wwPDB EM Validation Summary Report (i)

May 20, 2024 – 06:38 PM JST

PDB ID	:	8X19
EMDB ID	:	EMD-37988
Title	:	Structure of nucleosome-bound SRCAP-C in the ADP-BeFx-bound state
Authors	:	Yu, J.; Wang, Q.; Yu, Z.; Li, W.; Wang, L.; Xu, Y.
Deposited on	:	2023-11-06
Resolution	:	3.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

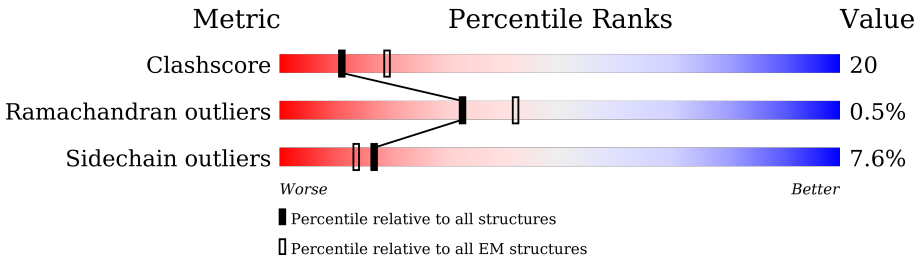
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	130	24% 50% 9% 17%
1	E	130	26% 43% 12% 19%
2	B	126	31% 37% 8% 24%
2	F	126	37% 33% 5% 25%
3	C	136	36% 28% 6% 30%
3	G	136	37% 32% •• 29%
4	D	103	57% 21% 21%
4	H	103	41% 28% 9% 22%
5	I	3230	21% 5% 73%

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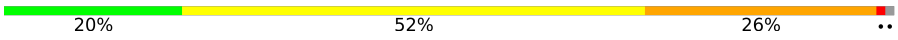
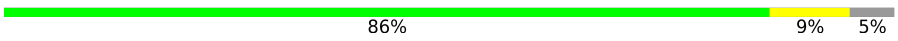
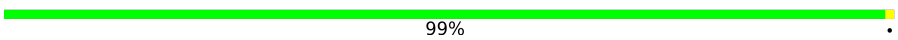
Mol	Chain	Length	Quality of chain
6	J	364	
7	K	396	
8	L	154	
9	M	456	
9	O	456	
9	Q	456	
10	N	463	
10	P	463	
10	R	463	
11	S	375	
11	U	375	
12	T	429	
13	V	467	
14	W	227	
15	X	147	
16	Y	147	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	BEF	I	3303	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 56704 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Histone H2A type 1-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	108	Total 833	C 525	N 165	O 143	0	0
1	E	105	Total 808	C 510	N 158	O 140	0	0

- Molecule 2 is a protein called Histone H2B type 1-C/E/F/G/I.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	96	Total 755	C 473	N 138	O 142	S 2	0	0
2	F	94	Total 736	C 461	N 134	O 139	S 2	0	0

- Molecule 3 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	95	Total 779	C 491	N 148	O 136	S 4	0	0
3	G	97	Total 801	C 505	N 155	O 137	S 4	0	0

- Molecule 4 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	81	Total 646	C 407	N 126	O 112	S 1	0	0
4	H	80	Total 638	C 401	N 125	O 111	S 1	0	0

- Molecule 5 is a protein called Helicase SRCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	864	Total	C	N	O	S	0	0
			7122	4533	1314	1236	39		

- Molecule 6 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	162	Total	C	N	O	S	0	0
			1350	846	260	239	5		

- Molecule 7 is a protein called Actin-related protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	394	Total	C	N	O	S	0	0
			3209	2054	526	611	18		

- Molecule 8 is a protein called Zinc finger HIT domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	113	Total	C	N	O	S	0	0
			893	546	173	165	9		

- Molecule 9 is a protein called RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	418	Total	C	N	O	S	0	0
			3213	2026	557	614	16		
9	O	435	Total	C	N	O	S	0	0
			3339	2105	571	646	17		
9	Q	440	Total	C	N	O	S	0	0
			3368	2121	579	651	17		

- Molecule 10 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	411	Total	C	N	O	S	0	0
			3185	1988	560	622	15		
10	P	427	Total	C	N	O	S	0	0
			3287	2054	576	642	15		
10	R	424	Total	C	N	O	S	0	0
			3293	2057	578	642	16		

- Molecule 11 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	375	Total	C	N	O	S	0	0
			2925	1850	491	561	23		
11	U	359	Total	C	N	O	S	0	0
			2802	1775	468	540	19		

- Molecule 12 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	403	Total	C	N	O	S	0	0
			3146	1988	535	599	24		

- Molecule 13 is a protein called DNA methyltransferase 1-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	204	Total	C	N	O	S	0	0
			1757	1117	327	309	4		

- Molecule 14 is a protein called YEATS domain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	187	Total	C	N	O	S	0	0
			1542	998	255	284	5		

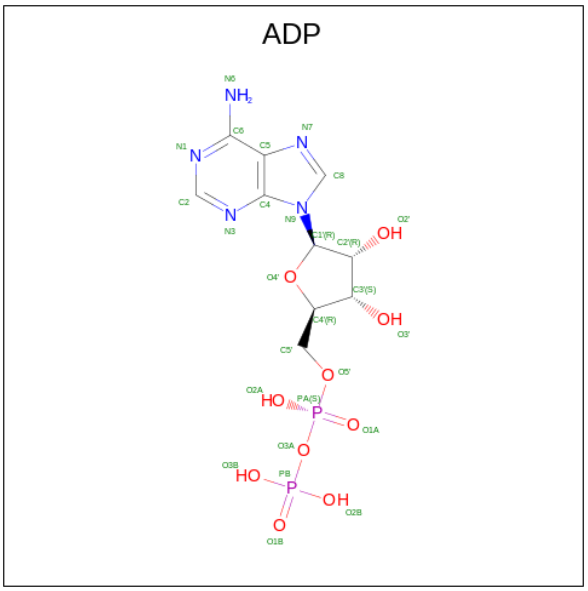
- Molecule 15 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	X	147	Total	C	N	O	P	0	0
			3031	1435	572	878	146		

- Molecule 16 is a DNA chain called DNA (147-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	147	Total	C	N	O	P	0	0
			2990	1422	540	882	146		

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

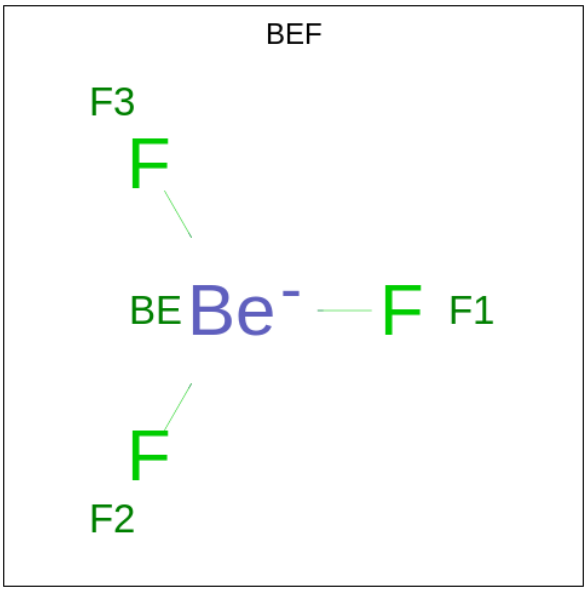


Mol	Chain	Residues	Atoms					AltConf
17	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	M	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	N	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	O	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	P	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	Q	1	Total	C	N	O	P	0
			27	10	5	10	2	
17	R	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

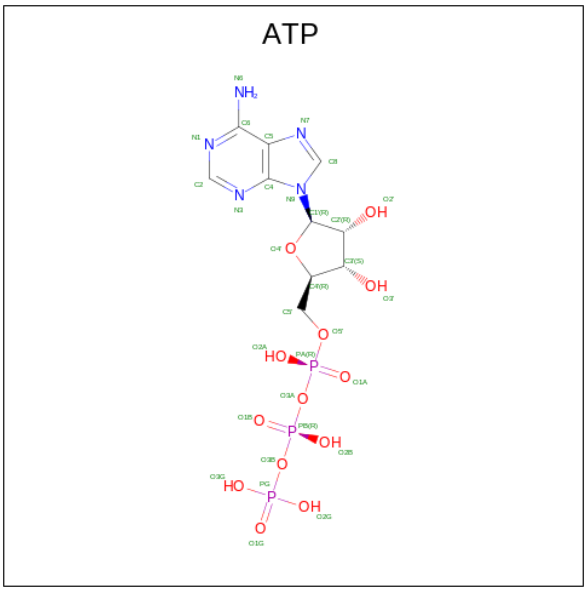
Mol	Chain	Residues	Atoms		AltConf
18	I	1	Total	Mg	0
			1	1	

- Molecule 19 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	I	1	Total	Be	F	0
			4	1	3	

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



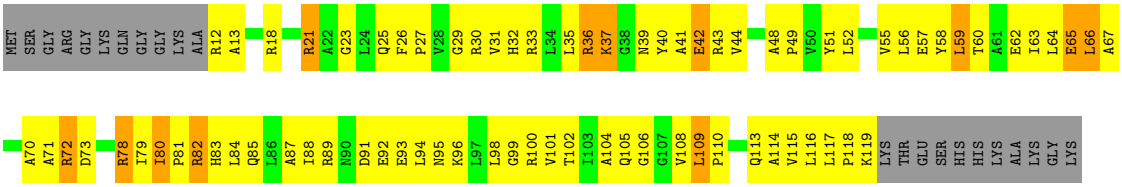
Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	N	O	P	0
			31	10	5	13	3	
20	U	1	Total	C	N	O	P	0
			31	10	5	13	3	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

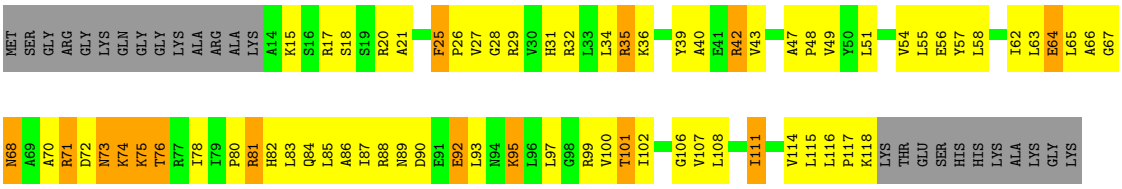
• Molecule 1: Histone H2A type 1-C

Chain A:



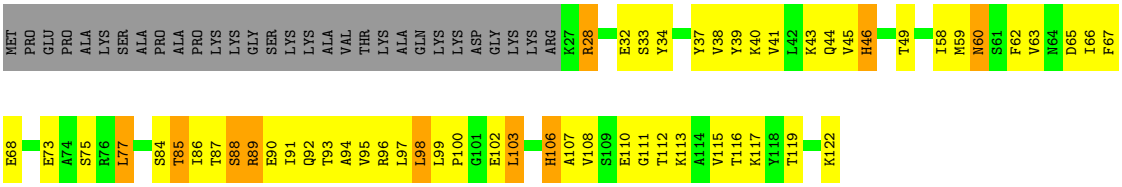
• Molecule 1: Histone H2A type 1-C

Chain E:



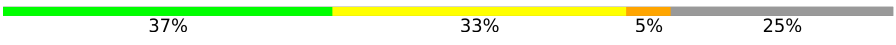
• Molecule 2: Histone H2B type 1-C/E/F/G/I

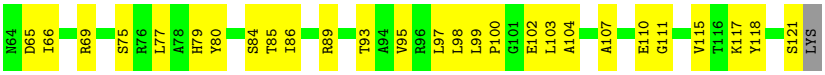
Chain B:



• Molecule 2: Histone H2B type 1-C/E/F/G/I

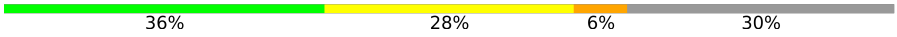
Chain F:

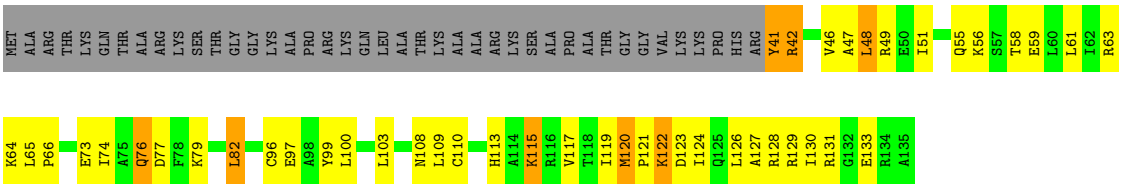




• Molecule 3: Histone H3.1

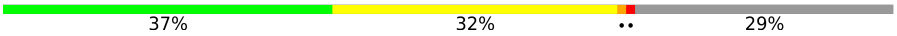
Chain C:

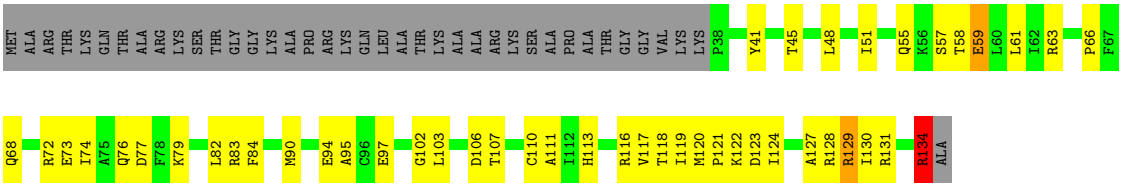




• Molecule 3: Histone H3.1

Chain G:



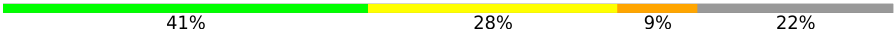


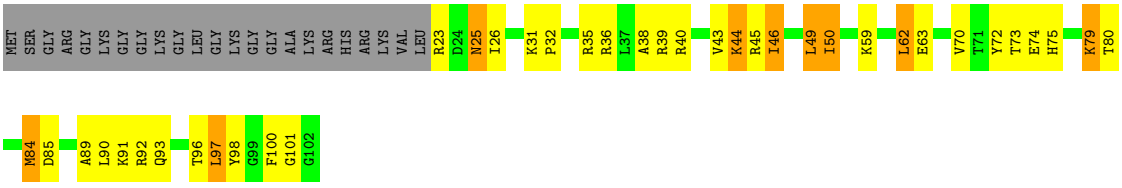
• Molecule 4: Histone H4

Chain D:

• Molecule 4: Histone H4

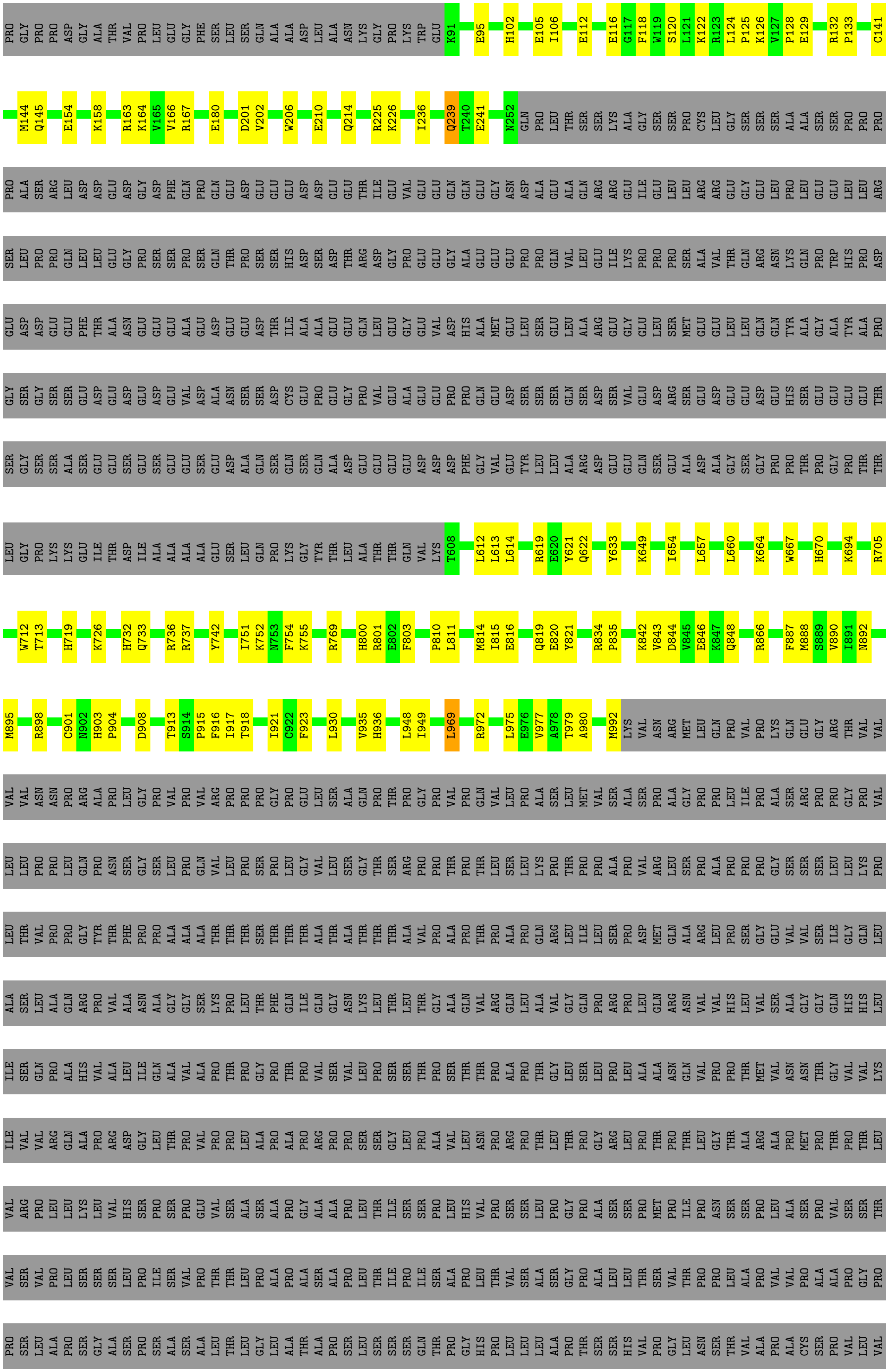
Chain H:





• Molecule 5: Helicase SRCAP

Chain I:


K91
E95
H102
E105
I106
E112
E116
G117
F118
W119
S120
L121
K122
R123
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P125
K126
V127
P128
E129
R132
P133
C141
M144
Q145
E154
K158
R163
K164
V165
V166
R167
E180
D201
V202
W206
E210
Q214
R225
K226
I236
Q239
T240
E241
N252
T608
L612
L613
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K755
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H800
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F803
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Q819
E820
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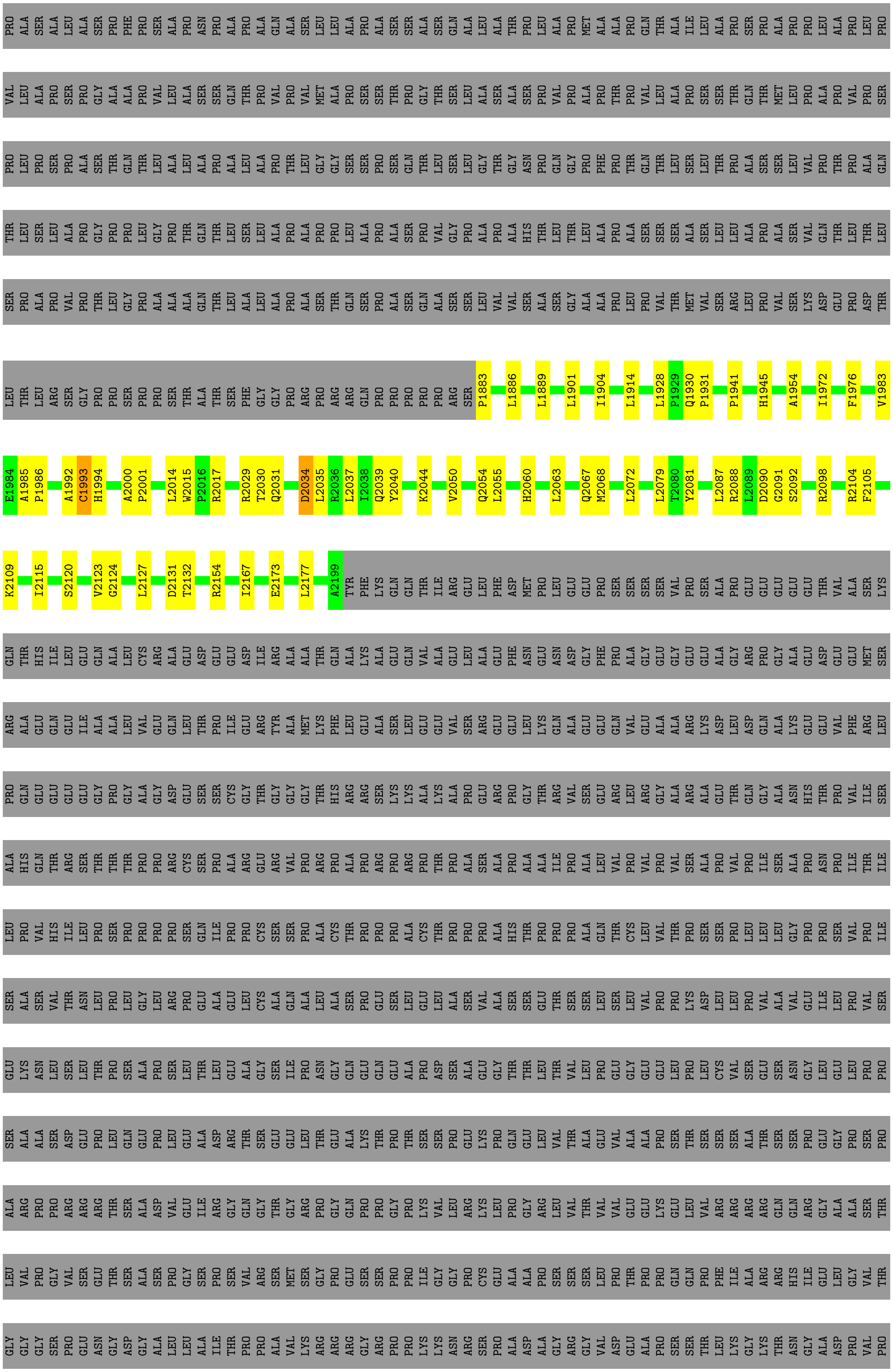
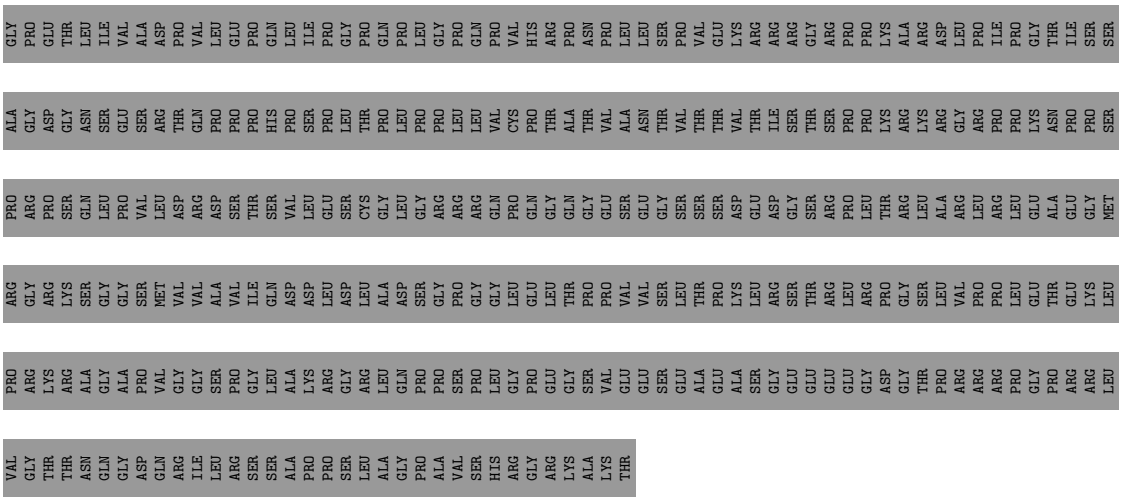
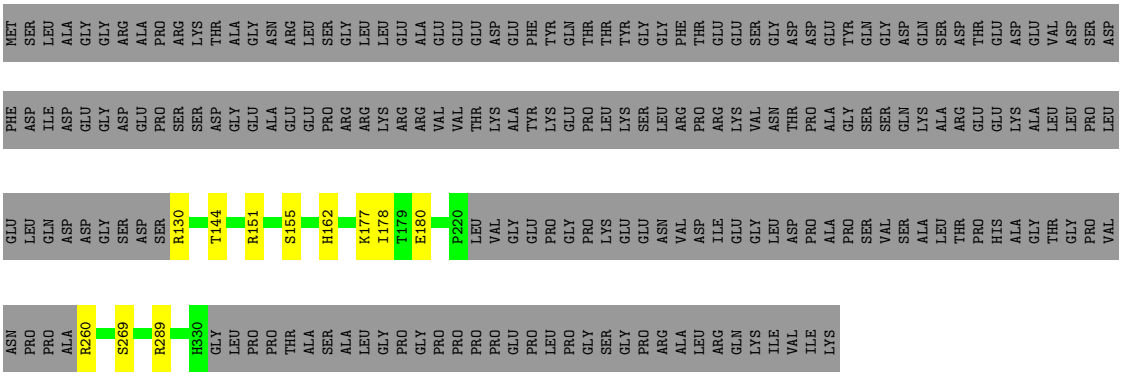

PRO ALA SER ALA LEU ALA SER PRO PHE PRO SER ALA PRO ASN PRO ALA PRO ALA GLN ALA SER LEU LEU ALA PRO ALA SER SER ALA SER GLN ALA LEU ALA THR PRO LEU ALA PRO MET ALA ALA PRO GLN THR ALA ILE LEU ALA PRO SER PRO ALA PRO PRO LEU ALA PRO LEU PRO
VAL LEU ALA PRO SER PRO GLY ALA ALA PRO VAL LEU ALA SER SER GLN THR PRO VAL PRO VAL MET ALA PRO SER SER THR PRO GLY THR SER LEU ALA SER ALA SER PRO VAL PRO ALA PRO THR PRO VAL LEU ALA PRO SER SER THR GLN THR MET LEU PRO ALA PRO VAL PRO SER
PRO LEU PRO SER PRO ALA SER THR GLN THR LEU ALA LEU ALA PRO ALA LEU ALA PRO THR LEU GLY GLY SER SER PRO SER GLN THR LEU SER LEU GLY THR GLY ASN PRO GLN GLY PRO PHE PRO THR GLN THR LEU SER LEU THR PRO ALA SER SER LEU VAL PRO THR PRO ALA GLN
THR LEU SER LEU ALA PRO GLY PRO PRO LEU GLY PRO THR GLN THR LEU SER LEU ALA PRO ALA PRO PRO LEU ALA PRO ALA SER PRO VAL GLY PRO ALA PRO ALA HIS THR LEU THR LEU ALA PRO ALA SER SER SER ALA SER LEU LEU ALA PRO ALA SER VAL GLN THR LEU THR LEU
SER PRO ALA PRO VAL PRO THR LEU GLY PRO ALA ALA ALA GLN THR LEU ALA LEU ALA PRO ALA SER THR GLN SER PRO ALA SER GLN ALA SER SER LEU VAL VAL SER ALA SER GLY ALA ALA PRO LEU PRO VAL THR MET VAL SER ARG LEU PRO VAL SER LYS ASP GLU PRO ASP THR
LEU THR LEU ARG SER GLY PRO PRO SER PRO PRO SER THR ALA THR SER PHE GLY GLY PRO ARG PRO ARG ARG GLN PRO PRO PRO PRO PRO ARG SER P1883 L1886 L1889 L1901 I1904 L1914 L1928 P1929 Q1930 P1931 P1941 H1945 A1954 I1972 F1976 V1983
E1984 A1985 P1986 A1992 C1993 H1994 A2000 P2001 L2014 W2015 P2016 R2017 R2029 T2030 Q2031 D2034 L2035 R2036 L2037 I2038 Q2039 Y2040 K2044 V2050 Q2054 L2055 H2060 L2063 Q2067 M2068 L2072 L2079 T2080 Y2081 L2087 R2088 L2089 D2090 G2091 S2092 R2098 R2104 F2105
K2109 I2115 S2120 V2123 G2124 L2127 D2131 T2132 R2154 I2167 E2173 L2177 A2199 TYR PHE LYS GLN GLN THR ILE ARG GLU LEU PHE ASP MET PRO LEU GLU GLU PRO SER SER SER SER VAL PRO SER ALA PRO GLU GLU GLU GLU GLU THR VAL ALA SER LYS
GLN THR HIS ILE LEU GLU GLN ALA LEU CYS ARG ALA GLU ASP GLU GLU ASP ILE ARG ALA ALA THR GLN ALA LYS ALA GLU GLN VAL ALA GLU LEU ALA GLU PHE ASN GLU ASN ASP GLY PHE PRO ALA GLY GLU GLY GLU GLU ALA GLY ARG PRO GLY ALA GLU ASP GLU MET SER
ARG ALA GLU GLN GLU ILE ALA ALA LEU VAL GLU GLN LEU THR PRO ILE GLU ARG TYR ALA MET LYS PHE LEU GLU ALA SER LEU GLU GLU VAL SER ARG GLU GLU LEU LYS GLN ALA GLU GLU GLN VAL GLU ALA ALA ARG LYS ASP LEU ASP GLN ALA LYS GLU GLU VAL PHE ARG LEU
PRO GLN GLU GLU GLU GLU GLY PRO GLY ALA GLY ASP GLU SER SER CYS GLY THR GLY GLY GLY THR HIS ARG ARG SER LYS LYS ALA LYS ALA PRO GLU ARG PRO GLY THR ARG VAL SER GLU ARG LEU ARG GLY ALA ARG ALA GLU THR GLN GLY ALA ASN HIS THR PRO VAL ILE SER
ALA HIS GLN THR ARG SER THR THR THR PRO PRO ARG CYS SER PRO ALA ARG GLU ARG VAL PRO ARG PRO ALA PRO ARG PRO ARG PRO THR PRO ALA SER ALA PRO ALA ALA ILE PRO ALA LEU VAL PRO VAL PRO VAL SER ALA PRO VAL PRO ILE SER ALA PRO ASN PRO ILE THR ILE
LEU PRO VAL HIS ILE LEU PRO SER PRO PRO PRO PRO SER GLN ILE PRO PRO CYS SER SER PRO ALA CYS THR PRO PRO PRO ALA CYS THR PRO PRO PRO ALA HIS THR PRO PRO PRO ALA GLN THR CYS LEU VAL THR PRO SER SER PRO LEU LEU LEU GLY PRO PRO SER VAL PRO ILE
SER ALA SER VAL THR ASN LEU PRO LEU GLY LEU ARG PRO GLU ALA GLU LEU CYS ALA GLN ALA LEU ALA SER PRO GLU SER LEU GLU LEU ALA SER VAL ALA SER SER GLU THR SER SER LEU SER LEU VAL PRO PRO LYS ASP LEU LEU PRO VAL ALA VAL GLU ILE LEU PRO VAL SER
GLU LYS ASN LEU SER LEU THR PRO SER ALA PRO SER LEU THR LEU GLU ALA GLY SER ILE PRO ASN GLY GLN GLU GLN GLU ALA PRO ASP SER ALA GLU GLY THR THR LEU THR VAL LEU PRO GLU GLY GLU GLU LEU PRO LEU CYS VAL SER GLU SER ASN GLY LEU GLU LEU PRO PRO
SER ALA ALA SER ASP GLU PRO LEU GLN GLU PRO LEU GLU ALA ASP ARG THR SER GLU GLU LEU THR GLU ALA LYS THR PRO THR SER SER PRO GLU LYS PRO GLN GLU LEU VAL THR ALA GLU VAL ALA ALA PRO SER THR SER SER SER ALA THR SER SER PRO GLU GLY PRO SER PRO
ALA ARG PRO PRO ARG ARG ARG THR SER ALA ASP VAL GLU ILE ARG GLY GLN GLY THR GLY ARG PRO GLY GLN PRO PRO GLY PRO LYS VAL LEU ARG LYS LEU PRO GLY ARG LEU VAL THR VAL VAL GLU GLU LYS GLU LEU VAL ARG ARG ARG GLN GLN ARG GLY ALA ALA SER THR
LEU VAL PRO GLY VAL SER GLU THR SER ALA SER PRO GLY SER PRO SER VAL ARG SER MET SER GLY PRO GLU SER SER PRO PRO ILE GLY GLY PRO CYS GLU ALA ALA PRO SER SER SER LEU PRO THR PRO PRO GLN GLN PRO PHE ILE ALA ARG ARG HIS ILE GLU LEU GLY VAL THR
GLY GLY GLY SER PRO GLU ASN GLY ASP GLY ALA LEU LEU ALA ILE THR PRO PRO ALA VAL LYS ARG ARG ARG GLY ARG PRO PRO LYS LYS ASN ARG SER PRO ALA ASP ALA GLY ARG GLY VAL ASP GLU ALA PRO SER SER THR LEU LYS GLY LYS THR ASN GLY ALA ASP PRO VAL PRO



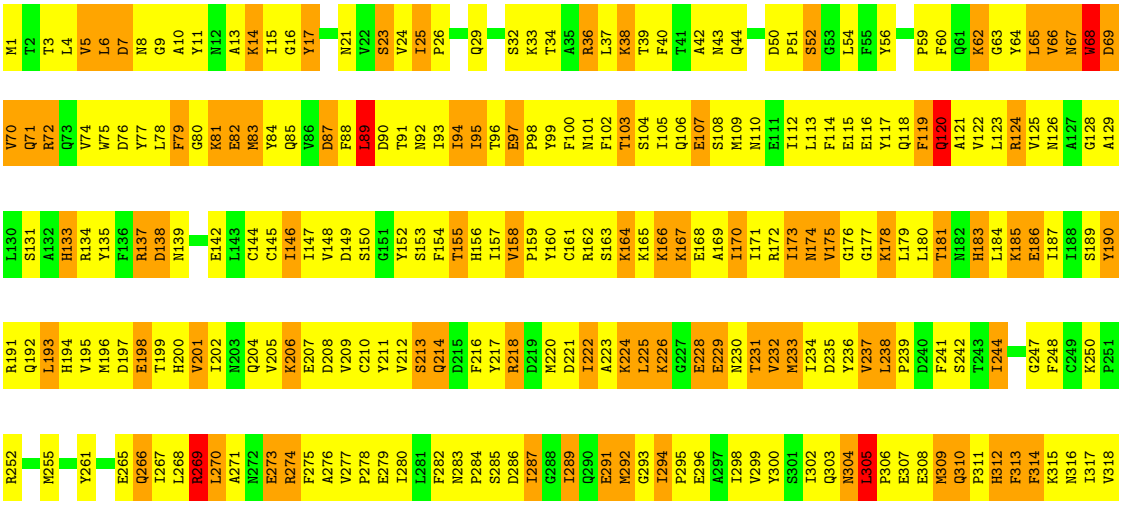
• Molecule 6: Vacuolar protein sorting-associated protein 72 homolog

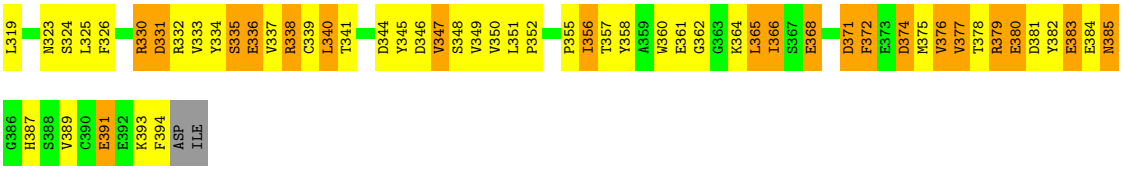
Chain J:



• Molecule 7: Actin-related protein 6

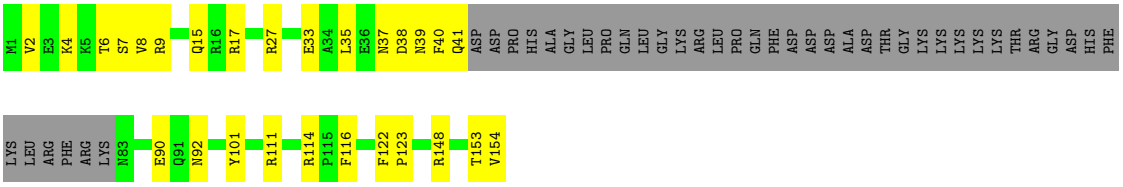
Chain K:





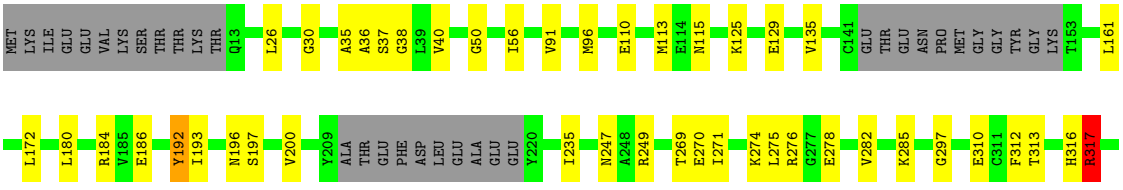
• Molecule 8: Zinc finger HIT domain-containing protein 1

Chain L:



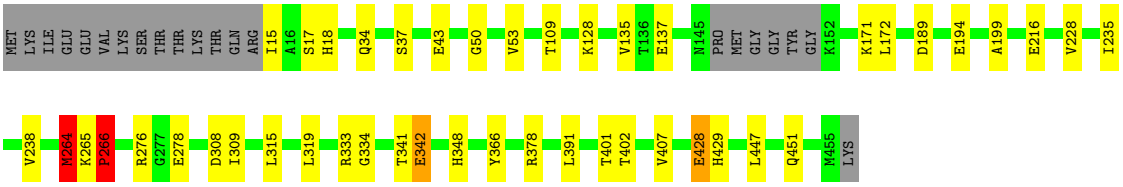
• Molecule 9: RuvB-like 1

Chain M:



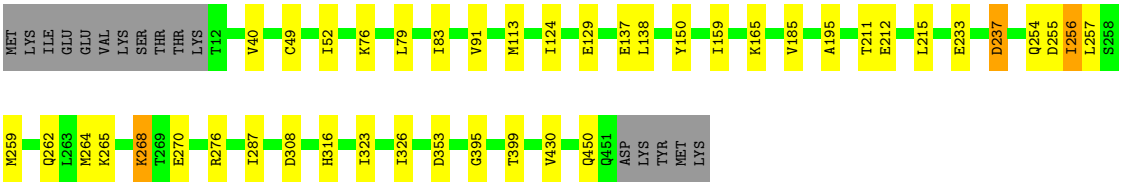
• Molecule 9: RuvB-like 1

Chain O:



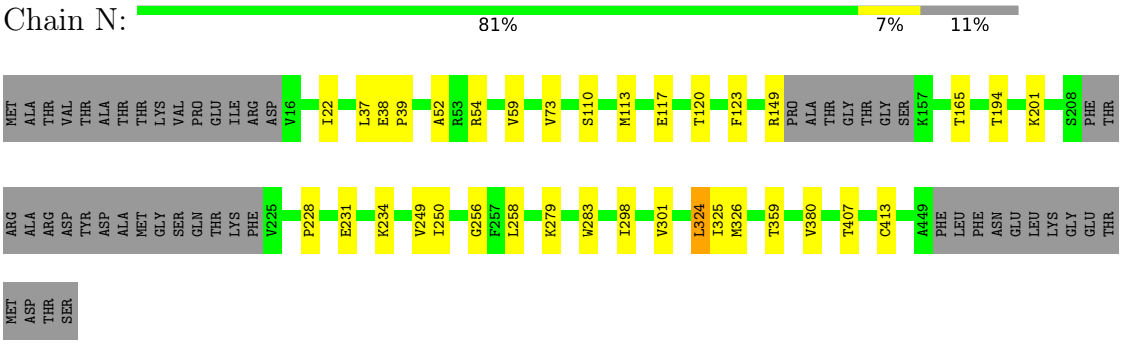
• Molecule 9: RuvB-like 1

Chain Q:



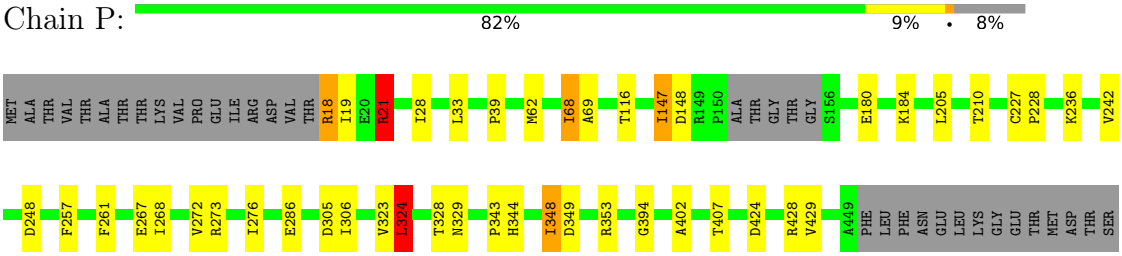
• Molecule 10: RuvB-like 2

Chain N:



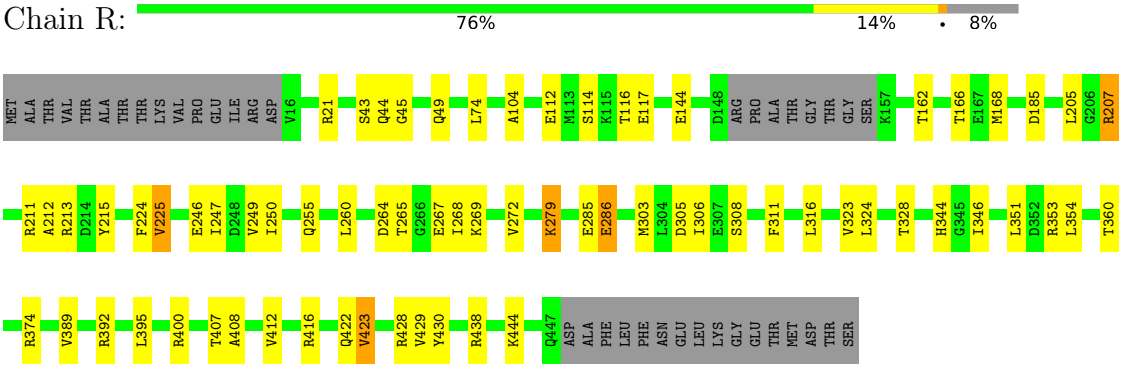
• Molecule 10: RuvB-like 2

Chain P:



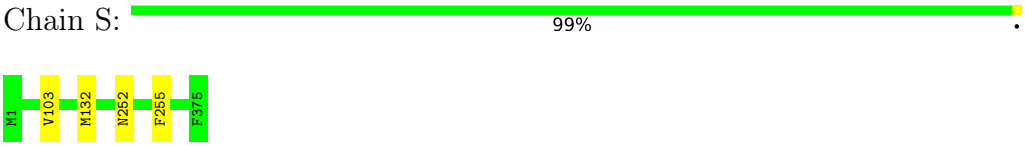
• Molecule 10: RuvB-like 2

Chain R:



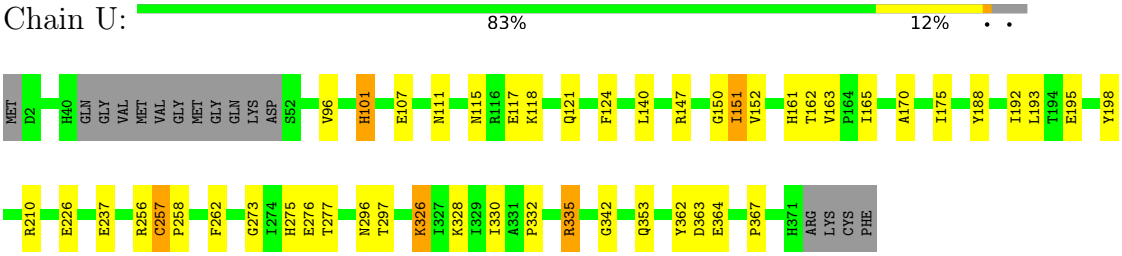
• Molecule 11: Actin, cytoplasmic 1

Chain S:



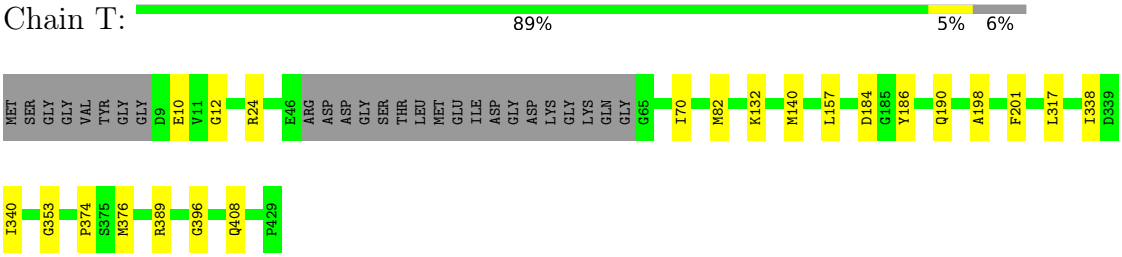
• Molecule 11: Actin, cytoplasmic 1

Chain U:



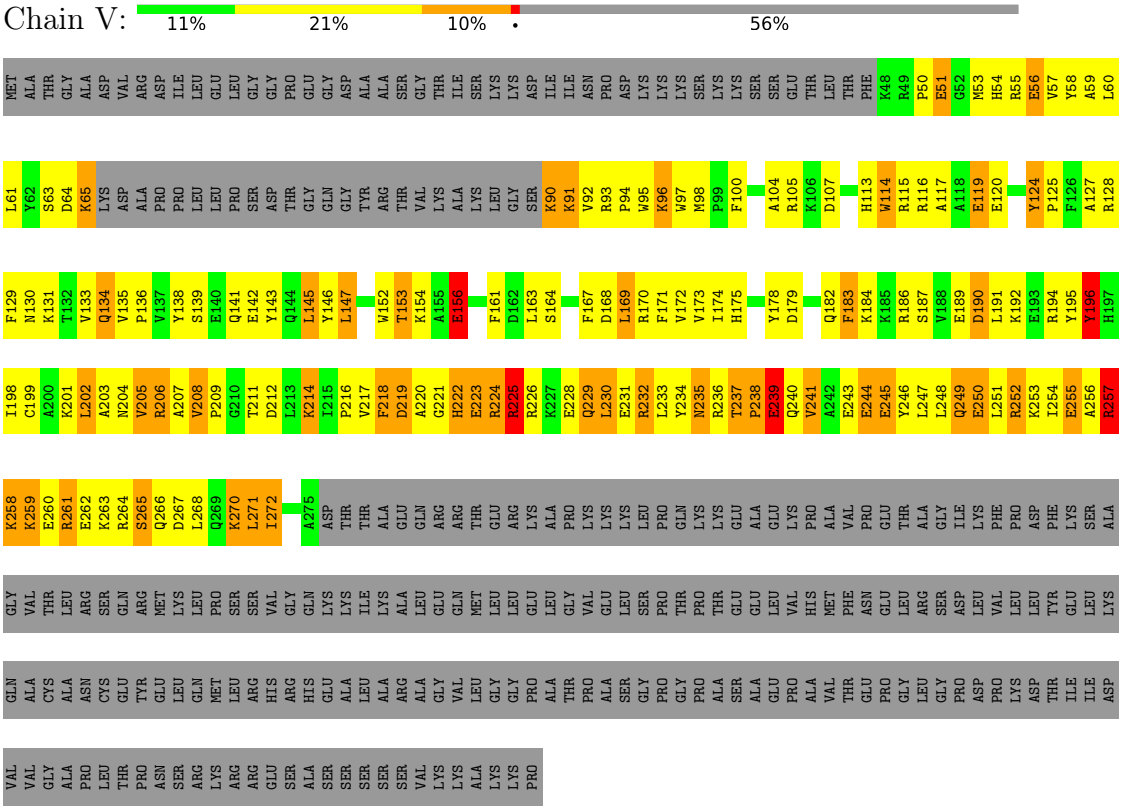
• Molecule 12: Actin-like protein 6A

Chain T:



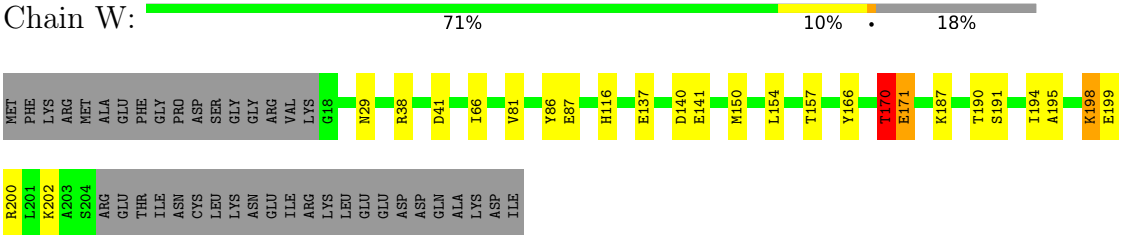
• Molecule 13: DNA methyltransferase 1-associated protein 1

Chain V:



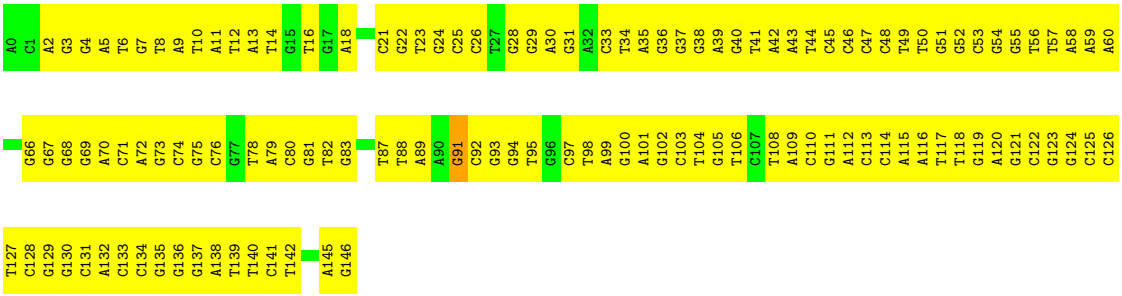
• Molecule 14: YEATS domain-containing protein 4

Chain W:



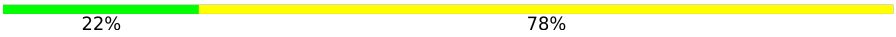
• Molecule 15: DNA (147-MER)

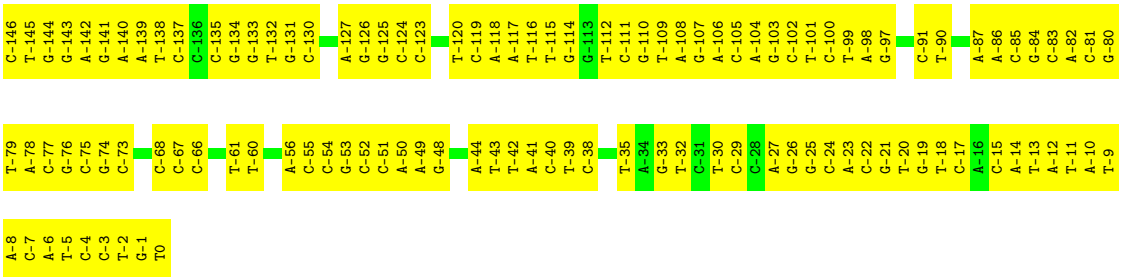
Chain X:



• Molecule 16: DNA (147-MER)

Chain Y:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	475617	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, BEF, ADP

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	0.31	0/843	0.58	0/1136
1	E	0.26	0/818	0.54	0/1104
2	B	0.27	0/766	0.50	0/1026
2	F	0.27	0/747	0.50	0/1004
3	C	0.28	0/789	0.56	0/1057
3	G	0.27	0/813	0.56	0/1090
4	D	0.30	0/653	0.58	0/873
4	H	0.25	0/645	0.56	0/862
5	I	0.32	0/7296	0.62	1/9855 (0.0%)
6	J	0.34	0/1381	0.62	0/1861
7	K	0.31	0/3283	0.55	2/4445 (0.0%)
8	L	0.35	0/909	0.63	0/1227
9	M	0.31	0/3253	0.58	0/4382
9	O	0.32	0/3382	0.57	0/4559
9	Q	0.31	0/3413	0.56	1/4603 (0.0%)
10	N	0.30	0/3217	0.60	1/4328 (0.0%)
10	P	0.30	0/3324	0.60	1/4477 (0.0%)
10	R	0.30	0/3329	0.60	0/4479
11	S	0.29	0/2988	0.50	0/4045
11	U	0.31	0/2863	0.56	0/3882
12	T	0.29	0/3217	0.50	0/4362
13	V	0.57	5/1801 (0.3%)	0.67	2/2419 (0.1%)
14	W	0.37	1/1578 (0.1%)	0.53	0/2128
15	X	0.58	0/3405	0.95	2/5259 (0.0%)
16	Y	0.56	0/3349	0.93	0/5162
All	All	0.36	6/58062 (0.0%)	0.64	10/79625 (0.0%)

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	G	0	1
5	I	0	1
9	M	0	1
10	P	0	2
10	R	0	1
13	V	0	3
14	W	0	1
All	All	0	10

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	V	156	GLU	CD-OE1	8.47	1.34	1.25
13	V	183	PHE	CD1-CE1	8.17	1.55	1.39
13	V	183	PHE	CE2-CZ	6.55	1.49	1.37
14	W	198	LYS	CD-CE	6.44	1.67	1.51
13	V	196	TYR	CD1-CE1	-5.59	1.30	1.39

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	K	89	LEU	CB-CG-CD2	-7.39	98.43	111.00
7	K	89	LEU	CA-CB-CG	6.25	129.68	115.30
15	X	89	DA	O4'-C1'-N9	6.19	112.33	108.00
13	V	156	GLU	CG-CD-OE2	-6.15	106.01	118.30
9	Q	79	LEU	CA-CB-CG	5.68	128.36	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	134	ARG	Sidechain
5	I	2029	ARG	Sidechain
9	M	317	ARG	Sidechain
10	P	18	ARG	Sidechain
10	P	21	ARG	Sidechain

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	A	833	0	895	184	0
1	E	808	0	864	118	0
2	B	755	0	782	136	0
2	F	736	0	756	68	0
3	C	779	0	816	72	0
3	G	801	0	839	93	0
4	D	646	0	687	36	0
4	H	638	0	676	63	0
5	I	7122	0	7212	309	0
6	J	1350	0	1370	28	0
7	K	3209	0	3132	518	0
8	L	893	0	880	52	0
9	M	3213	0	3331	90	0
9	O	3339	0	3425	28	0
9	Q	3368	0	3453	33	0
10	N	3185	0	3269	44	0
10	P	3287	0	3335	22	0
10	R	3293	0	3373	41	0
11	S	2925	0	2891	2	0
11	U	2802	0	2760	34	0
12	T	3146	0	3086	20	0
13	V	1757	0	1736	326	0
14	W	1542	0	1556	70	0
15	X	3031	0	1650	241	0
16	Y	2990	0	1652	182	0
17	I	27	0	12	6	0
17	M	27	0	12	0	0
17	N	27	0	12	0	0
17	O	27	0	12	1	0
17	P	27	0	12	0	0
17	Q	27	0	12	1	0
17	R	27	0	12	0	0
18	I	1	0	0	0	0
19	I	4	0	0	3	0
20	T	31	0	12	1	0
20	U	31	0	12	0	0
All	All	56704	0	54534	2263	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 20.

The worst 5 of 2263 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)
9:M:313:THR:HA	9:M:316:HIS:CE1	1.28	1.63
1:A:13:ALA:HB2	5:I:164:LYS:CD	1.25	1.61
9:M:413:ALA:HA	9:M:433:ILE:CD1	1.35	1.53
5:I:936:HIS:CE1	10:N:279:LYS:HZ3	1.29	1.48
5:I:936:HIS:HE1	10:N:279:LYS:NZ	1.08	1.47

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 PDB entries followed by that with respect to all EM entries.

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	106/130 (82%)	97 (92%)	9 (8%)	0	100 100
1	E	103/130 (79%)	93 (90%)	10 (10%)	0	100 100
2	B	94/126 (75%)	87 (93%)	7 (7%)	0	100 100
2	F	92/126 (73%)	88 (96%)	2 (2%)	2 (2%)	6 35
3	C	93/136 (68%)	91 (98%)	2 (2%)	0	100 100
3	G	95/136 (70%)	91 (96%)	4 (4%)	0	100 100
4	D	79/103 (77%)	78 (99%)	1 (1%)	0	100 100
4	H	78/103 (76%)	72 (92%)	6 (8%)	0	100 100
5	I	858/3230 (27%)	792 (92%)	63 (7%)	3 (0%)	41 74
6	J	158/364 (43%)	145 (92%)	13 (8%)	0	100 100
7	K	392/396 (99%)	295 (75%)	84 (21%)	13 (3%)	4 25
8	L	109/154 (71%)	96 (88%)	13 (12%)	0	100 100
9	M	412/456 (90%)	395 (96%)	16 (4%)	1 (0%)	47 79
9	O	431/456 (94%)	409 (95%)	19 (4%)	3 (1%)	22 61
9	Q	438/456 (96%)	417 (95%)	20 (5%)	1 (0%)	47 79
10	N	405/463 (88%)	386 (95%)	19 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	P	423/463 (91%)	396 (94%)	26 (6%)	1 (0%)	47 79
10	R	420/463 (91%)	393 (94%)	26 (6%)	1 (0%)	47 79
11	S	373/375 (100%)	366 (98%)	7 (2%)	0	100 100
11	U	355/375 (95%)	325 (92%)	29 (8%)	1 (0%)	41 74
12	T	399/429 (93%)	381 (96%)	18 (4%)	0	100 100
13	V	200/467 (43%)	178 (89%)	19 (10%)	3 (2%)	10 44
14	W	185/227 (82%)	182 (98%)	2 (1%)	1 (0%)	29 67
All	All	6298/9764 (64%)	5853 (93%)	415 (7%)	30 (0%)	32 67

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	820	GLU
7	K	89	LEU
7	K	103	THR
7	K	120	GLN
7	K	376	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 PDB entries followed by that with respect to all EM entries.

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	84/99 (85%)	64 (76%)	20 (24%)	0 3
1	E	82/99 (83%)	64 (78%)	18 (22%)	1 5
2	B	83/106 (78%)	71 (86%)	12 (14%)	3 15
2	F	81/106 (76%)	73 (90%)	8 (10%)	8 30
3	C	82/111 (74%)	68 (83%)	14 (17%)	2 10
3	G	85/111 (77%)	80 (94%)	5 (6%)	19 54
4	D	66/79 (84%)	66 (100%)	0	100 100
4	H	65/79 (82%)	54 (83%)	11 (17%)	2 10
5	I	775/2721 (28%)	759 (98%)	16 (2%)	53 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	J	148/312 (47%)	147 (99%)	1 (1%)	84 94
7	K	359/361 (99%)	238 (66%)	121 (34%)	0 0
8	L	98/133 (74%)	96 (98%)	2 (2%)	55 80
9	M	353/387 (91%)	346 (98%)	7 (2%)	55 80
9	O	364/387 (94%)	344 (94%)	20 (6%)	21 57
9	Q	366/387 (95%)	344 (94%)	22 (6%)	19 54
10	N	347/390 (89%)	340 (98%)	7 (2%)	55 80
10	P	352/390 (90%)	331 (94%)	21 (6%)	19 54
10	R	358/390 (92%)	329 (92%)	29 (8%)	11 42
11	S	318/318 (100%)	318 (100%)	0	100 100
11	U	305/318 (96%)	291 (95%)	14 (5%)	27 63
12	T	346/364 (95%)	338 (98%)	8 (2%)	50 78
13	V	183/400 (46%)	129 (70%)	54 (30%)	0 1
14	W	168/203 (83%)	164 (98%)	4 (2%)	49 77
All	All	5468/8251 (66%)	5054 (92%)	414 (8%)	17 45

5 of 414 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	M	192	TYR
9	Q	113	MET
13	V	252	ARG
10	N	283	TRP
9	O	428	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
9	Q	284	ASN
12	T	143	HIS
13	V	269	GLN
6	J	162	HIS
5	I	2060	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	BEF	I	3303	-	0,3,3	-	-	-		
20	ATP	U	401	-	26,33,33	0.63	1 (3%)	31,52,52	1.06	2 (6%)
17	ADP	I	3301	-	24,29,29	0.90	1 (4%)	29,45,45	1.64	5 (17%)
20	ATP	T	501	-	26,33,33	0.62	1 (3%)	31,52,52	1.12	4 (12%)
17	ADP	P	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.57	6 (20%)
17	ADP	Q	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.48	5 (17%)
17	ADP	M	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.42	3 (10%)
17	ADP	O	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	5 (17%)
17	ADP	R	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.40	5 (17%)
17	ADP	N	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.33	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	ATP	U	401	-	-	2/18/38/38	0/3/3/3
17	ADP	I	3301	-	-	5/12/32/32	0/3/3/3
20	ATP	T	501	-	-	1/18/38/38	0/3/3/3
17	ADP	P	501	-	-	2/12/32/32	0/3/3/3
17	ADP	Q	501	-	-	3/12/32/32	0/3/3/3
17	ADP	M	501	-	-	2/12/32/32	0/3/3/3
17	ADP	O	501	-	-	6/12/32/32	0/3/3/3
17	ADP	R	501	-	-	1/12/32/32	0/3/3/3
17	ADP	N	501	-	-	4/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	O	501	ADP	C5-C4	2.67	1.48	1.40
17	R	501	ADP	C5-C4	2.60	1.47	1.40
17	P	501	ADP	C5-C4	2.60	1.47	1.40
17	Q	501	ADP	C5-C4	2.59	1.47	1.40
17	M	501	ADP	C5-C4	2.58	1.47	1.40

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	I	3301	ADP	PA-O3A-PB	-4.37	117.84	132.83
17	P	501	ADP	C3'-C2'-C1'	3.73	106.60	100.98
17	Q	501	ADP	PA-O3A-PB	-3.64	120.34	132.83
17	I	3301	ADP	N3-C2-N1	-3.53	123.16	128.68
17	M	501	ADP	PA-O3A-PB	-3.51	120.79	132.83

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	I	3301	ADP	C5'-O5'-PA-O2A
17	N	501	ADP	C5'-O5'-PA-O1A
17	N	501	ADP	O4'-C4'-C5'-O5'
17	O	501	ADP	C5'-O5'-PA-O2A
17	P	501	ADP	PA-O3A-PB-O2B

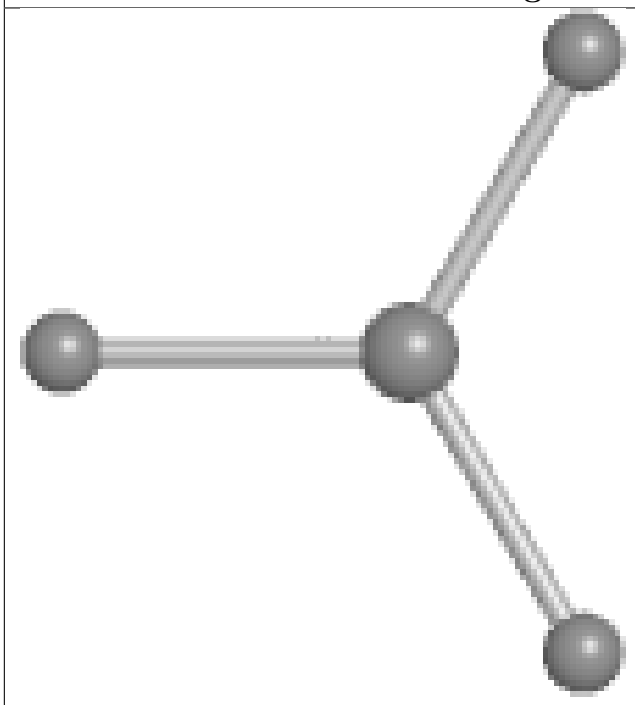
There are no ring outliers.

5 monomers are involved in 11 short contacts:

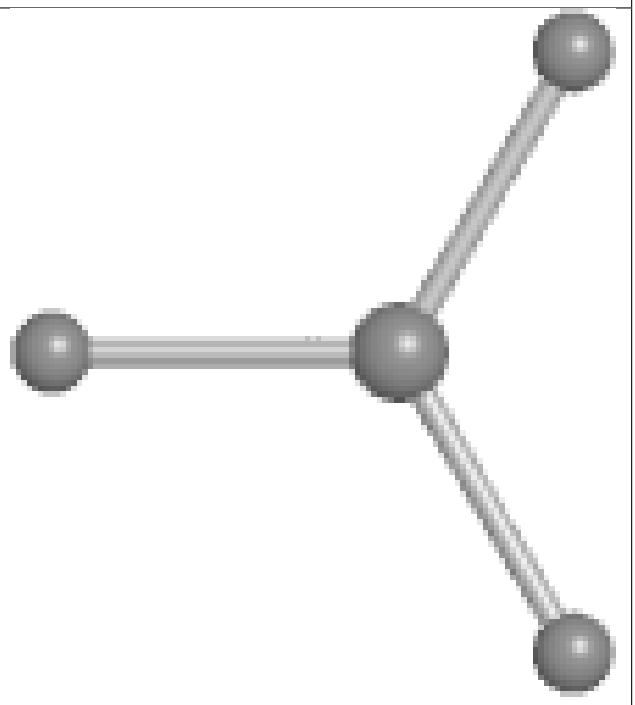
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	I	3303	BEF	3	0
17	I	3301	ADP	6	0
20	T	501	ATP	1	0
17	Q	501	ADP	1	0
17	O	501	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

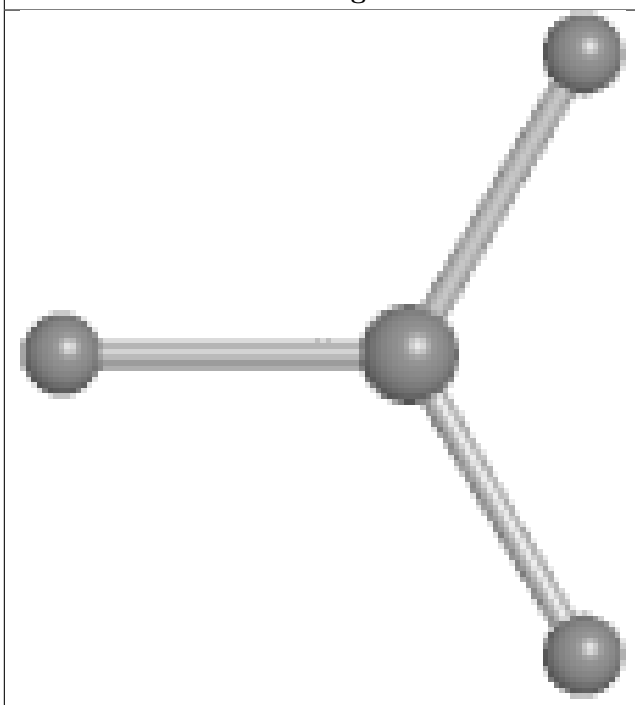
Ligand BEF I 3303



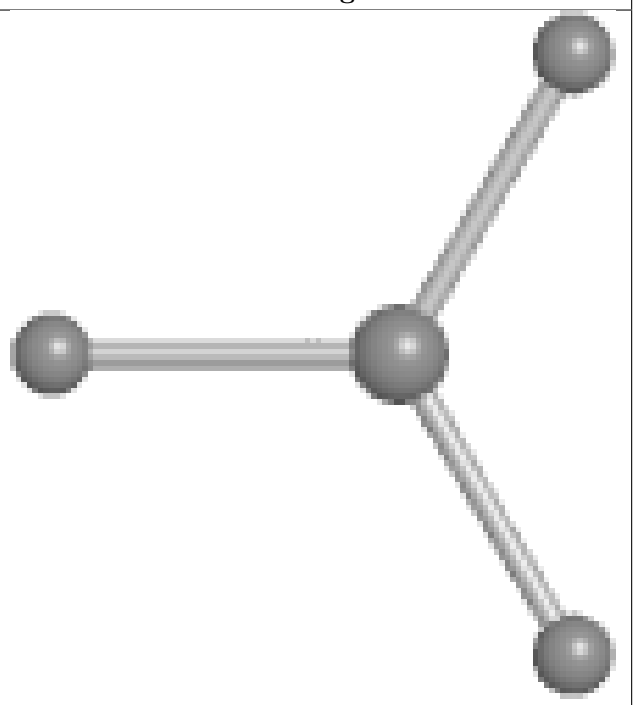
Bond lengths



Bond angles

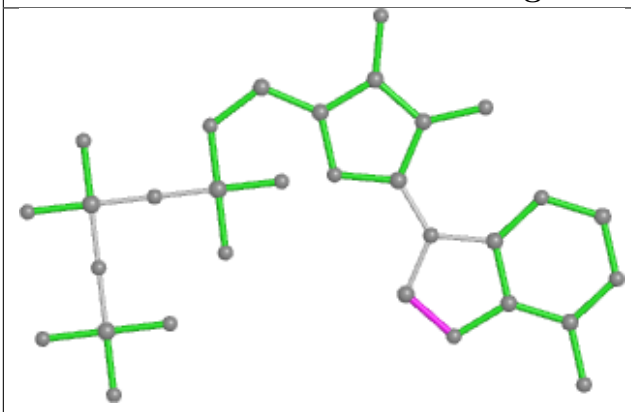


Torsions

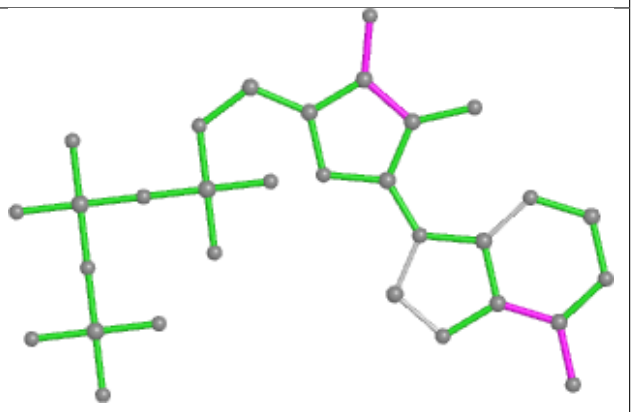


Rings

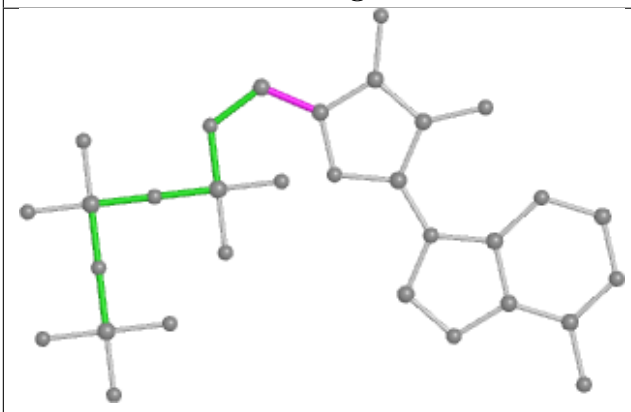
Ligand ATP U 401



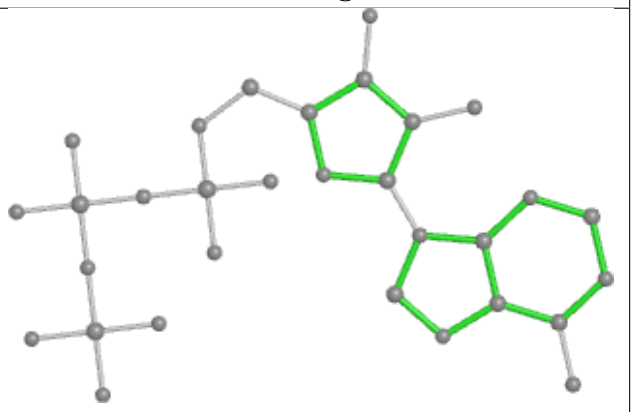
Bond lengths



Bond angles

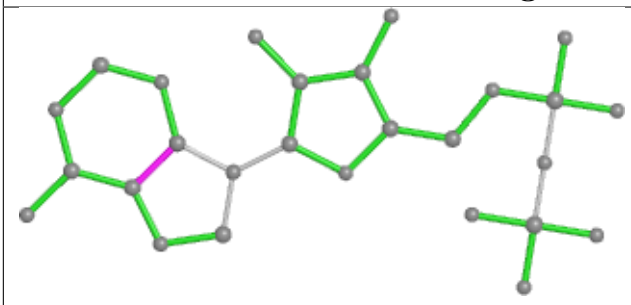


Torsions



Rings

Ligand ADP I 3301



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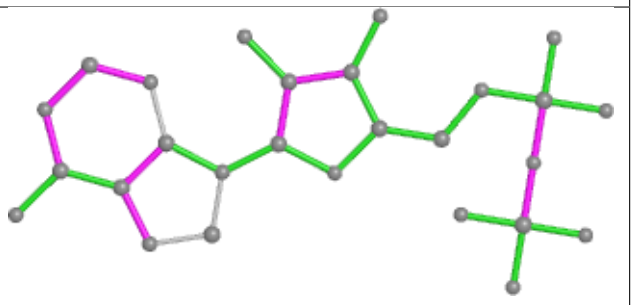
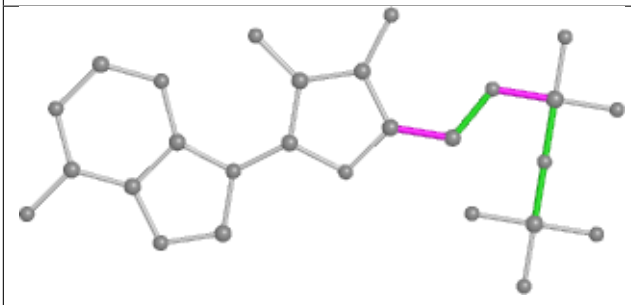


Bond angles



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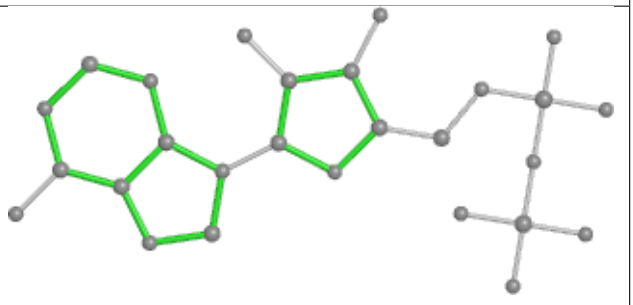
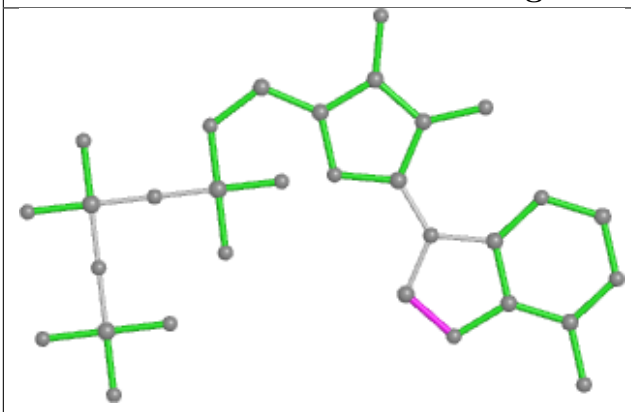


Rings

Ligand ATP T 501



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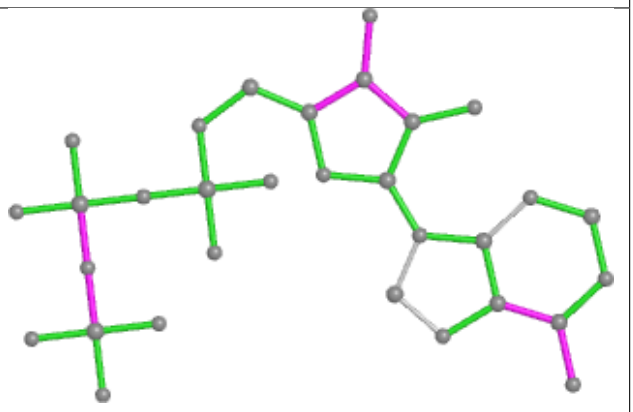
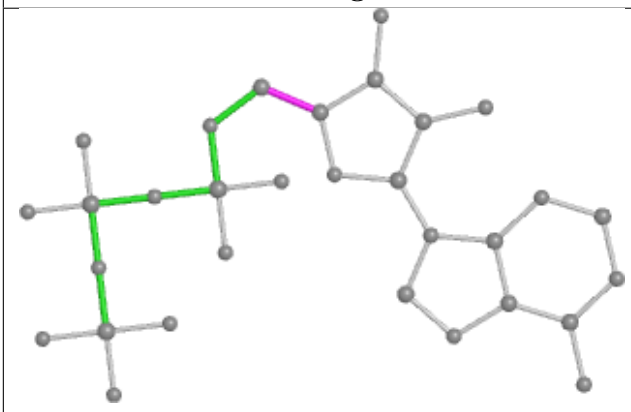
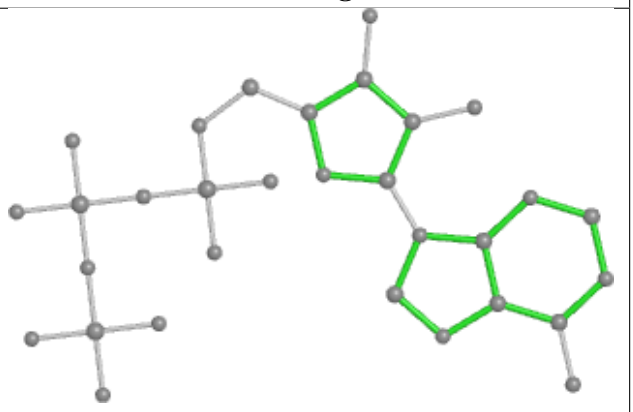


Bond angles

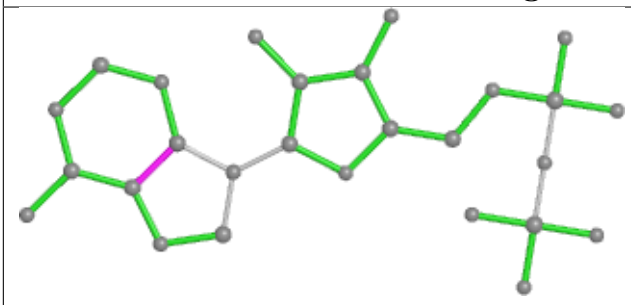


Torsions



Rings

Ligand ADP P 501



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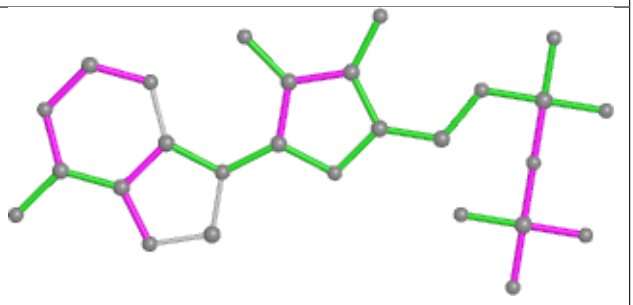

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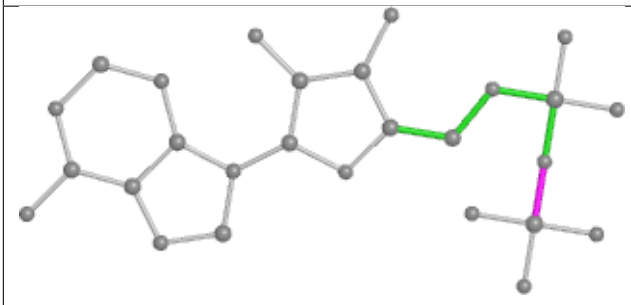

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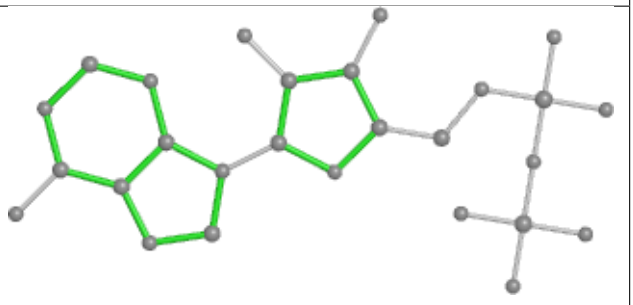
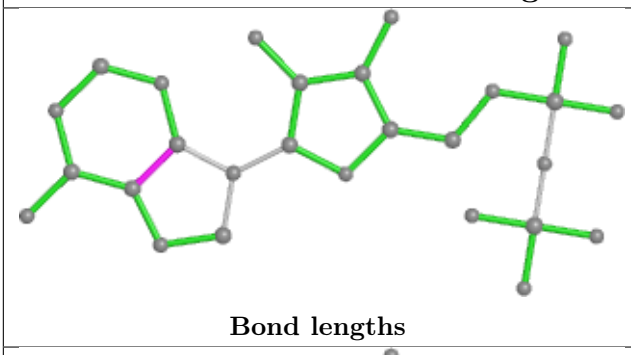


Rings

Ligand ADP Q 501



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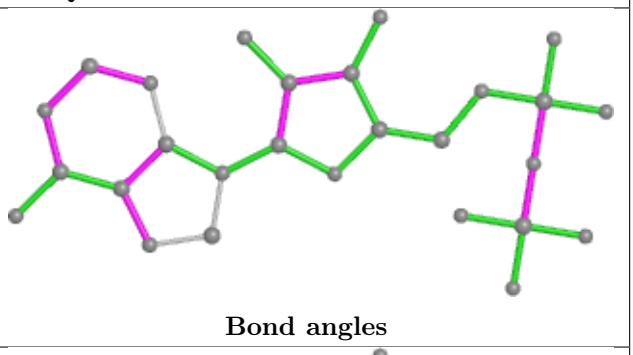

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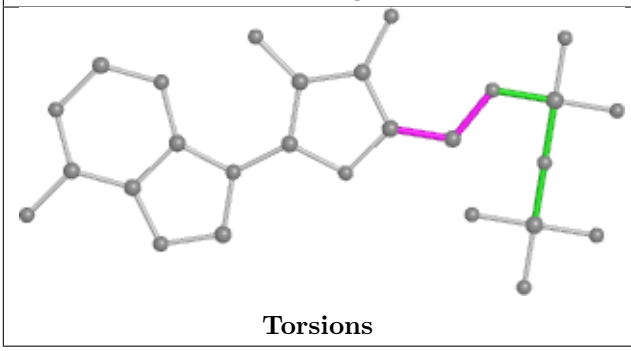

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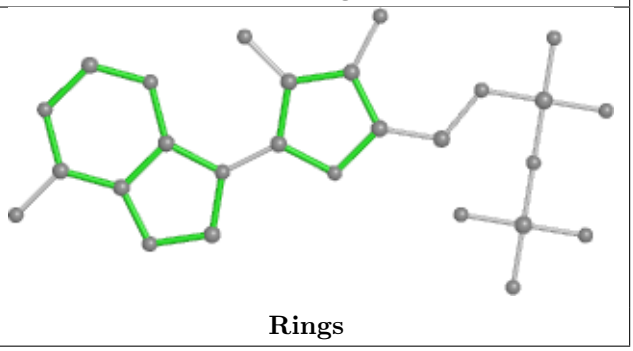
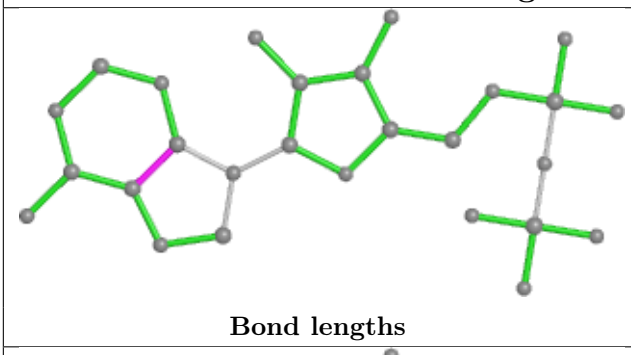


Rings

Ligand ADP M 501



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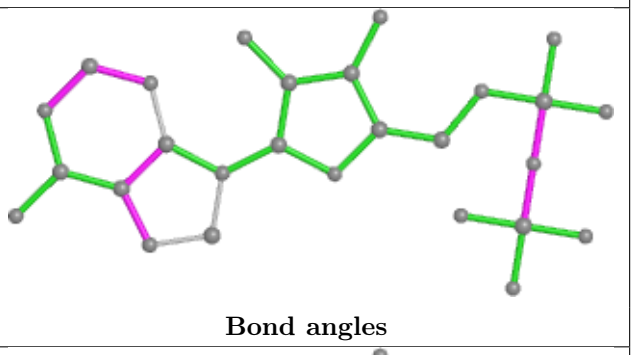

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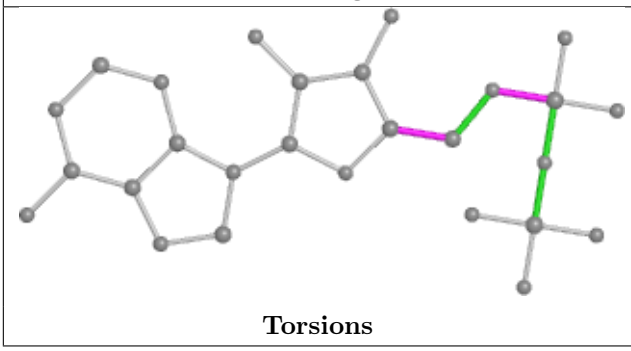

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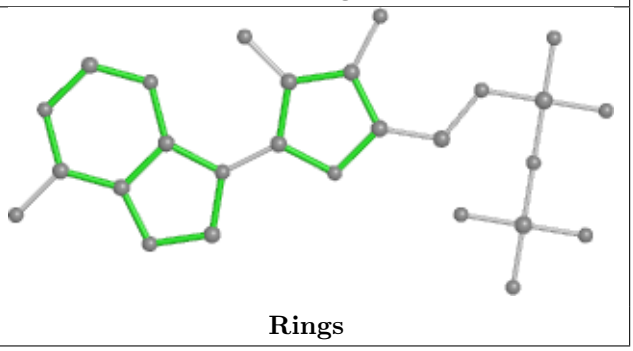
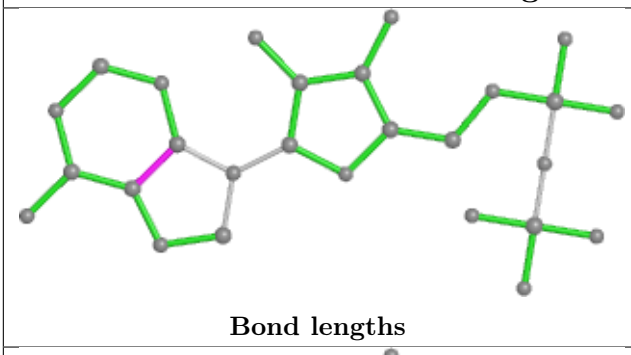
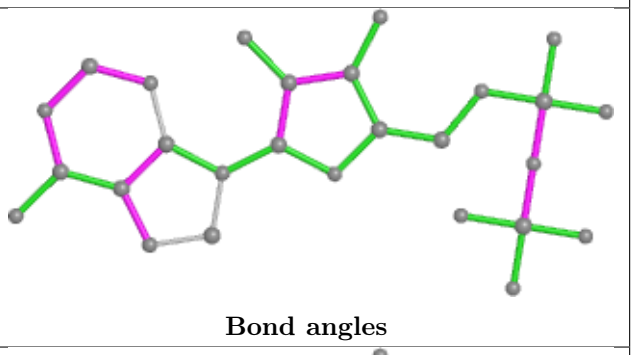


Rings

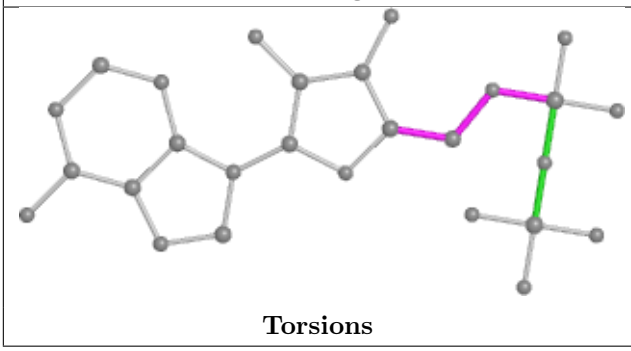
Ligand ADP O 501



Bond lengths



Bond angles



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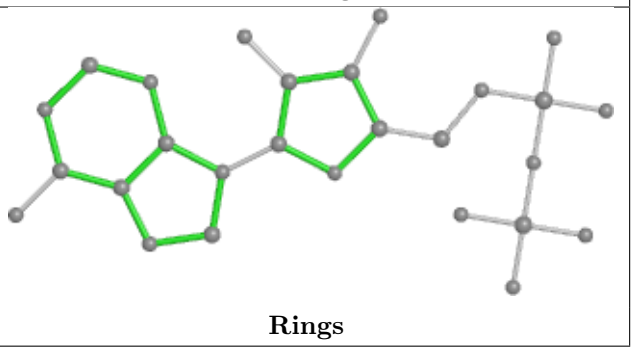
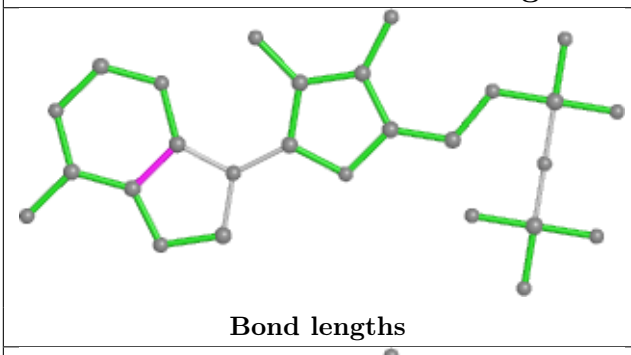
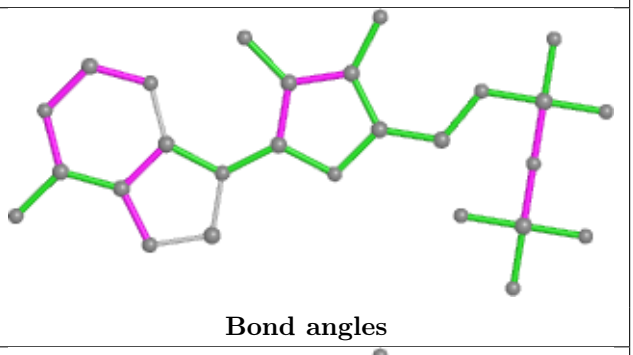


Rings

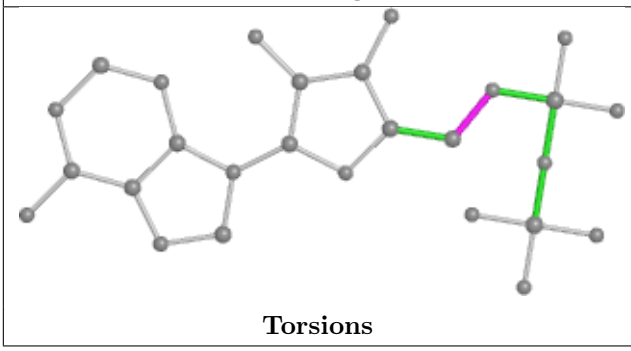
Ligand ADP R 501



Bond lengths



Bond angles



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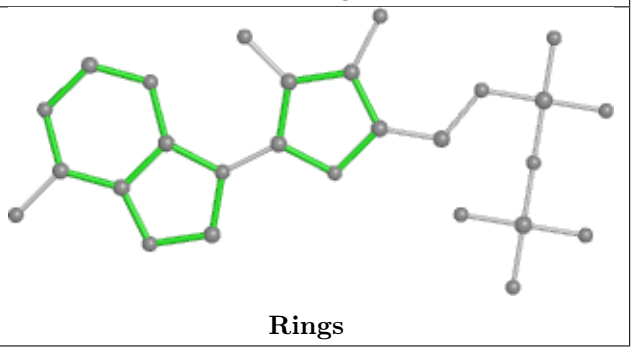
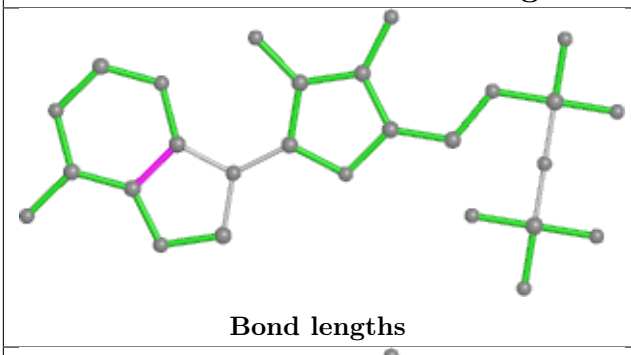
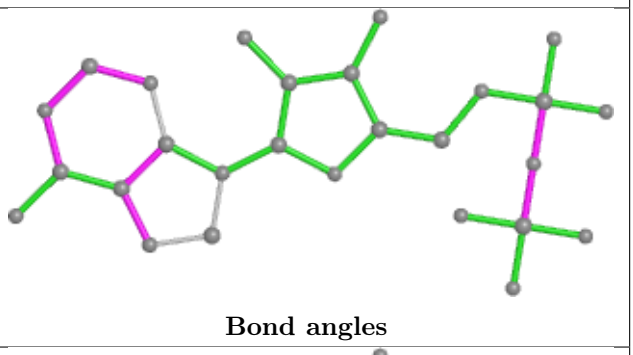


Rings

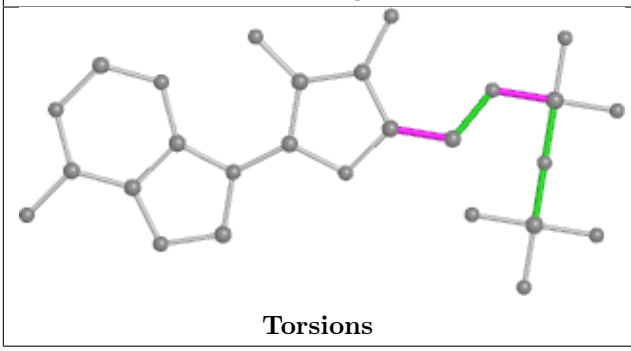
Ligand ADP N 501



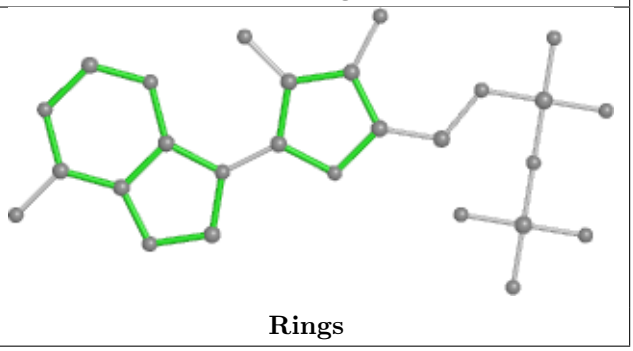
Bond lengths



Bond angles



Torsions



Rings

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.