



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:59 PM UTC

PDB ID : 1QVA / pdb_00001qva
Title : YEAST INITIATION FACTOR 4A N-TERMINAL DOMAIN
Authors : Johnson, E.R.; McKay, D.B.
Deposited on : 1999-07-07
Resolution : 2.50 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

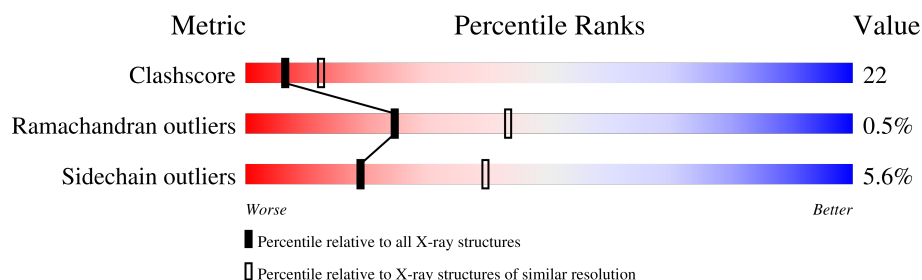
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	223	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1698 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 INITIATION FACTOR 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1643	1051	272	310	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASP	conflict	UNP P10081
A	31	GLN	ASN	conflict	UNP P10081

- Molecule 2 is water.

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

Note EDS was not executed.

Chain A: 55% 36%

Amino Acid	Category
SER	Green
GLY	Green
GLU	Green
ILE	Green
THR	Green
ASP	Green
ILE	Green
GLU	Green
SER	Green
Q11	Green
I12	Green
Q13	Green
T14	Green
Y16	Green
Q17	Green
Y21	Green
K22	Green
L28	Green
Y29	Green
E30	Green
V36	Green
F41	Green
S45	Green
A46	Green
L47	Green
Q48	Green
R49	Green
R50	Green
A51	Green
I52	Green
M53	Green
P54	Green
D60	Green
V61	Green
Q64	Green
A65	Green
Q66	Green
S67	Green
G68	Green
T69	Green
G70	Green
K71	Green
T74	Green

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.80Å 74.30Å 81.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50	Depositor
% Data completeness (in resolution range)	94.0 (40.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1698	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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	0.46	0/1670	0.94	6/2261 (0.3%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLN	N-CA-C	7.28	120.79	112.57
1	A	52	ILE	N-CA-C	6.88	117.00	110.53
1	A	60	ASP	N-CA-C	-6.26	101.02	110.28
1	A	61	VAL	N-CA-C	5.74	116.38	108.12
1	A	137	ARG	N-CA-C	5.35	116.97	111.03
1	A	219	VAL	N-CA-C	-5.06	102.33	109.21

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	1643	0	1654	72	0
2	A	55	0	0	3	0
All	All	1698	0	1654	72	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 22.

All (72) 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:127:THR:HG21	2:A:501:HOH:O	1.61	0.99
1:A:45:SER:H	1:A:48:GLN:HE21	1.22	0.86
1:A:153:ILE:HG21	1:A:189:LEU:HD13	1.61	0.80
1:A:99:ARG:HD2	1:A:148:ARG:HH21	1.47	0.80
1:A:113:ALA:HA	1:A:116:MET:HE3	1.67	0.77
1:A:45:SER:H	1:A:48:GLN:NE2	1.82	0.76
1:A:30:GLU:CD	1:A:30:GLU:H	1.95	0.73
1:A:191:PRO:O	1:A:194:THR:HG23	1.88	0.73
1:A:61:VAL:HG22	1:A:219:VAL:CG1	2.19	0.72
1:A:124:ILE:HA	1:A:148:ARG:HG3	1.71	0.71
1:A:165:MET:HE2	1:A:167:ILE:HD11	1.73	0.70
1:A:211:THR:HA	1:A:215:MET:HE3	1.73	0.69
1:A:113:ALA:HA	1:A:116:MET:CE	2.24	0.67
1:A:191:PRO:HG2	1:A:194:THR:CG2	2.25	0.66
1:A:21:TYR:O	1:A:22:LYS:HD2	1.97	0.64
1:A:14:THR:HA	1:A:220:ARG:O	1.98	0.64
1:A:41:PHE:HE2	1:A:69:THR:HG23	1.62	0.64
1:A:41:PHE:CE2	1:A:69:THR:HG23	2.35	0.62
1:A:66:GLN:CD	1:A:67:SER:H	2.10	0.59
1:A:120:VAL:HG22	1:A:141:ILE:HB	1.83	0.58
1:A:216:ARG:O	1:A:217:ASN:C	2.46	0.58
1:A:61:VAL:HG22	1:A:219:VAL:HG12	1.84	0.58
1:A:61:VAL:HG13	1:A:219:VAL:HG13	1.87	0.56
1:A:153:ILE:CG2	1:A:189:LEU:HD13	2.35	0.55
1:A:113:ALA:CA	1:A:116:MET:HE3	2.37	0.54
1:A:191:PRO:HG2	1:A:194:THR:HG22	1.89	0.54
1:A:108:VAL:O	1:A:112:LEU:HD23	2.07	0.54
1:A:16:TYR:HB2	1:A:219:VAL:HG23	1.89	0.54
1:A:30:GLU:CD	1:A:30:GLU:N	2.66	0.53
1:A:182:GLN:O	1:A:186:ILE:HG13	2.07	0.53
1:A:84:ASP:OD2	1:A:87:VAL:HG23	2.09	0.53
1:A:45:SER:N	1:A:48:GLN:HE21	2.00	0.52
1:A:125:GLY:N	1:A:148:ARG:HE	2.08	0.52
1:A:16:TYR:HB2	1:A:219:VAL:CG2	2.39	0.52
1:A:64:GLN:HB2	1:A:203:MET:HE3	1.92	0.52
1:A:101:LEU:HD13	1:A:170:GLU:OE1	2.10	0.52
1:A:174:MET:HG2	1:A:183:ILE:HD11	1.92	0.51
1:A:50:ARG:HH11	1:A:50:ARG:HG3	1.75	0.51
1:A:211:THR:O	1:A:215:MET:HB2	2.12	0.49
1:A:121:HIS:CD2	1:A:135:GLY:HA3	2.47	0.49
1:A:93:LEU:HD13	1:A:166:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:OG1	1:A:148:ARG:HG2	2.13	0.49
1:A:151:ASP:O	1:A:155:ARG:HB2	2.12	0.49
1:A:98:THR:OG1	1:A:100:GLU:HG2	2.14	0.48
1:A:36:VAL:HA	1:A:112:LEU:CD1	2.43	0.48
1:A:93:LEU:HD13	1:A:166:PHE:HE1	1.79	0.47
1:A:12:ILE:HG22	1:A:13:GLN:N	2.30	0.46
1:A:61:VAL:HG22	1:A:219:VAL:HG11	1.96	0.46
1:A:122:ALA:HA	1:A:143:VAL:O	2.14	0.46
1:A:198:LEU:C	1:A:198:LEU:HD23	2.40	0.46
1:A:89:ALA:O	1:A:91:GLN:HG3	2.17	0.45
1:A:199:LEU:HD22	1:A:199:LEU:N	2.32	0.45
1:A:71:LYS:O	1:A:74:THR:HB	2.17	0.45
1:A:148:ARG:HG2	1:A:148:ARG:HH11	1.82	0.45
1:A:209:GLU:O	1:A:213:LYS:HG3	2.16	0.45
1:A:113:ALA:CB	1:A:116:MET:HE3	2.48	0.44
1:A:83:ILE:HD12	1:A:140:GLN:HB3	2.00	0.43
1:A:125:GLY:CA	1:A:148:ARG:HE	2.31	0.43
1:A:131:GLU:HG3	2:A:536:HOH:O	2.18	0.43
1:A:67:SER:HA	1:A:71:LYS:NZ	2.33	0.43
1:A:82:ARG:HH11	1:A:195:GLN:NE2	2.17	0.43
1:A:66:GLN:CD	1:A:67:SER:N	2.76	0.42
1:A:106:GLN:NE2	1:A:120:VAL:O	2.53	0.42
1:A:158:PHE:C	1:A:158:PHE:CD1	2.98	0.42
1:A:53:MET:N	1:A:54:PRO:HD2	2.35	0.41
1:A:99:ARG:HG3	2:A:512:HOH:O	2.20	0.41
1:A:80:LEU:HD13	1:A:116:MET:HE1	2.03	0.41
1:A:183:ILE:HG22	1:A:187:PHE:HE1	1.87	0.40
1:A:50:ARG:HG3	1:A:50:ARG:NH1	2.36	0.40
1:A:99:ARG:CD	1:A:148:ARG:HH21	2.26	0.40
1:A:158:PHE:HD1	1:A:159:ARG:N	2.18	0.40
1:A:206:ASP:O	1:A:210:VAL:HG23	2.21	0.40

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	211/223 (95%)	203 (96%)	7 (3%)	1 (0%)	24	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	THR

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	177/192 (92%)	167 (94%)	10 (6%)	19	39

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	30	GLU
1	A	47	ILE
1	A	66	GLN
1	A	69	THR
1	A	85	THR
1	A	93	LEU
1	A	174	MET
1	A	175	LEU
1	A	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	59	HIS
1	A	121	HIS

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Mol	Chain	Res	Type
1	A	185	GLN
1	A	195	GLN
1	A	205	ASN
1	A	217	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.