



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:44 AM UTC

PDB ID : 6JLY / pdb_00006jly
Title : eIF2a - eIF2B complex
Authors : Kashiwagi, K.; Ito, T.
Deposited on : 2019-03-07
Resolution : 3.50 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
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

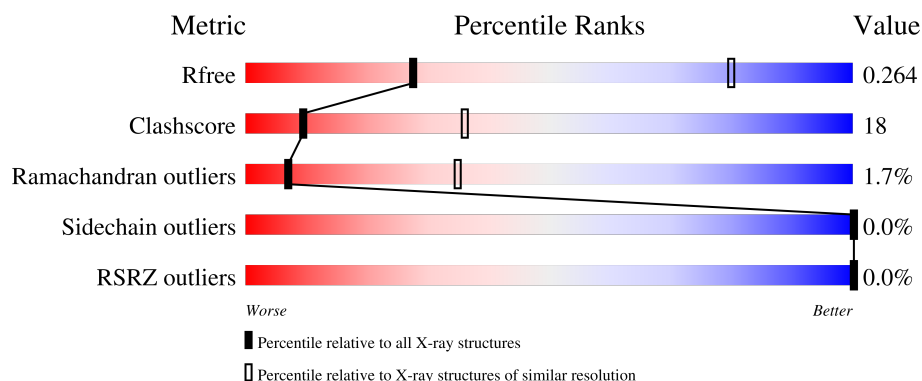
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

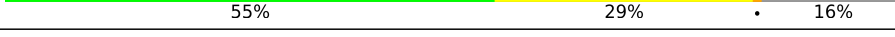
The reported resolution of this entry is 3.50 Å.

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.



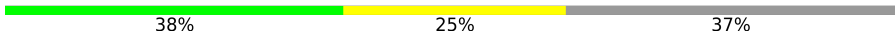
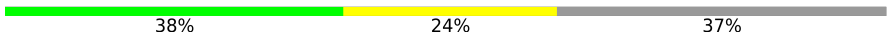
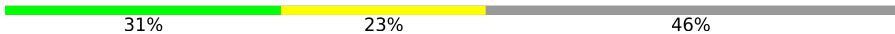
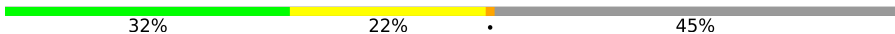
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	341	
1	B	341	
2	C	399	
2	D	399	
3	E	458	

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Mol	Chain	Length	Quality of chain
3	F	458	
4	G	467	
4	H	467	
5	I	678	
5	J	678	
6	L	304	
6	M	304	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31811 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2467	1568	431	455	13			
1	B	316	Total	C	N	O	S	0	0	0
			2465	1566	429	457	13			

- Molecule 2 is a protein called Probable translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	338	Total	C	N	O	S	0	0	0
			2617	1660	443	502	12			
2	D	337	Total	C	N	O	S	0	0	0
			2609	1654	442	501	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q9UT76
C	-4	PRO	-	expression tag	UNP Q9UT76
C	-3	ILE	-	expression tag	UNP Q9UT76
C	-2	SER	-	expression tag	UNP Q9UT76
C	-1	GLU	-	expression tag	UNP Q9UT76
C	0	PHE	-	expression tag	UNP Q9UT76
D	-5	GLY	-	expression tag	UNP Q9UT76
D	-4	PRO	-	expression tag	UNP Q9UT76
D	-3	ILE	-	expression tag	UNP Q9UT76
D	-2	SER	-	expression tag	UNP Q9UT76
D	-1	GLU	-	expression tag	UNP Q9UT76
D	0	PHE	-	expression tag	UNP Q9UT76

- Molecule 3 is a protein called Probable translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	414	Total	C	N	O	S	0	0	0
			3216	2040	555	604	17			
3	F	412	Total	C	N	O	S	0	0	0
			3204	2034	553	600	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	157	TYR	ILE	conflict	UNP P56288
E	158	THR	TYR	conflict	UNP P56288
E	159	VAL	GLY	conflict	UNP P56288
F	157	TYR	ILE	conflict	UNP P56288
F	158	THR	TYR	conflict	UNP P56288
F	159	VAL	GLY	conflict	UNP P56288

- Molecule 4 is a protein called Probable translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	363	Total	C	N	O	S	0	0	0
			2869	1834	486	536	13			
4	H	363	Total	C	N	O	S	0	0	0
			2869	1834	486	536	13			

- Molecule 5 is a protein called Probable translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	428	Total	C	N	O	S	0	0	0
			3377	2123	592	647	15			
5	J	426	Total	C	N	O	S	0	0	0
			3362	2115	587	645	15			

- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	165	Total	C	N	O	S	0	0	0
			1353	863	226	258	6			
6	M	166	Total	C	N	O	S	0	0	0
			1363	872	227	258	6			

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

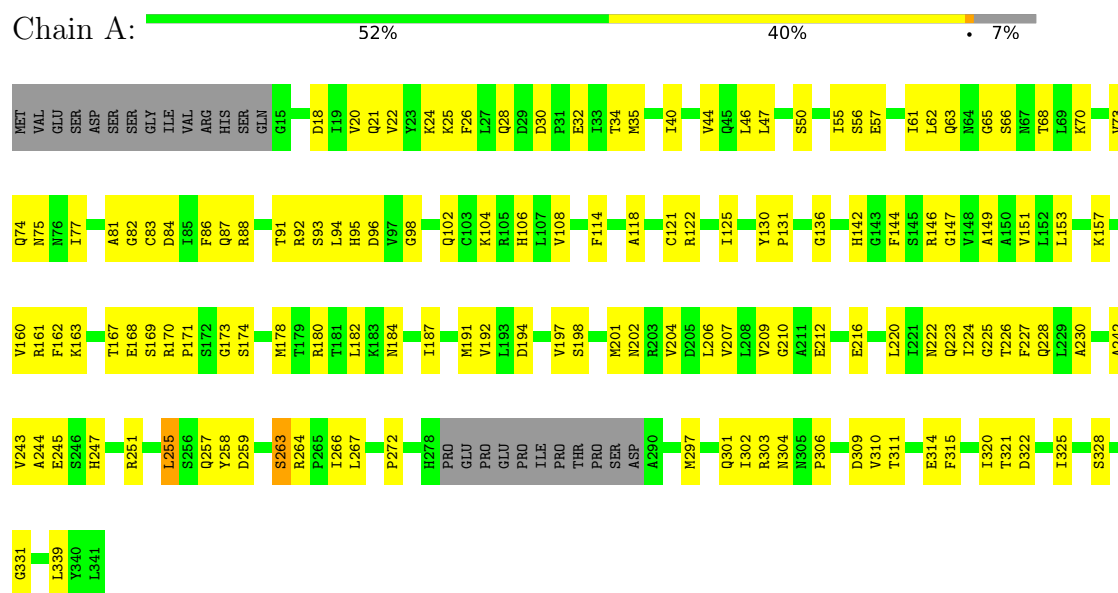


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		
7	E	1	Total	O	P	0	0
			5	4	1		
7	F	1	Total	O	P	0	0
			5	4	1		
7	F	1	Total	O	P	0	0
			5	4	1		
7	G	1	Total	O	P	0	0
			5	4	1		
7	H	1	Total	O	P	0	0
			5	4	1		

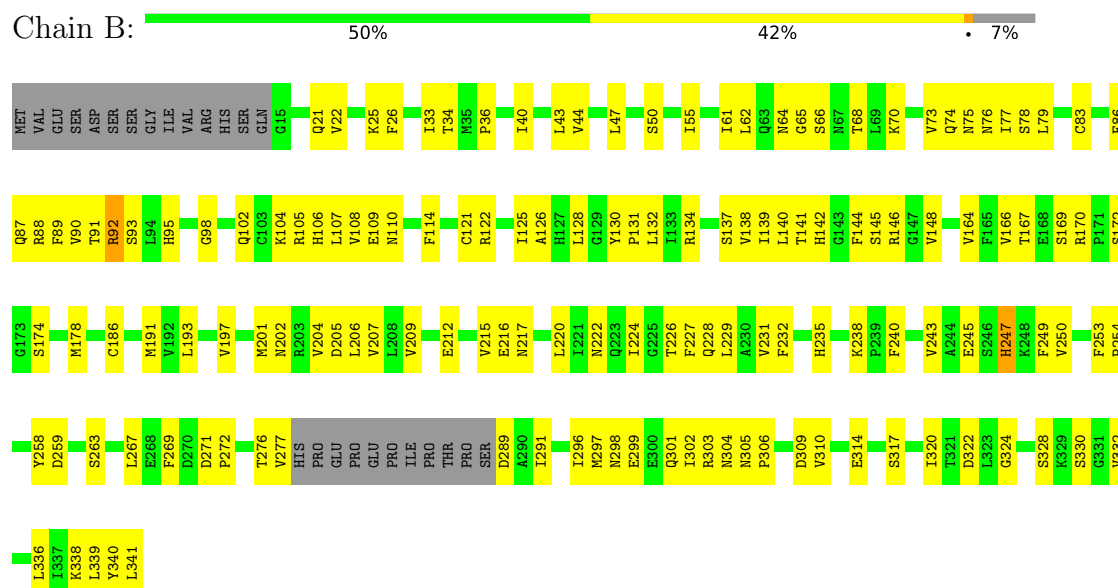
3 Residue-property plots

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.

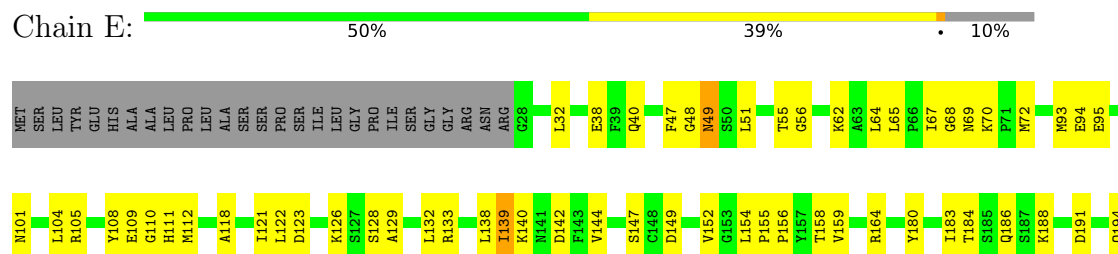
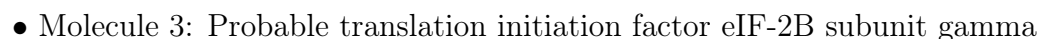
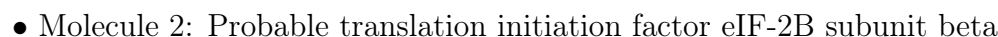
- Molecule 1: Translation initiation factor eIF-2B subunit alpha

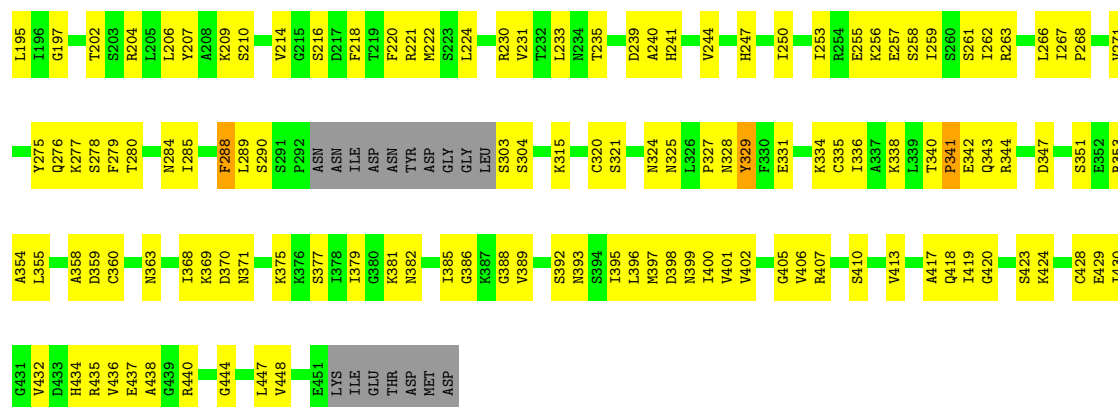


- Molecule 1: Translation initiation factor eIF-2B subunit alpha

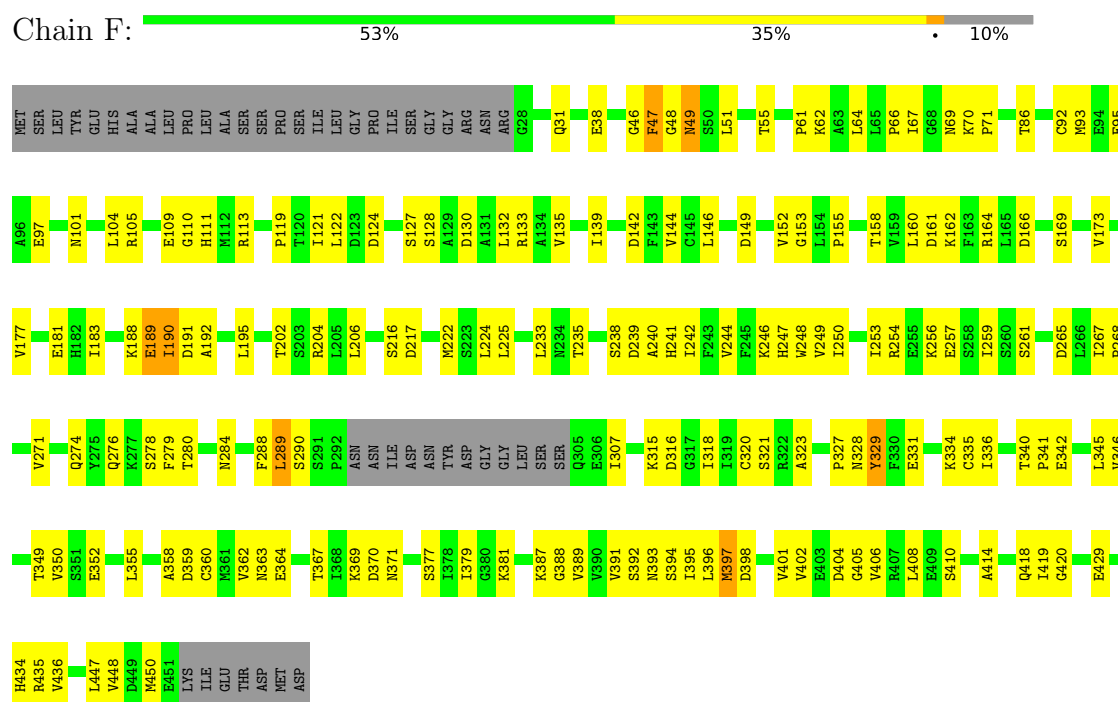


Chain C: 50% 34% 1% 15%

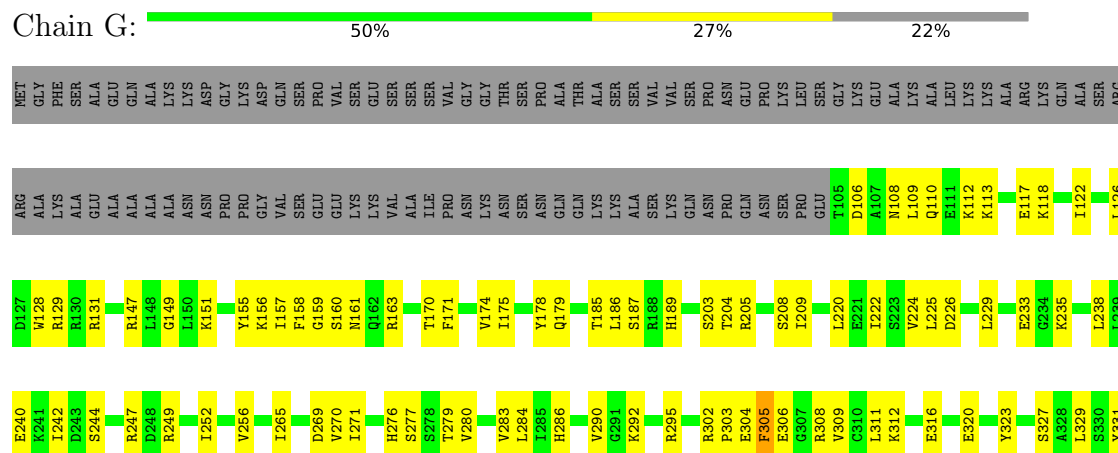




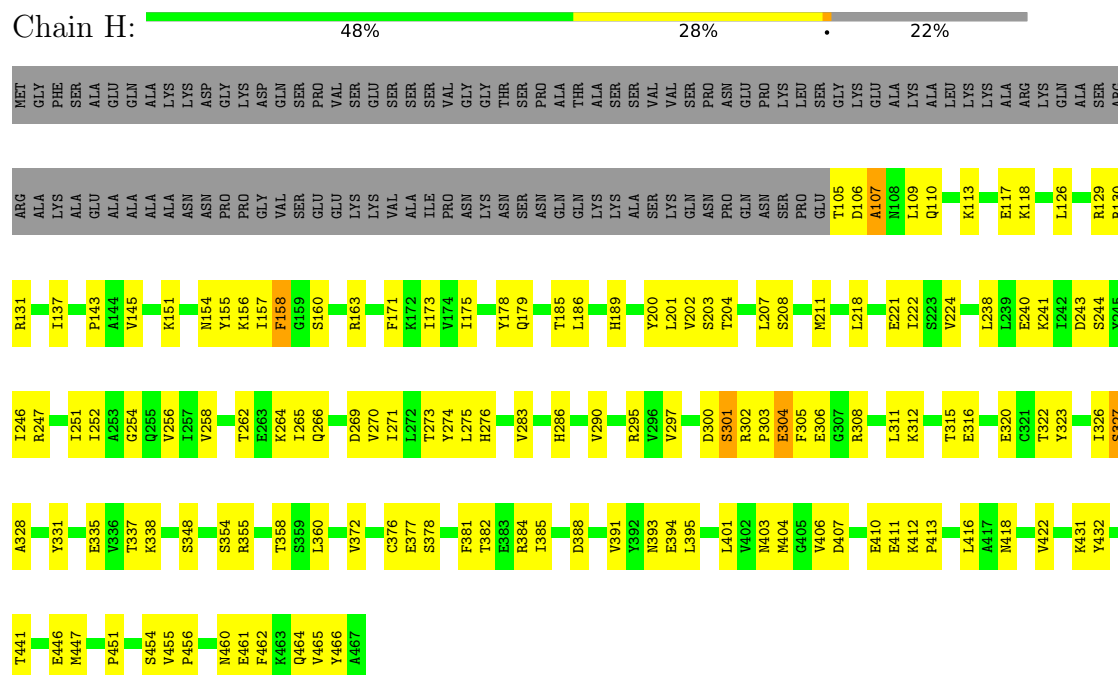
• Molecule 3: Probable translation initiation factor eIF-2B subunit gamma



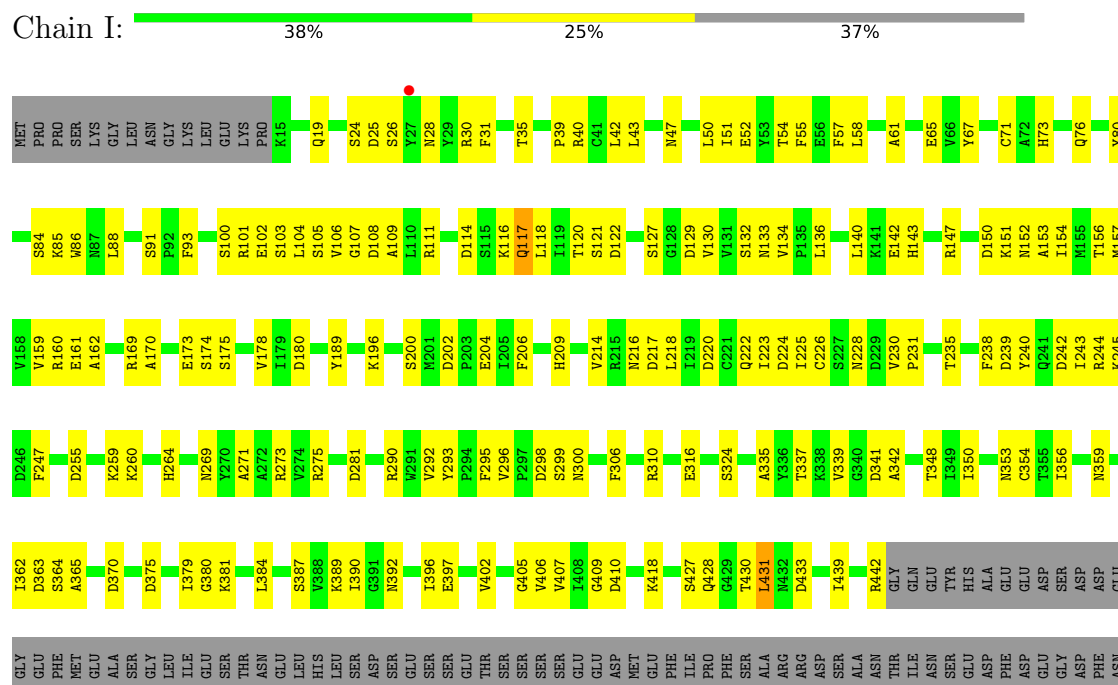
• Molecule 4: Probable translation initiation factor eIF-2B subunit delta



- Molecule 4: Probable translation initiation factor eIF-2B subunit delta

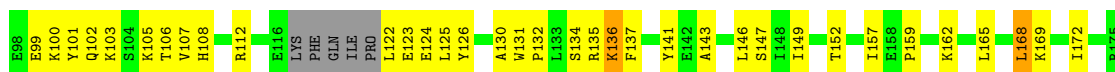


- Molecule 5: Probable translation initiation factor eIF-2B subunit epsilon



SER
GLU
ASP
ASP
GLU
ASP
GLU
SER
ASP
ASP
GLU

Chain M: 32% 22% . 45%

[illegible]

ASP
GLU
ASP
GLU
SER
ASP
ASP
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	155.56Å 207.99Å 155.59Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	49.31 – 3.50 49.31 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.31-3.50) 88.9 (49.31-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.53 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.224 , 0.260 0.227 , 0.264	Depositor DCC
R_{free} test set	1979 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å ²)	122.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 117.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.380 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31811	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: PO4

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	0.19	0/2513	0.40	0/3399
1	B	0.19	0/2510	0.38	0/3395
2	C	0.22	0/2661	0.40	0/3611
2	D	0.23	0/2653	0.39	0/3600
3	E	0.21	0/3272	0.45	0/4427
3	F	0.22	0/3260	0.47	0/4411
4	G	0.24	0/2917	0.40	0/3951
4	H	0.25	1/2917 (0.0%)	0.39	0/3951
5	I	0.20	0/3437	0.40	0/4658
5	J	0.20	0/3422	0.40	0/4639
6	L	0.16	0/1374	0.41	0/1845
6	M	0.16	0/1384	0.41	0/1859
All	All	0.21	1/32320 (0.0%)	0.41	0/43746

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	301	SER	C-N	-5.70	1.25	1.33

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	2467	0	2490	102	0
1	B	2465	0	2487	114	0
2	C	2617	0	2653	105	0
2	D	2609	0	2642	85	0
3	E	3216	0	3273	140	0
3	F	3204	0	3263	122	0
4	G	2869	0	2958	96	0
4	H	2869	0	2958	90	0
5	I	3377	0	3361	137	0
5	J	3362	0	3345	125	0
6	L	1353	0	1374	54	0
6	M	1363	0	1391	51	0
7	C	5	0	0	1	0
7	D	5	0	0	0	0
7	E	10	0	0	1	0
7	F	10	0	0	0	0
7	G	5	0	0	1	0
7	H	5	0	0	1	0
All	All	31811	0	32195	1144	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 18.

The worst 5 of 1144 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)
4:H:126:LEU:HB3	4:H:395:LEU:HD11	1.55	0.89
3:E:139:ILE:HG12	3:E:250:ILE:HG12	1.56	0.87
5:I:143:HIS:HD1	5:I:156:THR:HG1	1.21	0.83
5:J:101:ARG:H	5:J:101:ARG:HD3	1.44	0.83
3:E:402:VAL:HG23	3:E:419:ILE:HD11	1.62	0.81

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	312/341 (92%)	271 (87%)	36 (12%)	5 (2%)	7	36
1	B	312/341 (92%)	268 (86%)	39 (12%)	5 (2%)	7	36
2	C	334/399 (84%)	299 (90%)	33 (10%)	2 (1%)	21	54
2	D	333/399 (84%)	300 (90%)	27 (8%)	6 (2%)	6	34
3	E	410/458 (90%)	327 (80%)	72 (18%)	11 (3%)	4	27
3	F	408/458 (89%)	344 (84%)	51 (12%)	13 (3%)	3	24
4	G	361/467 (77%)	321 (89%)	36 (10%)	4 (1%)	11	43
4	H	361/467 (77%)	330 (91%)	20 (6%)	11 (3%)	3	25
5	I	426/678 (63%)	369 (87%)	54 (13%)	3 (1%)	18	51
5	J	424/678 (62%)	378 (89%)	43 (10%)	3 (1%)	18	51
6	L	159/304 (52%)	134 (84%)	23 (14%)	2 (1%)	9	39
6	M	160/304 (53%)	133 (83%)	23 (14%)	4 (2%)	4	28
All	All	4000/5294 (76%)	3474 (87%)	457 (11%)	69 (2%)	7	35

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	289	LEU
3	E	359	ASP
4	G	303	PRO
4	H	303	PRO
6	M	61	LEU

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	274/298 (92%)	274 (100%)	0	100	100
1	B	274/298 (92%)	274 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	291/350 (83%)	291 (100%)	0	100	100
2	D	290/350 (83%)	290 (100%)	0	100	100
3	E	359/395 (91%)	358 (100%)	1 (0%)	86	83
3	F	357/395 (90%)	357 (100%)	0	100	100
4	G	326/408 (80%)	326 (100%)	0	100	100
4	H	326/408 (80%)	326 (100%)	0	100	100
5	I	379/596 (64%)	379 (100%)	0	100	100
5	J	378/596 (63%)	378 (100%)	0	100	100
6	L	152/274 (56%)	152 (100%)	0	100	100
6	M	153/274 (56%)	153 (100%)	0	100	100
All	All	3559/4642 (77%)	3558 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	49	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	310	ASN
6	M	102	GLN
4	G	179	GLN
5	J	190	GLN
3	F	418	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	PO4	E	502	-	4,4,4	0.99	0	6,6,6	0.48	0
7	PO4	D	401	-	4,4,4	1.02	0	6,6,6	0.42	0
7	PO4	G	501	-	4,4,4	1.02	0	6,6,6	0.53	0
7	PO4	E	501	-	4,4,4	1.03	0	6,6,6	0.48	0
7	PO4	F	502	-	4,4,4	0.99	0	6,6,6	0.48	0
7	PO4	H	501	-	4,4,4	1.03	0	6,6,6	0.47	0
7	PO4	C	401	-	4,4,4	1.01	0	6,6,6	0.46	0
7	PO4	F	501	-	4,4,4	1.05	0	6,6,6	0.42	0

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.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	502	PO4	1	0
7	G	501	PO4	1	0
7	H	501	PO4	1	0
7	C	401	PO4	1	0

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	316/341 (92%)	-1.23	0 100 100	109, 145, 196, 237	0
1	B	316/341 (92%)	-1.18	0 100 100	106, 146, 196, 238	0
2	C	338/399 (84%)	-1.20	0 100 100	79, 121, 185, 214	0
2	D	337/399 (84%)	-1.25	0 100 100	76, 120, 189, 232	0
3	E	414/458 (90%)	-1.07	0 100 100	88, 139, 206, 234	0
3	F	412/458 (89%)	-1.08	0 100 100	93, 138, 205, 236	0
4	G	363/467 (77%)	-1.14	0 100 100	87, 122, 187, 235	0
4	H	363/467 (77%)	-1.21	0 100 100	88, 119, 191, 228	0
5	I	428/678 (63%)	-1.13	1 (0%) 91 82	101, 141, 187, 209	0
5	J	426/678 (62%)	-1.22	0 100 100	100, 141, 184, 222	0
6	L	165/304 (54%)	-0.84	0 100 100	121, 203, 232, 244	0
6	M	166/304 (54%)	-0.99	0 100 100	121, 202, 236, 253	0
All	All	4044/5294 (76%)	-1.15	1 (0%) 100 100	76, 137, 209, 253	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	27	TYR	2.1

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(Å ²)	Q<0.9
7	PO4	D	401	5/5	0.97	0.06	80,107,166,167	0
7	PO4	C	401	5/5	0.98	0.05	98,137,158,184	0
7	PO4	E	502	5/5	0.98	0.05	171,171,195,223	0
7	PO4	F	502	5/5	0.98	0.04	172,179,190,228	0
7	PO4	H	501	5/5	0.98	0.06	105,106,166,171	0
7	PO4	E	501	5/5	0.99	0.10	114,122,147,186	0
7	PO4	G	501	5/5	0.99	0.05	115,136,151,154	0
7	PO4	F	501	5/5	0.99	0.13	113,128,142,183	0

6.5 Other polymers [i](#)

There are no such residues in this entry.