



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 19, 2026 – 07:30 AM UTC

PDB ID : 7Y18 / pdb_00007y18
Title : Crystal structure of ribosomal ITS2 pre-rRNA processing complex from *Saccharomyces cerevisiae*
Authors : Chen, J.; Liu, L.
Deposited on : 2022-06-07
Resolution : 3.69 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

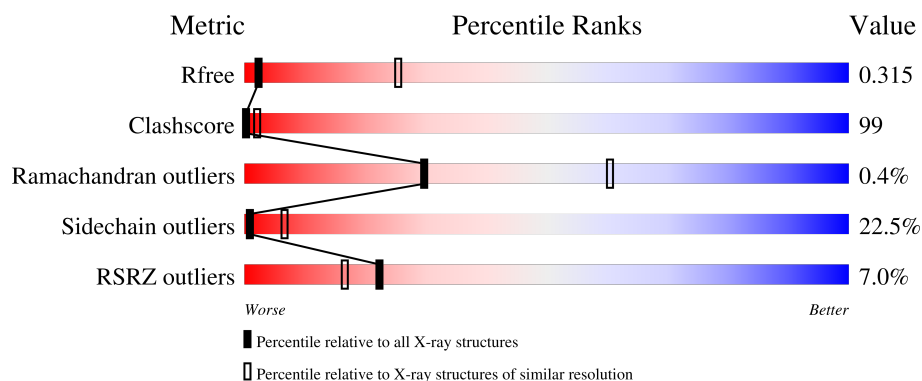
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.69 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	632	4% 17% 45% 21% • 16%
1	B	632	12% 23% 41% 18% • 16%
1	E	632	3% 22% 44% 17% • 17%
2	C	502	4% 32% 38% 14% • 14%
2	D	502	5% 34% 39% 11% • 15%

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Mol	Chain	Length	Quality of chain
2	F	502	6% 33% 34% 11% • 21%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23039 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 Polynucleotide 5'-hydroxyl-kinase GRC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4122	2649	693	771	9			
1	B	528	Total	C	N	O	S	0	0	0
			4069	2607	693	759	10			
1	E	527	Total	C	N	O	S	0	0	0
			4076	2614	691	761	10			

- Molecule 2 is a protein called Protein LAS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	430	Total	C	N	O	S	0	0	0
			3614	2324	629	652	9			
2	D	429	Total	C	N	O	S	0	0	0
			3614	2325	628	652	9			
2	F	397	Total	C	N	O	S	0	0	0
			3364	2176	584	595	9			

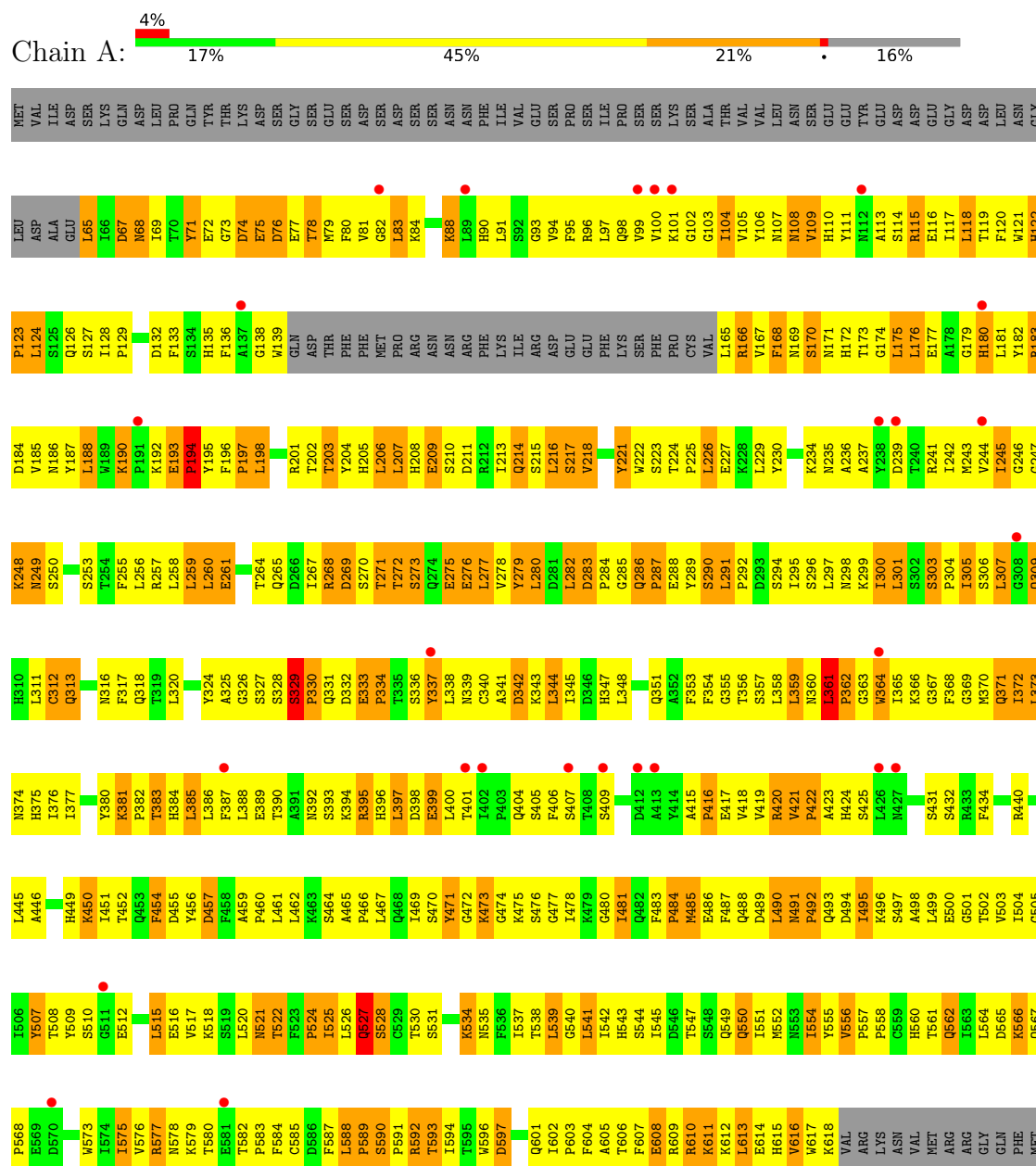
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	C	31	Total	O	0	0
			31	31		
3	D	21	Total	O	0	0
			21	21		
3	B	30	Total	O	0	0
			30	30		
3	E	43	Total	O	0	0
			43	43		
3	F	19	Total	O	0	0
			19	19		

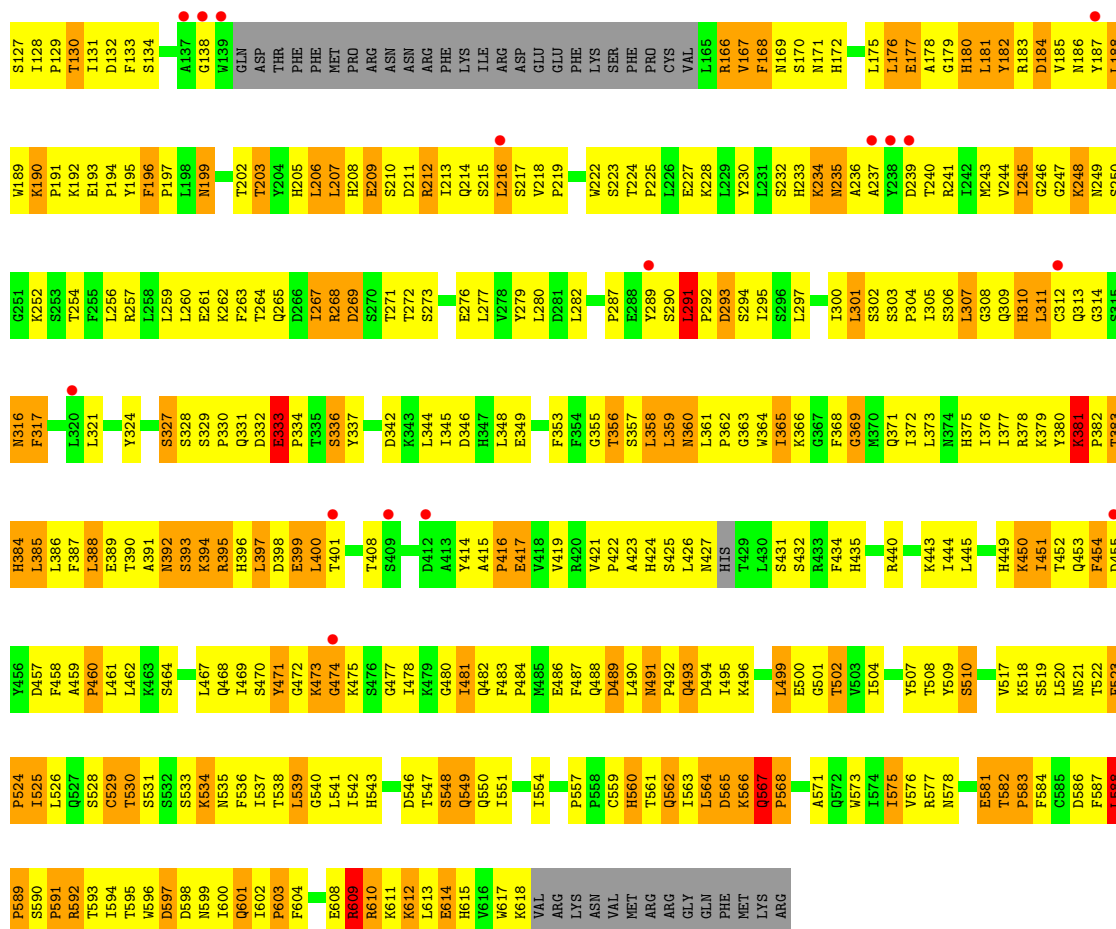
3 Residue-property plots

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.

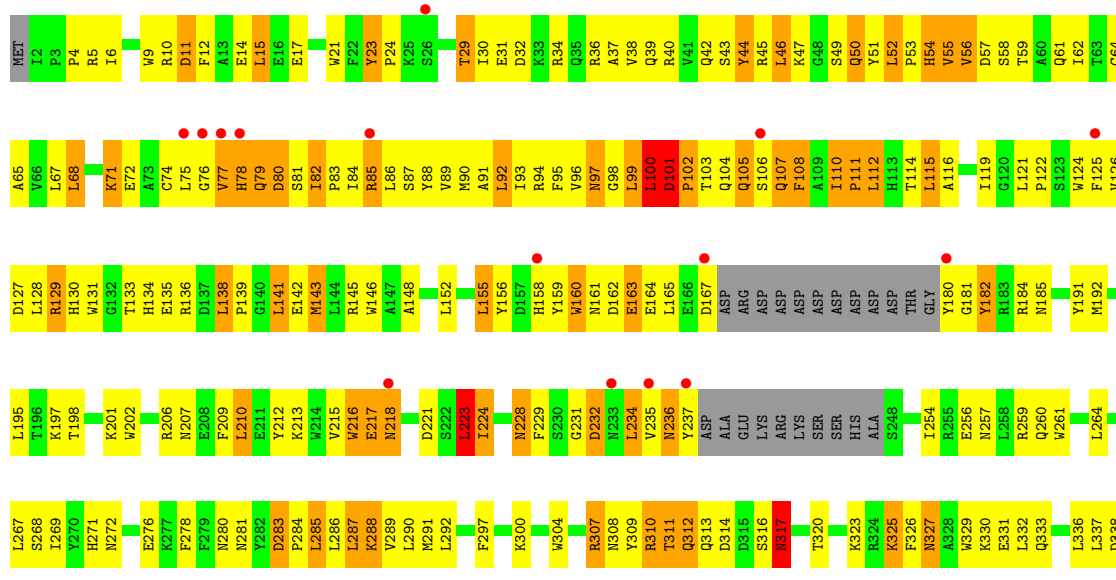
• Molecule 1: Polynucleotide 5'-hydroxyl-kinase GRC3

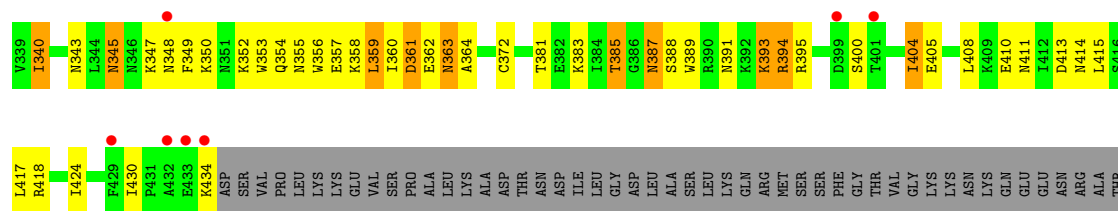


LEU	ASP	VAL	ASP	ASP	LEU	GLU	ASP	GLN	LYS	SER	LEU	GLU	ASP	ASP	GLN	PRO	LEU	THR	THR	LYS	ASP	SER	GLY	SER	SER	GLU	SER	ASP	ASP	ASP	SER	ASN	ASN	PHE	ILE	VAL	GLU	SER	PRO	PRO	THR	ALA	THR	VAL	VAL	LEU	ASN	ASN	SER	ASP	GLU	GLY	GLU	ASP	LEU	ASN	GLY	PI23
I66				I69	Y70	Y71	E72	G73	D74	E75	D76	E77	T78	F80	V81	G82	L83	K84	E85		K88	L89	H90	L91			F95	R96	L97	Q98	V99	V100	K101	G102	G103	I104	V105	V106	I107	M108	V109	H110	H111	N112	N113	S114	R115	E116	I117	L118	T119	F120	W121	H122	P123			

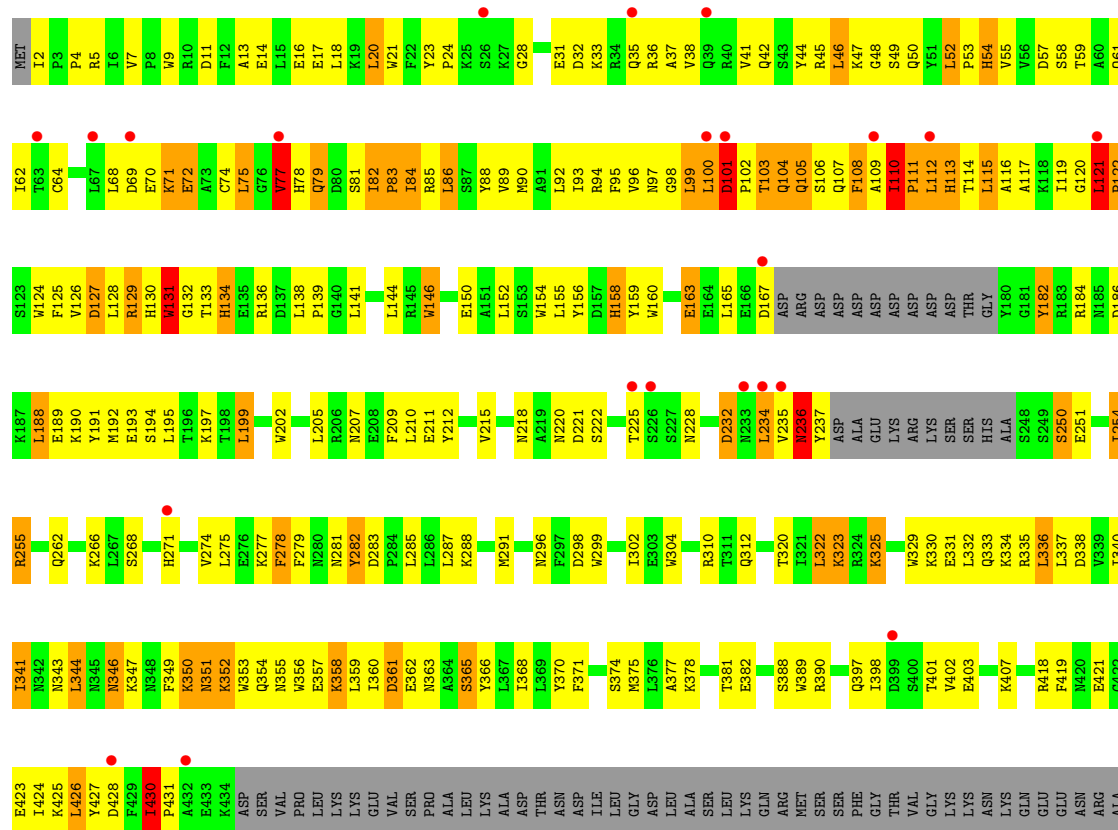


• Molecule 2: Protein LAS1

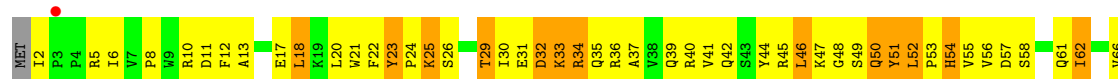


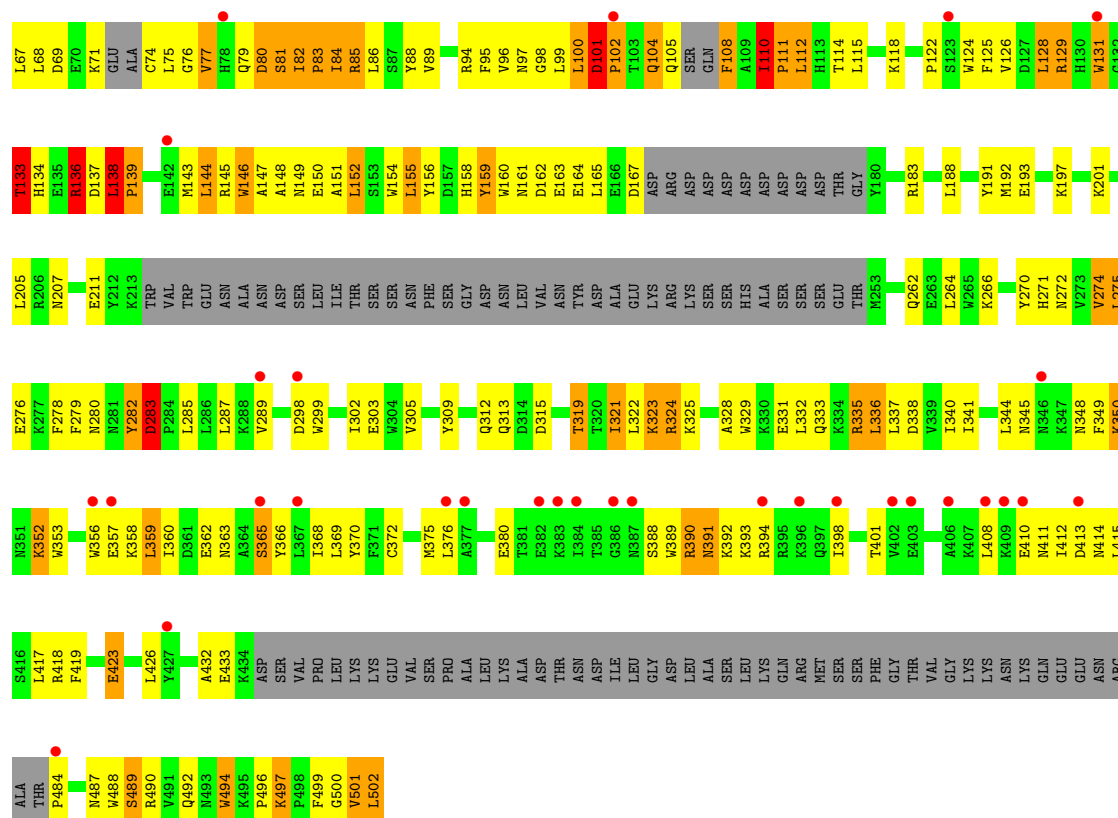


• Molecule 2: Protein LAS1



• Molecule 2: Protein LAS1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	233.56Å 116.14Å 159.31Å 90.00° 96.41° 90.00°	Depositor
Resolution (Å)	48.63 – 3.69 48.63 – 3.69	Depositor EDS
% Data completeness (in resolution range)	80.1 (48.63-3.69) 80.2 (48.63-3.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.278 , 0.318 0.278 , 0.315	Depositor DCC
R_{free} test set	1824 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 74.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	23039	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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	0.71	31/4230 (0.7%)	1.11	46/5764 (0.8%)
1	B	0.58	24/4169 (0.6%)	1.10	48/5676 (0.8%)
1	E	0.62	30/4179 (0.7%)	1.03	38/5690 (0.7%)
2	C	0.52	11/3703 (0.3%)	0.88	19/5016 (0.4%)
2	D	0.51	12/3704 (0.3%)	0.85	18/5017 (0.4%)
2	F	0.51	12/3445 (0.3%)	0.86	20/4658 (0.4%)
All	All	0.58	120/23430 (0.5%)	0.98	189/31821 (0.6%)

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	ASP	C-N	7.90	1.40	1.33
1	A	556	VAL	C-N	6.42	1.41	1.33
1	B	190	LYS	C-N	6.31	1.40	1.33
1	E	381	LYS	C-N	6.24	1.41	1.33
2	C	23	TYR	C-N	6.24	1.41	1.33

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	PRO	N-CA-C	-17.90	76.42	111.69
1	B	198	LEU	N-CA-CB	-12.20	90.87	110.51
1	B	617	TRP	N-CA-C	-11.63	90.42	109.96
1	B	618	LYS	N-CA-C	-10.53	81.53	111.00
1	B	197	PRO	CB-CA-C	-10.49	93.57	110.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	4122	0	3931	1042	0
1	B	4069	0	3873	974	0
1	E	4076	0	3880	900	3
2	C	3614	0	3553	708	0
2	D	3614	0	3551	682	0
2	F	3364	0	3350	547	6
3	A	36	0	0	4	0
3	B	30	0	0	2	0
3	C	31	0	0	4	0
3	D	21	0	0	1	0
3	E	43	0	0	8	0
3	F	19	0	0	1	0
All	All	23039	0	22138	4466	6

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 99.

The worst 5 of 4466 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:84:LYS:CB	1:A:139:TRP:CD1	1.77	1.65
2:C:202:TRP:CZ3	2:C:209:PHE:CE1	1.77	1.62
2:D:4:PRO:HB3	1:B:607:PHE:CE1	1.10	1.62
1:E:331:GLN:HG3	1:E:364:TRP:CZ2	1.21	1.62
1:A:607:PHE:CE1	2:C:4:PRO:CB	1.82	1.62

The worst 5 of 6 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:E:331:GLN:O	2:F:143:MET:CE[2_555]	1.76	0.44
2:F:49:SER:C	2:F:136:ARG:NH2[2_555]	1.94	0.26
2:F:49:SER:O	2:F:136:ARG:NH2[2_555]	1.99	0.21
1:E:486:GLU:O	2:F:81:SER:OG[2_555]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:ARG:NH2	2:F:136:ARG:O[2_555]	2.08	0.12

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	525/632 (83%)	494 (94%)	29 (6%)	2 (0%)	30	60
1	B	522/632 (83%)	488 (94%)	31 (6%)	3 (1%)	21	52
1	E	521/632 (82%)	492 (94%)	28 (5%)	1 (0%)	43	72
2	C	422/502 (84%)	404 (96%)	18 (4%)	0	100	100
2	D	421/502 (84%)	399 (95%)	20 (5%)	2 (0%)	24	56
2	F	385/502 (77%)	372 (97%)	11 (3%)	2 (0%)	24	56
All	All	2796/3402 (82%)	2649 (95%)	137 (5%)	10 (0%)	30	60

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	PRO
2	D	131	TRP
1	B	416	PRO
1	E	416	PRO
2	F	501	VAL

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	441/579 (76%)	313 (71%)	128 (29%)	0	2
1	B	430/579 (74%)	327 (76%)	103 (24%)	1	5
1	E	433/579 (75%)	320 (74%)	113 (26%)	0	4
2	C	392/461 (85%)	318 (81%)	74 (19%)	1	10
2	D	391/461 (85%)	319 (82%)	72 (18%)	1	11
2	F	364/461 (79%)	302 (83%)	62 (17%)	2	13
All	All	2451/3120 (79%)	1899 (78%)	552 (22%)	1	6

5 of 552 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	534	LYS
1	E	582	THR
1	E	529	CYS
2	F	138	LEU
2	C	387	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	318	GLN
1	E	371	GLN
1	B	396	HIS
1	B	599	ASN
1	E	491	ASN

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 ⓘ

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	529/632 (83%)	0.63	27 (5%)	33	22	30, 74, 134, 150	0
1	B	528/632 (83%)	1.09	78 (14%)	5	7	28, 109, 157, 177	0
1	E	527/632 (83%)	0.64	16 (3%)	52	32	49, 89, 133, 163	0
2	C	430/502 (85%)	0.55	22 (5%)	33	22	29, 72, 158, 200	0
2	D	429/502 (85%)	0.68	23 (5%)	31	21	45, 93, 152, 198	0
2	F	397/502 (79%)	0.84	32 (8%)	18	14	45, 133, 176, 198	0
All	All	2840/3402 (83%)	0.74	198 (6%)	22	16	28, 91, 158, 200	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	LEU	5.9
1	B	301	LEU	4.9
1	B	280	LEU	4.6
1	A	401	THR	4.4
2	C	85	ARG	4.3

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.