



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 05:14 PM UTC

PDB ID : 3CW2 / pdb_00003cw2
Title : Crystal structure of the intact archaeal translation initiation factor 2 from *Sulfolobus solfataricus* .
Authors : Stolboushkina, E.A.; Nikonov, S.V.; Nikulin, A.D.; Blaesi, U.; Manstein, D.J.; Fedorov, R.V.; Garber, M.B.; Nikonov, O.S.
Deposited on : 2008-04-21
Resolution : 2.80 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

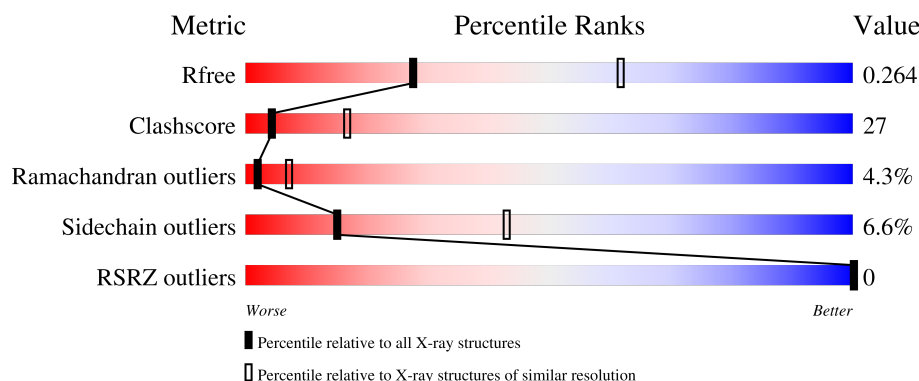
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	415	52% 42% 6%
1	B	415	50% 43% • •
1	E	415	51% 44% 5%
1	F	415	43% 52% 5%
2	C	266	52% 41% 6% •

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Mol	Chain	Length	Quality of chain
2	D	266	53%42%5%
2	G	266	53%40%7%
2	H	266	49%42%8%.
3	K	139	42%37%11%.8%
3	L	139	6%9%85%
3	M	139	51%33%12%..
3	N	139	12%7%.78%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23823 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 2 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3213	2058	548	595	12			
1	B	400	Total	C	N	O	S	0	0	0
			3096	1987	524	574	11			
1	E	414	Total	C	N	O	S	0	0	0
			3213	2058	548	595	12			
1	F	414	Total	C	N	O	S	0	0	0
			3213	2058	548	595	12			

- Molecule 2 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	266	Total	C	N	O	S	0	0	0
			2134	1364	365	403	2			
2	D	266	Total	C	N	O	S	0	0	0
			2134	1364	365	403	2			
2	G	266	Total	C	N	O	S	0	0	0
			2134	1364	365	403	2			
2	H	266	Total	C	N	O	S	0	0	0
			2134	1364	365	403	2			

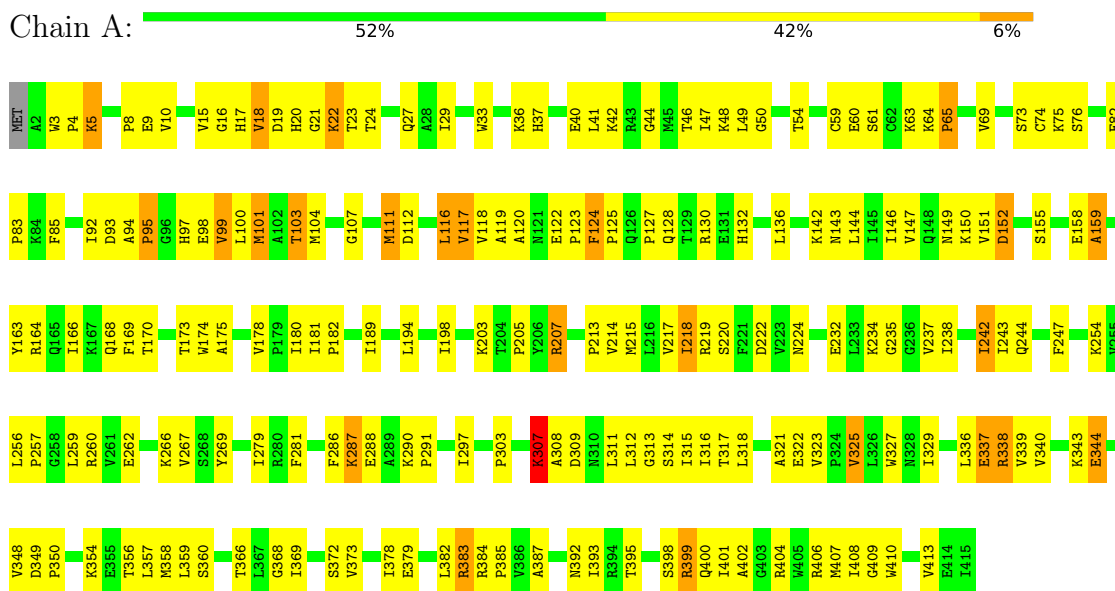
- Molecule 3 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	128	Total	C	N	O	S	0	0	0
			1032	655	174	194	9			
3	L	21	Total	C	N	O	S	0	0	0
			174	110	27	36	1			
3	M	138	Total	C	N	O	S	0	0	0
			1102	699	186	207	10			
3	N	30	Total	C	N	O	S	0	0	0
			244	152	41	50	1			

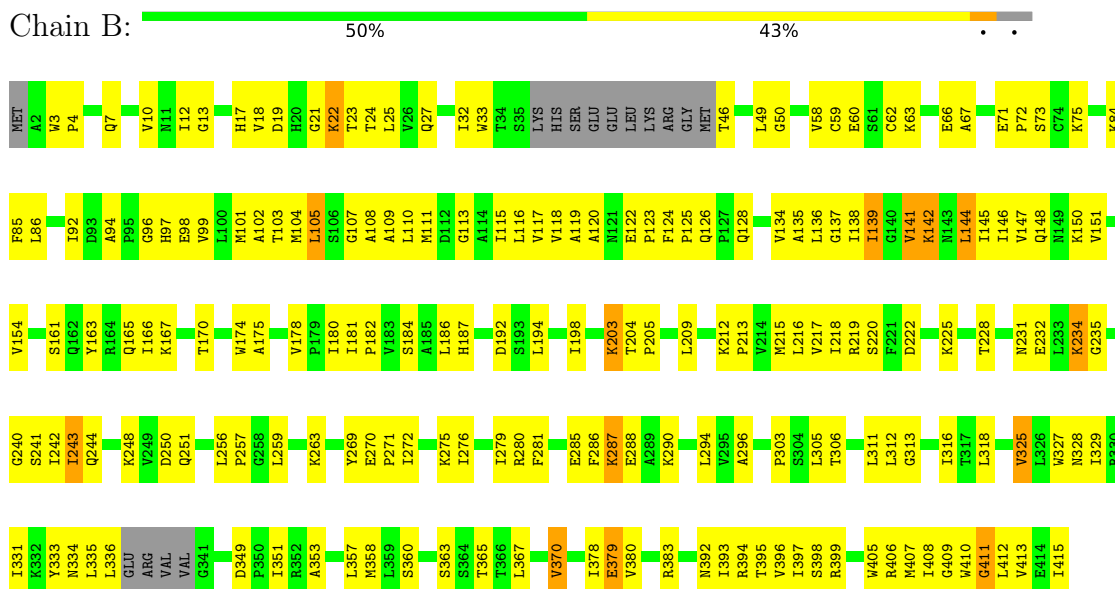
3 Residue-property plots

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.

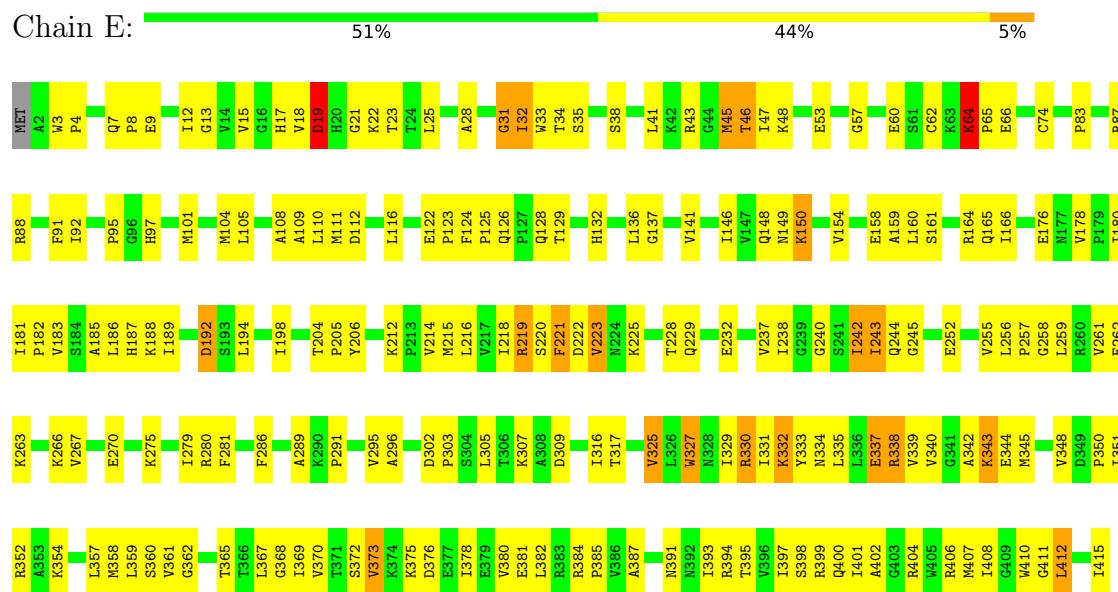
- Molecule 1: Translation initiation factor 2 subunit gamma



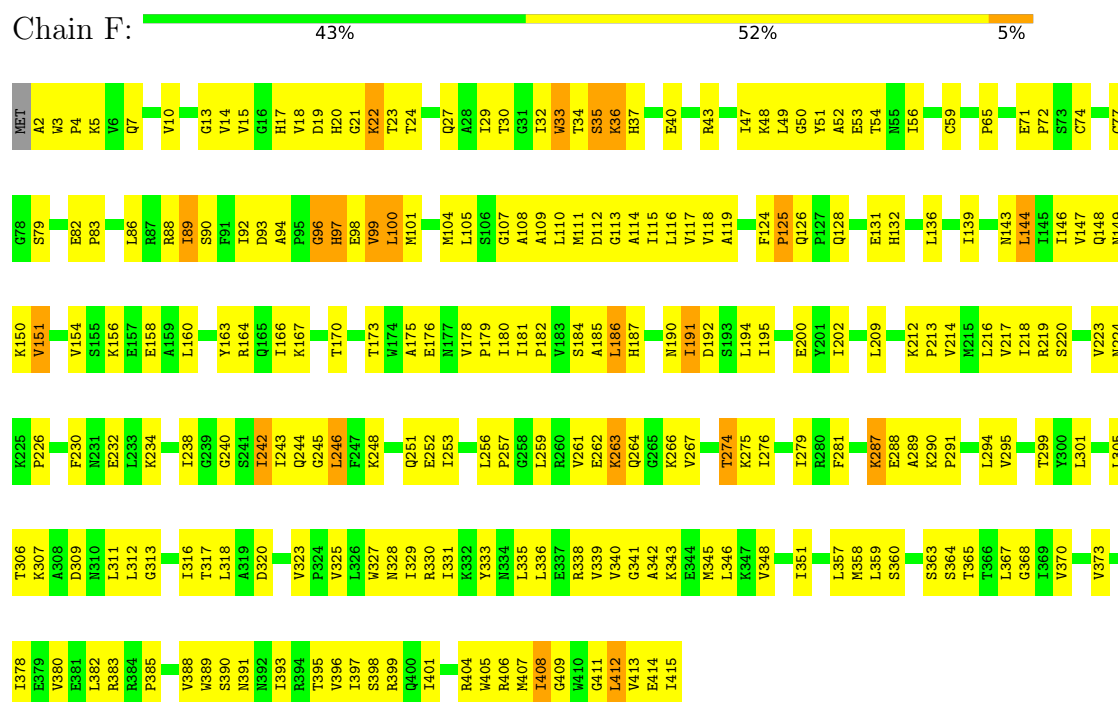
- Molecule 1: Translation initiation factor 2 subunit gamma



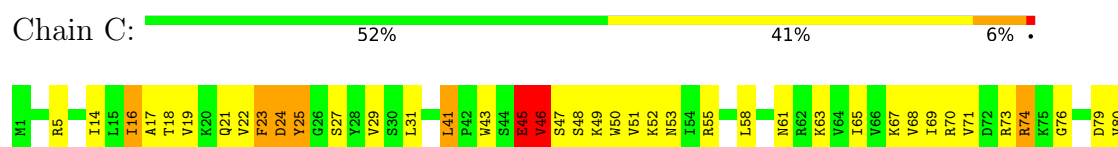
• Molecule 1: Translation initiation factor 2 subunit gamma

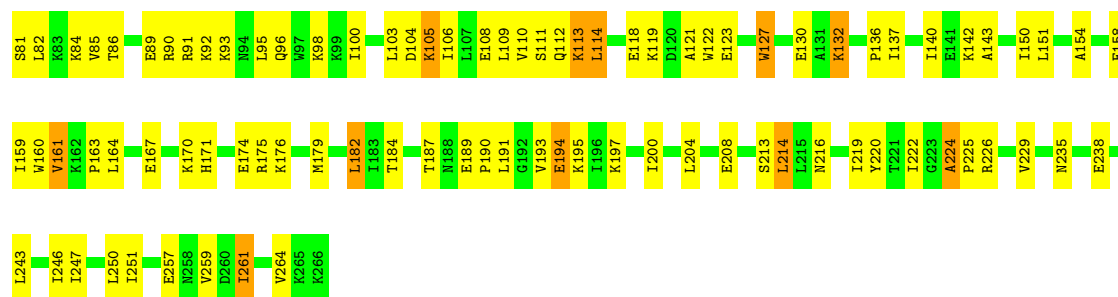


• Molecule 1: Translation initiation factor 2 subunit gamma



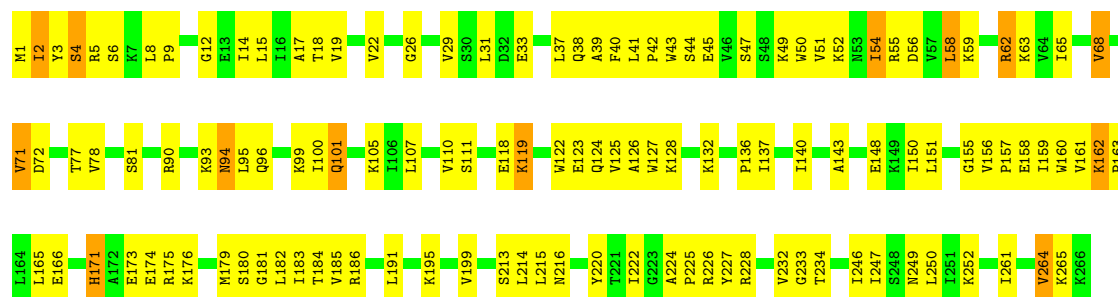
• Molecule 2: Translation initiation factor 2 subunit alpha





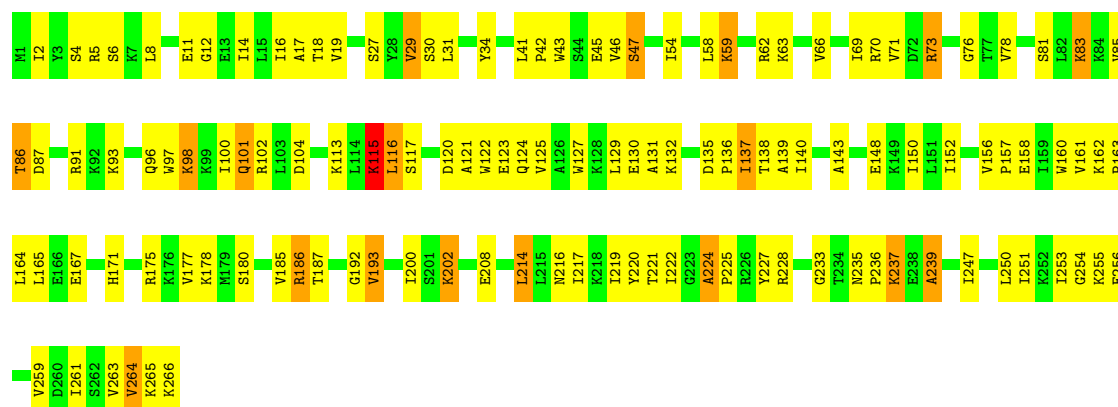
• Molecule 2: Translation initiation factor 2 subunit alpha

Chain D: 53% 42% 5%



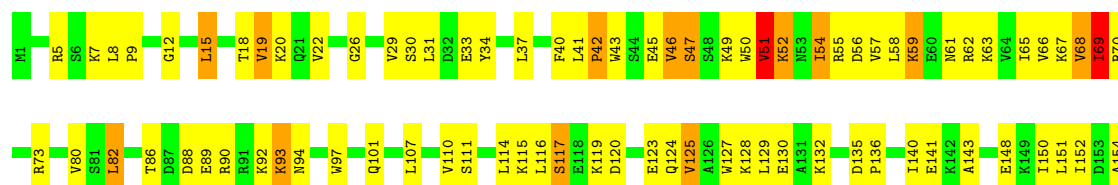
• Molecule 2: Translation initiation factor 2 subunit alpha

Chain G: 53% 40% 7%

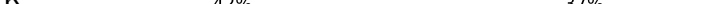


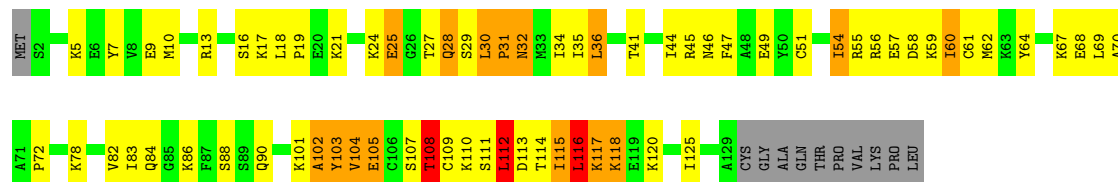
• Molecule 2: Translation initiation factor 2 subunit alpha

Chain H: 49% 42% 8%



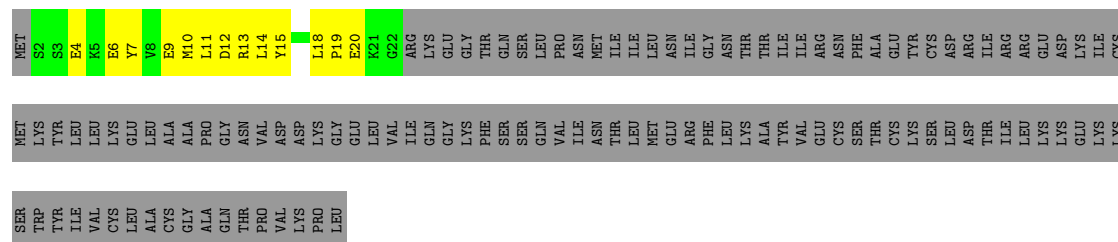
- Molecule 3: Translation initiation factor 2 subunit beta

Chain K:  42% 37% 11% 8%



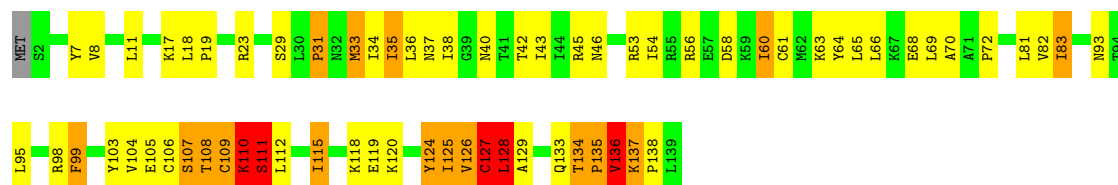
- Molecule 3: Translation initiation factor 2 subunit beta

Chain L: 6% 9% 85%

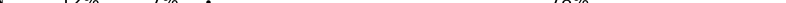


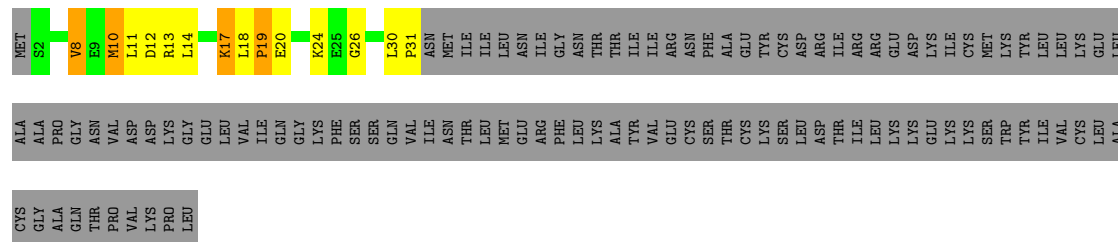
- Molecule 3: Translation initiation factor 2 subunit beta

Chain M: 51% 33% 12% .



- Molecule 3: Translation initiation factor 2 subunit beta

Chain N:  12% 7% • 78%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.20Å 162.92Å 161.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.80 19.91 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (19.91-2.80) 98.5 (19.91-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.79Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.225 , 0.276 0.227 , 0.264	Depositor DCC
R_{free} test set	4941 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	72.0	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.449 for h,-k,-l	Xtriage
Reported twinning fraction	0.459 for h,-k,-l	Depositor
Outliers	0 of 98811 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	23823	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.72% 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

5.1 Standard geometry

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	0.29	0/3272	0.74	0/4430
1	B	0.28	0/3152	0.78	2/4269 (0.0%)
1	E	0.29	0/3272	0.75	3/4430 (0.1%)
1	F	0.28	0/3272	0.74	0/4430
2	C	0.27	0/2164	0.70	0/2914
2	D	0.27	0/2164	0.76	1/2914 (0.0%)
2	G	0.29	0/2164	0.77	2/2914 (0.1%)
2	H	0.27	0/2164	0.74	3/2914 (0.1%)
3	K	0.27	0/1045	0.74	0/1399
3	L	0.23	0/176	0.78	0/233
3	M	0.28	0/1117	0.80	1/1497 (0.1%)
3	N	0.28	0/247	0.75	0/328
All	All	0.28	0/24209	0.75	12/32672 (0.0%)

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	1
1	F	0	1
2	C	0	3
2	D	0	1
3	K	0	10
3	M	0	3
All	All	0	19

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	337	GLU	N-CA-C	6.10	113.78	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	251	ILE	N-CA-C	-5.97	108.04	113.71
2	D	158	GLU	CB-CA-C	-5.93	109.72	116.54
2	H	135	ASP	CA-C-N	5.67	125.14	119.24
2	H	135	ASP	C-N-CA	5.67	125.14	119.24

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	ARG	Peptide
2	C	158	GLU	Peptide
2	C	45	GLU	Peptide
2	C	46	VAL	Peptide
2	D	2	ILE	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	3213	0	3332	164	0
1	B	3096	0	3207	165	0
1	E	3213	0	3332	211	0
1	F	3213	0	3334	211	0
2	C	2134	0	2242	98	0
2	D	2134	0	2242	108	0
2	G	2134	0	2242	111	0
2	H	2134	0	2242	106	0
3	K	1032	0	1073	61	0
3	L	174	0	173	11	0
3	M	1102	0	1148	90	0
3	N	244	0	246	13	0
All	All	23823	0	24813	1307	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 27.

The worst 5 of 1307 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)
2:D:5:ARG:HA	2:D:127:TRP:HE1	1.09	1.13
3:M:109:CYS:SG	3:M:127:CYS:HA	1.91	1.11
2:C:48:SER:HB2	2:C:50:TRP:HD1	1.18	1.08
3:M:111:SER:HB3	3:M:112:LEU:CG	1.84	1.07
1:E:330:ARG:HG3	1:E:330:ARG:HH11	1.16	1.06

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	412/415 (99%)	312 (76%)	82 (20%)	18 (4%)	2	7
1	B	394/415 (95%)	322 (82%)	67 (17%)	5 (1%)	9	31
1	E	412/415 (99%)	325 (79%)	73 (18%)	14 (3%)	3	11
1	F	412/415 (99%)	323 (78%)	77 (19%)	12 (3%)	3	13
2	C	264/266 (99%)	212 (80%)	40 (15%)	12 (4%)	2	7
2	D	264/266 (99%)	224 (85%)	34 (13%)	6 (2%)	5	18
2	G	264/266 (99%)	219 (83%)	34 (13%)	11 (4%)	2	7
2	H	264/266 (99%)	202 (76%)	42 (16%)	20 (8%)	1	2
3	K	126/139 (91%)	74 (59%)	41 (32%)	11 (9%)	0	1
3	L	19/139 (14%)	12 (63%)	6 (32%)	1 (5%)	1	5
3	M	136/139 (98%)	85 (62%)	36 (26%)	15 (11%)	0	1
3	N	28/139 (20%)	20 (71%)	5 (18%)	3 (11%)	0	1
All	All	2995/3280 (91%)	2330 (78%)	537 (18%)	128 (4%)	2	7

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	MET

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Mol	Chain	Res	Type
1	A	307	LYS
1	B	102	ALA
2	C	24	ASP
2	D	54	ILE

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	356/357 (100%)	332 (93%)	24 (7%)	15	42
1	B	343/357 (96%)	326 (95%)	17 (5%)	22	54
1	E	356/357 (100%)	338 (95%)	18 (5%)	21	54
1	F	356/357 (100%)	329 (92%)	27 (8%)	12	36
2	C	237/239 (99%)	220 (93%)	17 (7%)	13	39
2	D	237/239 (99%)	222 (94%)	15 (6%)	16	45
2	G	237/239 (99%)	221 (93%)	16 (7%)	14	42
2	H	237/239 (99%)	218 (92%)	19 (8%)	11	34
3	K	117/126 (93%)	108 (92%)	9 (8%)	12	36
3	L	20/126 (16%)	20 (100%)	0	100	100
3	M	125/126 (99%)	114 (91%)	11 (9%)	9	29
3	N	28/126 (22%)	26 (93%)	2 (7%)	13	39
All	All	2649/2888 (92%)	2474 (93%)	175 (7%)	15	43

5 of 175 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	223	VAL
2	H	15	LEU
1	F	274	THR
2	G	83	LYS
2	H	69	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	101	GLN
2	G	235	ASN
3	M	37	ASN
2	C	216	ASN
2	C	209	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 [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	414/415 (99%)	-1.37	0 100 100	46, 105, 152, 162	0
1	B	400/415 (96%)	-1.38	0 100 100	37, 109, 149, 173	0
1	E	414/415 (99%)	-1.38	0 100 100	46, 106, 150, 165	0
1	F	414/415 (99%)	-1.40	0 100 100	47, 107, 147, 163	0
2	C	266/266 (100%)	-1.48	0 100 100	42, 95, 133, 151	0
2	D	266/266 (100%)	-1.45	0 100 100	38, 98, 135, 169	0
2	G	266/266 (100%)	-1.45	0 100 100	41, 90, 120, 138	0
2	H	266/266 (100%)	-1.43	0 100 100	36, 102, 135, 146	0
3	K	128/139 (92%)	-1.38	0 100 100	124, 148, 168, 175	0
3	L	21/139 (15%)	-1.43	0 100 100	89, 119, 133, 134	0
3	M	138/139 (99%)	-1.38	0 100 100	108, 147, 172, 181	0
3	N	30/139 (21%)	-1.51	0 100 100	100, 139, 154, 155	0
All	All	3023/3280 (92%)	-1.41	0 100 100	36, 106, 153, 181	0

There are no RSRZ outliers to report.

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.