



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3ER0
Title : Crystal structure of the full length eIF5A from *Saccharomyces cerevisiae*
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Deposited on : 2008-10-01
Resolution : 3.35 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

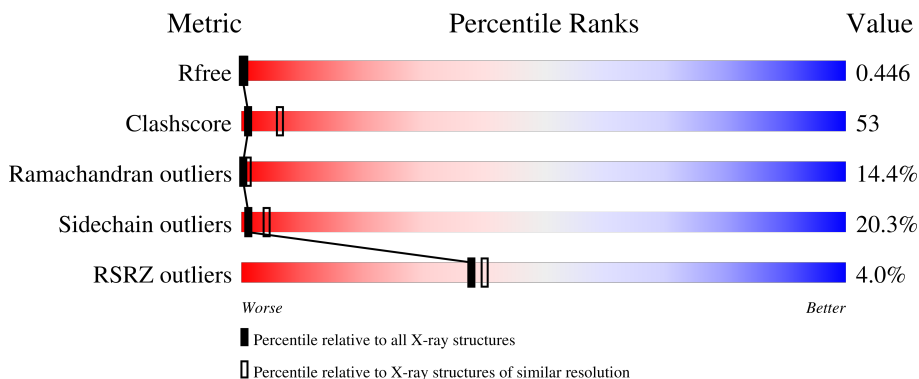
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	167	
1	B	167	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2105 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 Eukaryotic translation initiation factor 5A-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	146	1104	685	186	224	9	0	0	0
1	B	131	1001	628	164	200	9	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP P23301
A	-8	ARG	-	expression tag	UNP P23301
A	-7	GLY	-	expression tag	UNP P23301
A	-6	SER	-	expression tag	UNP P23301
A	-5	HIS	-	expression tag	UNP P23301
A	-4	HIS	-	expression tag	UNP P23301
A	-3	HIS	-	expression tag	UNP P23301
A	-2	HIS	-	expression tag	UNP P23301
A	-1	HIS	-	expression tag	UNP P23301
A	0	HIS	-	expression tag	UNP P23301
B	-9	MET	-	expression tag	UNP P23301
B	-8	ARG	-	expression tag	UNP P23301
B	-7	GLY	-	expression tag	UNP P23301
B	-6	SER	-	expression tag	UNP P23301
B	-5	HIS	-	expression tag	UNP P23301
B	-4	HIS	-	expression tag	UNP P23301
B	-3	HIS	-	expression tag	UNP P23301
B	-2	HIS	-	expression tag	UNP P23301
B	-1	HIS	-	expression tag	UNP P23301
B	0	HIS	-	expression tag	UNP P23301

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	59.66Å 59.66Å 339.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.45 – 3.35 49.43 – 3.35	Depositor EDS
% Data completeness (in resolution range)	91.9 (49.45-3.35) 91.9 (49.43-3.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.33Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.386 , 0.448 0.382 , 0.446	Depositor DCC
R_{free} test set	528 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å ²)	114.4	Xtrriage
Anisotropy	0.074	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 103.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	2105	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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	0.71	3/1119 (0.3%)	1.04	4/1505 (0.3%)
1	B	0.47	0/1013	0.94	1/1360 (0.1%)
All	All	0.61	3/2132 (0.1%)	0.99	5/2865 (0.2%)

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	A	0	18
1	B	0	17
All	All	0	35

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	GLU	CD-OE1	15.09	1.42	1.25
1	A	152	GLU	CG-CD	6.86	1.62	1.51
1	A	152	GLU	CB-CG	6.11	1.63	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	GLU	OE1-CD-OE2	-10.52	110.68	123.30
1	A	152	GLU	CG-CD-OE2	8.19	134.68	118.30
1	A	128	PHE	N-CA-C	-6.59	93.21	111.00
1	B	102	LEU	CB-CA-C	5.79	121.20	110.20
1	A	118	GLY	N-CA-C	-5.37	99.67	113.10

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	18	THR	Peptide
1	A	19	TYR	Peptide
1	A	49	THR	Peptide
1	A	50	GLY	Peptide
1	A	97	ASP	Peptide

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	1104	0	1096	100	1
1	B	1001	0	1011	94	1
All	All	2105	0	2107	194	1

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 53.

The worst 5 of 194 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:98:GLY:HA2	1:B:99:PHE:CG	1.77	1.19
1:B:100:LEU:H	1:B:101:SER:HA	1.02	1.13
1:A:114:LYS:O	1:A:116:PRO:HD2	1.51	1.10
1:B:17:ALA:CB	1:B:18:THR:HA	1.77	1.09
1:A:17:ALA:CB	1:A:18:THR:HA	1.83	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:SER:OG	1:B:119:GLU:OE1[10_455]	2.06	0.14

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	144/167 (86%)	94 (65%)	28 (19%)	22 (15%)	0	1
1	B	127/167 (76%)	87 (68%)	23 (18%)	17 (13%)	0	1
All	All	271/334 (81%)	181 (67%)	51 (19%)	39 (14%)	0	1

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	17	ALA
1	A	20	PRO
1	A	51	LYS
1	A	100	LEU

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	123/142 (87%)	96 (78%)	27 (22%)	1	3
1	B	114/142 (80%)	93 (82%)	21 (18%)	1	6
All	All	237/284 (84%)	189 (80%)	48 (20%)	1	4

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	21	MET

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Mol	Chain	Res	Type
1	B	99	PHE
1	B	37	ARG
1	B	73	LEU
1	B	106	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	125	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 monosaccharides 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	146/167 (87%)	0.47	7 (4%) 30 33	82, 84, 87, 91	37 (25%)
1	B	131/167 (78%)	0.29	4 (3%) 49 52	82, 84, 85, 86	29 (22%)
All	All	277/334 (82%)	0.38	11 (3%) 38 40	82, 84, 86, 91	66 (23%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	PRO	4.5
1	A	96	ASP	4.0
1	A	136	VAL	3.2
1	B	84	VAL	3.0
1	A	156	THR	2.9

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 monosaccharides 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.