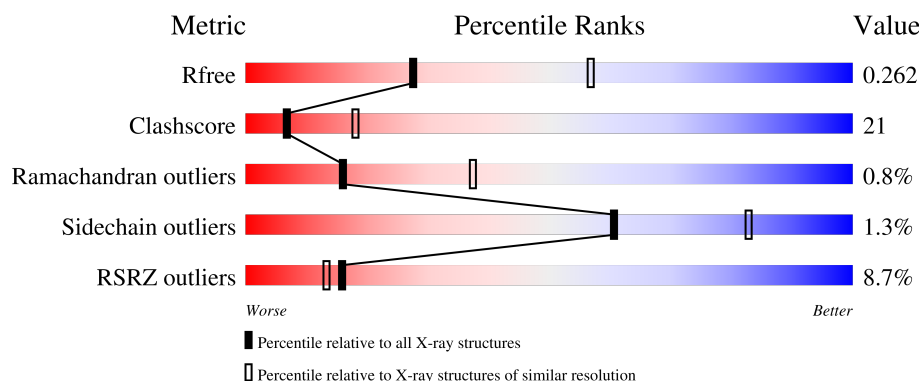
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	C	908	10% 70% 28% .
2	A	81	9% 32% 23% . 42%
3	P	111	% 62% 19% . 18%
4	R	77	3% 62% 27% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9128 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 CTR9-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	906	Total	C	N	O	S	0	0	0
			7363	4694	1248	1399	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP A0A0L8RHL9

- Molecule 2 is a protein called CDC73-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	47	Total	C	N	O	S	0	0	0
			366	229	67	69	1			

- Molecule 3 is a protein called PAF1-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	91	Total	C	N	O	S	0	0	0
			726	464	120	140	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	0	SER	-	expression tag	UNP A0A0L8RM45

- Molecule 4 is a protein called RTF1-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	69	Total	C	N	O	S	0	0	0
			594	373	107	112	2			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	56	Total 56	O 56	0	0
5	P	18	Total 18	O 18	0	0
5	R	5	Total 5	O 5	0	0

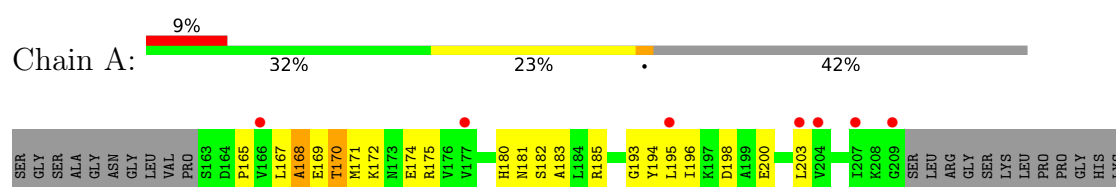
3 Residue-property plots

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: CTR9-like protein



• Molecule 2: CDC73-like protein



GLY
ALA
HIS
GLY
ARG
VAL
SER
THR
ASN
GLY
SER

● Molecule 3: PAF1-like protein



SER MET LYS LYS GLN GLU TYR ILE ALA PRO ILE LYS TYR GLN ASN S16 L17 P18 Q21 L22 E34 T35 N36 N51 I52 Q58 D67 L68 M69 K70 F71 L74 S80 K81 L82 L83 F86 D87 N88 V89 P102 R103 R106 LEU THR LYS THR

● Molecule 4: RTF1-like protein



SER LYS SER ASP PRO PHE SER ARG L502 Y509 Y513 E528 K529 L530 Q531 E532 D533 R534 E535 T536 K537 E538 R539 R540 E541 L545 L546 A547 Q548 F549 R550 R551 L552 G553 G554 K565 F566 F570

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.78Å 88.48Å 127.78Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	34.47 – 2.70 34.47 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.47-2.70) 99.6 (34.47-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.225 , 0.263 0.225 , 0.262	Depositor DCC
R_{free} test set	2133 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9128	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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	C	0.40	7/7499 (0.1%)	0.60	8/10111 (0.1%)
2	A	0.47	0/370	0.83	2/497 (0.4%)
3	P	0.66	3/740 (0.4%)	0.56	1/1006 (0.1%)
4	R	0.28	0/599	0.56	0/789
All	All	0.43	10/9208 (0.1%)	0.60	11/12403 (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	C	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	LEU	C-O	-7.54	1.14	1.23
1	C	239	LYS	C-O	-6.96	1.16	1.24
1	C	204	LYS	C-O	-6.33	1.16	1.24
3	P	103	ARG	C-N	-6.09	1.27	1.34
3	P	86	PHE	C-O	-5.88	1.16	1.23

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	627	LYS	N-CA-C	8.97	121.05	111.28
1	C	623	SER	N-CA-C	8.35	121.43	111.33
2	A	172	LYS	N-CA-C	7.29	122.36	113.17
1	C	88	ASN	N-CA-C	7.26	120.35	108.08
3	P	88	ASN	N-CA-C	6.64	120.71	111.74

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	775	LEU	Peptide
1	C	815	PHE	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	C	7363	0	7426	346	0
2	A	366	0	377	21	0
3	P	726	0	746	23	0
4	R	594	0	610	23	0
5	C	56	0	0	1	0
5	P	18	0	0	2	0
5	R	5	0	0	0	0
All	All	9128	0	9159	389	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 21.

The worst 5 of 389 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:C:613:ARG:HD2	1:C:616:TYR:CE1	1.36	1.55
1:C:613:ARG:CG	1:C:639:THR:HG22	1.54	1.36
1:C:613:ARG:CD	1:C:616:TYR:HE1	1.39	1.35
1:C:782:ARG:HB3	1:C:787:ARG:NH2	1.41	1.33
1:C:613:ARG:CG	1:C:639:THR:CG2	2.24	1.16

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	C	904/908 (100%)	817 (90%)	78 (9%)	9 (1%)	12	32
2	A	45/81 (56%)	39 (87%)	6 (13%)	0	100	100
3	P	89/111 (80%)	85 (96%)	4 (4%)	0	100	100
4	R	67/77 (87%)	63 (94%)	4 (6%)	0	100	100
All	All	1105/1177 (94%)	1004 (91%)	92 (8%)	9 (1%)	16	37

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	777	ARG
1	C	782	ARG
1	C	455	LYS
1	C	684	ALA
1	C	641	VAL

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	C	819/821 (100%)	810 (99%)	9 (1%)	65	85
2	A	40/64 (62%)	37 (92%)	3 (8%)	12	31
3	P	86/105 (82%)	85 (99%)	1 (1%)	63	84
4	R	62/70 (89%)	62 (100%)	0	100	100
All	All	1007/1060 (95%)	994 (99%)	13 (1%)	61	83

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	680	SER
1	C	816	ILE
3	P	103	ARG
2	A	170	THR
2	A	171	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	827	GLN
2	A	178	GLN
3	P	36	ASN
1	C	457	ASN
1	C	443	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 ⓘ

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	C	906/908 (99%)	0.40	87 (9%) 13 11	24, 76, 223, 317	0
2	A	47/81 (58%)	0.90	7 (14%) 5 4	80, 109, 134, 138	0
3	P	91/111 (81%)	-0.29	1 (1%) 78 76	29, 43, 99, 112	0
4	R	69/77 (89%)	0.06	2 (2%) 53 50	41, 59, 102, 109	0
All	All	1113/1177 (94%)	0.34	97 (8%) 16 13	24, 72, 216, 317	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	707	ILE	6.0
1	C	654	LEU	5.4
1	C	582	TYR	4.8
1	C	778	ALA	4.7
1	C	685	ILE	4.6

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.