wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2017 – 03:38 am GMT

PDB ID	:	3P6Y
Title	:	CF Im25-CF Im68-UGUAA complex
Authors	:	Li, H.; Tong, S.; Li, X.; Shi, H.; Gao, Y.; Ge, H.; Niu, L.; Teng, M.
Deposited on	:	2010-10-11
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.90 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.
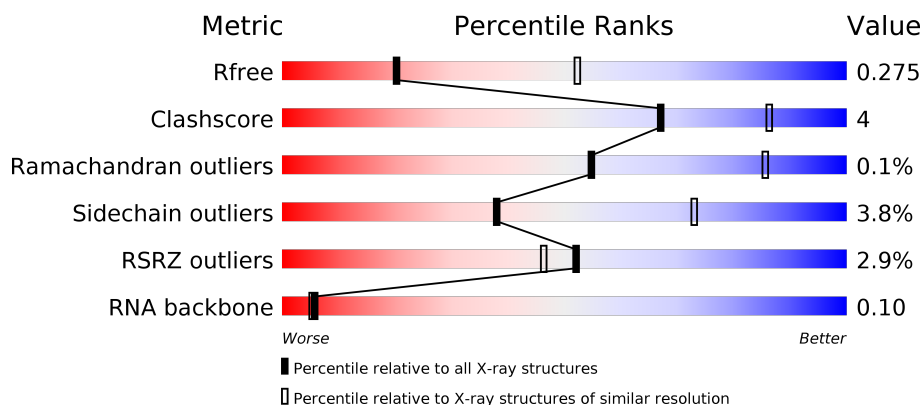
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	202	88% 8% •
1	B	202	% 87% 9% ••
1	E	202	86% 10% •
1	F	202	90% 7% •

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	202	87% 8%
1	J	202	87% 9%
1	M	202	87% 9%
1	N	202	86% 10%
2	C	90	74% 10% 12%
2	D	90	4% 78% 9% 13%
2	G	90	82% 11%
2	H	90	17% 76% 7% 18%
2	K	90	74% 11% 11%
2	L	90	77% 10% 11%
2	O	90	73% 13% 11%
2	P	90	27% 79% 17%
3	Q	5	20% 40% 60%
3	R	5	60% 40% 60%
3	S	5	40% 20% 40%
3	T	5	20% 40% 20% 20% 20%
3	U	5	40% 20% 40% 20% 20%
3	V	5	20% 40% 20% 40%
3	W	5	20% 20% 80%

2　Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 17567 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 Cleavage and polyadenylation specificity factor subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1568	1022	267	275	4			
1	B	197	Total	C	N	O	S	0	0	0
			1579	1028	268	279	4			
1	E	195	Total	C	N	O	S	0	0	0
			1571	1024	267	276	4			
1	F	197	Total	C	N	O	S	0	0	0
			1583	1033	265	281	4			
1	I	195	Total	C	N	O	S	0	0	0
			1553	1014	266	269	4			
1	J	197	Total	C	N	O	S	0	0	0
			1581	1033	265	279	4			
1	M	196	Total	C	N	O	S	0	0	0
			1570	1023	268	275	4			
1	N	197	Total	C	N	O	S	0	0	0
			1580	1029	268	279	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	LEU	-	EXPRESSION TAG	UNP O43809
A	229	GLU	-	EXPRESSION TAG	UNP O43809
A	230	HIS	-	EXPRESSION TAG	UNP O43809
A	231	HIS	-	EXPRESSION TAG	UNP O43809
A	232	HIS	-	EXPRESSION TAG	UNP O43809
A	233	HIS	-	EXPRESSION TAG	UNP O43809
A	234	HIS	-	EXPRESSION TAG	UNP O43809
A	235	HIS	-	EXPRESSION TAG	UNP O43809
B	228	LEU	-	EXPRESSION TAG	UNP O43809
B	229	GLU	-	EXPRESSION TAG	UNP O43809
B	230	HIS	-	EXPRESSION TAG	UNP O43809
B	231	HIS	-	EXPRESSION TAG	UNP O43809
B	232	HIS	-	EXPRESSION TAG	UNP O43809

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	233	HIS	-	EXPRESSION TAG	UNP O43809
B	234	HIS	-	EXPRESSION TAG	UNP O43809
B	235	HIS	-	EXPRESSION TAG	UNP O43809
E	228	LEU	-	EXPRESSION TAG	UNP O43809
E	229	GLU	-	EXPRESSION TAG	UNP O43809
E	230	HIS	-	EXPRESSION TAG	UNP O43809
E	231	HIS	-	EXPRESSION TAG	UNP O43809
E	232	HIS	-	EXPRESSION TAG	UNP O43809
E	233	HIS	-	EXPRESSION TAG	UNP O43809
E	234	HIS	-	EXPRESSION TAG	UNP O43809
E	235	HIS	-	EXPRESSION TAG	UNP O43809
F	228	LEU	-	EXPRESSION TAG	UNP O43809
F	229	GLU	-	EXPRESSION TAG	UNP O43809
F	230	HIS	-	EXPRESSION TAG	UNP O43809
F	231	HIS	-	EXPRESSION TAG	UNP O43809
F	232	HIS	-	EXPRESSION TAG	UNP O43809
F	233	HIS	-	EXPRESSION TAG	UNP O43809
F	234	HIS	-	EXPRESSION TAG	UNP O43809
F	235	HIS	-	EXPRESSION TAG	UNP O43809
I	228	LEU	-	EXPRESSION TAG	UNP O43809
I	229	GLU	-	EXPRESSION TAG	UNP O43809
I	230	HIS	-	EXPRESSION TAG	UNP O43809
I	231	HIS	-	EXPRESSION TAG	UNP O43809
I	232	HIS	-	EXPRESSION TAG	UNP O43809
I	233	HIS	-	EXPRESSION TAG	UNP O43809
I	234	HIS	-	EXPRESSION TAG	UNP O43809
I	235	HIS	-	EXPRESSION TAG	UNP O43809
J	228	LEU	-	EXPRESSION TAG	UNP O43809
J	229	GLU	-	EXPRESSION TAG	UNP O43809
J	230	HIS	-	EXPRESSION TAG	UNP O43809
J	231	HIS	-	EXPRESSION TAG	UNP O43809
J	232	HIS	-	EXPRESSION TAG	UNP O43809
J	233	HIS	-	EXPRESSION TAG	UNP O43809
J	234	HIS	-	EXPRESSION TAG	UNP O43809
J	235	HIS	-	EXPRESSION TAG	UNP O43809
M	228	LEU	-	EXPRESSION TAG	UNP O43809
M	229	GLU	-	EXPRESSION TAG	UNP O43809
M	230	HIS	-	EXPRESSION TAG	UNP O43809
M	231	HIS	-	EXPRESSION TAG	UNP O43809
M	232	HIS	-	EXPRESSION TAG	UNP O43809
M	233	HIS	-	EXPRESSION TAG	UNP O43809
M	234	HIS	-	EXPRESSION TAG	UNP O43809

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	235	HIS	-	EXPRESSION TAG	UNP O43809
N	228	LEU	-	EXPRESSION TAG	UNP O43809
N	229	GLU	-	EXPRESSION TAG	UNP O43809
N	230	HIS	-	EXPRESSION TAG	UNP O43809
N	231	HIS	-	EXPRESSION TAG	UNP O43809
N	232	HIS	-	EXPRESSION TAG	UNP O43809
N	233	HIS	-	EXPRESSION TAG	UNP O43809
N	234	HIS	-	EXPRESSION TAG	UNP O43809
N	235	HIS	-	EXPRESSION TAG	UNP O43809

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	79	Total 570	C 366	N 98	O 105	S 1	0	0	0
2	D	78	Total 557	C 358	N 93	O 105	S 1	0	0	0
2	G	80	Total 583	C 374	N 101	O 107	S 1	0	0	0
2	H	74	Total 509	C 323	N 88	O 98		0	0	0
2	K	80	Total 572	C 367	N 99	O 105	S 1	0	0	0
2	L	80	Total 570	C 367	N 97	O 105	S 1	0	0	0
2	O	80	Total 581	C 377	N 100	O 103	S 1	0	0	0
2	P	75	Total 522	C 333	N 89	O 99	S 1	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
C	162	LEU	-	EXPRESSION TAG	UNP Q16630
C	163	GLU	-	EXPRESSION TAG	UNP Q16630
C	164	HIS	-	EXPRESSION TAG	UNP Q16630
C	165	HIS	-	EXPRESSION TAG	UNP Q16630
C	166	HIS	-	EXPRESSION TAG	UNP Q16630
C	167	HIS	-	EXPRESSION TAG	UNP Q16630
C	168	HIS	-	EXPRESSION TAG	UNP Q16630
C	169	HIS	-	EXPRESSION TAG	UNP Q16630

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
D	162	LEU	-	EXPRESSION TAG	UNP Q16630
D	163	GLU	-	EXPRESSION TAG	UNP Q16630
D	164	HIS	-	EXPRESSION TAG	UNP Q16630
D	165	HIS	-	EXPRESSION TAG	UNP Q16630
D	166	HIS	-	EXPRESSION TAG	UNP Q16630
D	167	HIS	-	EXPRESSION TAG	UNP Q16630
D	168	HIS	-	EXPRESSION TAG	UNP Q16630
D	169	HIS	-	EXPRESSION TAG	UNP Q16630
G	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
G	162	LEU	-	EXPRESSION TAG	UNP Q16630
G	163	GLU	-	EXPRESSION TAG	UNP Q16630
G	164	HIS	-	EXPRESSION TAG	UNP Q16630
G	165	HIS	-	EXPRESSION TAG	UNP Q16630
G	166	HIS	-	EXPRESSION TAG	UNP Q16630
G	167	HIS	-	EXPRESSION TAG	UNP Q16630
G	168	HIS	-	EXPRESSION TAG	UNP Q16630
G	169	HIS	-	EXPRESSION TAG	UNP Q16630
H	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
H	162	LEU	-	EXPRESSION TAG	UNP Q16630
H	163	GLU	-	EXPRESSION TAG	UNP Q16630
H	164	HIS	-	EXPRESSION TAG	UNP Q16630
H	165	HIS	-	EXPRESSION TAG	UNP Q16630
H	166	HIS	-	EXPRESSION TAG	UNP Q16630
H	167	HIS	-	EXPRESSION TAG	UNP Q16630
H	168	HIS	-	EXPRESSION TAG	UNP Q16630
H	169	HIS	-	EXPRESSION TAG	UNP Q16630
K	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
K	162	LEU	-	EXPRESSION TAG	UNP Q16630
K	163	GLU	-	EXPRESSION TAG	UNP Q16630
K	164	HIS	-	EXPRESSION TAG	UNP Q16630
K	165	HIS	-	EXPRESSION TAG	UNP Q16630
K	166	HIS	-	EXPRESSION TAG	UNP Q16630
K	167	HIS	-	EXPRESSION TAG	UNP Q16630
K	168	HIS	-	EXPRESSION TAG	UNP Q16630
K	169	HIS	-	EXPRESSION TAG	UNP Q16630
L	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
L	162	LEU	-	EXPRESSION TAG	UNP Q16630
L	163	GLU	-	EXPRESSION TAG	UNP Q16630
L	164	HIS	-	EXPRESSION TAG	UNP Q16630
L	165	HIS	-	EXPRESSION TAG	UNP Q16630
L	166	HIS	-	EXPRESSION TAG	UNP Q16630

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	167	HIS	-	EXPRESSION TAG	UNP Q16630
L	168	HIS	-	EXPRESSION TAG	UNP Q16630
L	169	HIS	-	EXPRESSION TAG	UNP Q16630
O	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
O	162	LEU	-	EXPRESSION TAG	UNP Q16630
O	163	GLU	-	EXPRESSION TAG	UNP Q16630
O	164	HIS	-	EXPRESSION TAG	UNP Q16630
O	165	HIS	-	EXPRESSION TAG	UNP Q16630
O	166	HIS	-	EXPRESSION TAG	UNP Q16630
O	167	HIS	-	EXPRESSION TAG	UNP Q16630
O	168	HIS	-	EXPRESSION TAG	UNP Q16630
O	169	HIS	-	EXPRESSION TAG	UNP Q16630
P	159	SER	CYS	ENGINEERED MUTATION	UNP Q16630
P	162	LEU	-	EXPRESSION TAG	UNP Q16630
P	163	GLU	-	EXPRESSION TAG	UNP Q16630
P	164	HIS	-	EXPRESSION TAG	UNP Q16630
P	165	HIS	-	EXPRESSION TAG	UNP Q16630
P	166	HIS	-	EXPRESSION TAG	UNP Q16630
P	167	HIS	-	EXPRESSION TAG	UNP Q16630
P	168	HIS	-	EXPRESSION TAG	UNP Q16630
P	169	HIS	-	EXPRESSION TAG	UNP Q16630

- Molecule 3 is a RNA chain called 5'-R(*UP*GP*UP*AP*A)-3'.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Q	2	Total 32	C 14	N 7	O 10	P 1	0	0	0
3	R	5	Total 89	C 42	N 14	O 30	P 3	0	0	0
3	S	5	Total 104	C 48	N 19	O 33	P 4	0	0	0
3	T	4	Total 77	C 37	N 14	O 24	P 2	0	0	0
3	U	4	Total 70	C 33	N 14	O 21	P 2	0	0	0
3	V	3	Total 60	C 28	N 9	O 21	P 2	0	0	0
3	W	1	Total 17	C 9	N 2	O 6		0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	3	Total 3	O 3	0	0
4	C	3	Total 3	O 3	0	0
4	D	4	Total 4	O 4	0	0
4	E	3	Total 3	O 3	0	0
4	F	9	Total 9	O 9	0	0
4	G	7	Total 7	O 7	0	0
4	H	4	Total 4	O 4	0	0
4	I	3	Total 3	O 3	0	0
4	J	7	Total 7	O 7	0	0
4	K	4	Total 4	O 4	0	0
4	L	3	Total 3	O 3	0	0
4	M	6	Total 6	O 6	0	0
4	N	7	Total 7	O 7	0	0
4	O	3	Total 3	O 3	0	0
4	P	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Cleavage and polyadenylation specificity factor subunit 5

Chain A:

• Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain B:

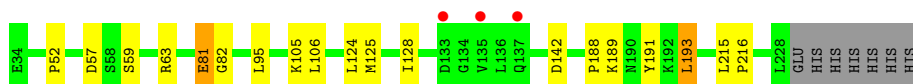• Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain E:

• Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain F:

• Molecule 1: Cleavage and polyadenylation specificity factor subunit 5
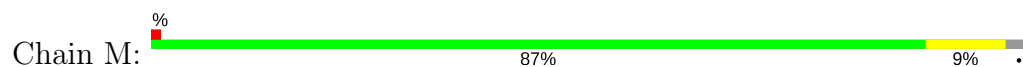
Chain I:

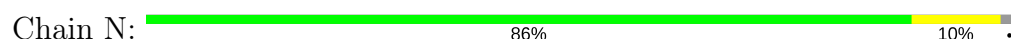• Molecule 1: Cleavage and polyadenylation specificity factor subunit 5
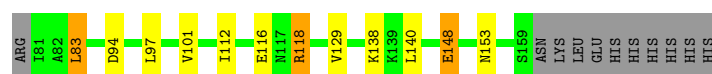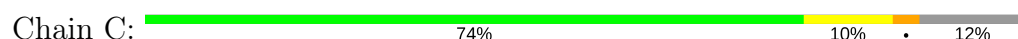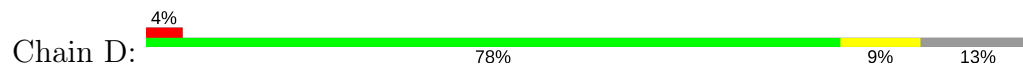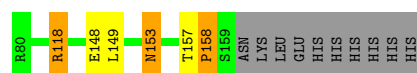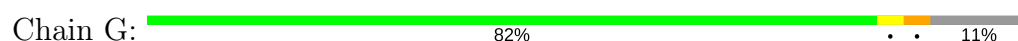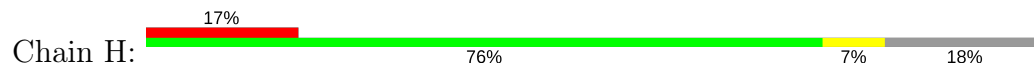
Chain J:

E34 T46 T49 D57 F64 R68 E81 G82 V83 L97 T101 V118 L121 M125 L129 L136 I141 D142 I145 R150 E154 L193 H230 HIS HIS HIS HIS

• Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain M:

%

87% 9% •

E34 T46 P52 D57 S58 S59 A62 D72 G82 L97 Q98 L99 G100 T101 V118 E119 M125 I128 D133 Q137 I141 D142 D143 C144 L176 L184 K189 N190 Y191 E229 HIS HIS HIS HIS HIS

• Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain N:

86% 10% •

E34 T46 F47 F64 R68 G82 V83 L84 L99 T102 M125 R131 Q132 D133 L136 Q137 I145 W148 F153 K169 L179 A183 L184 F185 I211 E229 H230 HIS HIS HIS HIS

• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain C:

74% 10% • 12%

ARG I81 A82 L83 D94 L97 V101 I112 E116 N117 R118 V129 K138 K139 L140 E148 N153 S159 ASN LYS LEU GLU HIS HIS HIS HIS HIS

• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain D:

4%

78% 9% 13%

ARG I81 A82 L83 Y84 I85 G86 D94 I112 E116 F126 A127 L128 V129 G130 V131 GLY S133 V156 T157 P158 S159 ASN LYS LEU GLU HIS HIS HIS HIS HIS

• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain G:

82% • • 11%

R80 R118 E148 L149 N153 T157 P158 S159 ASN LYS LEU GLU HIS HIS HIS HIS HIS

• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain H:

17%

76% 7% 18%

ARG ILE ALA L83 Y84 I85 G86 N87 D94 L97 L104 GLY V106 I112 K113 F114 F115 E116 F126 V131 GLY S133 E134 A135 K139 L143 R147 G151 Q152 N153 V156 T157 P158 SER ASN LYS LEU GLU HIS HIS HIS HIS HIS

• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain K:

74% 11% • 11%

ARG I81 D96 E116 N117 R118 D142 K146 R147 E148 L149 H150 N153 P154 P158 S159 N160 LYS LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain L: 77% 10% • 11%

R80 V101 I109 I112 E116 V129 G130 V131 S137 K138 K139 L140 M141 D142 L143 S159 ASN LYS LEU GLU HIS HIS HIS HIS HIS
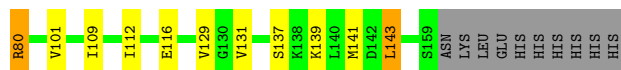
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain O: 73% 13% • 11%

ARG I81 T98 V101 H102 V106 L110 E116 N117 R118 L144 P145 E148 N153 P154 S159 N160 LYS LEU GLU HIS HIS HIS HIS HIS HIS
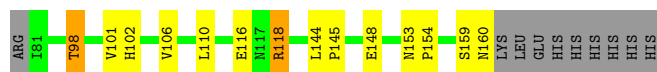
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

Chain P: 27% 79% • 17%

ARG ILE ALA LEU Y84 I85 L88 L104 G105 V106 F114 F115 E116 F126 A127 L128 V129 G132 A135 K138 K139 L140 M141 L144 P145 K146 R147 E148 L149 N153 P154 V155 V156 T157 P158 SER ASN LYS LEU GLU HIS HIS HIS HIS HIS
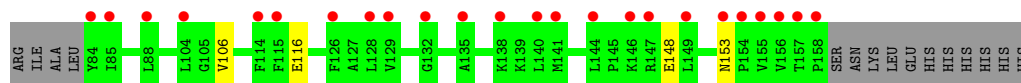
• Molecule 3: 5'-R(*UP*GP*UP*AP*A)-3'

Chain Q: 20% 40% 60%

U1 G2 U A A
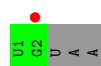
• Molecule 3: 5'-R(*UP*GP*UP*AP*A)-3'

Chain R: 60% 40% 60%

U1 G2 U3 A4 A5

• Molecule 3: 5'-R(*UP*GP*UP*AP*A)-3'

Chain S: 40% 20% 40%

U1 G2 U3 A4 A5

• Molecule 3: 5'-R(*UP*GP*UP*AP*A)-3'

Chain T: 20% 40% 20% 20% 20%

U1 G2 U3 A A5

• Molecule 3: 5'-R(*UP*GP*UP*AP*A)-3'

Chain U:
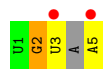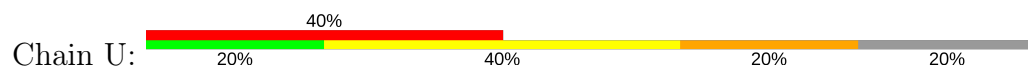
• Molecule 3: 5'-R(*UP*GP*UP*AP*A)-3'
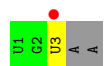
Chain V:

• Molecule 3: 5'-R(*UP*GP*UP*AP*A)-3'

Chain W:

4   Data and refinement statistics   (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.78Å 129.42Å 111.16Å 90.00° 94.01° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-2.90) 95.9 (48.60-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.12 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.226 , 0.275 0.226 , 0.275	Depositor DCC
R_{free} test set	3182 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 48.8	EDS
L-test for twinning[2]	$<\lvert L\rvert> = 0.47$, $<L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	17567	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.65 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4953e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<\lvert L\rvert>$, $<L^2>$ 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	0.34	0/1614	0.49	0/2196
1	B	0.35	0/1626	0.52	1/2215 (0.0%)
1	E	0.34	0/1617	0.50	0/2200
1	F	0.34	0/1630	0.50	0/2221
1	I	0.33	0/1599	0.48	0/2177
1	J	0.35	0/1628	0.51	1/2218 (0.0%)
1	M	0.34	0/1616	0.48	0/2200
1	N	0.35	0/1627	0.51	1/2216 (0.0%)
2	C	0.36	0/582	0.52	0/795
2	D	0.35	0/568	0.51	0/776
2	G	0.32	0/595	0.51	0/812
2	H	0.31	0/519	0.45	0/711
2	K	0.36	0/584	0.54	0/799
2	L	0.32	0/582	0.51	0/796
2	O	0.36	0/593	0.52	0/810
2	P	0.32	0/534	0.46	0/733
3	Q	0.83	0/34	0.96	0/50
3	R	0.62	0/98	1.57	3/149 (2.0%)
3	S	0.63	0/116	1.18	2/179 (1.1%)
3	T	0.72	0/85	1.23	0/129
3	U	0.66	0/77	1.34	0/116
3	V	0.69	0/66	1.12	0/101
3	W	0.91	0/18	1.29	0/26
All	All	0.35	0/18008	0.54	8/24625 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	R	2	G	O4'-C1'-N9	7.95	114.56	108.20
3	R	2	G	C1'-O4'-C4'	-7.00	104.30	109.90
1	N	136	LEU	CA-CB-CG	5.78	128.59	115.30
3	R	2	G	C3'-C2'-C1'	-5.59	97.03	101.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136	LEU	CA-CB-CG	5.30	127.48	115.30

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	1568	0	1533	9	0
1	B	1579	0	1521	13	0
1	E	1571	0	1534	13	0
1	F	1583	0	1532	11	0
1	I	1553	0	1509	10	0
1	J	1581	0	1532	10	0
1	M	1570	0	1528	16	0
1	N	1580	0	1523	14	0
2	C	570	0	528	8	0
2	D	557	0	493	3	0
2	G	583	0	546	5	0
2	H	509	0	412	2	0
2	K	572	0	523	9	0
2	L	570	0	519	7	0
2	O	581	0	557	9	0
2	P	522	0	448	1	0
3	Q	32	0	15	0	0
3	R	89	0	48	4	0
3	S	104	0	55	3	0
3	T	77	0	42	5	0
3	U	70	0	37	5	0
3	V	60	0	33	0	0
3	W	17	0	12	5	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	9	0	0	0	0
4	G	7	0	0	0	0
4	H	4	0	0	0	0
4	I	3	0	0	1	0
4	J	7	0	0	2	0
4	K	4	0	0	0	0
4	L	3	0	0	0	0
4	M	6	0	0	1	0
4	N	7	0	0	0	0
4	O	3	0	0	0	0
4	P	1	0	0	0	0
All	All	17567	0	16480	151	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 4.

The worst 5 of 151 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)
3:U:2:G:H1'	3:U:5:A:N6	1.54	1.21
2:K:118:ARG:HG3	2:K:118:ARG:HH11	1.22	1.03
2:G:118:ARG:HH11	2:G:118:ARG:HG3	1.24	1.01
2:C:118:ARG:HH11	2:C:118:ARG:HG3	1.27	0.99
3:U:2:G:H1'	3:U:5:A:H61	1.22	0.92

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	193/202 (96%)	186 (96%)	7 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	195/202 (96%)	190 (97%)	5 (3%)	0	100	100
1	E	193/202 (96%)	188 (97%)	5 (3%)	0	100	100
1	F	195/202 (96%)	190 (97%)	5 (3%)	0	100	100
1	I	193/202 (96%)	186 (96%)	7 (4%)	0	100	100
1	J	195/202 (96%)	189 (97%)	6 (3%)	0	100	100
1	M	194/202 (96%)	184 (95%)	10 (5%)	0	100	100
1	N	195/202 (96%)	189 (97%)	6 (3%)	0	100	100
2	C	77/90 (86%)	75 (97%)	2 (3%)	0	100	100
2	D	74/90 (82%)	70 (95%)	4 (5%)	0	100	100
2	G	78/90 (87%)	75 (96%)	2 (3%)	1 (1%)	14	43
2	H	68/90 (76%)	67 (98%)	1 (2%)	0	100	100
2	K	78/90 (87%)	75 (96%)	2 (3%)	1 (1%)	14	43
2	L	78/90 (87%)	76 (97%)	2 (3%)	0	100	100
2	O	78/90 (87%)	78 (100%)	0	0	100	100
2	P	73/90 (81%)	70 (96%)	2 (3%)	1 (1%)	13	41
All	All	2157/2336 (92%)	2088 (97%)	66 (3%)	3 (0%)	55	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	158	PRO
2	K	158	PRO
2	P	106	VAL

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	163/181 (90%)	159 (98%)	4 (2%)	53	83
1	B	162/181 (90%)	159 (98%)	3 (2%)	62	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	163/181 (90%)	159 (98%)	4 (2%)	53	83
1	F	164/181 (91%)	162 (99%)	2 (1%)	75	93
1	I	158/181 (87%)	153 (97%)	5 (3%)	44	78
1	J	163/181 (90%)	155 (95%)	8 (5%)	29	63
1	M	162/181 (90%)	156 (96%)	6 (4%)	39	74
1	N	162/181 (90%)	158 (98%)	4 (2%)	53	83
2	C	53/78 (68%)	48 (91%)	5 (9%)	10	30
2	D	49/78 (63%)	47 (96%)	2 (4%)	35	70
2	G	55/78 (70%)	51 (93%)	4 (7%)	16	43
2	H	41/78 (53%)	39 (95%)	2 (5%)	29	63
2	K	52/78 (67%)	47 (90%)	5 (10%)	10	29
2	L	51/78 (65%)	47 (92%)	4 (8%)	15	39
2	O	55/78 (70%)	50 (91%)	5 (9%)	11	32
2	P	45/78 (58%)	44 (98%)	1 (2%)	57	86
All	All	1698/2072 (82%)	1634 (96%)	64 (4%)	38	73

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	63	ARG
1	J	136	LEU
2	O	110	LEU
1	I	81	GLU
1	J	49	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	89	HIS
1	J	112	ASN
1	M	157	GLN
2	G	153	ASN
2	O	102	HIS

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	Q	0/5	-	-
3	R	3/5 (60%)	3 (100%)	0
3	S	4/5 (80%)	3 (75%)	0
3	T	2/5 (40%)	1 (50%)	0
3	U	2/5 (40%)	2 (100%)	0
3	V	2/5 (40%)	1 (50%)	0
3	W	0/5	-	-
All	All	13/35 (37%)	10 (76%)	0

5 of 10 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	2	G
3	R	3	U
3	R	4	A
3	S	2	G
3	S	4	A

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	195/202 (96%)	-0.13	0	100	100	30, 51, 79, 97	0
1	B	197/202 (97%)	-0.11	2 (1%)	82	81	25, 45, 71, 77	0
1	E	195/202 (96%)	-0.06	1 (0%)	90	90	34, 57, 81, 97	0
1	F	197/202 (97%)	-0.16	0	100	100	29, 52, 82, 89	0
1	I	195/202 (96%)	-0.06	3 (1%)	74	72	34, 59, 87, 109	0
1	J	197/202 (97%)	-0.08	3 (1%)	74	72	31, 50, 88, 97	0
1	M	196/202 (97%)	0.14	3 (1%)	74	72	35, 65, 104, 117	0
1	N	197/202 (97%)	-0.15	1 (0%)	90	90	26, 54, 72, 83	0
2	C	79/90 (87%)	-0.34	0	100	100	33, 47, 60, 66	0
2	D	78/90 (86%)	0.27	4 (5%)	29	24	50, 82, 95, 115	0
2	G	80/90 (88%)	-0.10	0	100	100	29, 56, 78, 86	0
2	H	74/90 (82%)	1.23	15 (20%)	1	1	97, 142, 190, 200	0
2	K	80/90 (88%)	-0.20	0	100	100	37, 55, 74, 80	0
2	L	80/90 (88%)	0.11	0	100	100	53, 79, 105, 117	0
2	O	80/90 (88%)	-0.24	0	100	100	29, 46, 61, 80	0
2	P	75/90 (83%)	1.48	24 (32%)	0	0	90, 137, 166, 175	0
3	Q	2/5 (40%)	1.57	1 (50%)	0	0	53, 53, 53, 60	2 (100%)
3	R	5/5 (100%)	3.39	3 (60%)	0	0	73, 76, 90, 104	2 (40%)
3	S	5/5 (100%)	1.01	0	100	100	91, 96, 120, 121	0
3	T	4/5 (80%)	1.18	1 (25%)	1	0	53, 54, 54, 60	4 (100%)
3	U	4/5 (80%)	1.65	2 (50%)	0	0	53, 54, 54, 63	3 (75%)
3	V	3/5 (60%)	1.66	1 (33%)	0	0	51, 51, 52, 53	3 (100%)
3	W	1/5 (20%)	3.69	1 (100%)	0	0	57, 57, 57, 57	1 (100%)
All	All	2219/2371 (93%)	0.04	65 (2%)	52	46	25, 56, 117, 200	15 (0%)

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	84	TYR	6.4
3	R	5	A	5.3
2	P	147	ARG	5.2
2	P	156	VAL	5.2
2	H	85	ILE	4.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.