wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:26 AM GMT

PDB ID	:	2GTT
Title	:	Crystal structure of the rabies virus nucleoprotein-RNA complex
Authors	:	Albertini, A.A.V.; Wernimont, A.K.; Muziol, T.; Ravelli, R.B.G.; Weissenhorn, W.; Ruigrok, R.W.H.
Deposited on	:	2006-04-28
Resolution	:	3.49 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 (1)) were used in the production of this report:

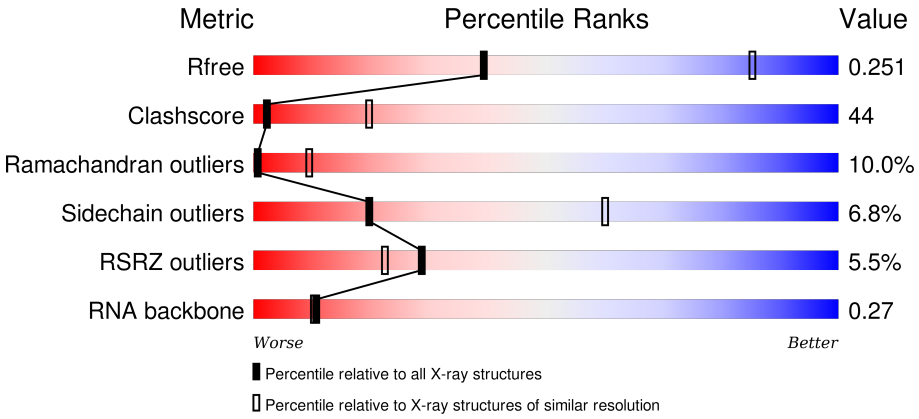
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.49 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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 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	W	99	3% 17% 30% 30% 22%
2	X	99	4% 14% 33% 34% 18%
3	A	450	5% 41% 38% 9% • 11%
3	B	450	5% 36% 43% 9% • 11%

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Mol	Chain	Length	Quality of chain
3	C	450	4% 43% 36% 10% • 10%
3	D	450	4% 44% 38% 7% • 11%
3	E	450	9% 40% 40% 9% 11%
3	F	450	6% 41% 40% 8% • 10%
3	G	450	6% 39% 42% 8% • 11%
3	H	450	6% 42% 39% 7% • 11%
3	I	450	4% 39% 41% 8% • 10%
3	J	450	6% 44% 37% 9% • 10%
3	K	450	3% 39% 41% 9% 11%
3	L	450	3% 36% 44% 10% • 10%
3	M	450	4% 39% 42% 8% 10%
3	N	450	5% 38% 42% 9% • 10%
3	O	450	7% 42% 38% 8% • 11%
3	P	450	4% 39% 41% 8% 11%
3	Q	450	3% 38% 40% 11% 11%
3	R	450	8% 44% 37% 8% 11%
3	S	450	6% 37% 43% 8% • 11%
3	T	450	3% 39% 39% 10% • 11%
3	U	450	5% 39% 40% 10% • 10%
3	V	450	5% 35% 43% 12% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 74551 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 RNA chain called RNA (99-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	W	99	Total	C	N	O	P	0	0	0
			2059	932	379	650	98			

- Molecule 2 is a RNA chain called RNA (99-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	99	Total	C	N	O	P	0	0	0
			2045	925	365	657	98			

- Molecule 3 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	401	Total	C	N	O	S	0	0	0
			3192	2042	549	584	17			
3	B	401	Total	C	N	O	S	0	0	0
			3196	2045	550	584	17			
3	C	404	Total	C	N	O	S	0	0	0
			3217	2058	553	589	17			
3	D	400	Total	C	N	O	S	0	0	0
			3187	2039	548	583	17			
3	E	400	Total	C	N	O	S	0	0	0
			3187	2039	548	583	17			
3	F	405	Total	C	N	O	S	0	0	0
			3223	2062	553	591	17			
3	G	400	Total	C	N	O	S	0	0	0
			3183	2037	548	581	17			
3	H	400	Total	C	N	O	S	0	0	0
			3191	2042	549	583	17			
3	I	403	Total	C	N	O	S	0	0	0
			3209	2053	551	588	17			
3	J	405	Total	C	N	O	S	0	0	0
			3225	2063	554	591	17			

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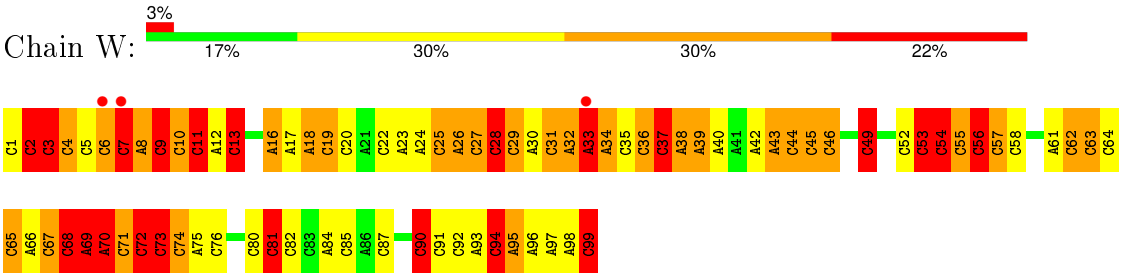
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	401	Total	C	N	O	S	0	0	0
			3192	2043	550	582	17			
3	L	406	Total	C	N	O	S	0	0	0
			3234	2068	555	594	17			
3	M	404	Total	C	N	O	S	0	0	0
			3217	2058	553	589	17			
3	N	405	Total	C	N	O	S	0	0	0
			3223	2062	553	591	17			
3	O	400	Total	C	N	O	S	0	0	0
			3183	2037	548	581	17			
3	P	399	Total	C	N	O	S	0	0	0
			3182	2037	548	580	17			
3	Q	402	Total	C	N	O	S	0	0	0
			3200	2048	550	585	17			
3	R	401	Total	C	N	O	S	0	0	0
			3192	2043	550	582	17			
3	S	401	Total	C	N	O	S	0	0	0
			3192	2043	550	582	17			
3	T	400	Total	C	N	O	S	0	0	0
			3187	2040	549	581	17			
3	U	403	Total	C	N	O	S	0	0	0
			3209	2054	552	586	17			
3	V	405	Total	C	N	O	S	0	0	0
			3226	2063	554	592	17			

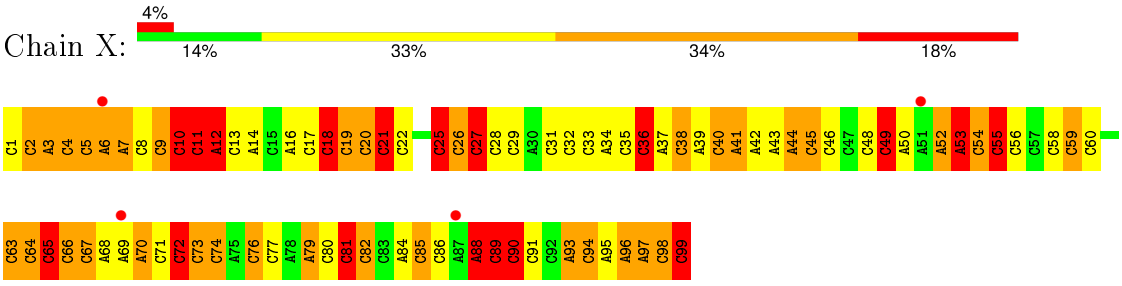
3 Residue-property plots (i)

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.

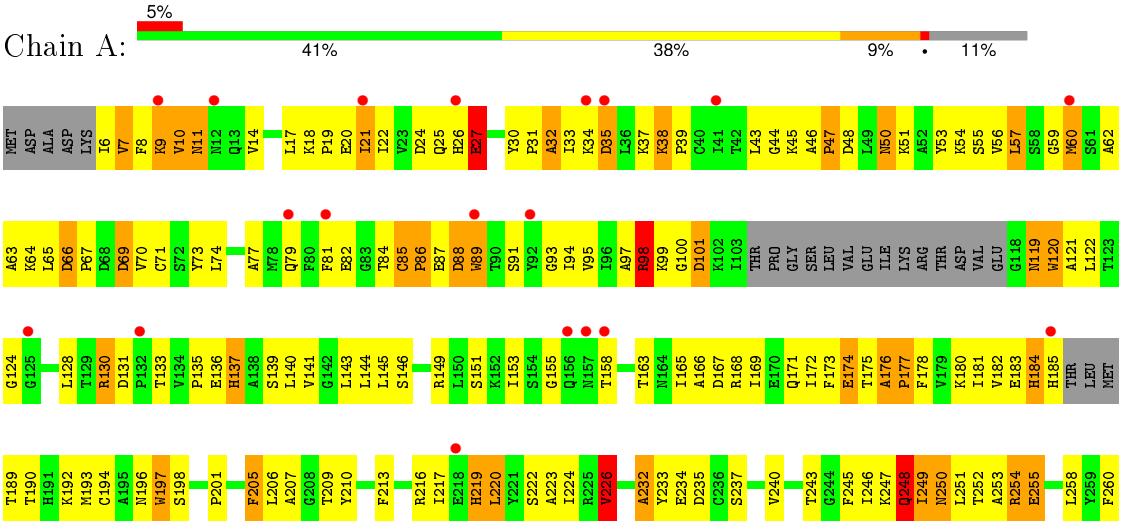
- Molecule 1: RNA (99-MER)

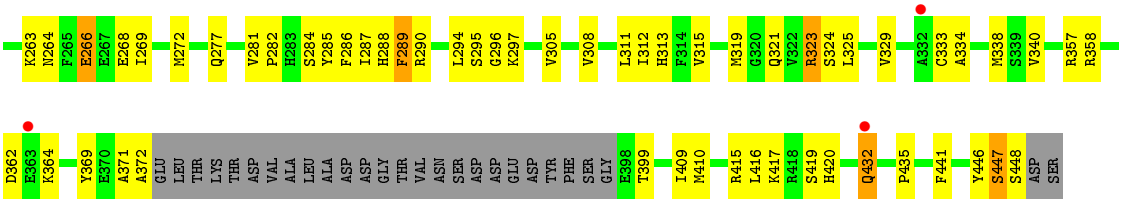


- Molecule 2: RNA (99-MER)



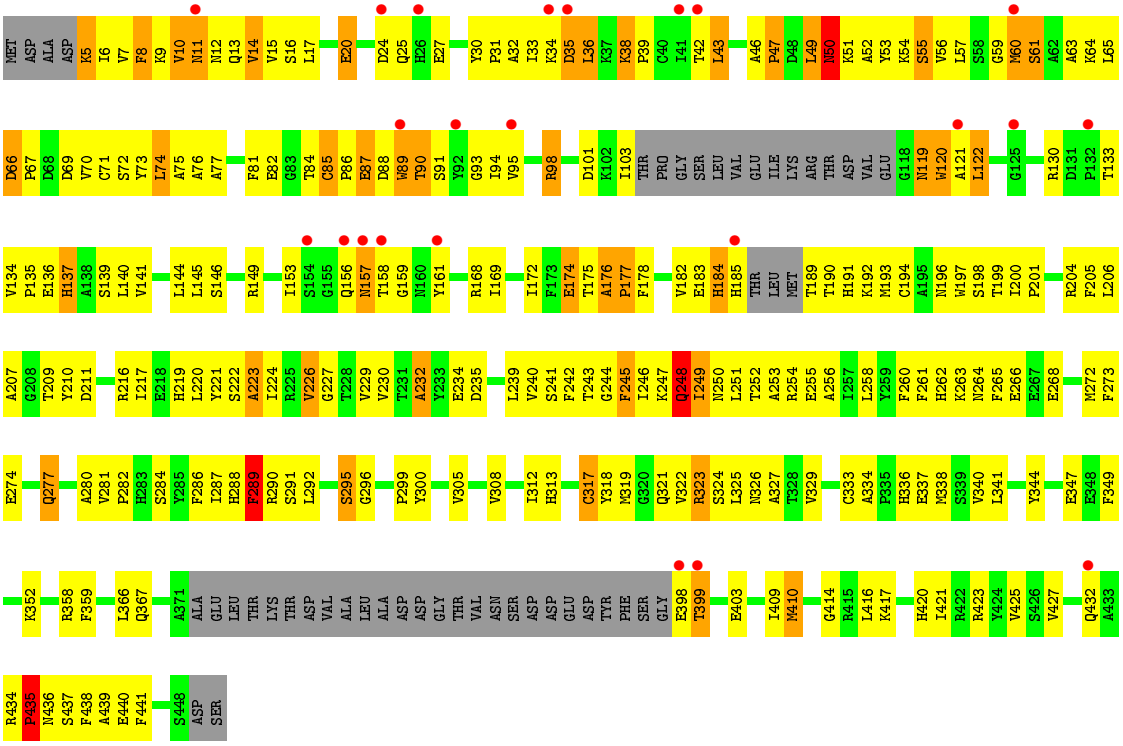
- Molecule 3: Nucleoprotein





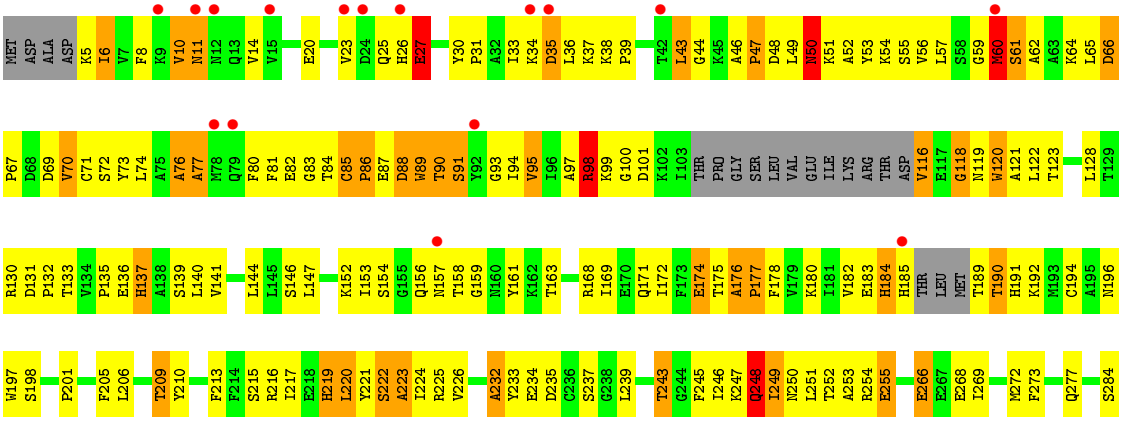
• Molecule 3: Nucleoprotein

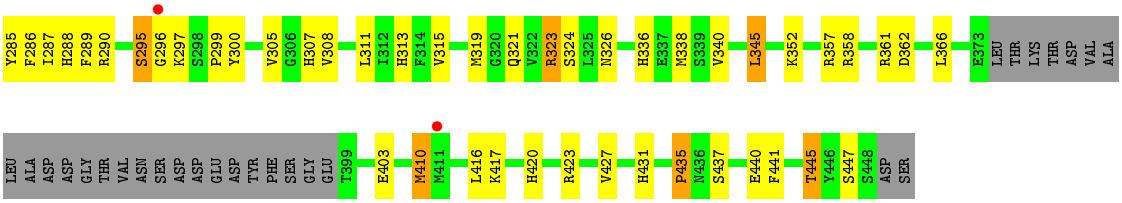
Chain B:



• Molecule 3: Nucleoprotein

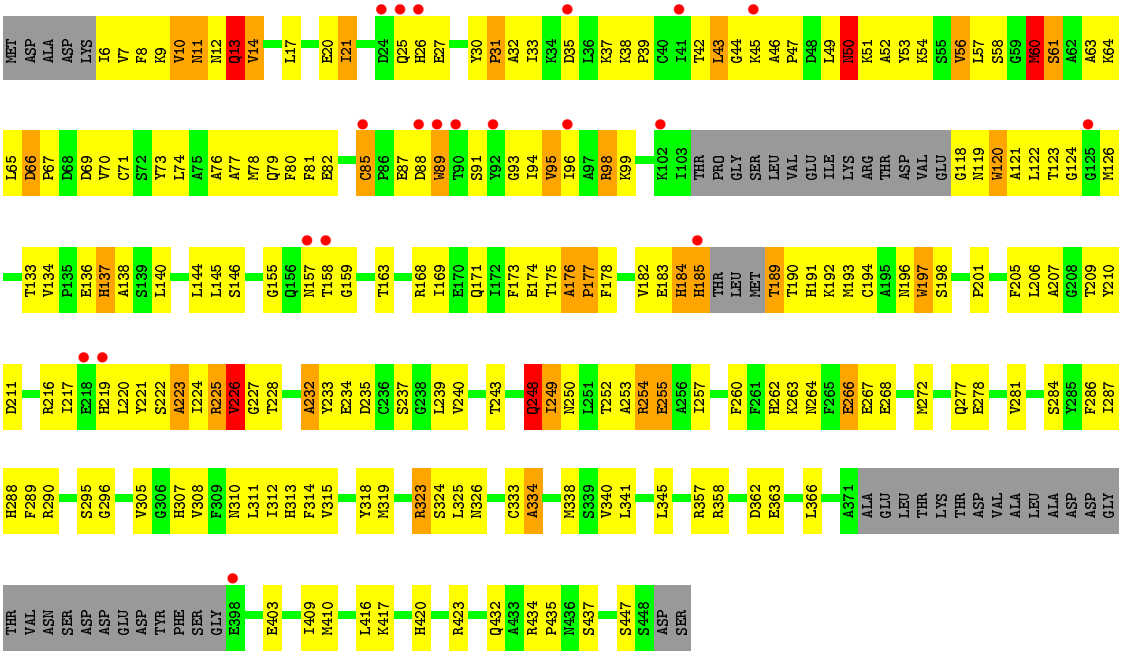
Chain C:





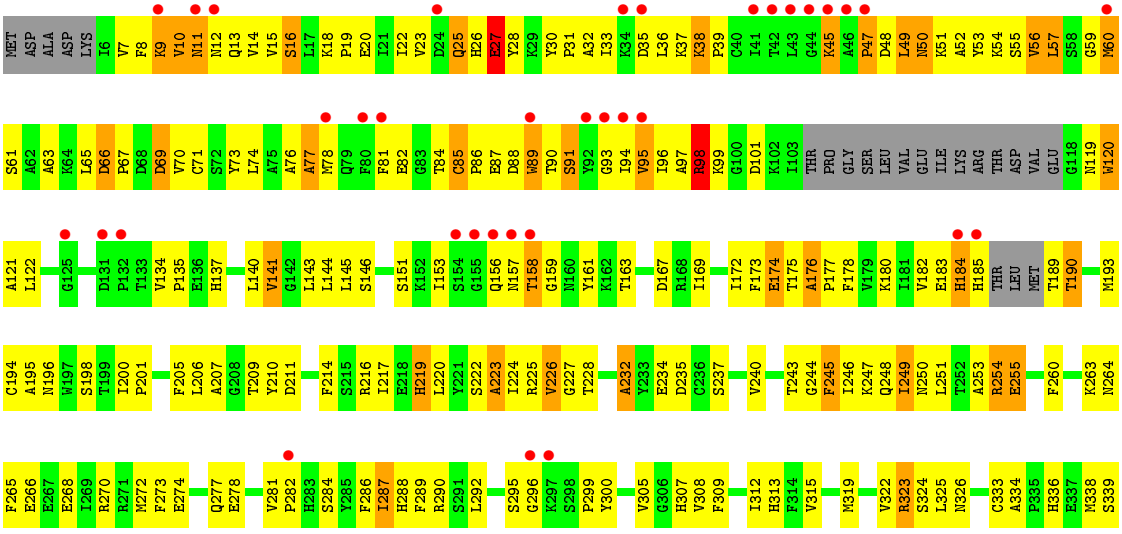
• Molecule 3: Nucleoprotein

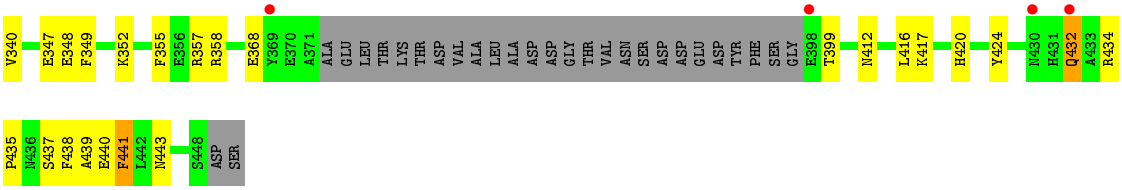
Chain D:



• Molecule 3: Nucleoprotein

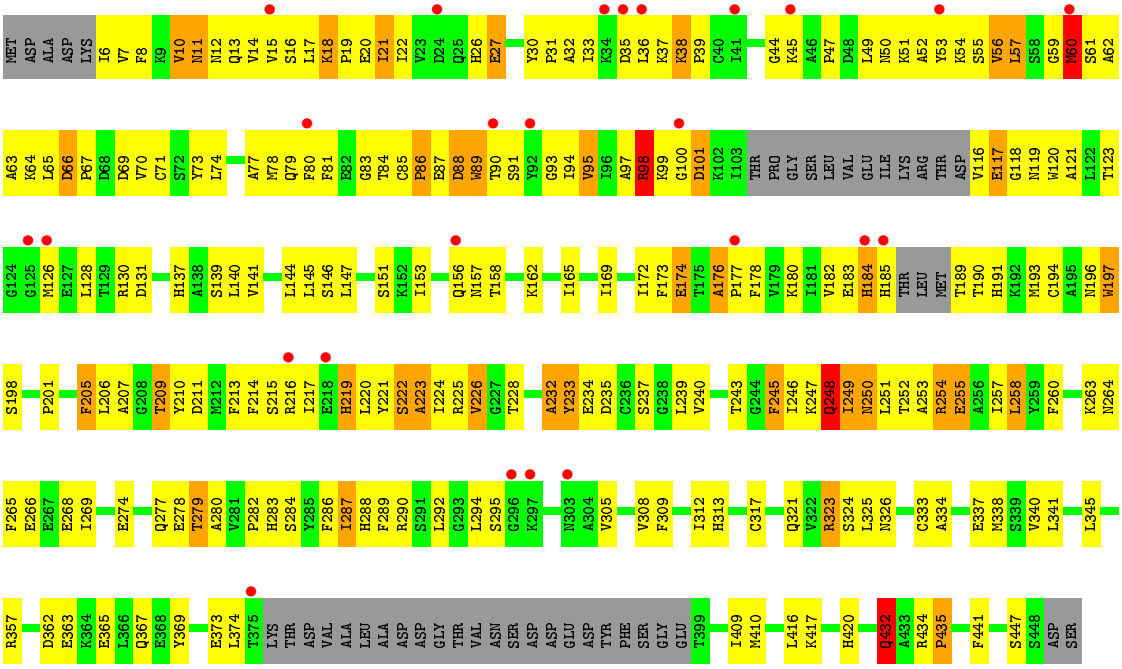
Chain E:





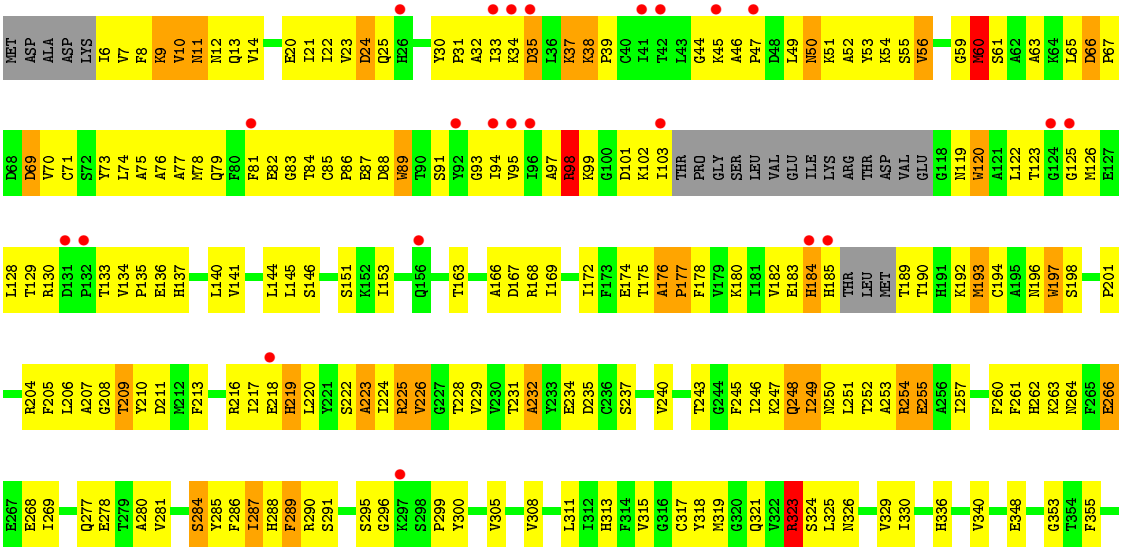
• Molecule 3: Nucleoprotein

Chain F:



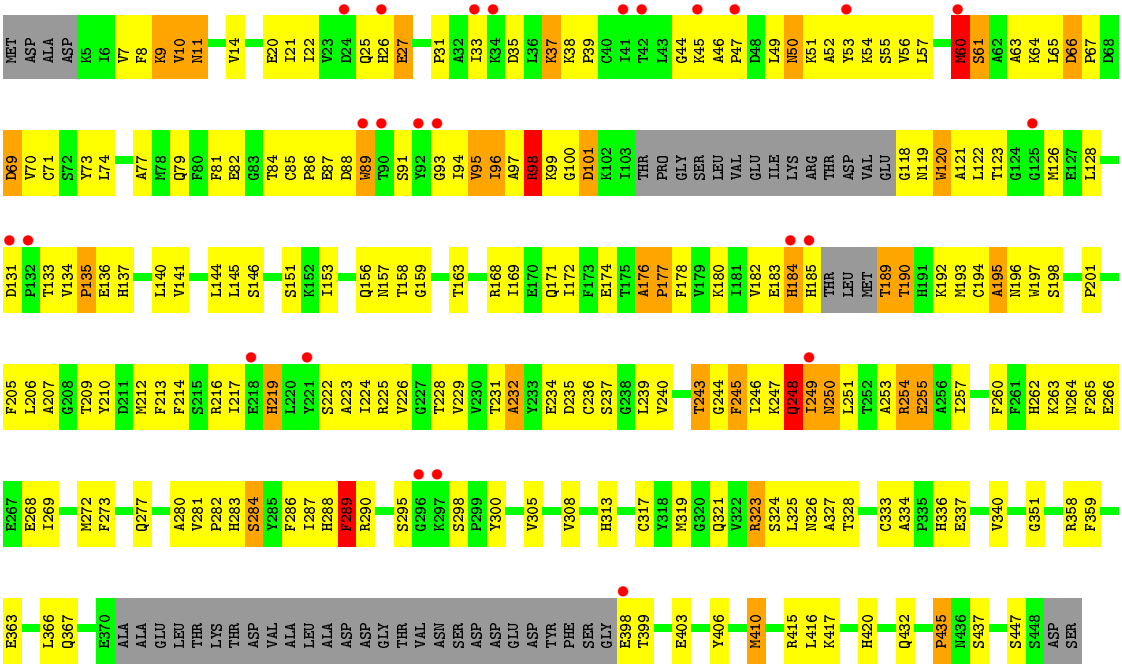
• Molecule 3: Nucleoprotein

Chain G:



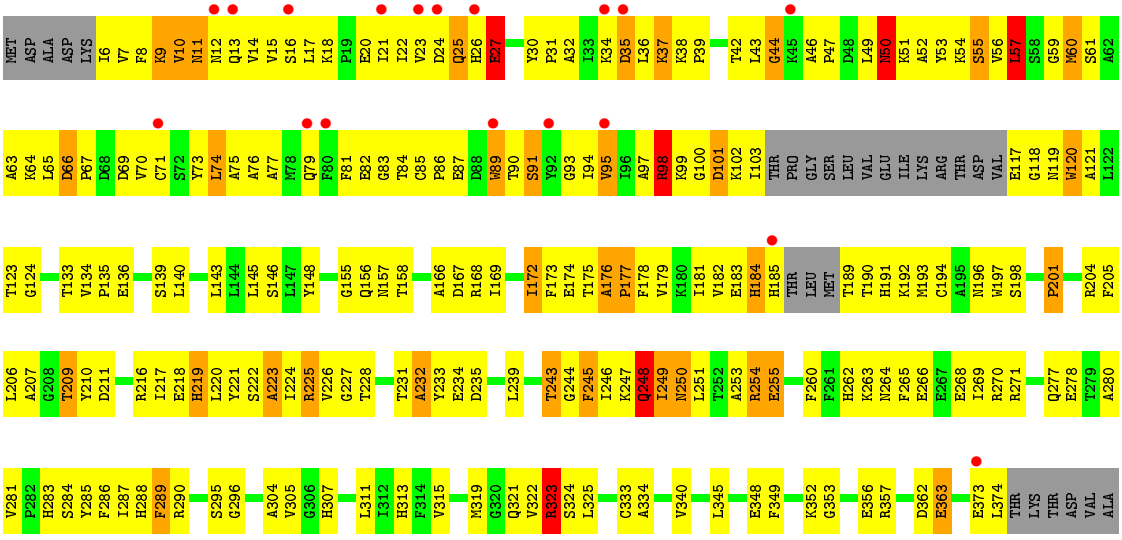
• Molecule 3: Nucleoprotein

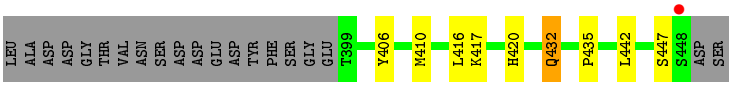
Chain H:



• Molecule 3: Nucleoprotein

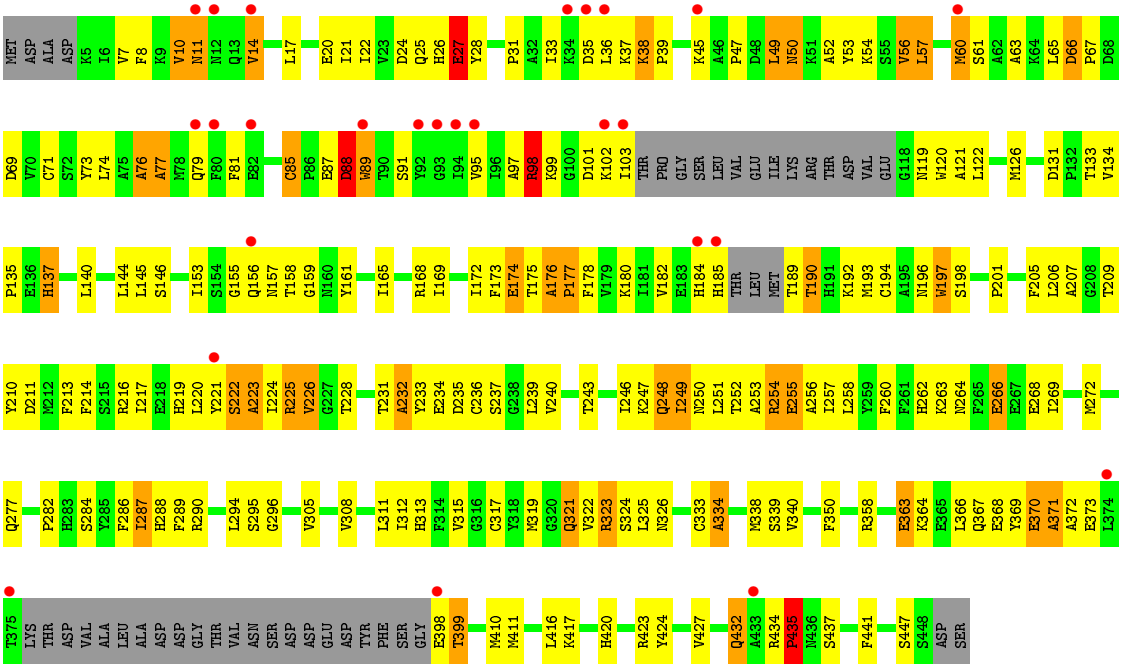
Chain I:





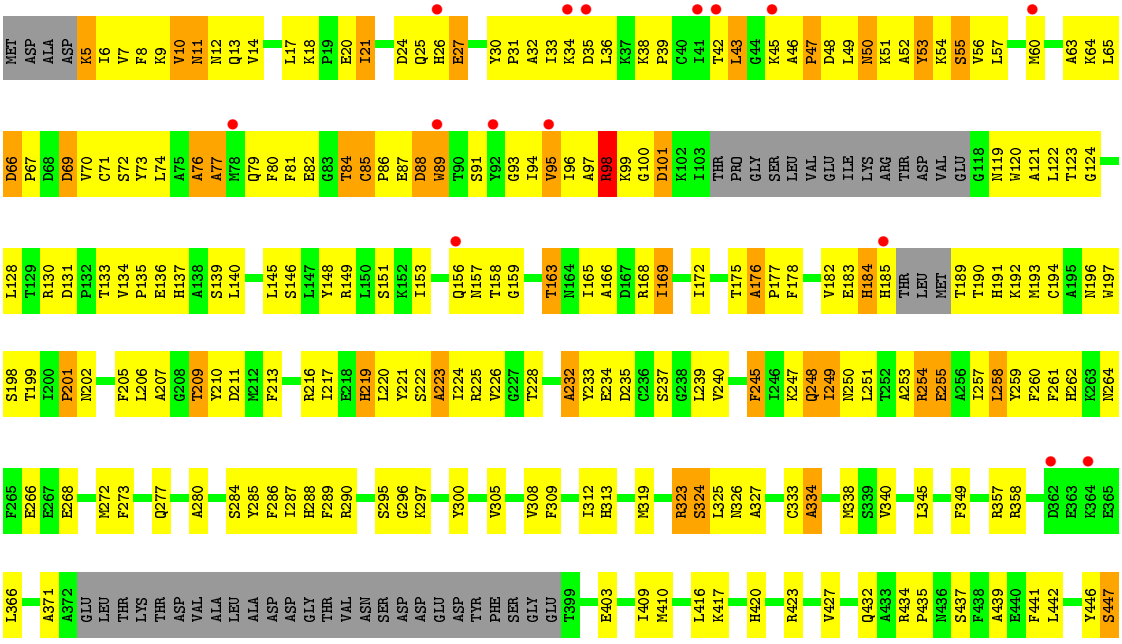
- Molecule 3: Nucleoprotein

Chain J:



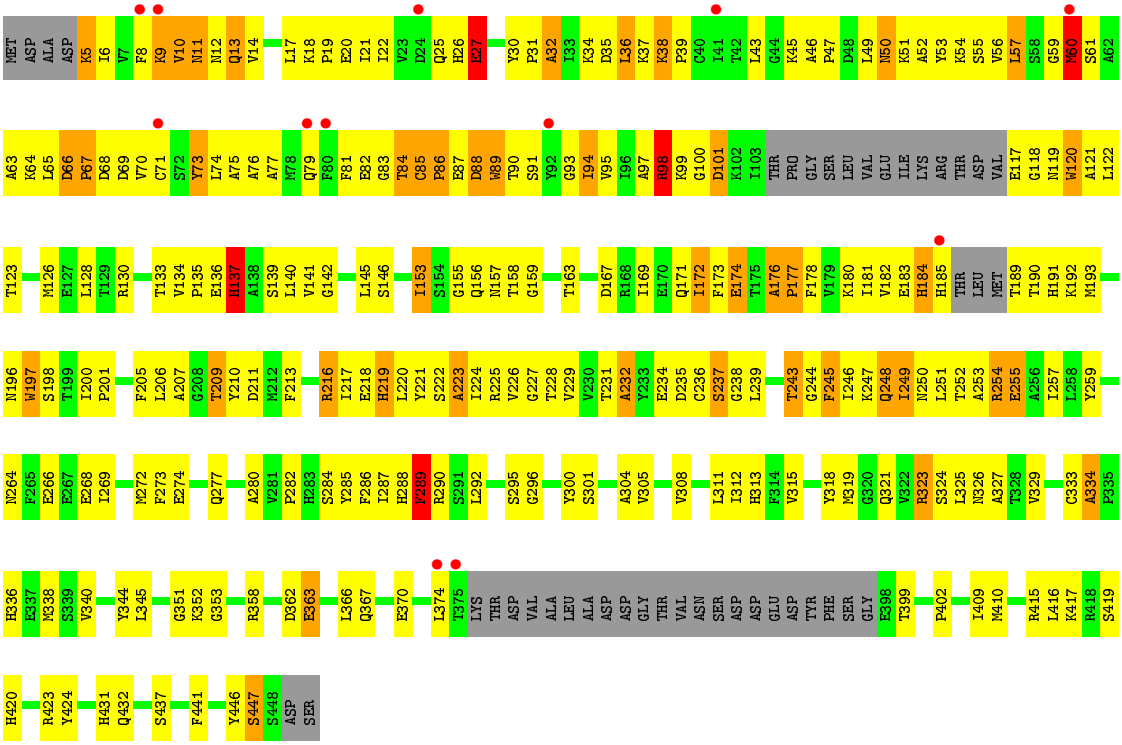
- Molecule 3: Nucleoprotein

Chain K:



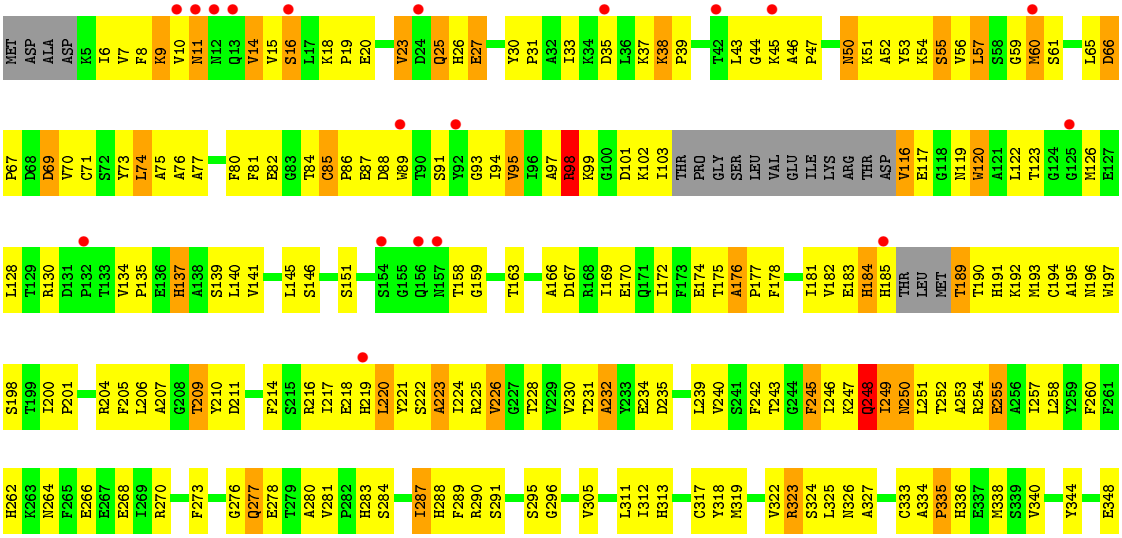
- Molecule 3: Nucleoprotein

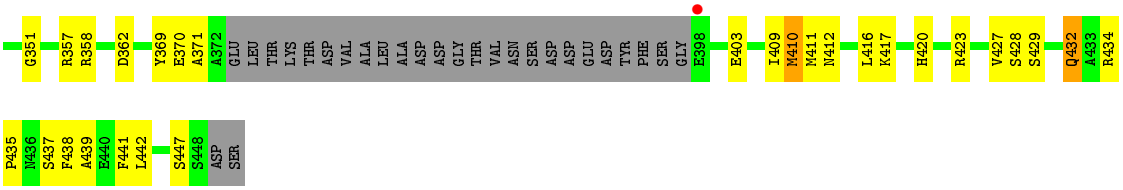
Chain L:



- Molecule 3: Nucleoprotein

Chain M:





- Molecule 3: Nucleoprotein

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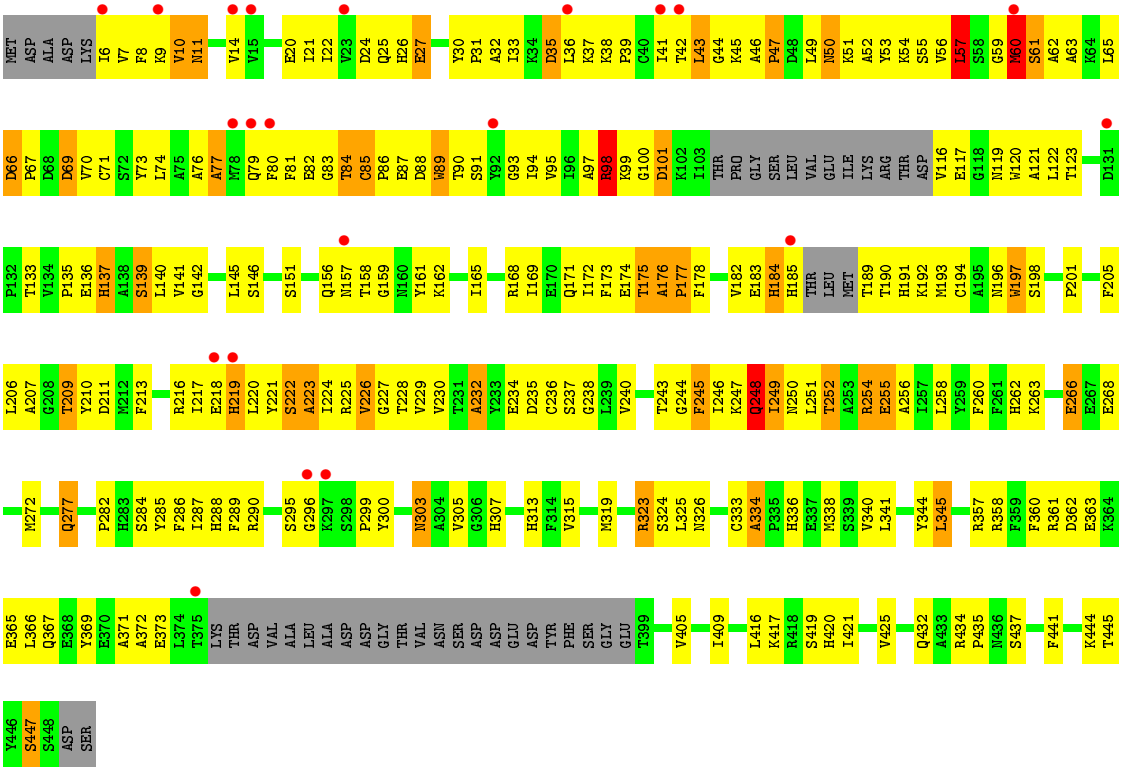
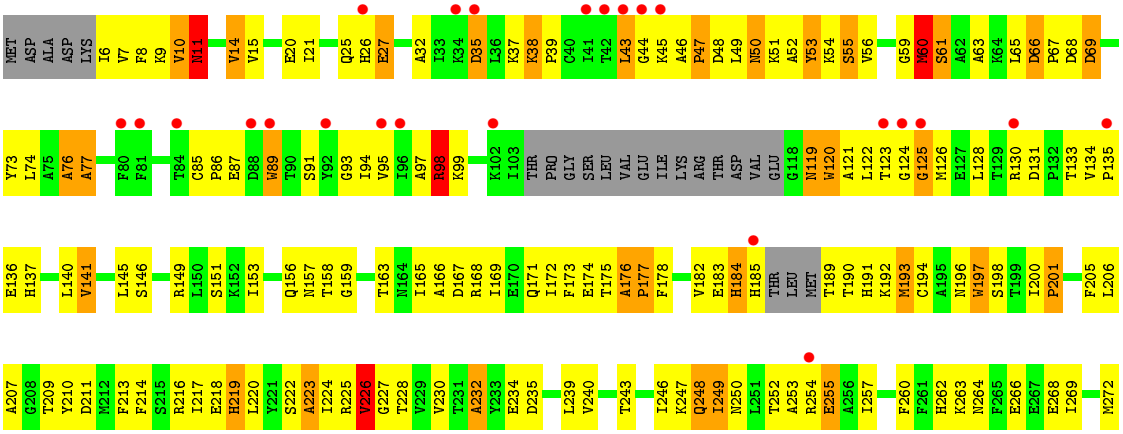
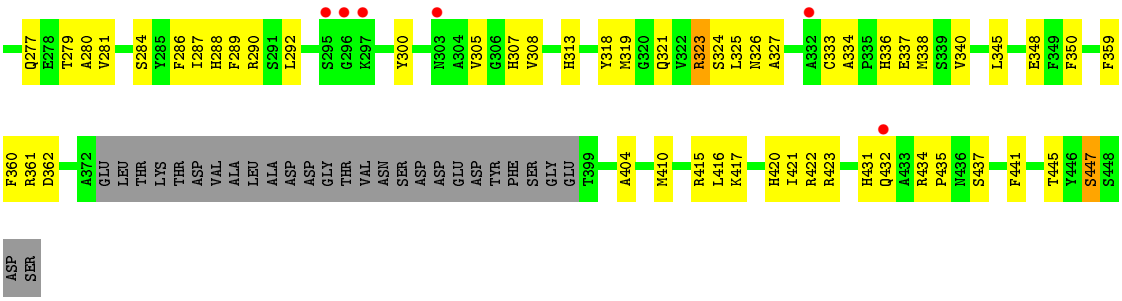


- Molecule 3: Nucleoprotein

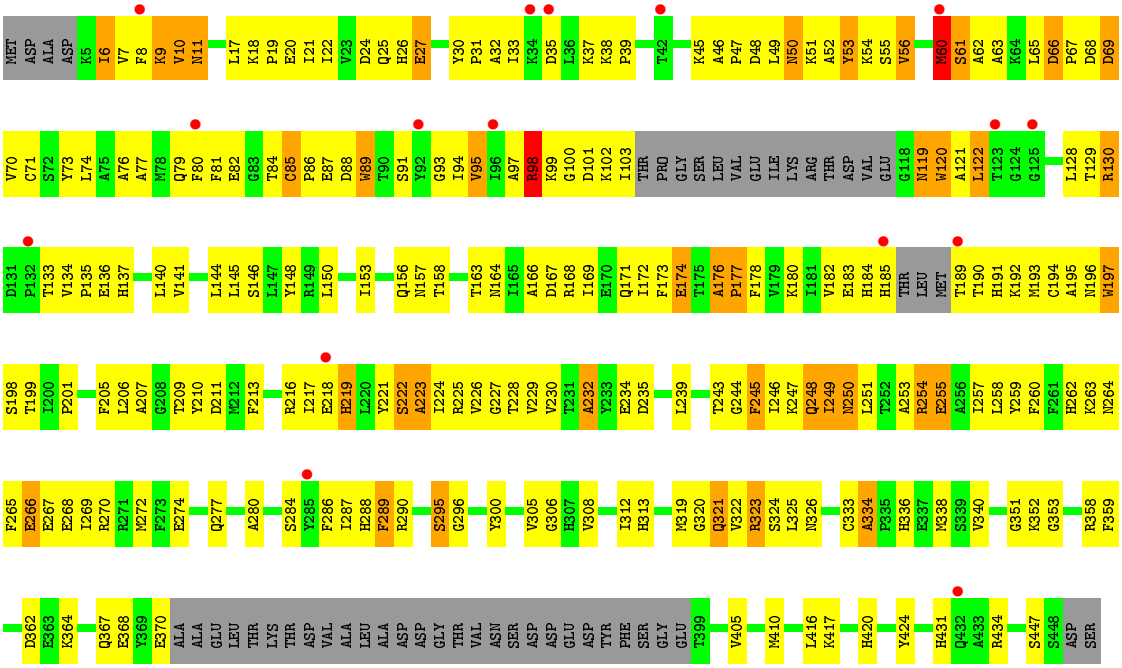
Chain O:





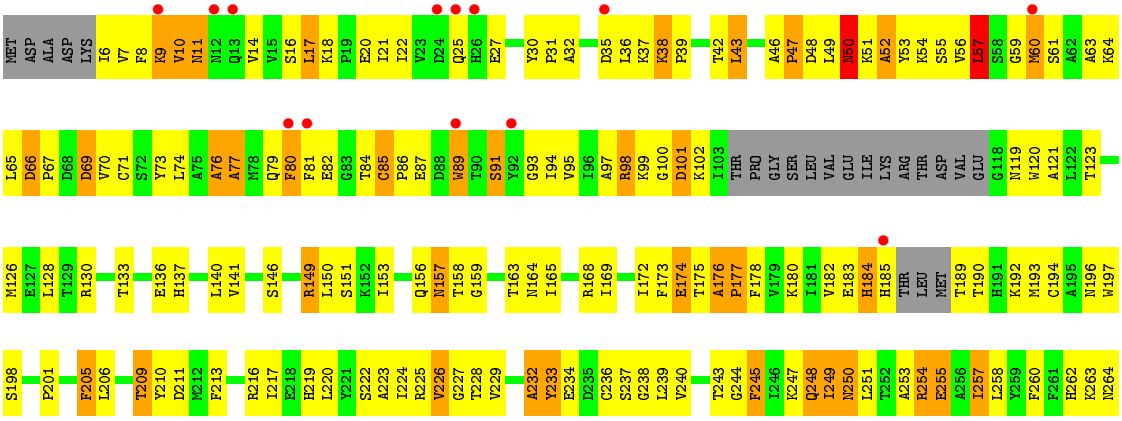
• Molecule 3: Nucleoprotein

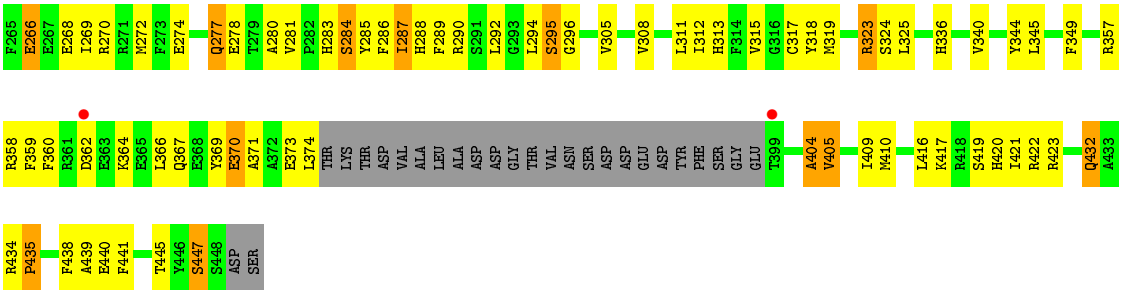
Chain P:

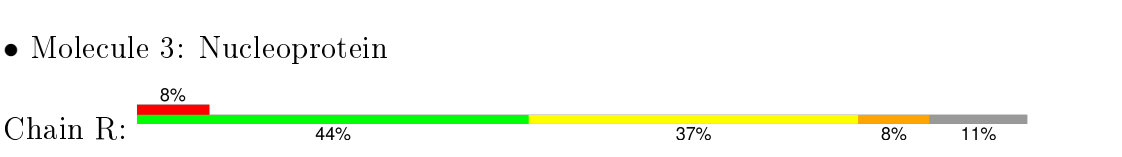


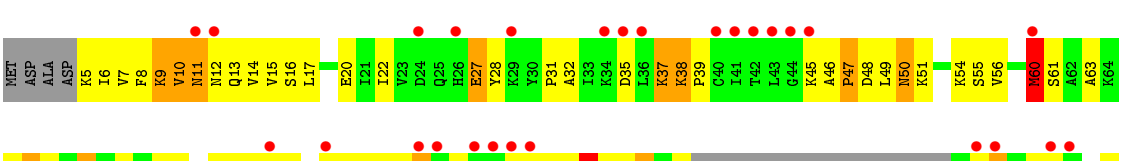
• Molecule 3: Nucleoprotein

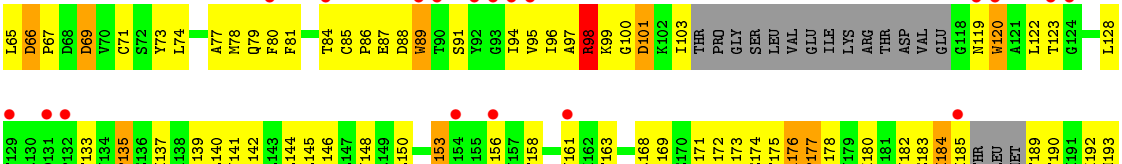
Chain Q:

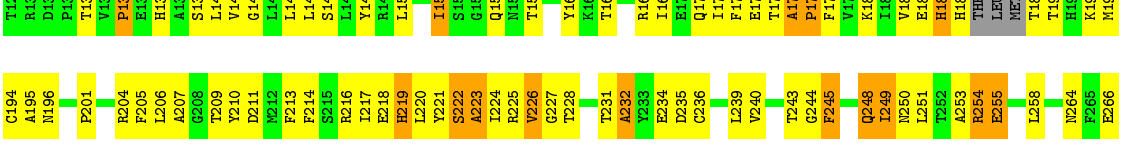


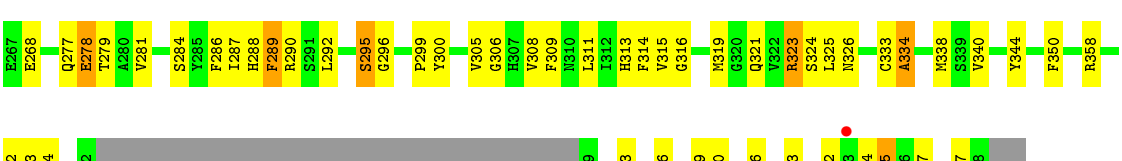


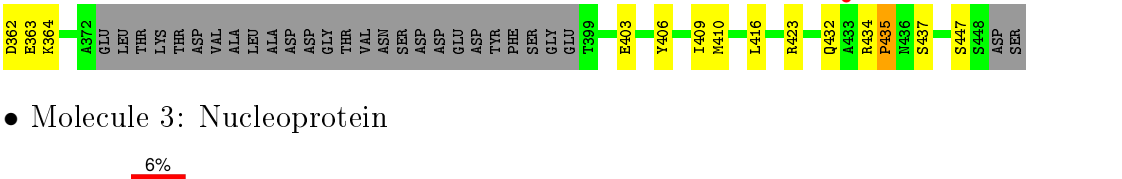


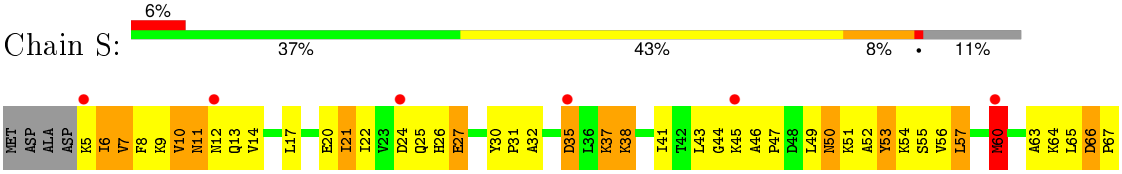


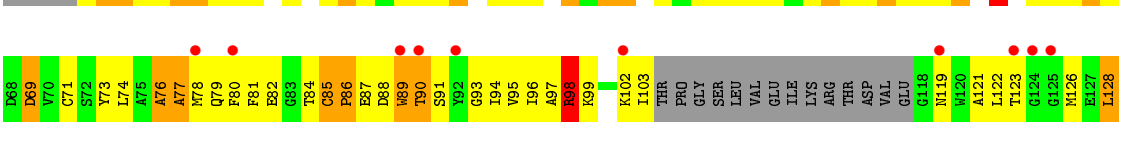


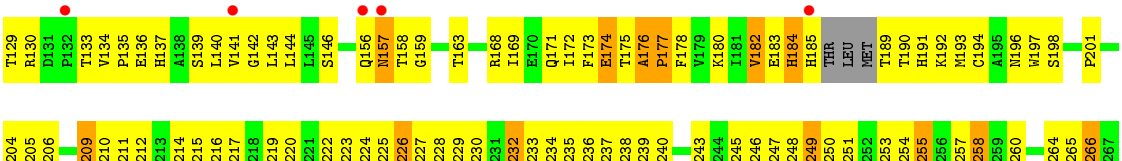










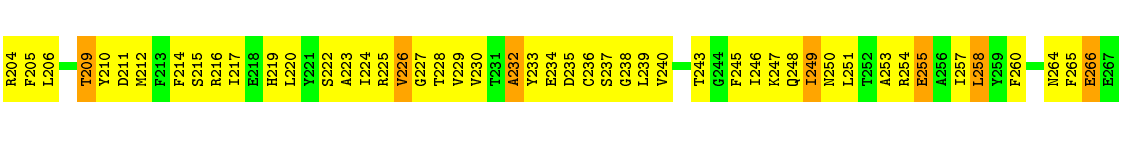


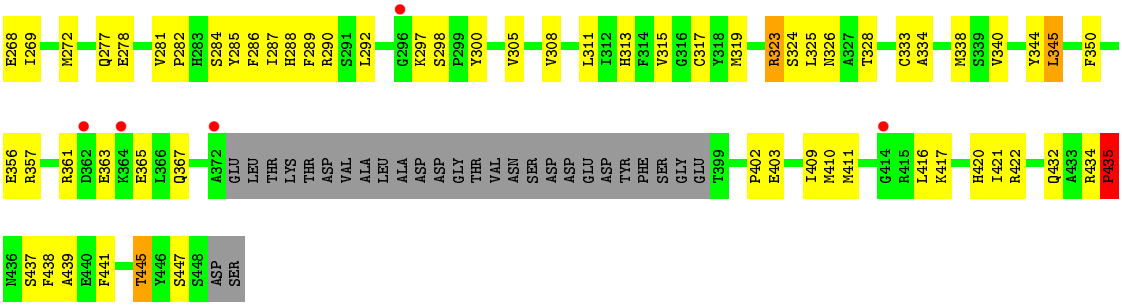
- Molecule 3: Nucleoprotein

Chain R:

- Molecule 3: Nucleoprotein

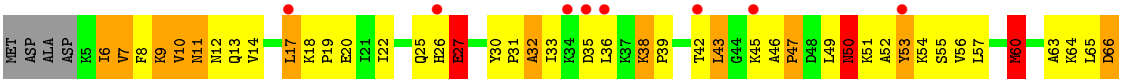
Chain S:

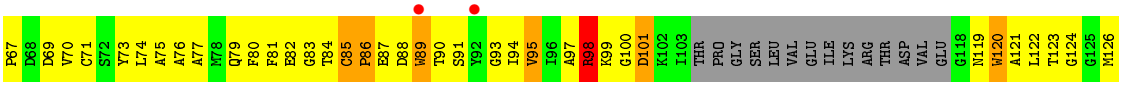


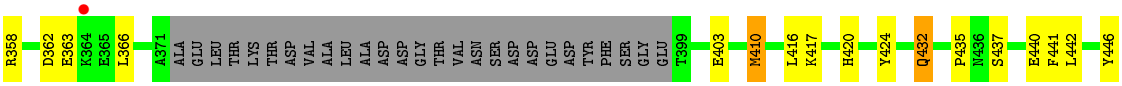


• Molecule 3: Nucleoprotein

Chain T:

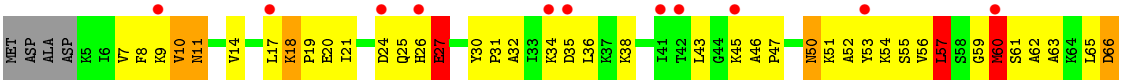


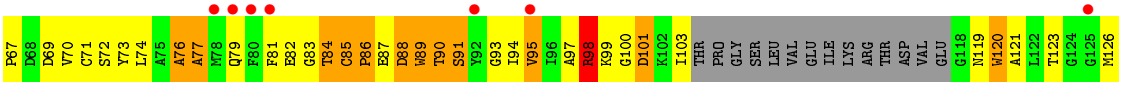


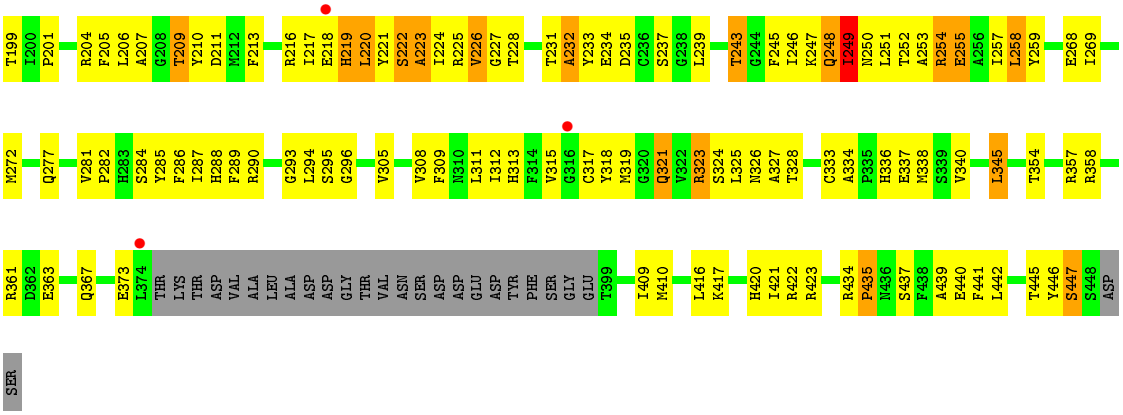


• Molecule 3: Nucleoprotein

Chain U:

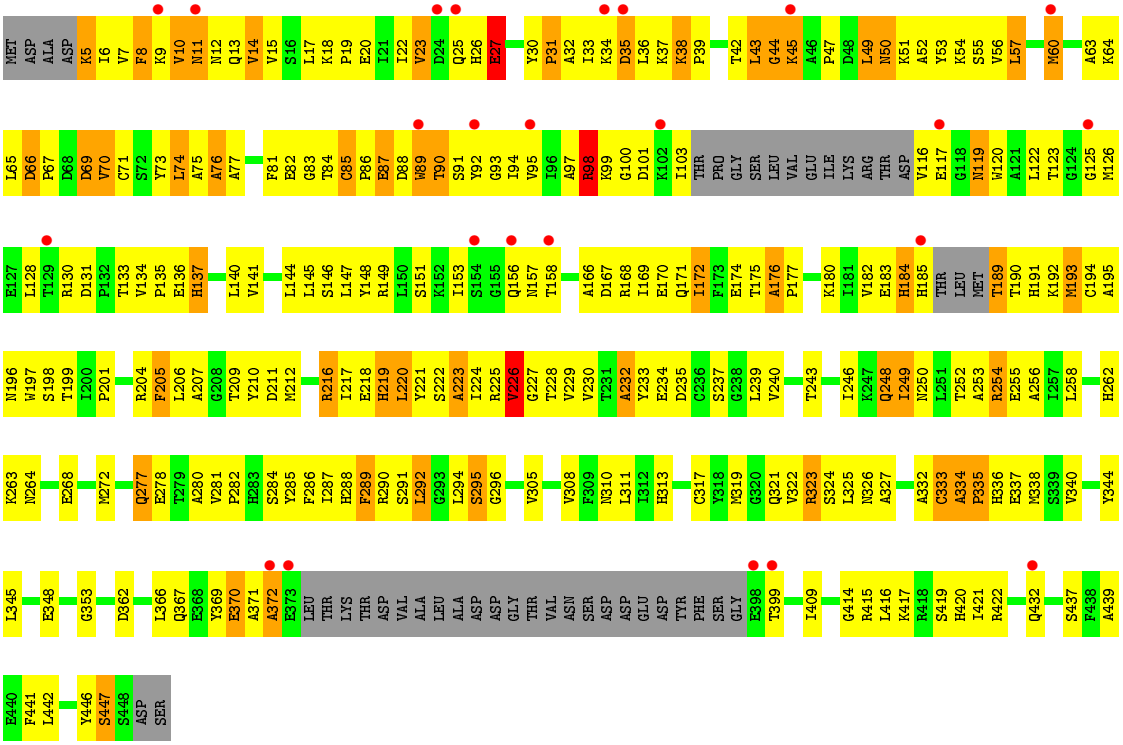






• Molecule 3: Nucleoprotein

Chain V:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	270.43Å 281.00Å 236.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.49 24.95 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-3.49) 99.3 (24.95-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 3.46Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.269 , 0.313 0.253 , 0.251	Depositor DCC
R_{free} test set	11041 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	105.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 101.9	EDS
Estimated twinning fraction	0.057 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 226047 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	74551	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	W	1.36	11/2297 (0.5%)	1.82	66/3563 (1.9%)
2	X	1.43	15/2276 (0.7%)	1.92	89/3528 (2.5%)
3	A	0.91	2/3269 (0.1%)	0.77	1/4413 (0.0%)
3	B	0.90	2/3273 (0.1%)	0.78	1/4417 (0.0%)
3	C	0.94	3/3294 (0.1%)	0.78	1/4446 (0.0%)
3	D	0.85	1/3264 (0.0%)	0.74	2/4406 (0.0%)
3	E	0.77	1/3264 (0.0%)	0.69	0/4406
3	F	0.85	1/3300 (0.0%)	0.75	1/4456 (0.0%)
3	G	0.78	0/3260	0.70	0/4401
3	H	0.83	0/3268	0.73	0/4410
3	I	0.94	3/3286 (0.1%)	0.78	1/4436 (0.0%)
3	J	0.84	2/3302 (0.1%)	0.72	0/4457
3	K	0.91	1/3269 (0.0%)	0.77	0/4412
3	L	1.06	5/3311 (0.2%)	0.83	0/4469
3	M	0.95	0/3294	0.77	0/4446
3	N	0.92	2/3300 (0.1%)	0.77	0/4456
3	O	0.80	0/3260	0.72	1/4401 (0.0%)
3	P	0.80	0/3259	0.72	0/4398
3	Q	0.89	1/3277 (0.0%)	0.78	1/4424 (0.0%)
3	R	0.79	0/3269	0.69	0/4412
3	S	0.83	1/3269 (0.0%)	0.75	0/4412
3	T	1.02	4/3264 (0.1%)	0.86	1/4405 (0.0%)
3	U	0.99	3/3286 (0.1%)	0.81	0/4435
3	V	0.96	3/3303 (0.1%)	0.79	0/4458
All	All	0.93	61/76714 (0.1%)	0.88	165/104467 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	1

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	11	C	C1'-N1	9.74	1.63	1.48
2	X	90	C	P-O5'	7.30	1.67	1.59
1	W	6	C	C1'-N1	7.24	1.59	1.48
3	L	57	LEU	C-N	6.88	1.49	1.34
3	T	57	LEU	C-N	6.55	1.49	1.34

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	2	C	O4'-C1'-N1	14.51	119.81	108.20
2	X	11	C	O4'-C1'-N1	13.06	118.65	108.20
1	W	2	C	C1'-O4'-C4'	-12.35	100.02	109.90
2	X	7	A	O4'-C1'-N9	12.30	118.04	108.20
1	W	53	C	C4'-C3'-C2'	-12.27	90.33	102.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	L	57	LEU	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	2059	0	1091	114	0
2	X	2045	0	1091	121	0
3	A	3192	0	3137	284	0
3	B	3196	0	3145	325	0
3	C	3217	0	3165	311	0
3	D	3187	0	3132	286	0
3	E	3187	0	3132	285	0
3	F	3223	0	3170	296	0
3	G	3183	0	3131	280	0
3	H	3191	0	3140	278	0
3	I	3209	0	3154	331	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	3225	0	3174	286	0
3	K	3192	0	3144	312	0
3	L	3234	0	3180	379	0
3	M	3217	0	3165	342	0
3	N	3223	0	3170	310	0
3	O	3183	0	3131	283	0
3	P	3182	0	3134	316	0
3	Q	3200	0	3148	336	0
3	R	3192	0	3144	254	0
3	S	3192	0	3144	284	0
3	T	3187	0	3139	328	0
3	U	3209	0	3161	321	0
3	V	3226	0	3171	327	0
All	All	74551	0	71493	6394	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 44.

The worst 5 of 6394 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:P:189:THR:CG2	3:P:192:LYS:HB3	1.35	1.56
3:A:255:GLU:HA	3:K:8:PHE:CZ	1.39	1.54
3:L:255:GLU:HA	3:V:8:PHE:CZ	1.35	1.54
3:E:8:PHE:CZ	3:F:255:GLU:HA	1.37	1.53
3:H:8:PHE:CZ	3:I:255:GLU:HA	1.45	1.50

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
3	A	393/450 (87%)	258 (66%)	93 (24%)	42 (11%)	0 8
3	B	393/450 (87%)	268 (68%)	87 (22%)	38 (10%)	1 10
3	C	396/450 (88%)	273 (69%)	79 (20%)	44 (11%)	0 7
3	D	392/450 (87%)	278 (71%)	80 (20%)	34 (9%)	1 12
3	E	392/450 (87%)	269 (69%)	86 (22%)	37 (9%)	1 10
3	F	397/450 (88%)	273 (69%)	84 (21%)	40 (10%)	1 9
3	G	392/450 (87%)	258 (66%)	93 (24%)	41 (10%)	1 8
3	H	392/450 (87%)	274 (70%)	86 (22%)	32 (8%)	1 13
3	I	395/450 (88%)	275 (70%)	81 (20%)	39 (10%)	1 10
3	J	397/450 (88%)	268 (68%)	84 (21%)	45 (11%)	0 7
3	K	393/450 (87%)	269 (68%)	95 (24%)	29 (7%)	1 16
3	L	398/450 (88%)	271 (68%)	85 (21%)	42 (11%)	0 8
3	M	396/450 (88%)	268 (68%)	92 (23%)	36 (9%)	1 11
3	N	397/450 (88%)	263 (66%)	94 (24%)	40 (10%)	1 9
3	O	392/450 (87%)	265 (68%)	89 (23%)	38 (10%)	1 10
3	P	391/450 (87%)	263 (67%)	90 (23%)	38 (10%)	1 10
3	Q	394/450 (88%)	268 (68%)	82 (21%)	44 (11%)	0 7
3	R	393/450 (87%)	273 (70%)	81 (21%)	39 (10%)	1 10
3	S	393/450 (87%)	273 (70%)	78 (20%)	42 (11%)	0 8
3	T	392/450 (87%)	276 (70%)	83 (21%)	33 (8%)	1 13
3	U	395/450 (88%)	263 (67%)	90 (23%)	42 (11%)	0 8
3	V	397/450 (88%)	251 (63%)	97 (24%)	49 (12%)	0 6
All	All	8670/9900 (88%)	5897 (68%)	1909 (22%)	864 (10%)	1 9

5 of 864 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	10	VAL
3	A	11	ASN
3	A	35	ASP
3	A	43	LEU
3	A	45	LYS

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	
3	A	343/386 (89%)	316 (92%)	27 (8%)	15	53
3	B	344/386 (89%)	320 (93%)	24 (7%)	19	59
3	C	346/386 (90%)	326 (94%)	20 (6%)	25	65
3	D	343/386 (89%)	323 (94%)	20 (6%)	25	65
3	E	343/386 (89%)	323 (94%)	20 (6%)	25	65
3	F	347/386 (90%)	325 (94%)	22 (6%)	22	63
3	G	342/386 (89%)	323 (94%)	19 (6%)	26	66
3	H	344/386 (89%)	319 (93%)	25 (7%)	17	57
3	I	345/386 (89%)	323 (94%)	22 (6%)	22	62
3	J	347/386 (90%)	322 (93%)	25 (7%)	18	57
3	K	343/386 (89%)	317 (92%)	26 (8%)	16	55
3	L	348/386 (90%)	320 (92%)	28 (8%)	15	52
3	M	346/386 (90%)	317 (92%)	29 (8%)	14	50
3	N	347/386 (90%)	319 (92%)	28 (8%)	15	52
3	O	342/386 (89%)	323 (94%)	19 (6%)	26	66
3	P	343/386 (89%)	324 (94%)	19 (6%)	27	67
3	Q	344/386 (89%)	316 (92%)	28 (8%)	15	52
3	R	343/386 (89%)	327 (95%)	16 (5%)	32	72
3	S	343/386 (89%)	320 (93%)	23 (7%)	20	61
3	T	343/386 (89%)	314 (92%)	29 (8%)	13	49
3	U	345/386 (89%)	320 (93%)	25 (7%)	18	57
3	V	347/386 (90%)	323 (93%)	24 (7%)	19	59
All	All	7578/8492 (89%)	7060 (93%)	518 (7%)	20	60

5 of 518 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	66	ASP
3	M	85	CYS
3	U	89	TRP
3	K	163	THR
3	L	117	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 229 such sidechains are listed below:

Mol	Chain	Res	Type
3	K	50	ASN
3	N	50	ASN
3	U	184	HIS
3	K	248	GLN
3	L	248	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	W	98/99 (98%)	44 (44%)	4 (4%)
2	X	98/99 (98%)	40 (40%)	3 (3%)
All	All	196/198 (98%)	84 (42%)	7 (3%)

5 of 84 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	W	2	C
1	W	3	C
1	W	4	C
1	W	6	C
1	W	7	C

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	W	94	C
2	X	72	C
2	X	21	C
1	W	53	C
2	X	65	C

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	W	99/99 (100%)	0.16	3 (3%)	54	43	50, 73, 96, 128	0
2	X	99/99 (100%)	0.19	4 (4%)	42	33	39, 68, 93, 114	0
3	A	401/450 (89%)	0.17	22 (5%)	29	22	28, 83, 106, 112	0
3	B	401/450 (89%)	0.23	23 (5%)	27	21	28, 83, 105, 112	0
3	C	404/450 (89%)	0.14	18 (4%)	37	29	27, 81, 104, 115	0
3	D	400/450 (88%)	0.18	20 (5%)	32	25	28, 84, 107, 115	0
3	E	400/450 (88%)	0.36	39 (9%)	10	9	29, 87, 111, 117	0
3	F	405/450 (90%)	0.30	25 (6%)	24	19	28, 83, 107, 113	0
3	G	400/450 (88%)	0.25	25 (6%)	23	18	28, 86, 108, 115	0
3	H	400/450 (88%)	0.19	25 (6%)	23	18	28, 85, 106, 114	0
3	I	403/450 (89%)	0.14	19 (4%)	35	28	28, 82, 105, 117	0
3	J	405/450 (90%)	0.21	26 (6%)	23	17	28, 85, 110, 120	0
3	K	401/450 (89%)	0.09	15 (3%)	45	36	27, 82, 106, 114	0
3	L	406/450 (90%)	0.11	12 (2%)	54	43	27, 80, 102, 114	0
3	M	404/450 (89%)	0.24	20 (4%)	32	25	28, 84, 107, 113	0
3	N	405/450 (90%)	0.20	21 (5%)	31	24	27, 81, 105, 112	0
3	O	400/450 (88%)	0.27	30 (7%)	17	14	28, 86, 106, 115	0
3	P	399/450 (88%)	0.21	16 (4%)	42	33	28, 85, 106, 113	0
3	Q	402/450 (89%)	0.12	15 (3%)	45	36	28, 82, 104, 115	0
3	R	401/450 (89%)	0.31	35 (8%)	13	12	29, 87, 111, 117	0
3	S	401/450 (89%)	0.22	26 (6%)	22	17	28, 83, 105, 112	0
3	T	400/450 (88%)	0.10	14 (3%)	48	38	27, 81, 104, 116	0
3	U	403/450 (89%)	0.15	24 (5%)	25	19	28, 82, 106, 118	0
3	V	405/450 (90%)	0.24	24 (5%)	26	20	28, 82, 106, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	9044/10098 (89%)	0.20	501 (5%)	29	22	27, 83, 106, 128	0

The worst 5 of 501 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	125	GLY	9.1
3	O	185	HIS	8.4
3	R	35	ASP	8.1
3	D	92	TYR	6.9
3	J	375	THR	6.1

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.