Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:38 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

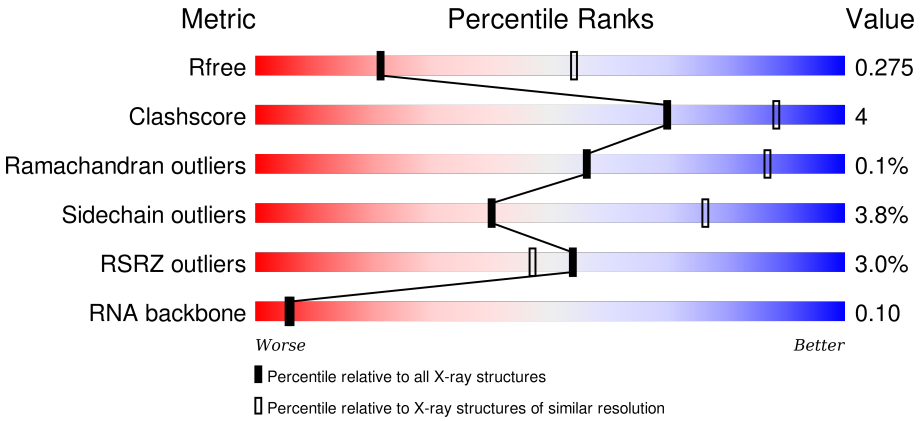
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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% •

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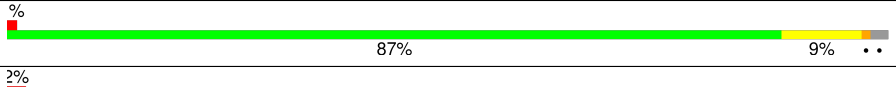
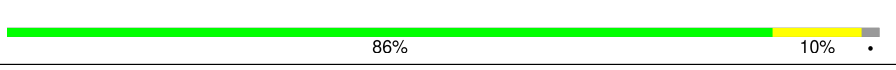
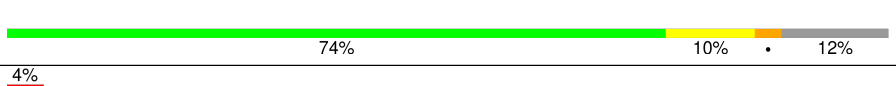
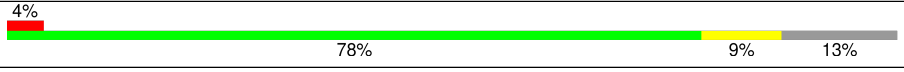
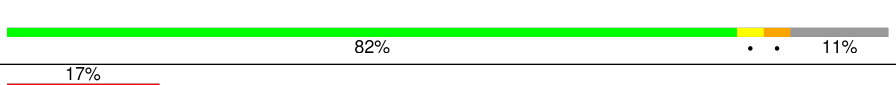
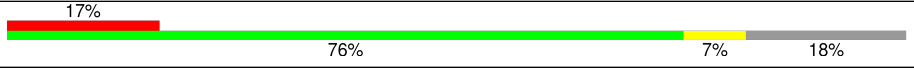
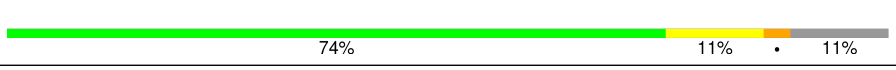
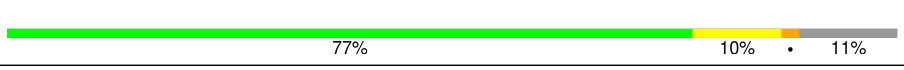
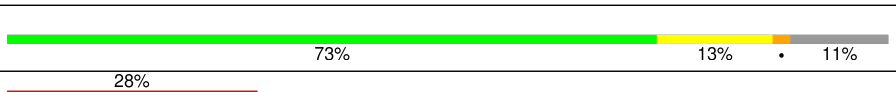
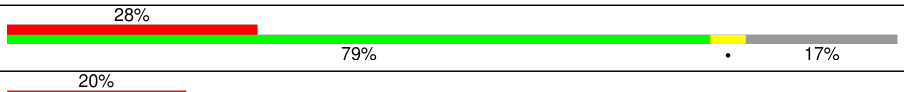
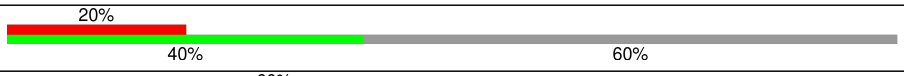
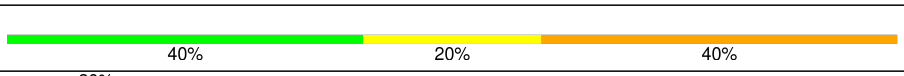
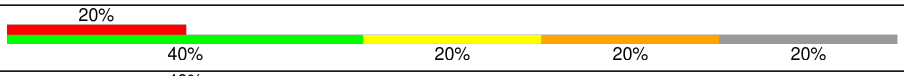
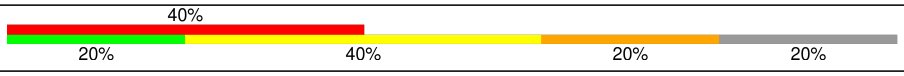
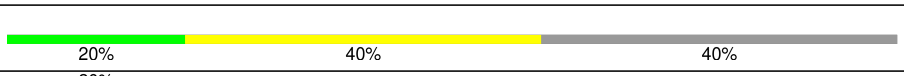
Mol	Chain	Length	Quality of chain
1	I	202	
1	J	202	
1	M	202	
1	N	202	
2	C	90	
2	D	90	
2	G	90	
2	H	90	
2	K	90	
2	L	90	
2	O	90	
2	P	90	
3	Q	5	
3	R	5	
3	S	5	
3	T	5	
3	U	5	
3	V	5	
3	W	5	

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

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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

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

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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

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

- Molecule 4 is water.

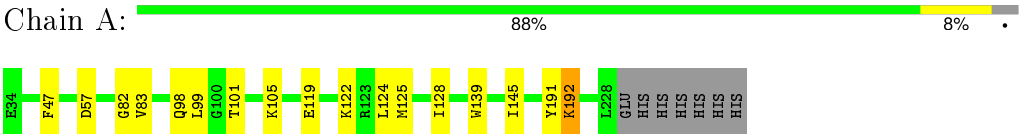
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	3	Total O 3 3	0	0
4	C	3	Total O 3 3	0	0
4	D	4	Total O 4 4	0	0
4	E	3	Total O 3 3	0	0
4	F	9	Total O 9 9	0	0
4	G	7	Total O 7 7	0	0
4	H	4	Total O 4 4	0	0
4	I	3	Total O 3 3	0	0
4	J	7	Total O 7 7	0	0
4	K	4	Total O 4 4	0	0
4	L	3	Total O 3 3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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

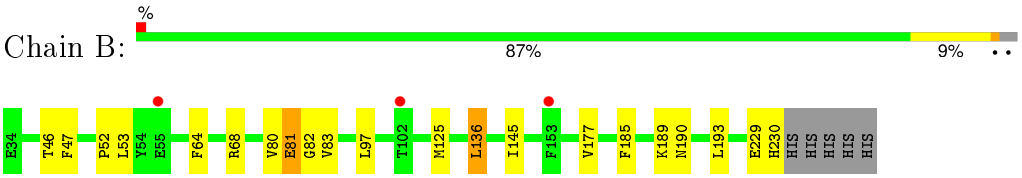
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain A:



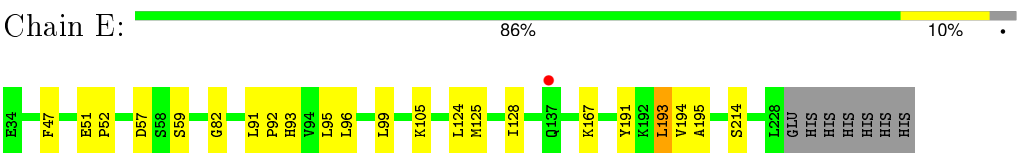
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain B:



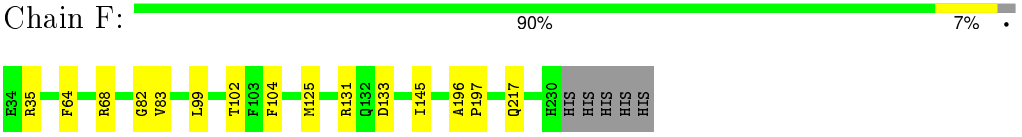
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain E:



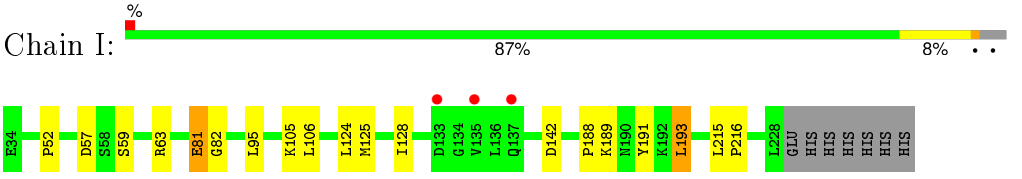
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain F:



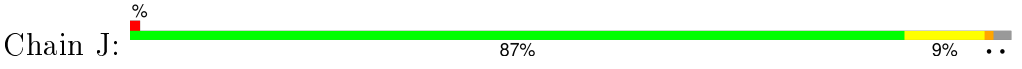
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

Chain I:



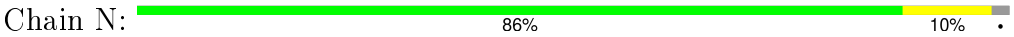
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

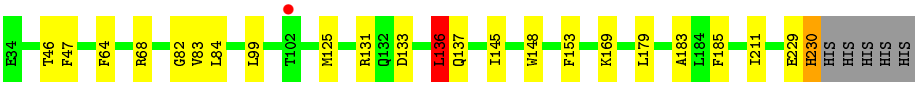
Chain J:



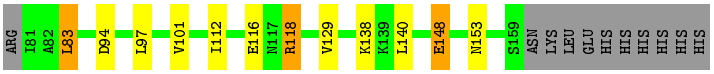
• Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

• Molecule 1: Cleavage and polyadenylation specificity factor subunit 5

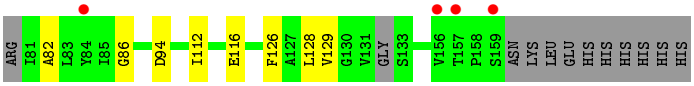




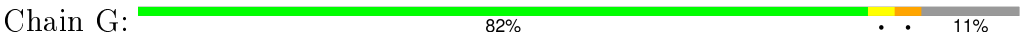
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



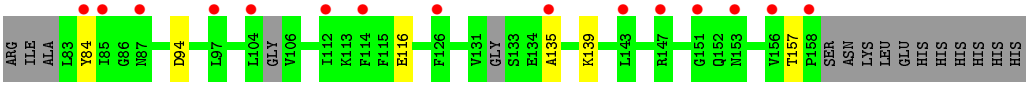
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



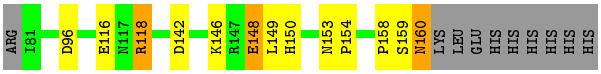
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



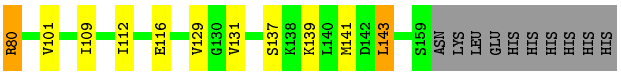
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



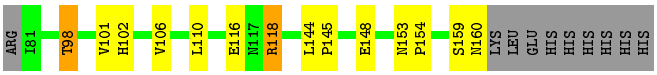
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



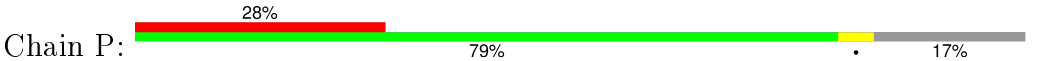
• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6

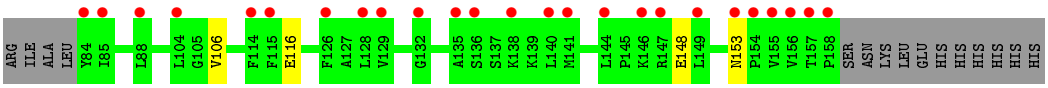


• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6



• Molecule 2: Cleavage and polyadenylation specificity factor subunit 6





• Molecule 3: 5'-R(*UP*GP*UP*AP*A)-3'

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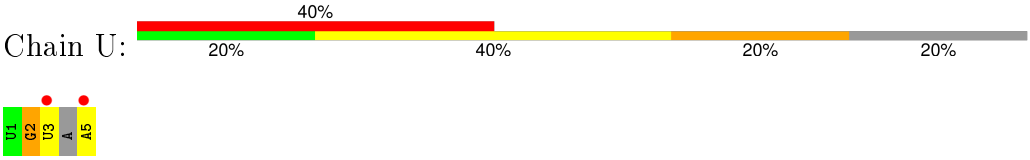
• Molecule 3: 5'-R(*UP*GP*UP*AP*A)-3'

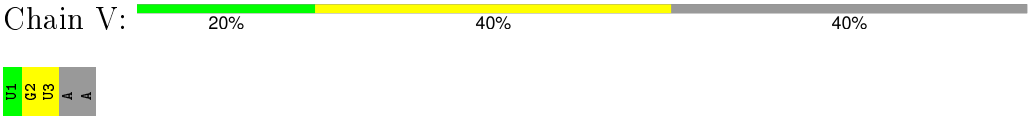
- Molecule 3: 5'-R(*UP*GP*UP*AP*A)-3'

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 , 48.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 62789 reflections (0.002%)	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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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.

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	136	LEU	CA-CB-CG	5.30	127.48	115.30
1	J	136	LEU	CA-CB-CG	5.28	127.44	115.30
3	S	5	A	C1'-O4'-C4'	-5.18	105.75	109.90
3	S	5	A	O4'-C1'-N9	5.07	112.26	108.20

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	3	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
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.

All (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
3:U:2:G:C1'	3:U:5:A:N6	2.33	0.91
2:K:159:SER:HB2	2:K:160:ASN:HA	1.57	0.85
2:O:118:ARG:HH11	2:O:118:ARG:HG3	1.40	0.84
2:O:118:ARG:CG	2:O:118:ARG:HH11	1.95	0.80
2:G:118:ARG:HH11	2:G:118:ARG:CG	1.93	0.79
1:F:104:PHE:O	3:W:1:U:N3	2.18	0.75
1:N:229:GLU:O	1:N:230:HIS:HB2	1.86	0.75
2:K:118:ARG:CG	2:K:118:ARG:HH11	1.97	0.74
1:E:82:GLY:HA3	1:E:125:MET:CE	2.18	0.72
1:M:99:LEU:HD11	1:M:191:TYR:CE2	2.26	0.70
3:U:2:G:C1'	3:U:5:A:H61	1.96	0.69
2:L:80:ARG:HB2	3:S:4:A:H61	1.57	0.69
1:A:82:GLY:HA3	1:A:125:MET:CE	2.23	0.69
1:E:124:LEU:O	1:E:128:ILE:HG12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:2:G:H21	3:T:5:A:H62	1.43	0.67
2:G:118:ARG:HG3	2:G:118:ARG:NH1	2.04	0.65
2:C:118:ARG:NH1	2:C:118:ARG:HG3	2.02	0.65
1:N:82:GLY:HA3	1:N:125:MET:HE1	1.79	0.65
1:B:125:MET:HE3	1:B:177:VAL:HG21	1.79	0.64
1:B:83:VAL:HG21	1:B:145:ILE:HD11	1.79	0.64
1:I:82:GLY:HA3	1:I:125:MET:HE1	1.80	0.63
1:N:64:PHE:O	1:N:68:ARG:HG3	1.98	0.63
3:T:5:A:H8	3:T:5:A:H3'	1.64	0.63
1:M:82:GLY:HA3	1:M:125:MET:CE	2.29	0.62
2:D:82:ALA:HB1	2:D:128:LEU:HD11	1.81	0.62
3:T:5:A:H3'	3:T:5:A:C8	2.34	0.62
1:N:82:GLY:HA3	1:N:125:MET:CE	2.29	0.62
1:J:142:ASP:HB3	4:J:33:HOH:O	2.00	0.62
1:I:82:GLY:HA3	1:I:125:MET:CE	2.29	0.62
1:F:82:GLY:HA3	1:F:125:MET:CE	2.29	0.62
2:O:159:SER:O	2:O:160:ASN:HB2	2.00	0.61
1:F:104:PHE:O	3:W:1:U:C2	2.54	0.61
3:T:5:A:C3'	3:T:5:A:C8	2.83	0.60
1:B:229:GLU:O	1:B:230:HIS:HB2	2.02	0.60
3:R:3:U:H6	3:R:3:U:H5"	1.66	0.60
1:N:137:GLN:HE22	1:N:183:ALA:HB1	1.67	0.60
1:A:122:LYS:HG2	1:A:139:TRP:HB2	1.86	0.58
1:M:142:ASP:HB3	4:M:32:HOH:O	2.03	0.57
3:R:4:A:O3'	3:R:5:A:H3'	2.03	0.57
1:F:64:PHE:O	1:F:68:ARG:HG3	2.05	0.56
1:B:52:PRO:HG3	1:B:189:LYS:HB2	1.86	0.56
1:M:118:VAL:HG13	1:M:141:ILE:HG12	1.88	0.55
2:K:118:ARG:HG3	2:K:118:ARG:NH1	2.02	0.54
2:O:98:THR:HG22	2:O:102:HIS:CE1	2.43	0.54
1:A:98:GLN:NE2	1:A:101:THR:HA	2.23	0.54
1:A:98:GLN:HE21	1:A:101:THR:HA	1.73	0.54
2:G:153:ASN:N	2:G:153:ASN:HD22	2.06	0.54
1:A:47:PHE:O	1:N:133:ASP:HB2	2.07	0.53
2:O:159:SER:O	2:O:160:ASN:CB	2.56	0.53
1:M:97:LEU:HB3	1:M:191:TYR:HD2	1.73	0.53
1:E:82:GLY:HA3	1:E:125:MET:HE1	1.90	0.53
1:B:47:PHE:CE1	1:B:185:PHE:HD2	2.26	0.52
1:M:118:VAL:HG22	1:M:141:ILE:HD11	1.92	0.52
3:R:1:U:H5"	3:R:1:U:H6	1.75	0.52
1:J:64:PHE:O	1:J:68:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:O	1:A:128:ILE:HG12	2.11	0.51
1:M:59:SER:OG	1:M:62:ALA:N	2.44	0.51
1:E:95:LEU:HD22	1:E:193:LEU:HD21	1.93	0.51
1:F:131:ARG:HD3	1:F:133:ASP:OD1	2.12	0.50
1:A:105:LYS:HE3	1:A:191:TYR:HE2	1.76	0.50
2:L:101:VAL:HG11	2:L:109:ILE:HD11	1.93	0.50
1:A:192:LYS:HB3	1:N:136:LEU:HB3	1.92	0.50
2:C:112:ILE:HG12	2:C:129:VAL:HG22	1.93	0.50
1:J:83:VAL:HG21	1:J:145:ILE:HD11	1.93	0.50
1:B:53:LEU:O	1:B:190:ASN:ND2	2.42	0.49
1:M:46:THR:HB	1:M:184:LEU:HD12	1.95	0.49
1:B:82:GLY:HA3	1:B:125:MET:CE	2.41	0.49
2:O:118:ARG:NH1	2:O:118:ARG:CG	2.63	0.49
2:L:139:LYS:O	2:L:143:LEU:HG	2.11	0.49
2:L:80:ARG:CB	3:S:4:A:H61	2.26	0.49
1:N:47:PHE:CE1	1:N:185:PHE:HD2	2.31	0.49
1:M:99:LEU:CD1	1:M:191:TYR:CE2	2.95	0.48
2:C:118:ARG:CG	2:C:118:ARG:NH1	2.74	0.48
1:N:131:ARG:HD3	1:N:133:ASP:OD1	2.14	0.48
2:K:118:ARG:NH1	2:K:118:ARG:CG	2.64	0.48
1:I:105:LYS:HE3	1:I:191:TYR:CE2	2.49	0.48
1:F:83:VAL:HG21	1:F:145:ILE:HD11	1.95	0.48
3:U:2:G:C1'	3:U:5:A:H62	2.23	0.47
1:I:124:LEU:O	1:I:128:ILE:HG12	2.13	0.47
1:M:82:GLY:HA3	1:M:125:MET:HE1	1.96	0.47
1:B:64:PHE:O	1:B:68:ARG:HG3	2.15	0.47
1:F:104:PHE:O	3:W:1:U:O2	2.32	0.47
1:E:99:LEU:HD13	1:E:191:TYR:CE2	2.49	0.47
2:L:80:ARG:HB2	3:S:4:A:N6	2.28	0.47
1:M:97:LEU:HD11	1:M:128:ILE:HG21	1.97	0.47
1:B:125:MET:CE	1:B:177:VAL:HG21	2.45	0.47
1:F:104:PHE:N	3:W:1:U:O2	2.46	0.46
2:H:135:ALA:O	2:H:139:LYS:CB	2.63	0.46
3:T:2:G:N2	3:T:5:A:H62	2.10	0.46
1:J:97:LEU:HD21	1:J:129:LEU:HD21	1.98	0.46
1:A:83:VAL:HG21	1:A:145:ILE:HD11	1.97	0.46
1:N:83:VAL:HG21	1:N:145:ILE:HD11	1.98	0.46
2:H:84:TYR:N	2:H:157:THR:O	2.49	0.46
2:K:96:ASP:OD2	2:K:150:HIS:HE1	1.99	0.45
1:M:59:SER:OG	1:M:62:ALA:CB	2.64	0.45
1:J:142:ASP:HB2	4:J:27:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:LEU:HD23	2:C:140:LEU:HD23	1.99	0.45
1:J:82:GLY:HA3	1:J:125:MET:CE	2.47	0.45
2:L:112:ILE:HG12	2:L:129:VAL:HG22	1.99	0.45
1:J:141:ILE:O	1:J:141:ILE:HG13	2.17	0.44
1:N:137:GLN:NE2	1:N:183:ALA:HB1	2.32	0.44
1:I:188:PRO:HB2	1:I:191:TYR:HD1	1.81	0.44
1:I:81:GLU:HG2	1:I:106:LEU:HB2	1.99	0.44
1:I:95:LEU:HD22	1:I:193:LEU:HD21	2.00	0.44
1:I:215:LEU:N	1:I:216:PRO:CD	2.81	0.44
1:I:52:PRO:HG3	1:I:189:LYS:HB2	2.01	0.43
1:I:142:ASP:HB3	4:I:236:HOH:O	2.19	0.43
1:E:93:HIS:HD2	1:E:195:ALA:O	2.02	0.43
1:B:82:GLY:HA3	1:B:125:MET:HE2	2.01	0.43
2:O:101:VAL:HG12	2:O:106:VAL:HB	2.00	0.42
2:D:86:GLY:HA2	2:D:126:PHE:HB3	2.01	0.42
2:P:148:GLU:HB3	2:P:153:ASN:ND2	2.34	0.42
1:M:99:LEU:HD11	1:M:191:TYR:CZ	2.54	0.42
1:J:118:VAL:HG13	1:J:141:ILE:HG12	2.00	0.42
2:D:112:ILE:HG12	2:D:129:VAL:HG22	2.00	0.42
2:L:137:SER:O	2:L:141:MET:HG3	2.19	0.42
2:C:97:LEU:O	2:C:101:VAL:HG23	2.19	0.42
1:N:84:LEU:HD23	1:N:179:LEU:HD21	2.01	0.42
1:B:80:VAL:C	1:B:81:GLU:HG2	2.39	0.42
1:B:47:PHE:CE1	1:B:185:PHE:CD2	3.06	0.42
2:K:153:ASN:HA	2:K:154:PRO:HD3	1.93	0.41
1:J:150:ARG:HD3	1:J:154:GLU:O	2.20	0.41
3:R:3:U:C6	3:R:3:U:H5"	2.52	0.41
1:B:97:LEU:HD23	1:B:193:LEU:HD12	2.02	0.41
1:N:153:PHE:CZ	1:N:169:LYS:HD2	2.55	0.41
1:F:102:THR:O	3:W:1:U:O2'	2.30	0.41
1:M:52:PRO:HG3	1:M:189:LYS:HB2	2.03	0.41
1:M:99:LEU:HD11	1:M:191:TYR:CD2	2.54	0.41
2:K:142:ASP:O	2:K:146:LYS:HG3	2.20	0.41
1:N:148:TRP:CD2	1:N:211:ILE:HG12	2.56	0.41
1:F:196:ALA:HA	1:F:197:PRO:HD2	1.94	0.41
1:E:91:LEU:HA	1:E:92:PRO:HD3	1.97	0.41
1:M:99:LEU:CD1	1:M:191:TYR:CD2	3.04	0.41
2:K:148:GLU:HA	2:K:153:ASN:ND2	2.35	0.41
1:E:51:GLU:HA	1:E:52:PRO:HD3	1.96	0.41
2:C:148:GLU:HA	2:C:153:ASN:HD22	1.86	0.41
1:E:214:SER:HB2	1:F:217:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:GLY:HA3	1:E:125:MET:HE3	2.00	0.41
1:E:105:LYS:HE3	1:E:191:TYR:HE2	1.86	0.41
2:O:144:LEU:HB3	2:O:145:PRO:HD3	2.03	0.41
2:C:138:LYS:HB3	2:C:138:LYS:HE2	1.89	0.41
1:E:47:PHE:CE1	1:E:193:LEU:HD22	2.57	0.40
2:G:157:THR:HA	2:G:158:PRO:HD3	1.93	0.40
1:E:96:LEU:HB2	1:E:194:VAL:HG23	2.03	0.40
2:O:153:ASN:HA	2:O:154:PRO:HD3	1.93	0.40
1:J:121:LEU:HD23	1:J:141:ILE:HD13	2.02	0.40

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	193/202 (96%)	186 (96%)	7 (4%)	0	100	100
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%)	15	46
2	H	68/90 (76%)	67 (98%)	1 (2%)	0	100	100
2	K	78/90 (87%)	75 (96%)	2 (3%)	1 (1%)	15	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	14 44
All	All	2157/2336 (92%)	2088 (97%)	66 (3%)	3 (0%)	56 87

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 (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	163/181 (90%)	159 (98%)	4 (2%)	55 85
1	B	162/181 (90%)	159 (98%)	3 (2%)	65 89
1	E	163/181 (90%)	159 (98%)	4 (2%)	55 85
1	F	164/181 (91%)	162 (99%)	2 (1%)	78 94
1	I	158/181 (87%)	153 (97%)	5 (3%)	46 81
1	J	163/181 (90%)	155 (95%)	8 (5%)	31 67
1	M	162/181 (90%)	156 (96%)	6 (4%)	41 77
1	N	162/181 (90%)	158 (98%)	4 (2%)	55 85
2	C	53/78 (68%)	48 (91%)	5 (9%)	11 32
2	D	49/78 (63%)	47 (96%)	2 (4%)	37 73
2	G	55/78 (70%)	51 (93%)	4 (7%)	17 45
2	H	41/78 (53%)	39 (95%)	2 (5%)	31 67
2	K	52/78 (67%)	47 (90%)	5 (10%)	10 31
2	L	51/78 (65%)	47 (92%)	4 (8%)	16 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	O	55/78 (70%)	50 (91%)	5 (9%)	12 34
2	P	45/78 (58%)	44 (98%)	1 (2%)	60 88
All	All	1698/2072 (82%)	1634 (96%)	64 (4%)	40 76

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASP
1	A	99	LEU
1	A	119	GLU
1	A	192	LYS
1	B	46	THR
1	B	81	GLU
1	B	136	LEU
2	C	83	LEU
2	C	94	ASP
2	C	116	GLU
2	C	118	ARG
2	C	148	GLU
2	D	94	ASP
2	D	116	GLU
1	E	57	ASP
1	E	59	SER
1	E	167	LYS
1	E	193	LEU
1	F	35	ARG
1	F	99	LEU
2	G	118	ARG
2	G	148	GLU
2	G	149	LEU
2	G	153	ASN
2	H	94	ASP
2	H	116	GLU
1	I	57	ASP
1	I	59	SER
1	I	63	ARG
1	I	81	GLU
1	I	193	LEU
1	J	46	THR
1	J	49	THR
1	J	81	GLU

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Mol	Chain	Res	Type
1	J	101	THR
1	J	136	LEU
1	J	141	ILE
1	J	193	LEU
1	J	230	HIS
2	K	116	GLU
2	K	118	ARG
2	K	148	GLU
2	K	149	LEU
2	K	160	ASN
2	L	80	ARG
2	L	116	GLU
2	L	131	VAL
2	L	143	LEU
1	M	57	ASP
1	M	72	ASP
1	M	101	THR
1	M	119	GLU
1	M	141	ILE
1	M	176	LEU
1	N	46	THR
1	N	99	LEU
1	N	136	LEU
1	N	230	HIS
2	O	98	THR
2	O	110	LEU
2	O	116	GLU
2	O	118	ARG
2	O	148	GLU
2	P	116	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	178	GLN
2	C	152	GLN
2	C	153	ASN
1	E	89	HIS
1	E	93	HIS
2	G	102	HIS
2	G	153	ASN
1	I	89	HIS

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Mol	Chain	Res	Type
1	J	112	ASN
2	K	150	HIS
2	K	153	ASN
1	M	98	GLN
1	M	157	GLN
2	O	102	HIS
2	O	153	ASN
2	P	153	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	Q	0/5	-	-
3	R	3/5 (60%)	3 (100%)	1 (33%)
3	S	4/5 (80%)	3 (75%)	0
3	T	2/5 (40%)	1 (50%)	0
3	U	2/5 (40%)	2 (100%)	1 (50%)
3	V	2/5 (40%)	1 (50%)	1 (50%)
3	W	0/5	-	-
All	All	13/35 (37%)	10 (76%)	3 (23%)

All (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
3	S	5	A
3	T	2	G
3	U	2	G
3	U	3	U
3	V	3	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	R	3	U
3	U	2	G
3	V	2	G

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, 95^{th} 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%)	-0.12	0 100 100	30, 51, 79, 97	0
1	B	197/202 (97%)	-0.10	3 (1%) 76 74	25, 45, 71, 77	0
1	E	195/202 (96%)	-0.05	1 (0%) 91 90	34, 57, 81, 97	0
1	F	197/202 (97%)	-0.15	0 100 100	29, 52, 82, 89	0
1	I	195/202 (96%)	-0.05	3 (1%) 76 74	34, 59, 87, 109	0
1	J	197/202 (97%)	-0.07	3 (1%) 76 74	31, 50, 88, 97	0
1	M	196/202 (97%)	0.15	4 (2%) 68 64	35, 65, 104, 117	0
1	N	197/202 (97%)	-0.14	1 (0%) 91 90	26, 54, 72, 83	0
2	C	79/90 (87%)	-0.33	0 100 100	33, 47, 60, 66	0
2	D	78/90 (86%)	0.29	4 (5%) 32 25	50, 82, 95, 115	0
2	G	80/90 (88%)	-0.09	0 100 100	29, 56, 78, 86	0
2	H	74/90 (82%)	1.27	15 (20%) 1 1	97, 142, 190, 200	0
2	K	80/90 (88%)	-0.19	0 100 100	37, 55, 74, 80	0
2	L	80/90 (88%)	0.13	0 100 100	53, 79, 105, 117	0
2	O	80/90 (88%)	-0.23	0 100 100	29, 46, 61, 80	0
2	P	75/90 (83%)	1.51	25 (33%) 0 0	90, 137, 166, 175	0
3	Q	2/5 (40%)	1.45	1 (50%) 0 0	53, 53, 53, 60	2 (100%)
3	R	5/5 (100%)	2.93	3 (60%) 0 0	73, 76, 90, 104	2 (40%)
3	S	5/5 (100%)	0.86	0 100 100	91, 96, 120, 121	0
3	T	4/5 (80%)	1.03	1 (25%) 1 0	53, 54, 54, 60	4 (100%)
3	U	4/5 (80%)	1.35	2 (50%) 0 0	53, 54, 54, 63	3 (75%)
3	V	3/5 (60%)	1.26	0 100 100	51, 51, 52, 53	3 (100%)
3	W	1/5 (20%)	2.55	1 (100%) 0 0	57, 57, 57, 57	1 (100%)
All	All	2219/2371 (93%)	0.05	67 (3%) 54 47	25, 56, 117, 200	15 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	84	TYR	6.6
2	P	156	VAL	5.2
2	P	147	ARG	5.0
3	R	5	A	4.9
2	H	85	ILE	4.9
2	H	84	TYR	4.6
3	R	4	A	4.4
2	P	85	ILE	4.3
2	P	140	LEU	4.2
1	I	137	GLN	4.0
2	P	144	LEU	3.9
2	H	97	LEU	3.9
2	P	104	LEU	3.8
2	H	112	ILE	3.5
2	H	158	PRO	3.4
2	P	154	PRO	3.3
1	M	137	GLN	3.3
2	P	146	LYS	3.3
2	H	114	PHE	3.0
2	D	159	SER	3.0
2	P	128	LEU	2.9
2	P	132	GLY	2.9
2	H	104	LEU	2.9
2	P	114	PHE	2.9
2	P	153	ASN	2.8
1	B	102	THR	2.8
1	I	133	ASP	2.7
2	P	115	PHE	2.7
2	P	149	LEU	2.7
2	H	151	GLY	2.7
1	J	101	THR	2.6
2	H	143	LEU	2.6
1	I	135	VAL	2.6
2	P	88	LEU	2.6
2	P	126	PHE	2.6
3	W	1	U	2.6
1	M	133	ASP	2.5
1	J	64	PHE	2.5
2	H	147	ARG	2.5
2	H	126	PHE	2.5
2	H	156	VAL	2.5
2	H	135	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	157	THR	2.4
1	N	102	THR	2.4
2	H	87	ASN	2.4
2	P	155	VAL	2.4
3	Q	2	G	2.4
3	R	3	U	2.3
2	H	153	ASN	2.3
1	E	137	GLN	2.3
1	J	57	ASP	2.3
2	D	156	VAL	2.3
2	D	84	TYR	2.3
2	P	135	ALA	2.2
3	T	5	A	2.2
2	P	158	PRO	2.2
1	B	153	PHE	2.2
2	P	141	MET	2.2
1	M	144	CYS	2.2
3	U	5	A	2.2
2	P	157	THR	2.1
2	P	129	VAL	2.1
3	U	3	U	2.1
2	P	138	LYS	2.0
1	B	55	GLU	2.0
2	P	136	SER	2.0
1	M	189	LYS	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 carbohydrates 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.