



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:14 PM UTC

PDB ID : 4U0B / pdb_00004u0b
Title : Hexamer HIV-1 CA in complex with CPSF6 peptide, P212121 crystal form
Authors : Price, A.J.; Jacques, D.A.; James, L.C.
Deposited on : 2014-07-11
Resolution : 2.80 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)	:	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

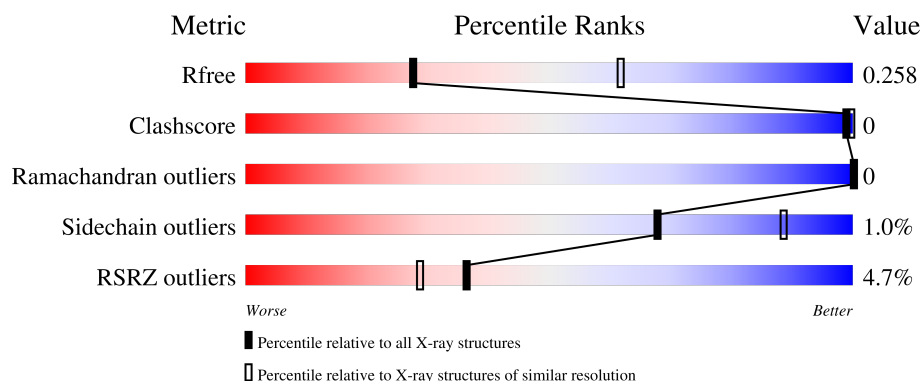
1 Overall quality at a glance

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.



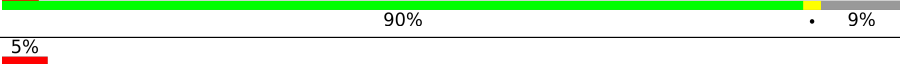
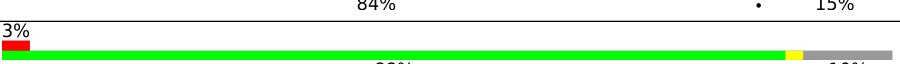
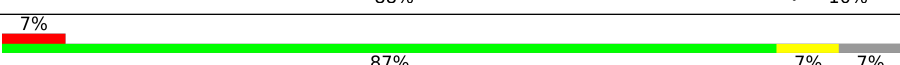
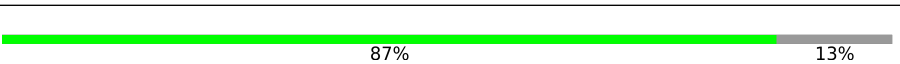
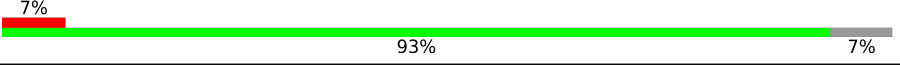
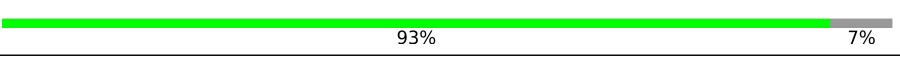
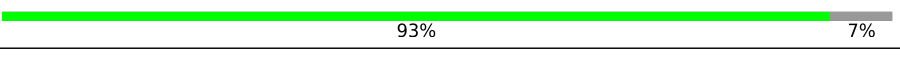
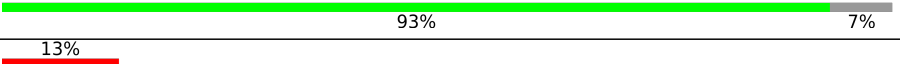
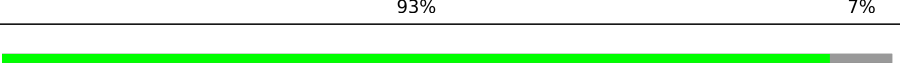
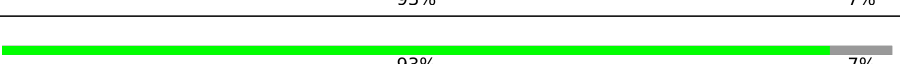
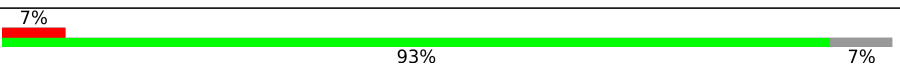
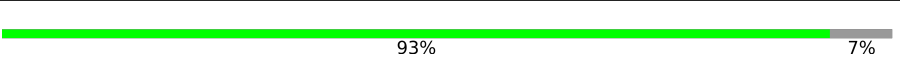
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	231	4% 89% 10%
1	B	231	6% 85% 13%
1	C	231	4% 83% 14%
1	D	231	6% 86% 12%
1	E	231	4% 85% 14%

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Mol	Chain	Length	Quality of chain
1	F	231	
1	G	231	
1	H	231	
1	I	231	
1	J	231	
1	K	231	
1	L	231	
2	M	15	
2	N	15	
2	O	15	
2	P	15	
2	Q	15	
2	R	15	
2	S	15	
2	T	15	
2	U	15	
2	V	15	
2	W	15	
2	X	15	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19958 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 Capsid protein p24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1601	1008	278	301	14			
1	B	201	Total	C	N	O	S	0	0	0
			1554	979	271	290	14			
1	C	198	Total	C	N	O	S	0	1	0
			1527	964	263	286	14			
1	D	203	Total	C	N	O	S	0	1	0
			1577	993	275	294	15			
1	E	198	Total	C	N	O	S	0	1	0
			1533	967	266	286	14			
1	F	207	Total	C	N	O	S	0	0	0
			1585	997	275	300	13			
1	G	198	Total	C	N	O	S	0	1	0
			1533	967	266	286	14			
1	H	202	Total	C	N	O	S	0	1	0
			1555	980	270	291	14			
1	I	211	Total	C	N	O	S	0	1	0
			1627	1025	285	302	15			
1	J	198	Total	C	N	O	S	0	1	0
			1533	967	266	286	14			
1	K	197	Total	C	N	O	S	0	1	0
			1526	962	265	285	14			
1	L	208	Total	C	N	O	S	0	0	0
			1604	1008	279	304	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	engineered mutation	UNP P12493
A	45	CYS	GLU	engineered mutation	UNP P12493
A	184	ALA	TRP	engineered mutation	UNP P12493
A	185	ALA	MET	engineered mutation	UNP P12493
B	14	CYS	ALA	engineered mutation	UNP P12493

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Chain	Residue	Modelled	Actual	Comment	Reference
B	45	CYS	GLU	engineered mutation	UNP P12493
B	184	ALA	TRP	engineered mutation	UNP P12493
B	185	ALA	MET	engineered mutation	UNP P12493
C	14	CYS	ALA	engineered mutation	UNP P12493
C	45	CYS	GLU	engineered mutation	UNP P12493
C	184	ALA	TRP	engineered mutation	UNP P12493
C	185	ALA	MET	engineered mutation	UNP P12493
D	14	CYS	ALA	engineered mutation	UNP P12493
D	45	CYS	GLU	engineered mutation	UNP P12493
D	184	ALA	TRP	engineered mutation	UNP P12493
D	185	ALA	MET	engineered mutation	UNP P12493
E	14	CYS	ALA	engineered mutation	UNP P12493
E	45	CYS	GLU	engineered mutation	UNP P12493
E	184	ALA	TRP	engineered mutation	UNP P12493
E	185	ALA	MET	engineered mutation	UNP P12493
F	14	CYS	ALA	engineered mutation	UNP P12493
F	45	CYS	GLU	engineered mutation	UNP P12493
F	184	ALA	TRP	engineered mutation	UNP P12493
F	185	ALA	MET	engineered mutation	UNP P12493
G	14	CYS	ALA	engineered mutation	UNP P12493
G	45	CYS	GLU	engineered mutation	UNP P12493
G	184	ALA	TRP	engineered mutation	UNP P12493
G	185	ALA	MET	engineered mutation	UNP P12493
H	14	CYS	ALA	engineered mutation	UNP P12493
H	45	CYS	GLU	engineered mutation	UNP P12493
H	184	ALA	TRP	engineered mutation	UNP P12493
H	185	ALA	MET	engineered mutation	UNP P12493
I	14	CYS	ALA	engineered mutation	UNP P12493
I	45	CYS	GLU	engineered mutation	UNP P12493
I	184	ALA	TRP	engineered mutation	UNP P12493
I	185	ALA	MET	engineered mutation	UNP P12493
J	14	CYS	ALA	engineered mutation	UNP P12493
J	45	CYS	GLU	engineered mutation	UNP P12493
J	184	ALA	TRP	engineered mutation	UNP P12493
J	185	ALA	MET	engineered mutation	UNP P12493
K	14	CYS	ALA	engineered mutation	UNP P12493
K	45	CYS	GLU	engineered mutation	UNP P12493
K	184	ALA	TRP	engineered mutation	UNP P12493
K	185	ALA	MET	engineered mutation	UNP P12493
L	14	CYS	ALA	engineered mutation	UNP P12493
L	45	CYS	GLU	engineered mutation	UNP P12493
L	184	ALA	TRP	engineered mutation	UNP P12493

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Chain	Residue	Modelled	Actual	Comment	Reference
L	185	ALA	MET	engineered mutation	UNP P12493

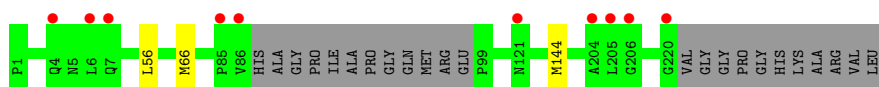
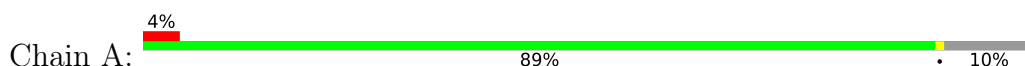
- Molecule 2 is a protein called Cleavage and polyadenylation specificity factor subunit 6.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	N	13	Total	C	N	O	0	0	0
			98	68	15	15			
2	O	14	Total	C	N	O	0	0	0
			103	71	16	16			
2	P	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	Q	14	Total	C	N	O	0	0	0
			103	71	16	16			
2	R	14	Total	C	N	O	0	0	0
			103	71	16	16			
2	S	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	T	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	U	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	V	14	Total	C	N	O	0	0	0
			103	71	16	16			
2	W	14	Total	C	N	O	0	0	0
			99	69	15	15			
2	X	14	Total	C	N	O	0	0	0
			99	69	15	15			

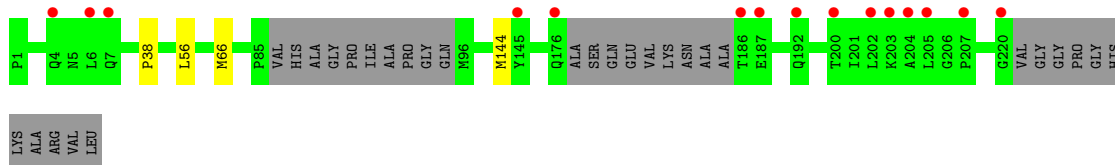
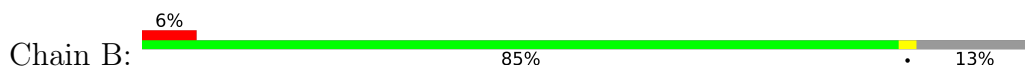
3 Residue-property plots [i](#)

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.

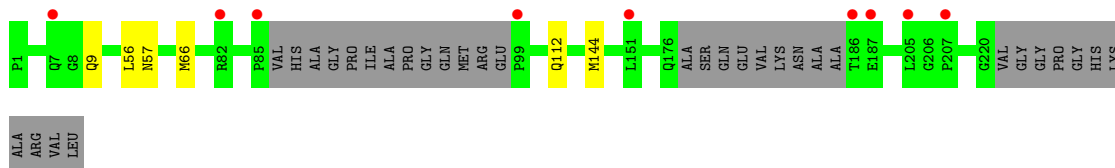
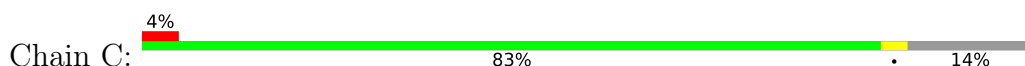
- Molecule 1: Capsid protein p24



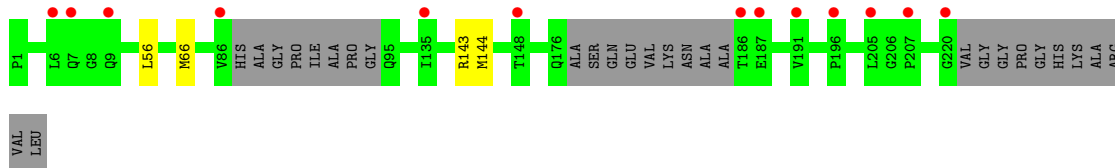
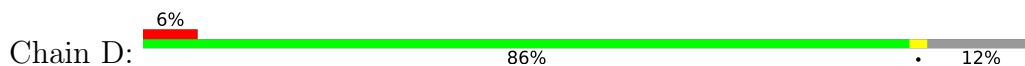
- Molecule 1: Capsid protein p24



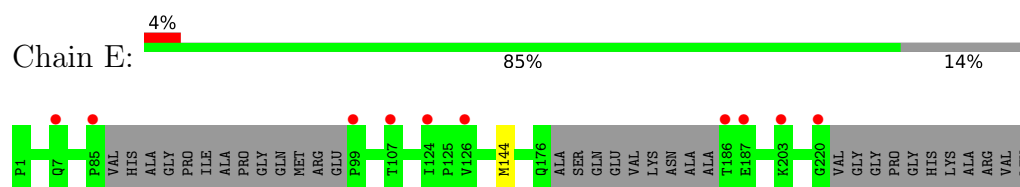
- Molecule 1: Capsid protein p24



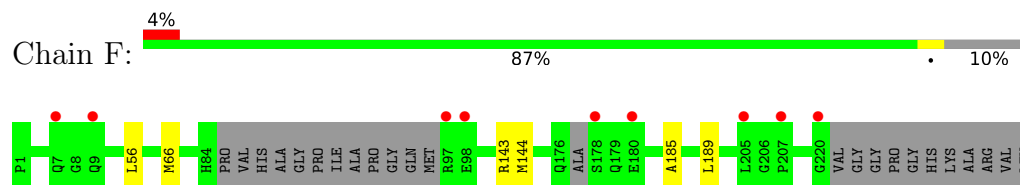
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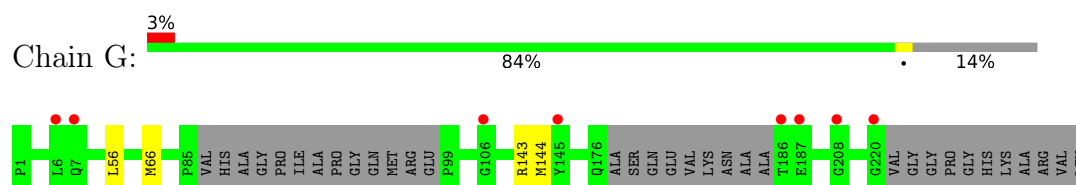
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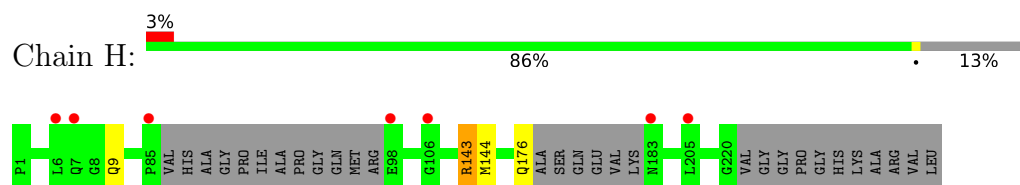
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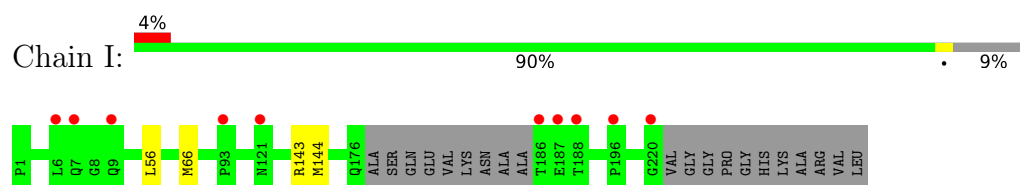
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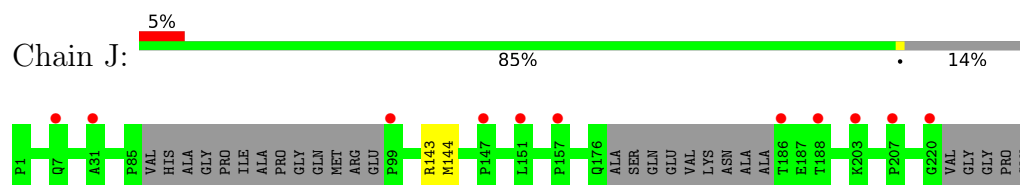
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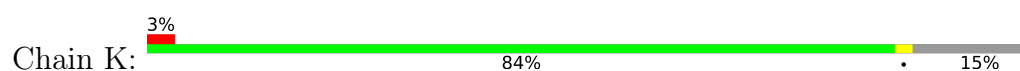


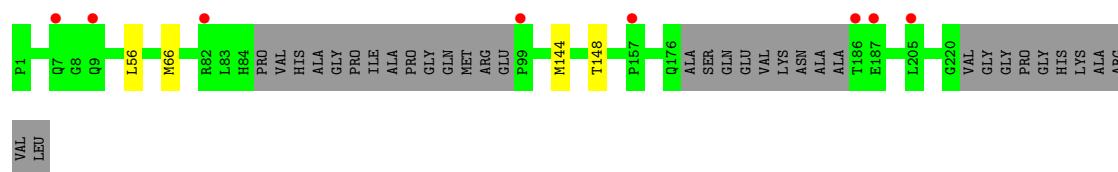
- Molecule 1: Capsid protein p24



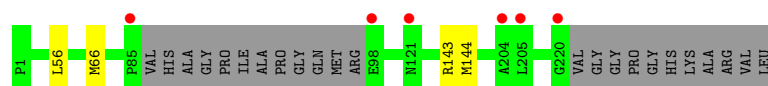
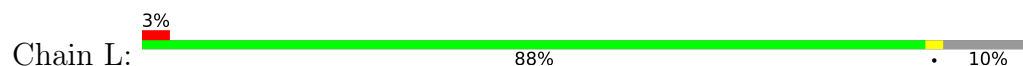
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- Molecule 1: Capsid protein p24

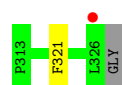
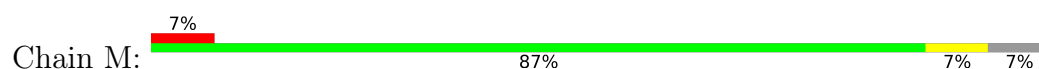




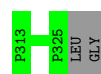
- Molecule 1: Capsid protein p24



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



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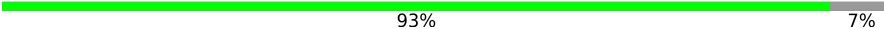
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



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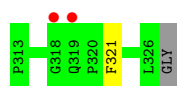
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain R:  93% 7%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain S:  13% 87% 7% 7%

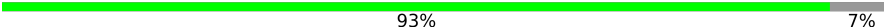


- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain T:  93% 7%

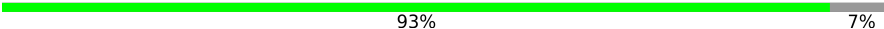


- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain U:  93% 7%

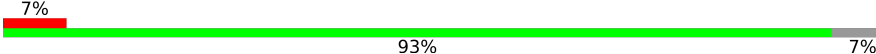


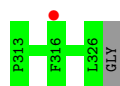
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain V:  93% 7%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain W:  7% 93% 7%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain X:  93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.13Å 135.89Å 208.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 2.80 48.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.60-2.80) 94.1 (48.60-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.230 , 0.262 0.229 , 0.258	Depositor DCC
R_{free} test set	4479 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.238 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19958	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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	0.38	0/1637	0.68	0/2225
1	B	0.38	0/1586	0.67	0/2153
1	C	0.37	0/1562	0.67	0/2122
1	D	0.38	0/1612	0.67	0/2188
1	E	0.38	0/1568	0.66	0/2129
1	F	0.38	0/1616	0.69	0/2196
1	G	0.38	0/1568	0.68	0/2129
1	H	0.38	0/1590	0.69	0/2161
1	I	0.38	0/1666	0.68	0/2265
1	J	0.37	0/1568	0.66	0/2129
1	K	0.37	0/1560	0.67	0/2117
1	L	0.38	0/1637	0.69	0/2225
2	M	0.46	0/105	0.67	0/145
2	N	0.41	0/104	0.62	0/143
2	O	0.44	0/109	0.60	0/150
2	P	0.48	0/105	0.64	0/145
2	Q	0.48	0/109	0.72	0/150
2	R	0.44	0/109	0.59	0/150
2	S	0.46	0/105	0.67	0/145
2	T	0.46	0/105	0.67	0/145
2	U	0.49	0/105	0.62	0/145
2	V	0.45	0/109	0.68	0/150
2	W	0.49	0/105	0.67	0/145
2	X	0.48	0/105	0.68	0/145
All	All	0.38	0/20445	0.67	0/27797

There are no bond length outliers.

There are no bond angle outliers.

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	1601	0	1588	2	0
1	B	1554	0	1534	2	0
1	C	1527	0	1507	3	0
1	D	1577	0	1562	1	0
1	E	1533	0	1518	0	0
1	F	1585	0	1551	2	0
1	G	1533	0	1518	2	0
1	H	1555	0	1536	2	0
1	I	1627	0	1611	1	0
1	J	1533	0	1518	0	0
1	K	1526	0	1511	1	0
1	L	1604	0	1586	1	0
2	M	99	0	91	1	0
2	N	98	0	95	0	0
2	O	103	0	97	0	0
2	P	99	0	91	0	0
2	Q	103	0	97	0	0
2	R	103	0	97	0	0
2	S	99	0	91	1	0
2	T	99	0	91	0	0
2	U	99	0	91	0	0
2	V	103	0	97	0	0
2	W	99	0	91	0	0
2	X	99	0	91	0	0
All	All	19958	0	19660	15	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 0.

All (15) 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:H:143:ARG:HD3	1:H:176:GLN:HG3	1.91	0.52
1:L:56:LEU:HD22	1:L:66:MET:HE1	1.92	0.52
1:A:56:LEU:HD22	1:A:66:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:LEU:HD22	1:G:66:MET:HE1	1.93	0.51
1:C:9:GLN:CD	1:H:9:GLN:HE22	2.20	0.49
1:B:56:LEU:HD22	1:B:66:MET:HE1	1.96	0.48
1:F:185:ALA:O	1:F:189:LEU:HB3	2.15	0.46
1:K:56:LEU:HD22	1:K:66:MET:HE1	1.97	0.45
1:F:56:LEU:HD22	1:F:66:MET:HE1	1.98	0.44
1:I:56:LEU:HD22	1:I:66:MET:HE1	1.99	0.44
1:A:66:MET:HE3	2:M:321:PHE:CE2	2.54	0.42
1:G:66:MET:HE3	2:S:321:PHE:CE2	2.54	0.42
1:C:56:LEU:HD22	1:C:66:MET:HE1	2.02	0.42
1:D:56:LEU:HD22	1:D:66:MET:HE1	2.03	0.41
1:B:38:PRO:HG3	1:C:57:ASN:HB3	2.02	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	205/231 (89%)	200 (98%)	5 (2%)	0	100	100
1	B	195/231 (84%)	191 (98%)	4 (2%)	0	100	100
1	C	193/231 (84%)	189 (98%)	4 (2%)	0	100	100
1	D	198/231 (86%)	193 (98%)	5 (2%)	0	100	100
1	E	193/231 (84%)	189 (98%)	4 (2%)	0	100	100
1	F	201/231 (87%)	198 (98%)	3 (2%)	0	100	100
1	G	193/231 (84%)	189 (98%)	4 (2%)	0	100	100
1	H	197/231 (85%)	193 (98%)	4 (2%)	0	100	100
1	I	208/231 (90%)	205 (99%)	3 (1%)	0	100	100
1	J	193/231 (84%)	188 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	192/231 (83%)	190 (99%)	2 (1%)	0	100	100
1	L	204/231 (88%)	202 (99%)	2 (1%)	0	100	100
2	M	12/15 (80%)	12 (100%)	0	0	100	100
2	N	11/15 (73%)	11 (100%)	0	0	100	100
2	O	12/15 (80%)	12 (100%)	0	0	100	100
2	P	12/15 (80%)	12 (100%)	0	0	100	100
2	Q	12/15 (80%)	12 (100%)	0	0	100	100
2	R	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
2	S	12/15 (80%)	12 (100%)	0	0	100	100
2	T	12/15 (80%)	12 (100%)	0	0	100	100
2	U	12/15 (80%)	12 (100%)	0	0	100	100
2	V	12/15 (80%)	12 (100%)	0	0	100	100
2	W	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
2	X	12/15 (80%)	12 (100%)	0	0	100	100
All	All	2515/2952 (85%)	2468 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	174/193 (90%)	173 (99%)	1 (1%)	78	92
1	B	168/193 (87%)	167 (99%)	1 (1%)	78	92
1	C	166/193 (86%)	164 (99%)	2 (1%)	63	87
1	D	172/193 (89%)	170 (99%)	2 (1%)	63	87
1	E	167/193 (86%)	166 (99%)	1 (1%)	78	92
1	F	169/193 (88%)	167 (99%)	2 (1%)	63	87
1	G	167/193 (86%)	165 (99%)	2 (1%)	63	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	168/193 (87%)	166 (99%)	2 (1%)	63	87
1	I	176/193 (91%)	174 (99%)	2 (1%)	65	87
1	J	167/193 (86%)	165 (99%)	2 (1%)	63	87
1	K	166/193 (86%)	164 (99%)	2 (1%)	63	87
1	L	174/193 (90%)	172 (99%)	2 (1%)	65	87
2	M	10/12 (83%)	10 (100%)	0	100	100
2	N	11/12 (92%)	11 (100%)	0	100	100
2	O	11/12 (92%)	11 (100%)	0	100	100
2	P	10/12 (83%)	10 (100%)	0	100	100
2	Q	11/12 (92%)	11 (100%)	0	100	100
2	R	11/12 (92%)	11 (100%)	0	100	100
2	S	10/12 (83%)	10 (100%)	0	100	100
2	T	10/12 (83%)	10 (100%)	0	100	100
2	U	10/12 (83%)	10 (100%)	0	100	100
2	V	11/12 (92%)	11 (100%)	0	100	100
2	W	10/12 (83%)	10 (100%)	0	100	100
2	X	10/12 (83%)	10 (100%)	0	100	100
All	All	2159/2460 (88%)	2138 (99%)	21 (1%)	68	88

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	MET
1	B	144	MET
1	C	112	GLN
1	C	144	MET
1	D	143	ARG
1	D	144	MET
1	E	144	MET
1	F	143	ARG
1	F	144	MET
1	G	143	ARG
1	G	144	MET
1	H	143	ARG
1	H	144	MET
1	I	143	ARG

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Mol	Chain	Res	Type
1	I	144	MET
1	J	143	ARG
1	J	144	MET
1	K	144	MET
1	K	148	THR
1	L	143	ARG
1	L	144	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	HIS
1	B	84	HIS
1	C	9	GLN
1	C	84	HIS
1	C	112	GLN
1	D	50	GLN
1	D	84	HIS
1	D	95	GLN
1	F	114	GLN
1	G	84	HIS
1	H	9	GLN
1	H	84	HIS
1	H	112	GLN
1	I	50	GLN
1	I	62	HIS
1	I	84	HIS
1	K	50	GLN
1	K	63	GLN
1	K	84	HIS
2	N	319	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](#)

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 ⓘ

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	208/231 (90%)	0.06	10 (4%) 35 28	43, 69, 129, 161	1 (0%)
1	B	201/231 (87%)	0.25	15 (7%) 20 15	42, 75, 162, 222	0
1	C	198/231 (85%)	0.31	9 (4%) 38 30	57, 86, 131, 145	1 (0%)
1	D	203/231 (87%)	0.33	13 (6%) 25 18	57, 87, 165, 185	1 (0%)
1	E	198/231 (85%)	0.26	10 (5%) 33 25	53, 86, 137, 156	1 (0%)
1	F	207/231 (89%)	0.16	9 (4%) 40 31	48, 72, 128, 158	0
1	G	198/231 (85%)	0.21	8 (4%) 42 33	41, 74, 142, 166	1 (0%)
1	H	202/231 (87%)	0.16	7 (3%) 47 38	54, 83, 124, 146	1 (0%)
1	I	211/231 (91%)	0.24	10 (4%) 36 29	52, 83, 149, 165	1 (0%)
1	J	198/231 (85%)	0.40	11 (5%) 30 23	55, 91, 159, 189	1 (0%)
1	K	197/231 (85%)	0.13	8 (4%) 41 33	48, 75, 133, 172	1 (0%)
1	L	208/231 (90%)	0.05	6 (2%) 53 43	41, 72, 132, 163	0
2	M	14/15 (93%)	0.00	1 (7%) 22 16	58, 73, 99, 117	0
2	N	13/15 (86%)	0.05	0 100 100	50, 76, 87, 89	0
2	O	14/15 (93%)	0.54	1 (7%) 22 16	64, 87, 114, 116	0
2	P	14/15 (93%)	0.65	0 100 100	72, 89, 109, 118	0
2	Q	14/15 (93%)	0.83	0 100 100	72, 97, 116, 123	0
2	R	14/15 (93%)	0.32	0 100 100	73, 87, 100, 124	0
2	S	14/15 (93%)	0.87	2 (14%) 6 5	65, 81, 95, 102	0
2	T	14/15 (93%)	0.57	0 100 100	65, 85, 108, 113	0
2	U	14/15 (93%)	0.63	0 100 100	70, 92, 118, 126	0
2	V	14/15 (93%)	0.39	0 100 100	69, 90, 115, 120	0
2	W	14/15 (93%)	0.81	1 (7%) 22 16	73, 98, 122, 123	0
2	X	14/15 (93%)	0.33	0 100 100	63, 82, 109, 123	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	2596/2952 (87%)	0.23	121 (4%)	36	29	41, 81, 144, 222	9 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	186	THR	7.2
1	K	186	THR	6.9
1	A	86	VAL	6.0
1	C	186	THR	5.8
1	B	186	THR	5.5
1	D	186	THR	5.5
1	E	186	THR	4.9
1	L	205	LEU	4.7
1	G	186	THR	4.7
1	G	145	TYR	4.5
1	B	220	GLY	4.2
1	F	97	ARG	4.1
1	I	186	THR	4.1
1	L	121	ASN	4.0
1	E	99	PRO	3.9
1	K	7	GLN	3.8
1	F	207	PRO	3.8
1	K	99	PRO	3.8
1	E	85	PRO	3.7
1	D	7	GLN	3.6
1	L	85	PRO	3.5
1	A	204	ALA	3.4
1	D	86	VAL	3.4
1	H	183	ASN	3.4
2	O	326	LEU	3.3
1	A	220	GLY	3.3
1	D	187	GLU	3.3
1	E	7	GLN	3.2
1	K	9	GLN	3.2
1	I	220	GLY	3.2
1	B	187	GLU	3.1
1	L	98	GLU	3.1
1	B	145	TYR	3.1
1	J	157	PRO	3.1
1	L	204	ALA	3.0
1	D	9	GLN	3.0
1	A	7	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	7	GLN	2.9
1	B	204	ALA	2.9
1	C	187	GLU	2.9
1	I	9	GLN	2.9
1	A	205	LEU	2.9
1	B	6	LEU	2.8
1	H	85	PRO	2.8
1	G	6	LEU	2.7
1	I	188	THR	2.7
1	E	187	GLU	2.7
2	S	319	GLN	2.7
1	C	205	LEU	2.6
1	F	180	GLU	2.6
1	I	187	GLU	2.6
1	F	9	GLN	2.6
1	I	196	PRO	2.6
1	I	7	GLN	2.6
1	B	207	PRO	2.6
1	D	135	ILE	2.5
1	G	220	GLY	2.5
1	K	187	GLU	2.5
1	F	205	LEU	2.5
1	H	205	LEU	2.5
1	J	207	PRO	2.5
2	S	318	GLY	2.4
1	I	121	ASN	2.4
1	D	148	THR	2.4
1	K	82	ARG	2.4
1	B	4	GLN	2.4
1	A	85	PRO	2.4
1	L	220	GLY	2.4
1	C	82	ARG	2.4
1	F	178	SER	2.4
1	B	202	LEU	2.4
1	D	205	LEU	2.4
1	B	192	GLN	2.3
1	A	6	LEU	2.3
1	J	151	LEU	2.3
1	C	99	PRO	2.3
1	E	220	GLY	2.3
1	J	7	GLN	2.3
1	J	188	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	7	GLN	2.3
1	K	157	PRO	2.3
1	F	220	GLY	2.3
1	G	187	GLU	2.3
1	K	205	LEU	2.3
1	A	206	GLY	2.3
1	J	220	GLY	2.3
1	H	6	LEU	2.2
1	B	176	GLN	2.2
1	B	200	THR	2.2
1	D	220	GLY	2.2
1	H	106	GLY	2.2
1	I	6	LEU	2.2
1	C	7	GLN	2.2
1	D	191	VAL	2.2
1	J	203	LYS	2.2
1	E	124	ILE	2.2
1	F	7	GLN	2.2
1	C	85	PRO	2.2
1	A	121	ASN	2.2
1	D	207	PRO	2.2
2	W	316	PHE	2.2
1	B	205	LEU	2.2
1	J	31	ALA	2.2
1	G	7	GLN	2.1
1	C	207	PRO	2.1
1	D	196	PRO	2.1
1	G	208	GLY	2.1
1	J	147	PRO	2.1
1	E	203	LYS	2.1
1	I	93	PRO	2.1
1	D	6	LEU	2.1
1	G	106	GLY	2.1
1	A	4	GLN	2.1
1	B	203	LYS	2.1
2	M	326	LEU	2.1
1	E	107	THR	2.1
1	F	98	GLU	2.1
1	E	126	VAL	2.0
1	J	99	PRO	2.0
1	H	98	GLU	2.0
1	C	151	LEU	2.0

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.