



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5ZYP / pdb_00005zyp
Title : Structure of the Yeast Ctr9/Paf1 complex
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Deposited on : 2018-05-28
Resolution : 2.53 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

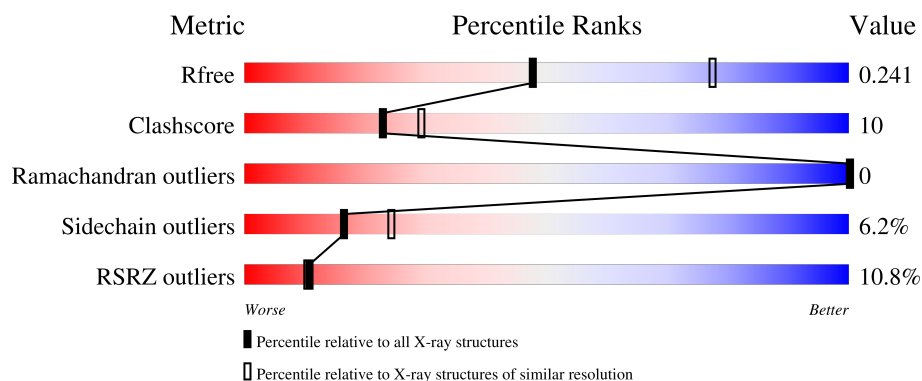
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	390	9% 66% 19% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2827 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 RNA polymerase-associated protein CTR9,RNA polymerase II-associated protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	Se	0	0	0
			2739	1758	453	518	3	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1027	GLU	-	linker	UNP P89105
A	1028	ASN	-	linker	UNP P89105
A	1029	LEU	-	linker	UNP P89105
A	1030	TYR	-	linker	UNP P89105
A	1031	PHE	-	linker	UNP P89105
A	1032	GLN	-	linker	UNP P89105
A	1033	SER	-	linker	UNP P89105

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ni	0	0
			3	3		

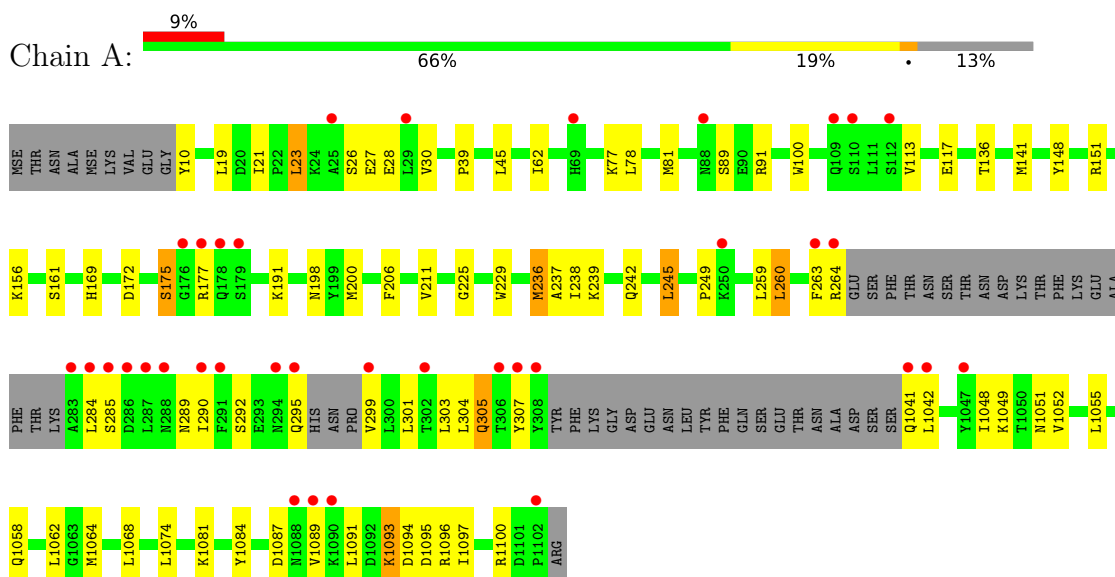
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total	O	0	0
			85	85		

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: RNA polymerase-associated protein CTR9, RNA polymerase II-associated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	95.95Å 95.95Å 115.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.98 – 2.53 47.98 – 2.53	Depositor EDS
% Data completeness (in resolution range)	90.1 (47.98-2.53) 82.2 (47.98-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10_2155_000)	Depositor
R, R_{free}	0.194 , 0.243 0.195 , 0.241	Depositor DCC
R_{free} test set	1798 reflections (9.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2827	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI

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	0.35	0/2784	0.54	0/3759

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 [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	2739	0	2766	57	0
2	A	3	0	0	0	0
3	A	85	0	0	9	0
All	All	2827	0	2766	57	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 10.

All (57) 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:172:ASP:OD2	1:A:177:ARG:NH1	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:SER:O	1:A:289:ASN:ND2	2.11	0.83
1:A:198:ASN:ND2	3:A:901:HOH:O	2.18	0.76
1:A:292:SER:O	1:A:295:GLN:NE2	2.21	0.73
1:A:39:PRO:HD2	1:A:45:LEU:HD11	1.71	0.72
1:A:236:MSE:HE3	1:A:239:LYS:HE3	1.73	0.70
1:A:260:LEU:HD12	1:A:1052:VAL:HG13	1.77	0.65
1:A:177:ARG:NH1	3:A:904:HOH:O	2.27	0.62
1:A:1091:LEU:O	1:A:1096:ARG:NH1	2.33	0.61
1:A:264:ARG:HH21	1:A:1049:LYS:NZ	1.99	0.60
1:A:264:ARG:HE	1:A:1049:LYS:HE3	1.66	0.59
1:A:299:VAL:HG23	1:A:1055:LEU:HD13	1.83	0.59
1:A:21:ILE:HB	1:A:30:VAL:HG13	1.86	0.58
1:A:91:ARG:NH2	3:A:909:HOH:O	2.40	0.54
1:A:1093:LYS:O	1:A:1097:ILE:HG13	2.07	0.54
1:A:169:HIS:HE1	3:A:964:HOH:O	1.91	0.53
1:A:211:VAL:HG23	1:A:1091:LEU:HD22	1.91	0.53
1:A:263:PHE:HE1	1:A:284:LEU:HB3	1.75	0.52
1:A:295:GLN:N	1:A:295:GLN:OE1	2.43	0.51
1:A:242:GLN:NE2	3:A:912:HOH:O	2.44	0.51
1:A:307:TYR:O	1:A:307:TYR:HD2	1.94	0.51
1:A:245:LEU:HD22	1:A:249:PRO:HA	1.92	0.50
1:A:169:HIS:CE1	3:A:964:HOH:O	2.63	0.50
1:A:23:LEU:HD13	1:A:28:GLU:HG3	1.93	0.49
1:A:1084:TYR:OH	3:A:902:HOH:O	2.18	0.49
1:A:229:TRP:HH2	1:A:264:ARG:HD3	1.78	0.47
1:A:264:ARG:HH21	1:A:1049:LYS:HZ1	1.62	0.47
1:A:78:LEU:HD12	1:A:81:MSE:HE3	1.99	0.45
1:A:206:PHE:CZ	1:A:1064:MSE:HE1	2.52	0.45
1:A:45:LEU:HD22	1:A:62:ILE:HG21	1.99	0.44
1:A:236:MSE:CE	1:A:239:LYS:HE3	2.46	0.44
1:A:301:LEU:O	1:A:304:LEU:N	2.49	0.44
1:A:1081:LYS:HE2	1:A:1081:LYS:HB3	1.75	0.44
1:A:175:SER:O	1:A:177:ARG:HG3	2.17	0.44
1:A:1051:ASN:ND2	3:A:917:HOH:O	2.48	0.44
1:A:78:LEU:HA	1:A:81:MSE:HE2	2.00	0.44
1:A:292:SER:C	1:A:295:GLN:HE22	2.20	0.43
1:A:117:GLU:OE1	1:A:151:ARG:NH2	2.47	0.43
1:A:1089:VAL:HG22	1:A:1091:LEU:HB2	2.01	0.43
1:A:100:TRP:CE2	1:A:1068:LEU:HG	2.54	0.43
1:A:191:LYS:HG2	1:A:1062:LEU:HD12	2.01	0.43
1:A:1091:LEU:HA	1:A:1091:LEU:HD12	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TYR:OH	1:A:156:LYS:HE3	2.19	0.42
1:A:225:GLY:HA2	1:A:237:ALA:HA	2.01	0.42
1:A:263:PHE:CE2	1:A:1048:ILE:HD11	2.54	0.42
1:A:136:THR:O	1:A:141:MSE:HE2	2.19	0.42
1:A:238:ILE:O	1:A:242:GLN:HG3	2.20	0.42
1:A:1068:LEU:HD13	1:A:1074:LEU:HD21	2.02	0.42
1:A:26:SER:OG	1:A:28:GLU:HG2	2.19	0.42
1:A:21:ILE:HB	1:A:30:VAL:CG1	2.50	0.42
1:A:77:LYS:O	1:A:81:MSE:HG3	2.19	0.42
1:A:10:TYR:OH	1:A:1095:ASP:OD1	2.33	0.41
1:A:301:LEU:HG	1:A:305:GLN:OE1	2.20	0.41
1:A:1055:LEU:HA	1:A:1058:GLN:HB2	2.02	0.41
1:A:1094:ASP:HA	1:A:1097:ILE:HD12	2.03	0.41
1:A:1089:VAL:HG13	1:A:1089:VAL:O	2.21	0.41
1:A:19:LEU:HA	3:A:921:HOH:O	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	332/390 (85%)	316 (95%)	16 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	308/344 (90%)	289 (94%)	19 (6%)	16	24

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

Mol	Chain	Res	Type
1	A	23	LEU
1	A	27	GLU
1	A	89	SER
1	A	113	VAL
1	A	161	SER
1	A	175	SER
1	A	200	MSE
1	A	236	MSE
1	A	245	LEU
1	A	259	LEU
1	A	260	LEU
1	A	290	ILE
1	A	303	LEU
1	A	305	GLN
1	A	1041	GLN
1	A	1042	LEU
1	A	1087	ASP
1	A	1093	LYS
1	A	1100	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	198	ASN
1	A	289	ASN
1	A	1051	ASN
1	A	1057	GLN

5.3.3 RNA ⓘ

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	333/390 (85%)	0.31	36 (10%)	11 10	12, 42, 95, 116	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	110	SER	7.3
1	A	1102	PRO	6.5
1	A	284	LEU	5.9
1	A	1041	GLN	5.4
1	A	283	ALA	5.4
1	A	308	TYR	5.2
1	A	1042	LEU	4.6
1	A	178	GLN	4.0
1	A	291	PHE	3.8
1	A	1089	VAL	3.8
1	A	177	ARG	3.8
1	A	29	LEU	3.7
1	A	295	GLN	3.7
1	A	179	SER	3.6
1	A	88	ASN	3.2
1	A	307	TYR	3.2
1	A	1047	TYR	3.2
1	A	302	THR	3.2
1	A	290	ILE	3.1
1	A	264	ARG	3.0
1	A	288	ASN	3.0
1	A	306	THR	2.9
1	A	1088	ASN	2.8
1	A	287	LEU	2.7
1	A	1090	LYS	2.6
1	A	286	ASP	2.5
1	A	109	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	25	ALA	2.5
1	A	263	PHE	2.4
1	A	250	LYS	2.3
1	A	299	VAL	2.2
1	A	294	ASN	2.2
1	A	112	SER	2.1
1	A	285	SER	2.1
1	A	176	GLY	2.0
1	A	69	HIS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	A	801	1/1	0.98	0.06	80,80,80,80	0
2	NI	A	803	1/1	0.98	0.04	37,37,37,37	0
2	NI	A	802	1/1	0.99	0.03	42,42,42,42	1

6.5 Other polymers [i](#)

There are no such residues in this entry.