



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:39 PM UTC

PDB ID : 4V81 / pdb_00004v81
Title : The crystal structure of yeast CCT reveals intrinsic asymmetry of eukaryotic cytosolic chaperonins
Authors : Dekker, C.; Roe, S.M.; McCormack, E.A.; Beuron, F.; Pearl, L.H.; Willison, K.R.
Deposited on : 2010-10-17
Resolution : 3.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

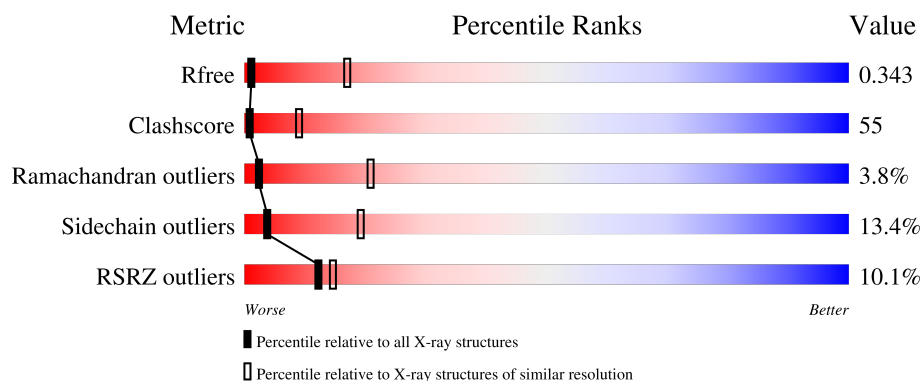
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	559	8% 51% 39% 6% . .
1	I	559	10% 52% 38% 6% . .
1	a	559	4% 52% 38% 6% . .
1	i	559	7% 52% 39% 6% . .

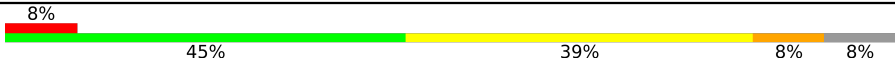
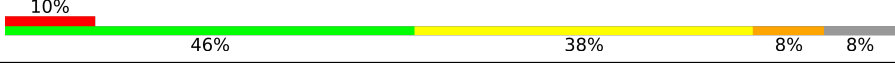
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Mol	Chain	Length	Quality of chain
2	B	527	
2	J	527	
2	b	527	
2	j	527	
3	C	590	
3	K	590	
3	c	590	
3	k	590	
4	D	528	
4	L	528	
4	d	528	
4	l	528	
5	E	562	
5	M	562	
5	e	562	
5	m	562	
6	F	546	
6	N	546	
6	f	546	
6	n	546	
7	G	550	
7	O	550	
7	g	550	
7	o	550	
8	H	568	

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Mol	Chain	Length	Quality of chain
8	P	568	
8	h	568	
8	p	568	

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
10	BEF	C	1102	-	-	X	-
10	BEF	F	602	-	-	X	-
10	BEF	N	602	-	-	X	-
10	BEF	n	1602	-	-	-	X
9	ADP	A	601	X	-	-	-
9	ADP	B	601	X	-	-	-
9	ADP	C	1101	X	-	-	-
9	ADP	D	601	X	-	-	-
9	ADP	E	601	X	-	-	-
9	ADP	G	601	X	-	-	-
9	ADP	H	601	X	-	-	-
9	ADP	J	601	X	-	-	-
9	ADP	M	601	X	-	-	-
9	ADP	N	601	X	-	-	-
9	ADP	P	601	X	-	-	-
9	ADP	a	1601	X	-	-	-
9	ADP	b	1601	X	-	-	-
9	ADP	e	1601	X	-	-	-
9	ADP	f	1601	X	-	-	-
9	ADP	g	1601	X	-	-	-
9	ADP	h	1601	X	-	-	-
9	ADP	k	2101	X	-	X	-
9	ADP	m	1601	X	-	-	-
9	ADP	n	1601	X	-	-	-
9	ADP	p	1601	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 111235 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			
1	I	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			
1	a	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			
1	i	544	Total	C	N	O	S	0	0	0
			3492	2146	600	732	14			

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	513	Total	C	N	O	S	0	0	0
			3459	2125	597	728	9			
2	J	513	Total	C	N	O	S	0	0	0
			3459	2125	597	728	9			
2	b	513	Total	C	N	O	S	0	0	0
			3460	2126	597	728	9			
2	j	513	Total	C	N	O	S	0	0	0
			3457	2123	597	728	9			

- Molecule 3 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	514	Total	C	N	O	S	0	0	0
			3392	2104	590	685	13			
3	K	514	Total	C	N	O	S	0	0	0
			3393	2104	590	685	14			
3	c	514	Total	C	N	O	S	0	0	0
			3395	2106	590	685	14			
3	k	514	Total	C	N	O	S	0	0	0
			3395	2106	590	685	14			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1001	GLY	-	SEE REMARK 999	UNP P39077
C	1002	SER	-	SEE REMARK 999	UNP P39077
C	1003	GLY	-	SEE REMARK 999	UNP P39077
C	1004	SER	-	SEE REMARK 999	UNP P39077
C	1005	GLY	-	SEE REMARK 999	UNP P39077
C	1006	TRP	-	SEE REMARK 999	UNP P39077
C	1007	SER	-	SEE REMARK 999	UNP P39077
C	1008	HIS	-	SEE REMARK 999	UNP P39077
C	1009	PRO	-	SEE REMARK 999	UNP P39077
C	1010	GLN	-	SEE REMARK 999	UNP P39077
C	1011	PHE	-	SEE REMARK 999	UNP P39077
C	1012	GLU	-	SEE REMARK 999	UNP P39077
C	1013	LYS	-	SEE REMARK 999	UNP P39077
C	1014	GLY	-	SEE REMARK 999	UNP P39077
C	1015	SER	-	SEE REMARK 999	UNP P39077
C	1016	GLY	-	SEE REMARK 999	UNP P39077
C	1017	LYS	-	SEE REMARK 999	UNP P39077
C	1018	ARG	-	SEE REMARK 999	UNP P39077
C	1019	ARG	-	SEE REMARK 999	UNP P39077
C	1020	TRP	-	SEE REMARK 999	UNP P39077
C	1021	LYS	-	SEE REMARK 999	UNP P39077
C	1022	LYS	-	SEE REMARK 999	UNP P39077
C	1023	ASN	-	SEE REMARK 999	UNP P39077
C	1024	PHE	-	SEE REMARK 999	UNP P39077
C	1025	ILE	-	SEE REMARK 999	UNP P39077
C	1026	ALA	-	SEE REMARK 999	UNP P39077
C	1027	VAL	-	SEE REMARK 999	UNP P39077
C	1028	SER	-	SEE REMARK 999	UNP P39077
C	1029	ALA	-	SEE REMARK 999	UNP P39077
C	1030	ALA	-	SEE REMARK 999	UNP P39077
C	1031	ASN	-	SEE REMARK 999	UNP P39077
C	1032	ARG	-	SEE REMARK 999	UNP P39077
C	1033	PHE	-	SEE REMARK 999	UNP P39077
C	1034	LYS	-	SEE REMARK 999	UNP P39077
C	1035	LYS	-	SEE REMARK 999	UNP P39077
C	1036	ILE	-	SEE REMARK 999	UNP P39077
C	1037	SER	-	SEE REMARK 999	UNP P39077
C	1038	SER	-	SEE REMARK 999	UNP P39077
C	1039	SER	-	SEE REMARK 999	UNP P39077
C	1040	GLY	-	SEE REMARK 999	UNP P39077
C	1041	ALA	-	SEE REMARK 999	UNP P39077
C	1042	LEU	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1043	GLY	-	SEE REMARK 999	UNP P39077
C	1044	SER	-	SEE REMARK 999	UNP P39077
C	1045	GLY	-	SEE REMARK 999	UNP P39077
C	1046	HIS	-	SEE REMARK 999	UNP P39077
C	1047	HIS	-	SEE REMARK 999	UNP P39077
C	1048	HIS	-	SEE REMARK 999	UNP P39077
C	1049	HIS	-	SEE REMARK 999	UNP P39077
C	1050	HIS	-	SEE REMARK 999	UNP P39077
C	1051	HIS	-	SEE REMARK 999	UNP P39077
C	1052	HIS	-	SEE REMARK 999	UNP P39077
C	1053	HIS	-	SEE REMARK 999	UNP P39077
C	1054	GLY	-	SEE REMARK 999	UNP P39077
C	1055	SER	-	SEE REMARK 999	UNP P39077
C	1056	GLY	-	SEE REMARK 999	UNP P39077
K	1001	GLY	-	SEE REMARK 999	UNP P39077
K	1002	SER	-	SEE REMARK 999	UNP P39077
K	1003	GLY	-	SEE REMARK 999	UNP P39077
K	1004	SER	-	SEE REMARK 999	UNP P39077
K	1005	GLY	-	SEE REMARK 999	UNP P39077
K	1006	TRP	-	SEE REMARK 999	UNP P39077
K	1007	SER	-	SEE REMARK 999	UNP P39077
K	1008	HIS	-	SEE REMARK 999	UNP P39077
K	1009	PRO	-	SEE REMARK 999	UNP P39077
K	1010	GLN	-	SEE REMARK 999	UNP P39077
K	1011	PHE	-	SEE REMARK 999	UNP P39077
K	1012	GLU	-	SEE REMARK 999	UNP P39077
K	1013	LYS	-	SEE REMARK 999	UNP P39077
K	1014	GLY	-	SEE REMARK 999	UNP P39077
K	1015	SER	-	SEE REMARK 999	UNP P39077
K	1016	GLY	-	SEE REMARK 999	UNP P39077
K	1017	LYS	-	SEE REMARK 999	UNP P39077
K	1018	ARG	-	SEE REMARK 999	UNP P39077
K	1019	ARG	-	SEE REMARK 999	UNP P39077
K	1020	TRP	-	SEE REMARK 999	UNP P39077
K	1021	LYS	-	SEE REMARK 999	UNP P39077
K	1022	LYS	-	SEE REMARK 999	UNP P39077
K	1023	ASN	-	SEE REMARK 999	UNP P39077
K	1024	PHE	-	SEE REMARK 999	UNP P39077
K	1025	ILE	-	SEE REMARK 999	UNP P39077
K	1026	ALA	-	SEE REMARK 999	UNP P39077
K	1027	VAL	-	SEE REMARK 999	UNP P39077
K	1028	SER	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1029	ALA	-	SEE REMARK 999	UNP P39077
K	1030	ALA	-	SEE REMARK 999	UNP P39077
K	1031	ASN	-	SEE REMARK 999	UNP P39077
K	1032	ARG	-	SEE REMARK 999	UNP P39077
K	1033	PHE	-	SEE REMARK 999	UNP P39077
K	1034	LYS	-	SEE REMARK 999	UNP P39077
K	1035	LYS	-	SEE REMARK 999	UNP P39077
K	1036	ILE	-	SEE REMARK 999	UNP P39077
K	1037	SER	-	SEE REMARK 999	UNP P39077
K	1038	SER	-	SEE REMARK 999	UNP P39077
K	1039	SER	-	SEE REMARK 999	UNP P39077
K	1040	GLY	-	SEE REMARK 999	UNP P39077
K	1041	ALA	-	SEE REMARK 999	UNP P39077
K	1042	LEU	-	SEE REMARK 999	UNP P39077
K	1043	GLY	-	SEE REMARK 999	UNP P39077
K	1044	SER	-	SEE REMARK 999	UNP P39077
K	1045	GLY	-	SEE REMARK 999	UNP P39077
K	1046	HIS	-	SEE REMARK 999	UNP P39077
K	1047	HIS	-	SEE REMARK 999	UNP P39077
K	1048	HIS	-	SEE REMARK 999	UNP P39077
K	1049	HIS	-	SEE REMARK 999	UNP P39077
K	1050	HIS	-	SEE REMARK 999	UNP P39077
K	1051	HIS	-	SEE REMARK 999	UNP P39077
K	1052	HIS	-	SEE REMARK 999	UNP P39077
K	1053	HIS	-	SEE REMARK 999	UNP P39077
K	1054	GLY	-	SEE REMARK 999	UNP P39077
K	1055	SER	-	SEE REMARK 999	UNP P39077
K	1056	GLY	-	SEE REMARK 999	UNP P39077
c	2001	GLY	-	SEE REMARK 999	UNP P39077
c	2002	SER	-	SEE REMARK 999	UNP P39077
c	2003	GLY	-	SEE REMARK 999	UNP P39077
c	2004	SER	-	SEE REMARK 999	UNP P39077
c	2005	GLY	-	SEE REMARK 999	UNP P39077
c	2006	TRP	-	SEE REMARK 999	UNP P39077
c	2007	SER	-	SEE REMARK 999	UNP P39077
c	2008	HIS	-	SEE REMARK 999	UNP P39077
c	2009	PRO	-	SEE REMARK 999	UNP P39077
c	2010	GLN	-	SEE REMARK 999	UNP P39077
c	2011	PHE	-	SEE REMARK 999	UNP P39077
c	2012	GLU	-	SEE REMARK 999	UNP P39077
c	2013	LYS	-	SEE REMARK 999	UNP P39077
c	2014	GLY	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
c	2015	SER	-	SEE REMARK 999	UNP P39077
c	2016	GLY	-	SEE REMARK 999	UNP P39077
c	2017	LYS	-	SEE REMARK 999	UNP P39077
c	2018	ARG	-	SEE REMARK 999	UNP P39077
c	2019	ARG	-	SEE REMARK 999	UNP P39077
c	2020	TRP	-	SEE REMARK 999	UNP P39077
c	2021	LYS	-	SEE REMARK 999	UNP P39077
c	2022	LYS	-	SEE REMARK 999	UNP P39077
c	2023	ASN	-	SEE REMARK 999	UNP P39077
c	2024	PHE	-	SEE REMARK 999	UNP P39077
c	2025	ILE	-	SEE REMARK 999	UNP P39077
c	2026	ALA	-	SEE REMARK 999	UNP P39077
c	2027	VAL	-	SEE REMARK 999	UNP P39077
c	2028	SER	-	SEE REMARK 999	UNP P39077
c	2029	ALA	-	SEE REMARK 999	UNP P39077
c	2030	ALA	-	SEE REMARK 999	UNP P39077
c	2031	ASN	-	SEE REMARK 999	UNP P39077
c	2032	ARG	-	SEE REMARK 999	UNP P39077
c	2033	PHE	-	SEE REMARK 999	UNP P39077
c	2034	LYS	-	SEE REMARK 999	UNP P39077
c	2035	LYS	-	SEE REMARK 999	UNP P39077
c	2036	ILE	-	SEE REMARK 999	UNP P39077
c	2037	SER	-	SEE REMARK 999	UNP P39077
c	2038	SER	-	SEE REMARK 999	UNP P39077
c	2039	SER	-	SEE REMARK 999	UNP P39077
c	2040	GLY	-	SEE REMARK 999	UNP P39077
c	2041	ALA	-	SEE REMARK 999	UNP P39077
c	2042	LEU	-	SEE REMARK 999	UNP P39077
c	2043	GLY	-	SEE REMARK 999	UNP P39077
c	2044	SER	-	SEE REMARK 999	UNP P39077
c	2045	GLY	-	SEE REMARK 999	UNP P39077
c	2046	HIS	-	SEE REMARK 999	UNP P39077
c	2047	HIS	-	SEE REMARK 999	UNP P39077
c	2048	HIS	-	SEE REMARK 999	UNP P39077
c	2049	HIS	-	SEE REMARK 999	UNP P39077
c	2050	HIS	-	SEE REMARK 999	UNP P39077
c	2051	HIS	-	SEE REMARK 999	UNP P39077
c	2052	HIS	-	SEE REMARK 999	UNP P39077
c	2053	HIS	-	SEE REMARK 999	UNP P39077
c	2054	GLY	-	SEE REMARK 999	UNP P39077
c	2055	SER	-	SEE REMARK 999	UNP P39077
c	2056	GLY	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
k	2001	GLY	-	SEE REMARK 999	UNP P39077
k	2002	SER	-	SEE REMARK 999	UNP P39077
k	2003	GLY	-	SEE REMARK 999	UNP P39077
k	2004	SER	-	SEE REMARK 999	UNP P39077
k	2005	GLY	-	SEE REMARK 999	UNP P39077
k	2006	TRP	-	SEE REMARK 999	UNP P39077
k	2007	SER	-	SEE REMARK 999	UNP P39077
k	2008	HIS	-	SEE REMARK 999	UNP P39077
k	2009	PRO	-	SEE REMARK 999	UNP P39077
k	2010	GLN	-	SEE REMARK 999	UNP P39077
k	2011	PHE	-	SEE REMARK 999	UNP P39077
k	2012	GLU	-	SEE REMARK 999	UNP P39077
k	2013	LYS	-	SEE REMARK 999	UNP P39077
k	2014	GLY	-	SEE REMARK 999	UNP P39077
k	2015	SER	-	SEE REMARK 999	UNP P39077
k	2016	GLY	-	SEE REMARK 999	UNP P39077
k	2017	LYS	-	SEE REMARK 999	UNP P39077
k	2018	ARG	-	SEE REMARK 999	UNP P39077
k	2019	ARG	-	SEE REMARK 999	UNP P39077
k	2020	TRP	-	SEE REMARK 999	UNP P39077
k	2021	LYS	-	SEE REMARK 999	UNP P39077
k	2022	LYS	-	SEE REMARK 999	UNP P39077
k	2023	ASN	-	SEE REMARK 999	UNP P39077
k	2024	PHE	-	SEE REMARK 999	UNP P39077
k	2025	ILE	-	SEE REMARK 999	UNP P39077
k	2026	ALA	-	SEE REMARK 999	UNP P39077
k	2027	VAL	-	SEE REMARK 999	UNP P39077
k	2028	SER	-	SEE REMARK 999	UNP P39077
k	2029	ALA	-	SEE REMARK 999	UNP P39077
k	2030	ALA	-	SEE REMARK 999	UNP P39077
k	2031	ASN	-	SEE REMARK 999	UNP P39077
k	2032	ARG	-	SEE REMARK 999	UNP P39077
k	2033	PHE	-	SEE REMARK 999	UNP P39077
k	2034	LYS	-	SEE REMARK 999	UNP P39077
k	2035	LYS	-	SEE REMARK 999	UNP P39077
k	2036	ILE	-	SEE REMARK 999	UNP P39077
k	2037	SER	-	SEE REMARK 999	UNP P39077
k	2038	SER	-	SEE REMARK 999	UNP P39077
k	2039	SER	-	SEE REMARK 999	UNP P39077
k	2040	GLY	-	SEE REMARK 999	UNP P39077
k	2041	ALA	-	SEE REMARK 999	UNP P39077
k	2042	LEU	-	SEE REMARK 999	UNP P39077

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Chain	Residue	Modelled	Actual	Comment	Reference
k	2043	GLY	-	SEE REMARK 999	UNP P39077
k	2044	SER	-	SEE REMARK 999	UNP P39077
k	2045	GLY	-	SEE REMARK 999	UNP P39077
k	2046	HIS	-	SEE REMARK 999	UNP P39077
k	2047	HIS	-	SEE REMARK 999	UNP P39077
k	2048	HIS	-	SEE REMARK 999	UNP P39077
k	2049	HIS	-	SEE REMARK 999	UNP P39077
k	2050	HIS	-	SEE REMARK 999	UNP P39077
k	2051	HIS	-	SEE REMARK 999	UNP P39077
k	2052	HIS	-	SEE REMARK 999	UNP P39077
k	2053	HIS	-	SEE REMARK 999	UNP P39077
k	2054	GLY	-	SEE REMARK 999	UNP P39077
k	2055	SER	-	SEE REMARK 999	UNP P39077
k	2056	GLY	-	SEE REMARK 999	UNP P39077

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			
4	L	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			
4	d	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			
4	l	522	Total	C	N	O	S	0	0	0
			3398	2092	609	686	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	345	ASP	GLY	engineered mutation	UNP P39078
L	345	ASP	GLY	engineered mutation	UNP P39078
d	1345	ASP	GLY	engineered mutation	UNP P39078
l	1345	ASP	GLY	engineered mutation	UNP P39078

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			
5	M	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	e	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			
5	m	525	Total	C	N	O	S	0	0	0
			3437	2110	599	720	8			

- Molecule 6 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	533	Total	C	N	O	S	0	0	0
			3631	2253	629	740	9			
6	N	533	Total	C	N	O	S	0	0	0
			3628	2250	629	740	9			
6	f	533	Total	C	N	O	S	0	0	0
			3633	2255	630	739	9			
6	n	533	Total	C	N	O	S	0	0	0
			3629	2252	629	739	9			

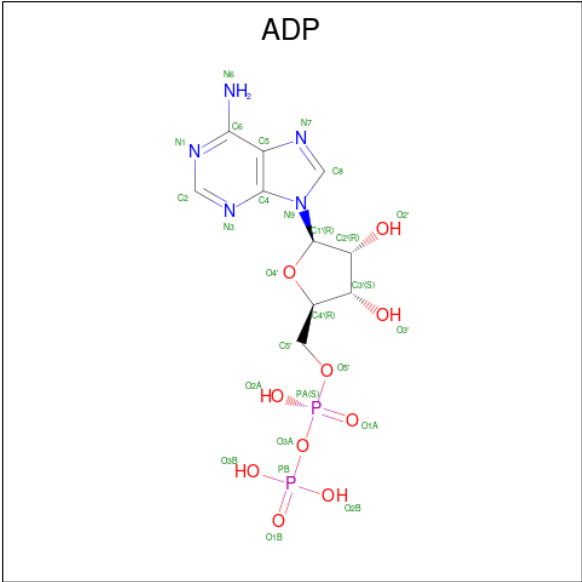
- Molecule 7 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	509	Total	C	N	O	S	0	0	0
			3317	2055	583	669	10			
7	O	509	Total	C	N	O	S	0	0	0
			3314	2052	583	669	10			
7	g	509	Total	C	N	O	S	0	0	0
			3314	2052	583	669	10			
7	o	509	Total	C	N	O	S	0	0	0
			3314	2052	583	669	10			

- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	525	Total	C	N	O	S	0	0	0
			3487	2161	608	705	13			
8	P	525	Total	C	N	O	S	0	0	0
			3487	2161	608	705	13			
8	h	525	Total	C	N	O	S	0	0	0
			3485	2159	608	705	13			
8	p	525	Total	C	N	O	S	0	0	0
			3487	2161	608	705	13			

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



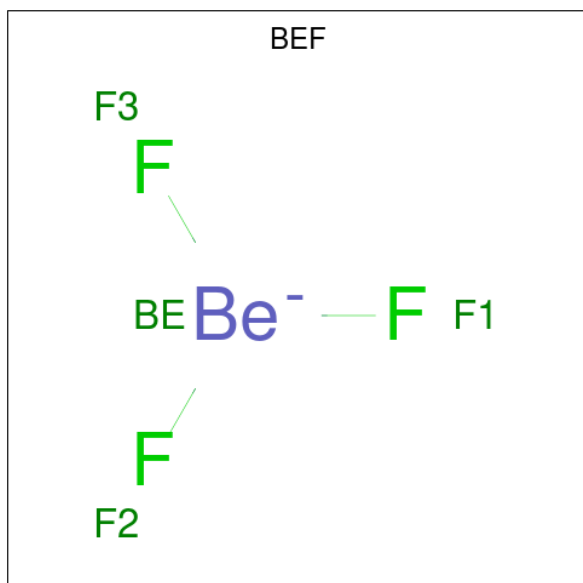
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	a	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	b	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	e	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	f	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	g	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	h	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	k	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	l	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	m	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	n	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	p	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 10 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	Be	F	0	0
			4	1	3		

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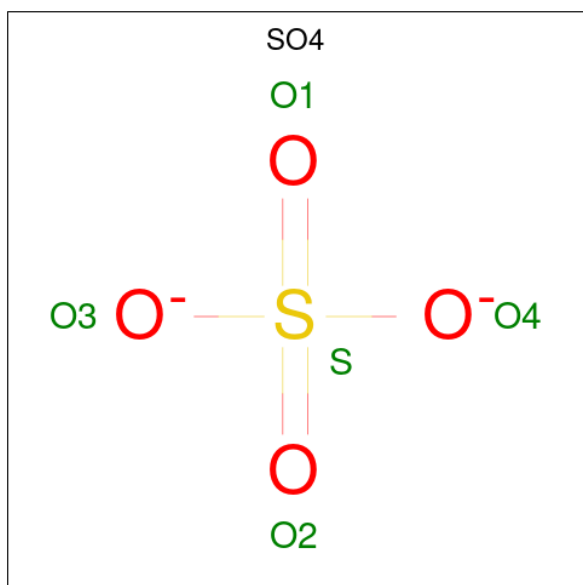
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total 4	Be 1	F 3	0	0
10	C	1	Total 4	Be 1	F 3	0	0
10	D	1	Total 4	Be 1	F 3	0	0
10	E	1	Total 4	Be 1	F 3	0	0
10	F	1	Total 4	Be 1	F 3	0	0
10	G	1	Total 4	Be 1	F 3	0	0
10	H	1	Total 4	Be 1	F 3	0	0
10	J	1	Total 4	Be 1	F 3	0	0
10	L	1	Total 4	Be 1	F 3	0	0
10	M	1	Total 4	Be 1	F 3	0	0
10	N	1	Total 4	Be 1	F 3	0	0
10	P	1	Total 4	Be 1	F 3	0	0
10	a	1	Total 4	Be 1	F 3	0	0
10	b	1	Total 4	Be 1	F 3	0	0
10	e	1	Total 4	Be 1	F 3	0	0
10	f	1	Total 4	Be 1	F 3	0	0
10	g	1	Total 4	Be 1	F 3	0	0
10	h	1	Total 4	Be 1	F 3	0	0
10	k	1	Total 4	Be 1	F 3	0	0
10	l	1	Total 4	Be 1	F 3	0	0
10	m	1	Total 4	Be 1	F 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	n	1	Total	Be	F	0	0
			4	1	3		
10	p	1	Total	Be	F	0	0
			4	1	3		

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	I	1	Total	O	S	0	0
			5	4	1		
11	K	1	Total	O	S	0	0
			5	4	1		
11	O	1	Total	O	S	0	0
			5	4	1		
11	c	1	Total	O	S	0	0
			5	4	1		
11	d	1	Total	O	S	0	0
			5	4	1		
11	i	1	Total	O	S	0	0
			5	4	1		
11	j	1	Total	O	S	0	0
			5	4	1		
11	o	1	Total	O	S	0	0
			5	4	1		

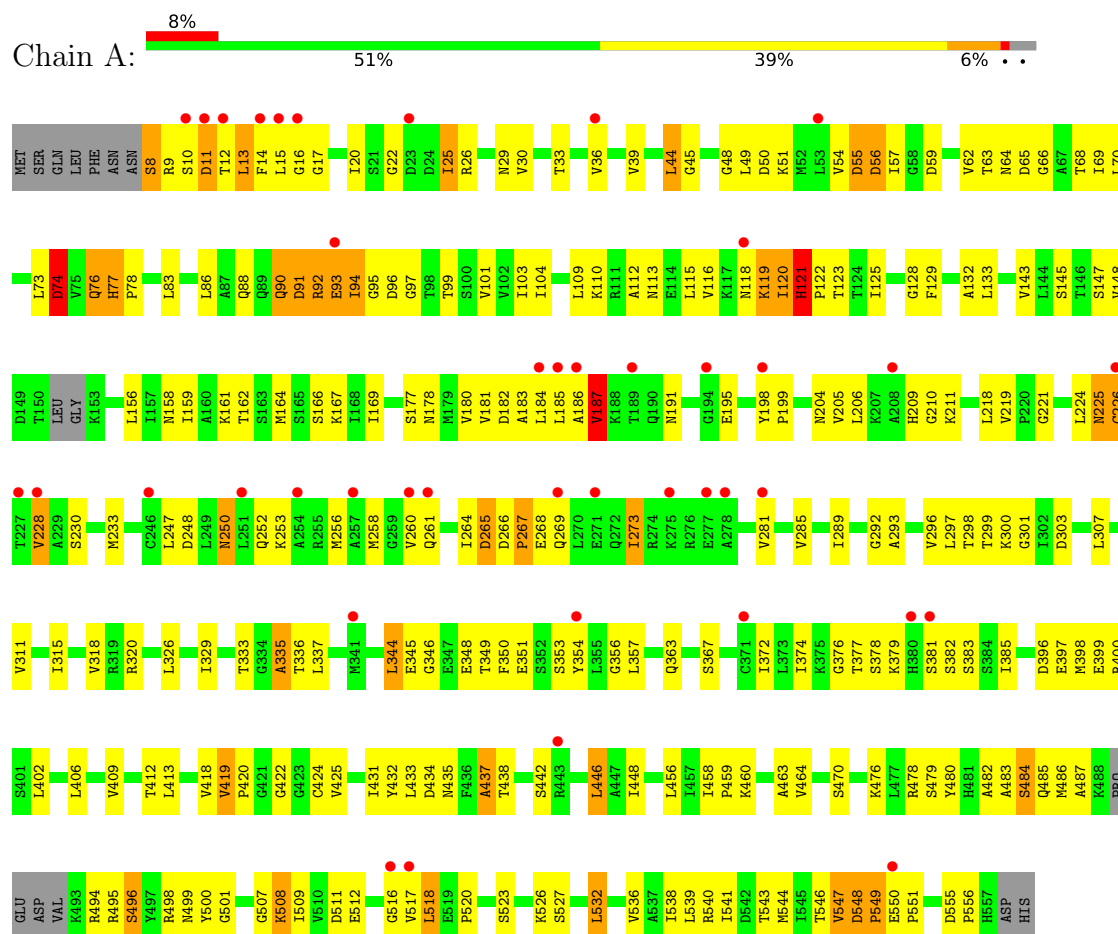
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total 1	O 1	0	0
12	E	1	Total 1	O 1	0	0
12	G	1	Total 1	O 1	0	0
12	M	1	Total 1	O 1	0	0
12	e	1	Total 1	O 1	0	0
12	g	1	Total 1	O 1	0	0
12	m	1	Total 1	O 1	0	0

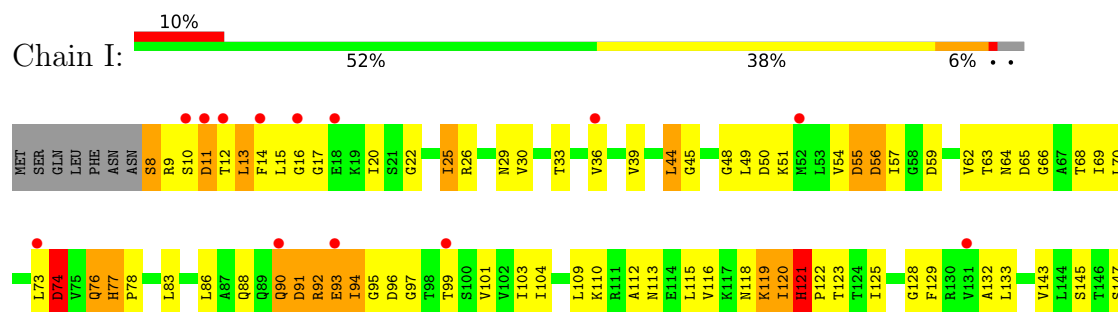
3 Residue-property plots

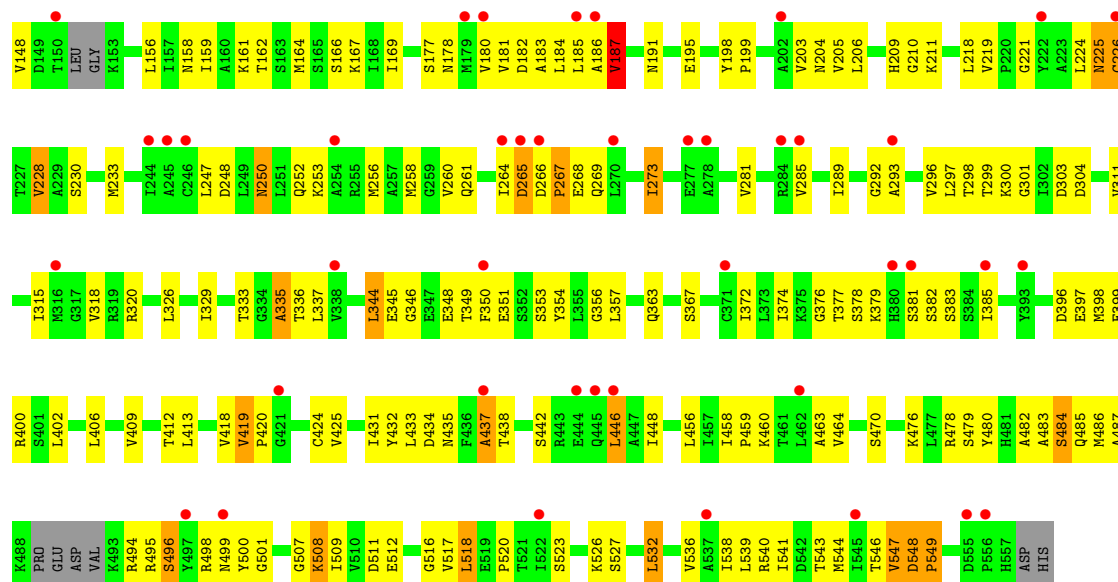
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: T-complex protein 1 subunit alpha

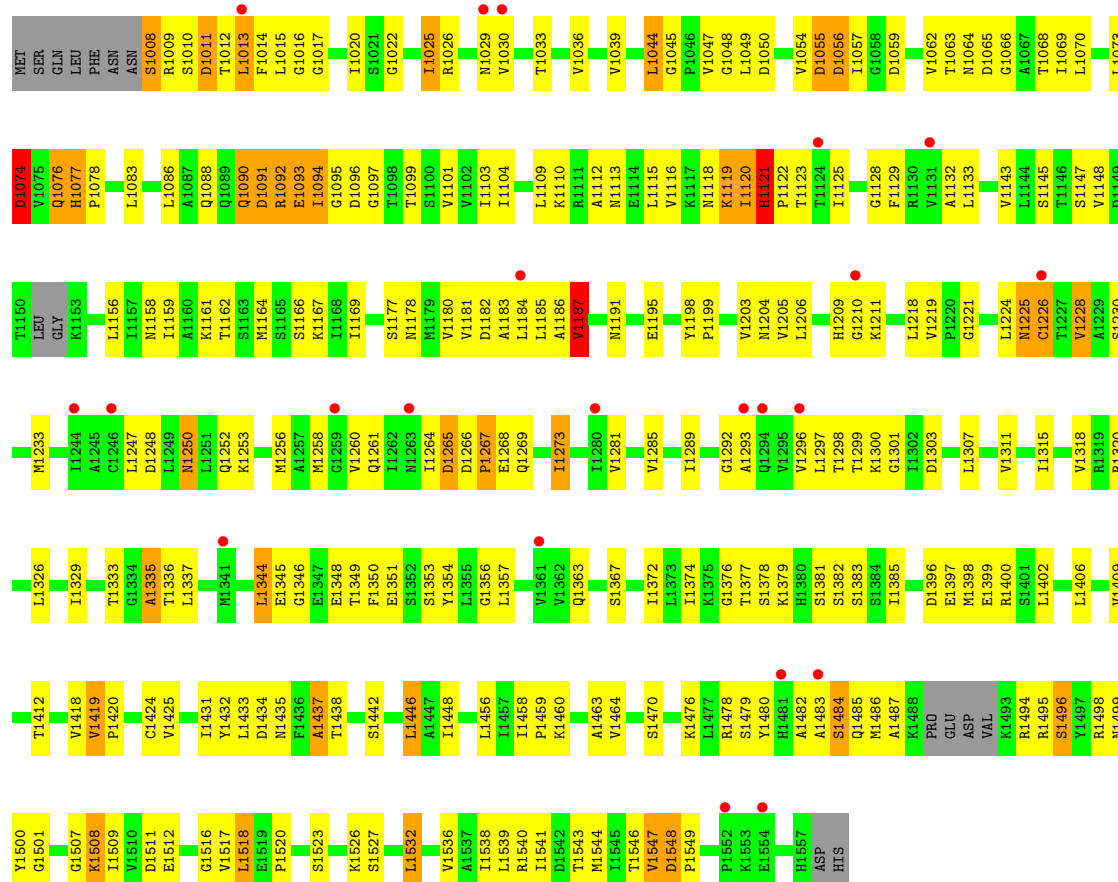


• Molecule 1: T-complex protein 1 subunit alpha



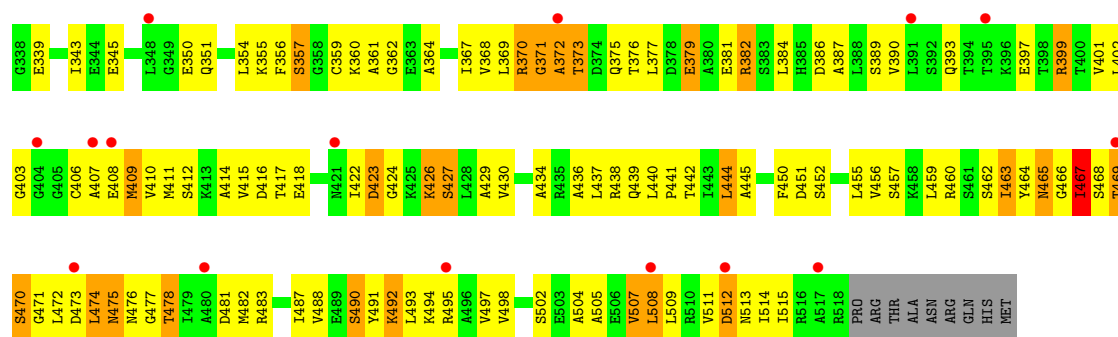


• Molecule 1: T-complex protein 1 subunit alpha

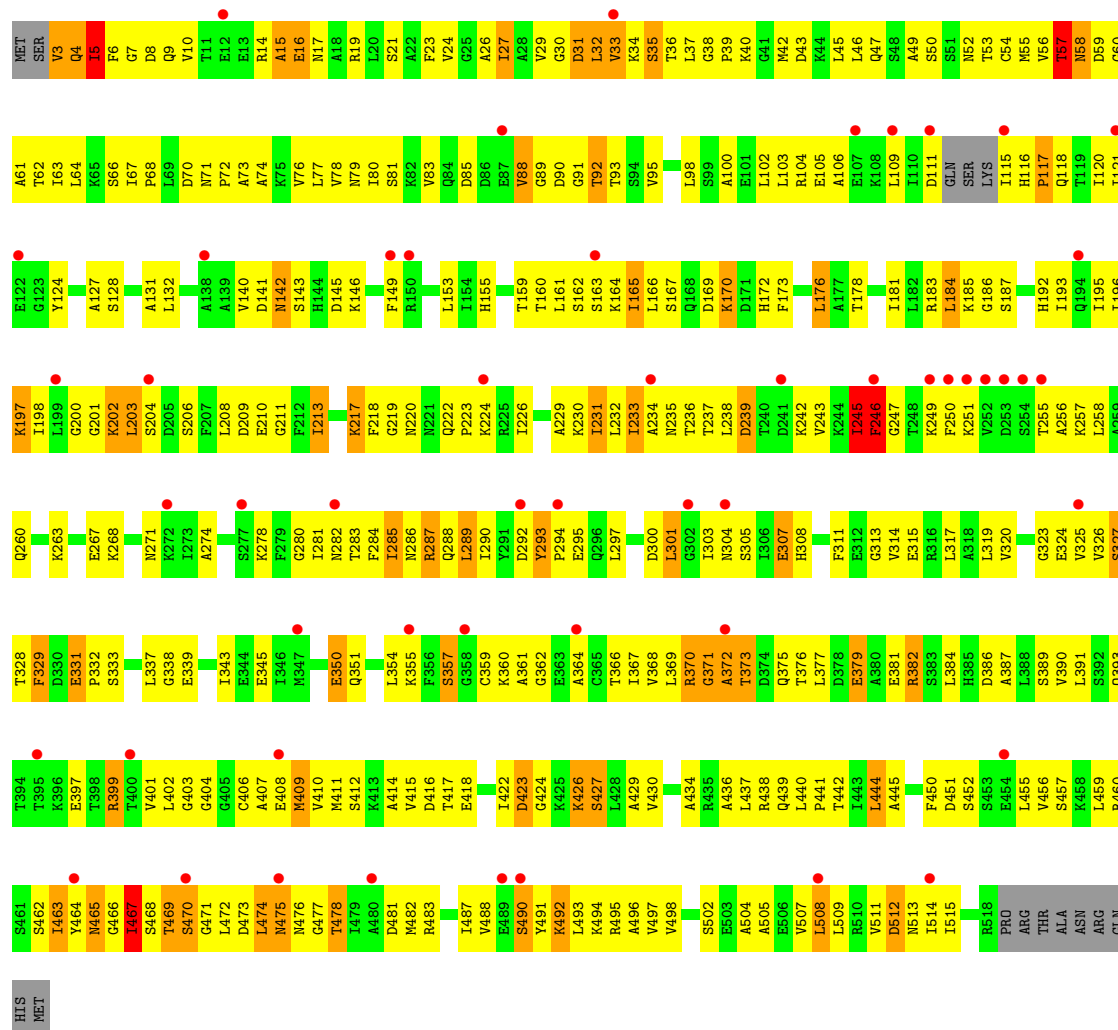


• Molecule 1: T-complex protein 1 subunit alpha



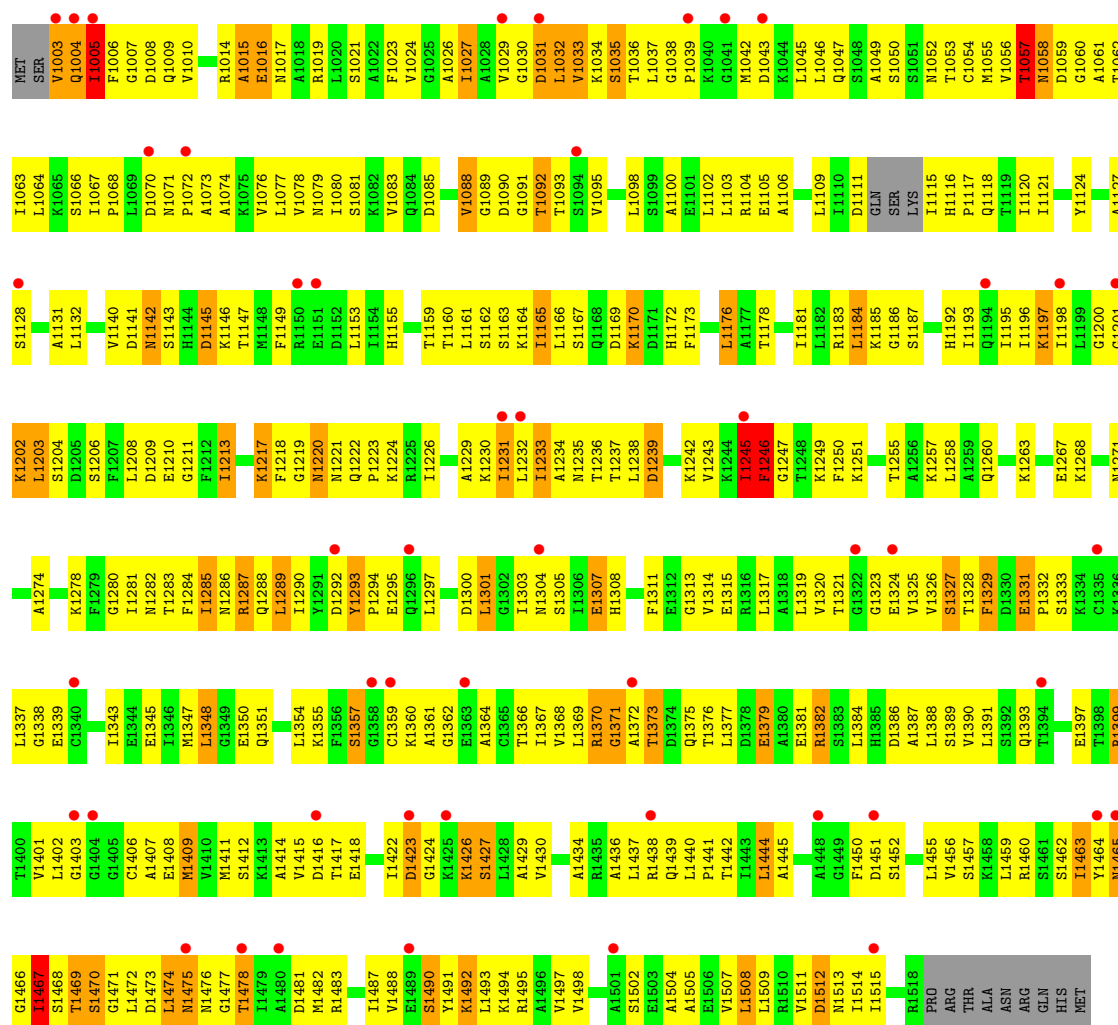


• Molecule 2: T-complex protein 1 subunit beta

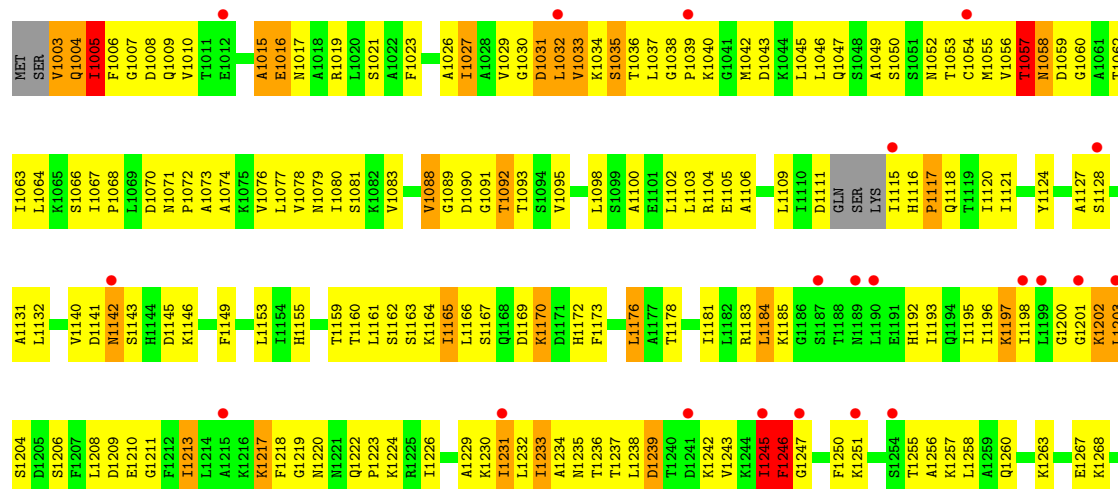


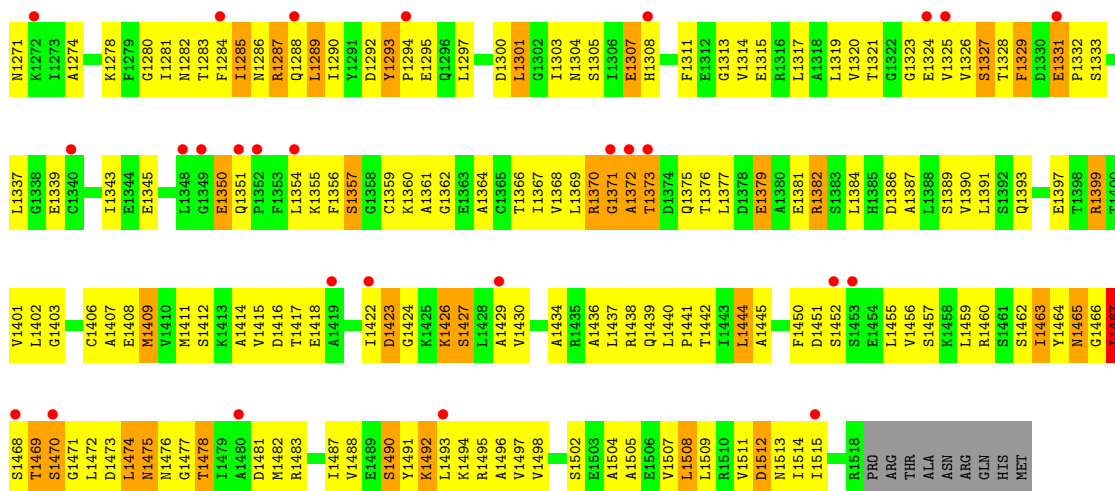
• Molecule 2: T-complex protein 1 subunit beta



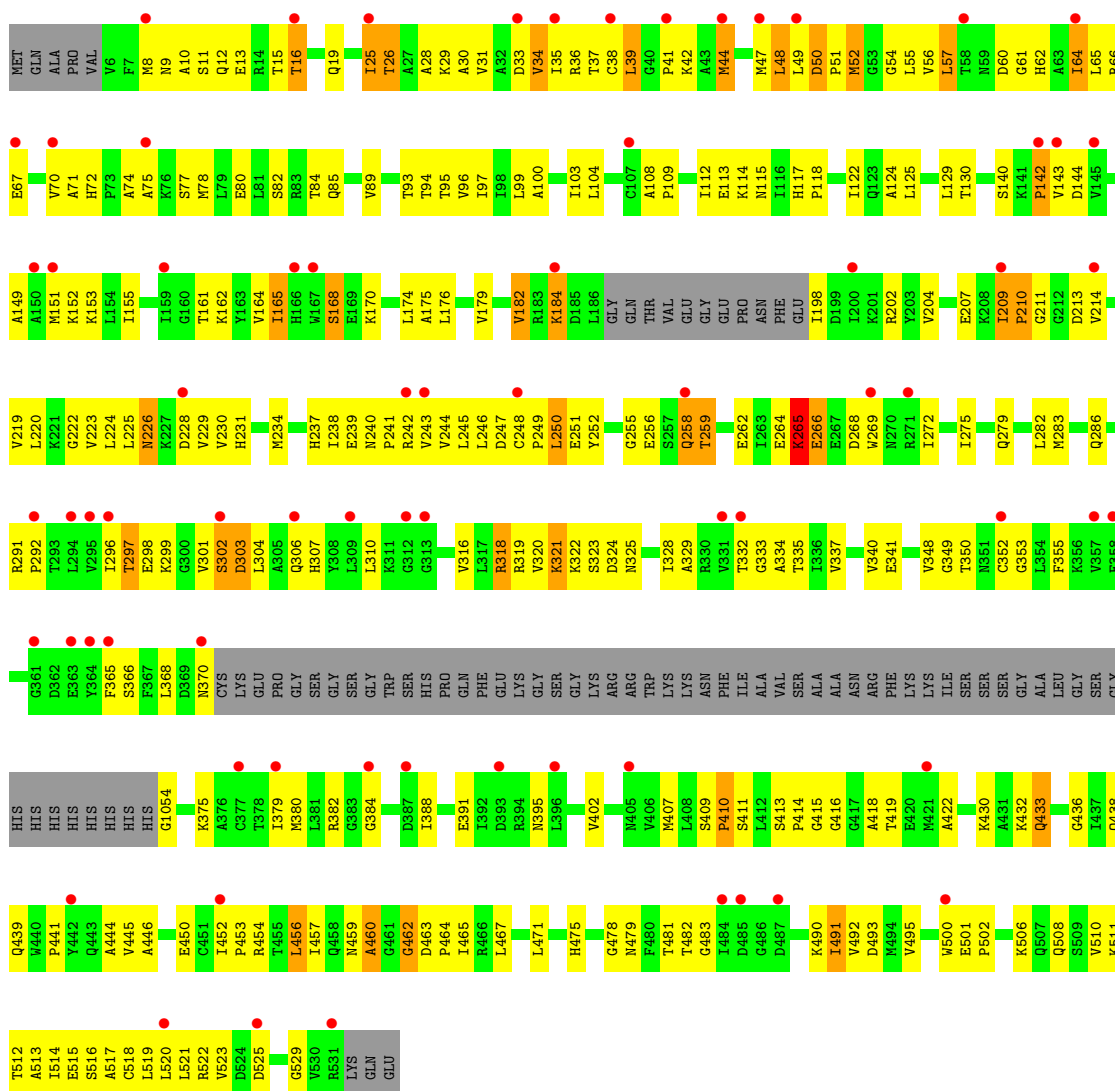


Chain j: 9% 35% 50% 11% ..





• Molecule 3: T-complex protein 1 subunit gamma

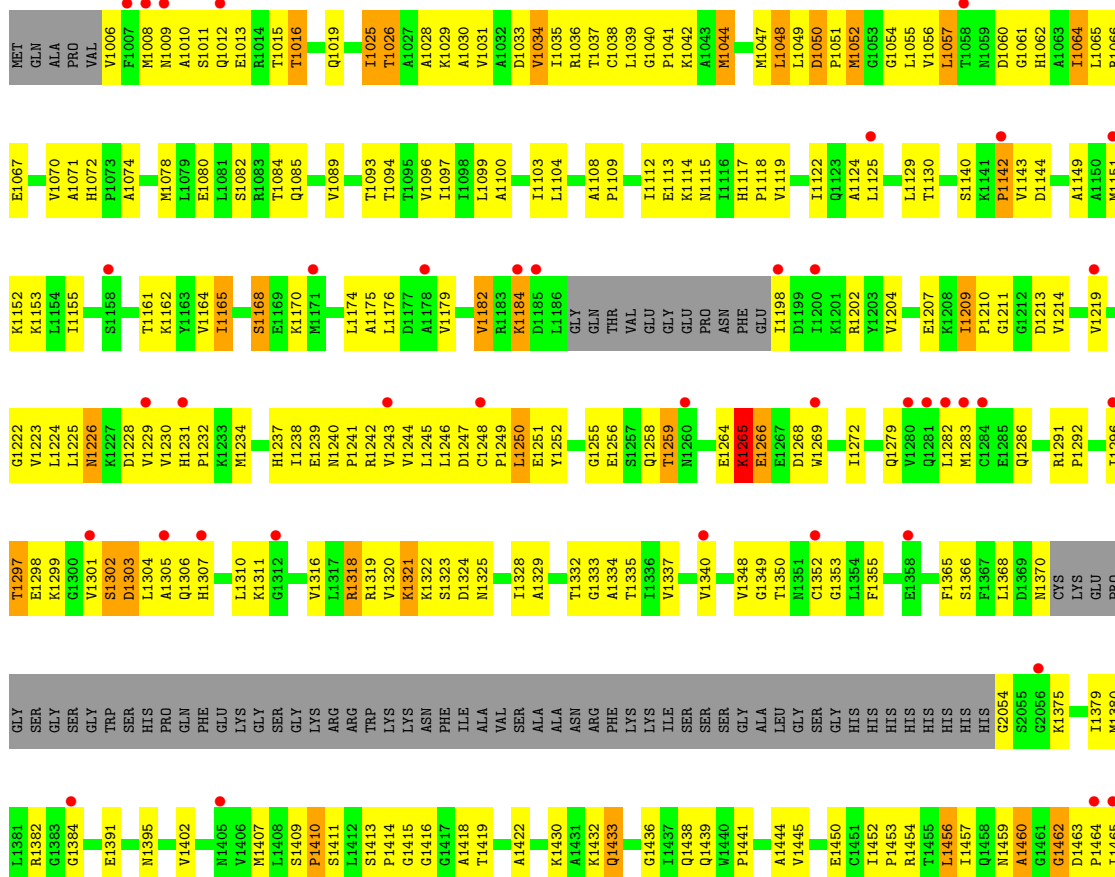


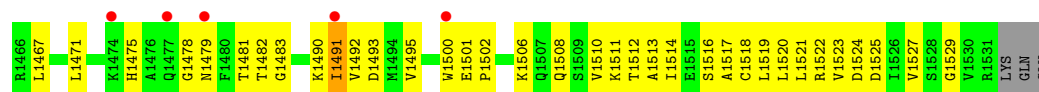
Chain K:

Residue Type	Count
Green	43
Yellow	39
Orange	5
Grey	13
Red Dot	9

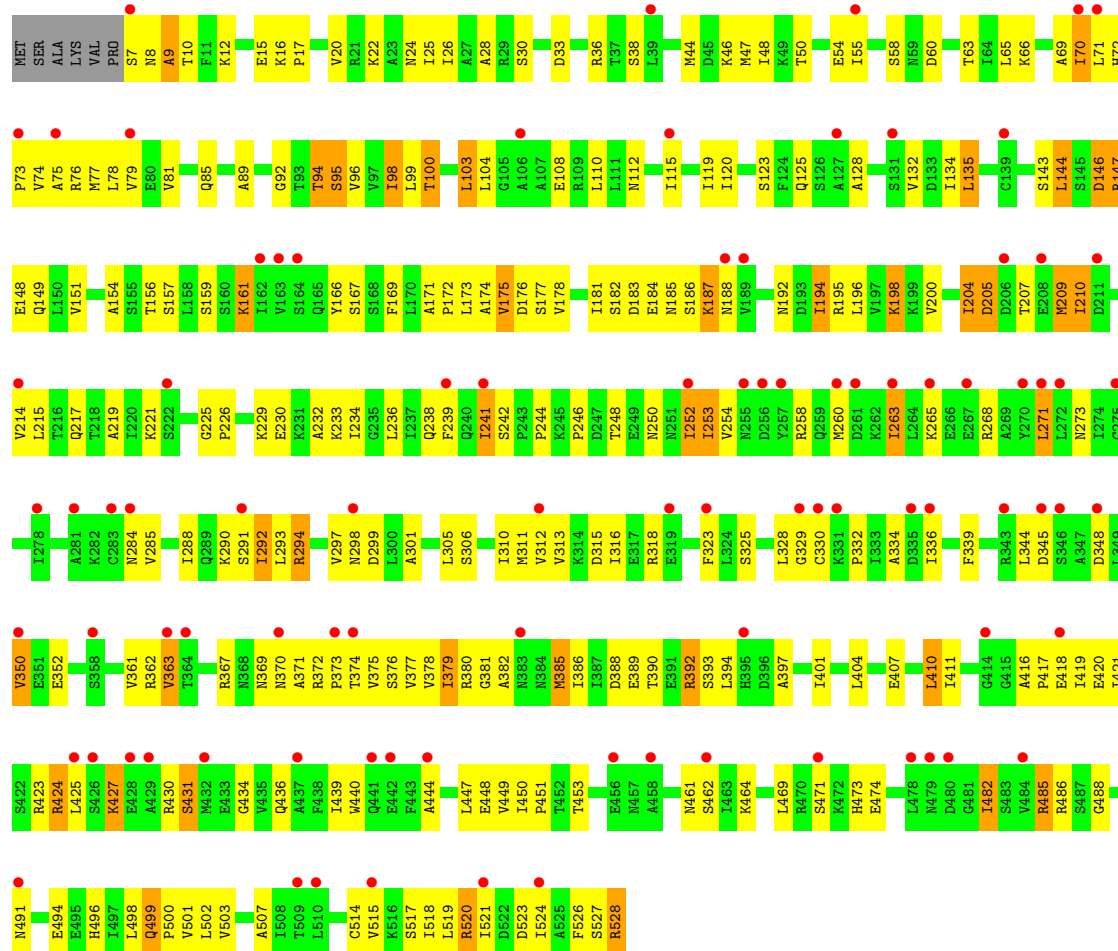
Chain c:

Amino Acid	Percentage
Met	7%
Gln	
Ala	
Pro	
Val	
Val006	
P1007	
M1008	
N1009	
A1010	
S1011	
Q1012	
E1013	
R1014	
T1015	
T1016	
Q1019	
T1025	
A1026	
A1028	
K1029	
A1030	
V1031	
A1032	
D1033	
V1034	
I1035	
K1036	
T1037	
C1038	
L1039	
G1040	
P1041	
K1042	
A1043	
M1044	
M1047	
L1048	
L1049	
D1050	
P1051	
M1052	
G1053	
G1054	
L1055	
V1056	
L1057	
T1058	
N1059	
D1060	
G1061	
H1062	
A1063	
I1064	
L1065	
P1066	
E1067	
V1070	
A1071	
H1072	
P1073	
A1074	
A1075	
K1076	
S1077	
E1080	
L1081	
S1082	
R1083	
T1084	
Q1085	
V1089	
T1093	
T1095	
V1096	
I1097	
I1098	
L1099	
A1100	
I1103	
L1104	
L1110	
A1108	
P1109	
L1112	
E1113	
K1114	
L1115	
I1116	
A1117	
P1118	
V1119	
T1120	
I1121	
I1122	
G1123	
L1124	
L1125	
L1129	
T1130	
S1140	
P1141	
T1142	
V1143	
D1144	
A1145	
V1146	
E1147	
D1148	
A1149	
A1150	
M1151	
K1152	
K1153	
L1154	
I1155	
T1161	
K1162	
T1163	
V1164	
I1165	
S1168	
E1169	
K1170	
M1171	
L1174	
A1175	
L1176	
V1179	
V1182	
R1183	
K1184	
D1185	
L1186	
GLY	
GLN	
THR	
VAL	
GLU	
GLY	
GLU	
PRO	
ASN	
PHE	
GLU	
I1198	
R1202	
V1203	
V1204	
E1207	
K1208	
I1209	
P1210	
D1213	
V1214	
V1219	
L1220	
V1223	

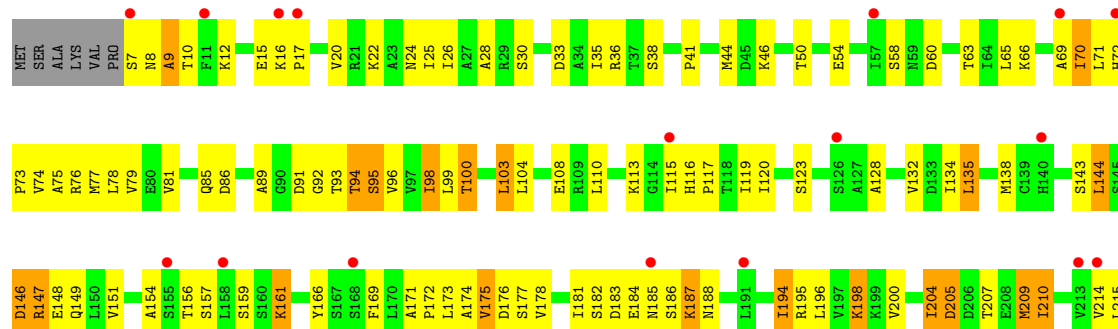


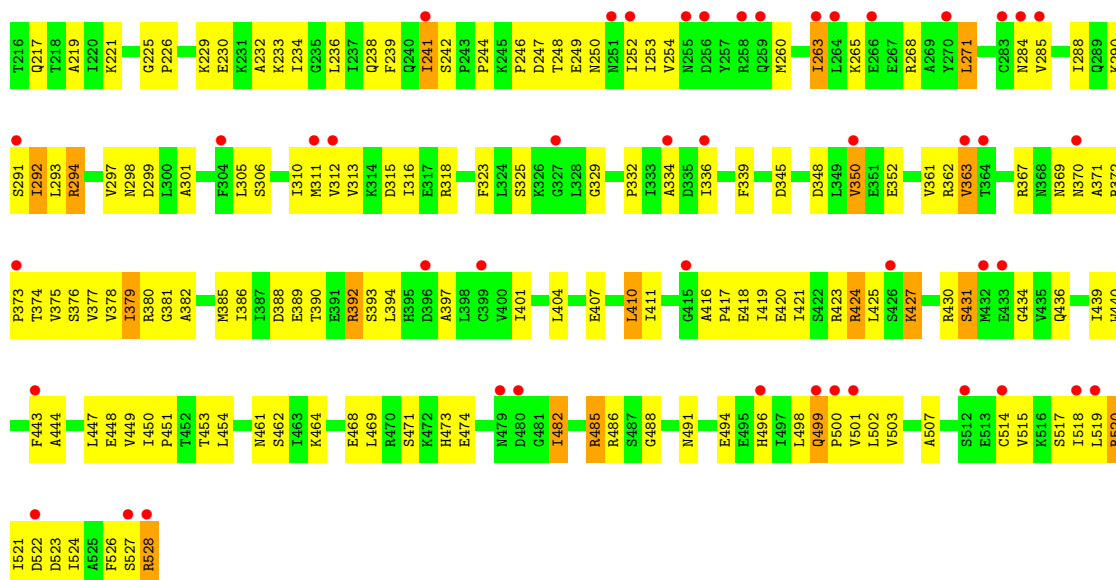


• Molecule 4: T-complex protein 1 subunit delta

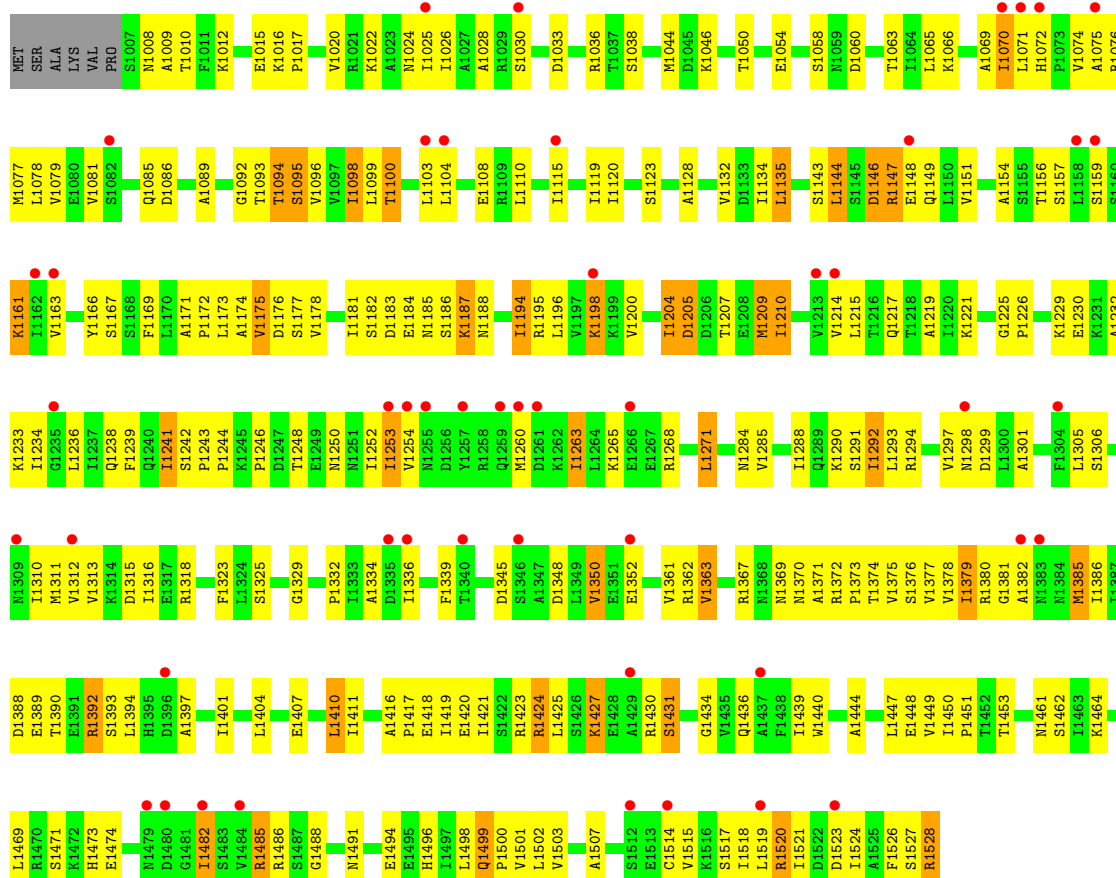


• Molecule 4: T-complex protein 1 subunit delta

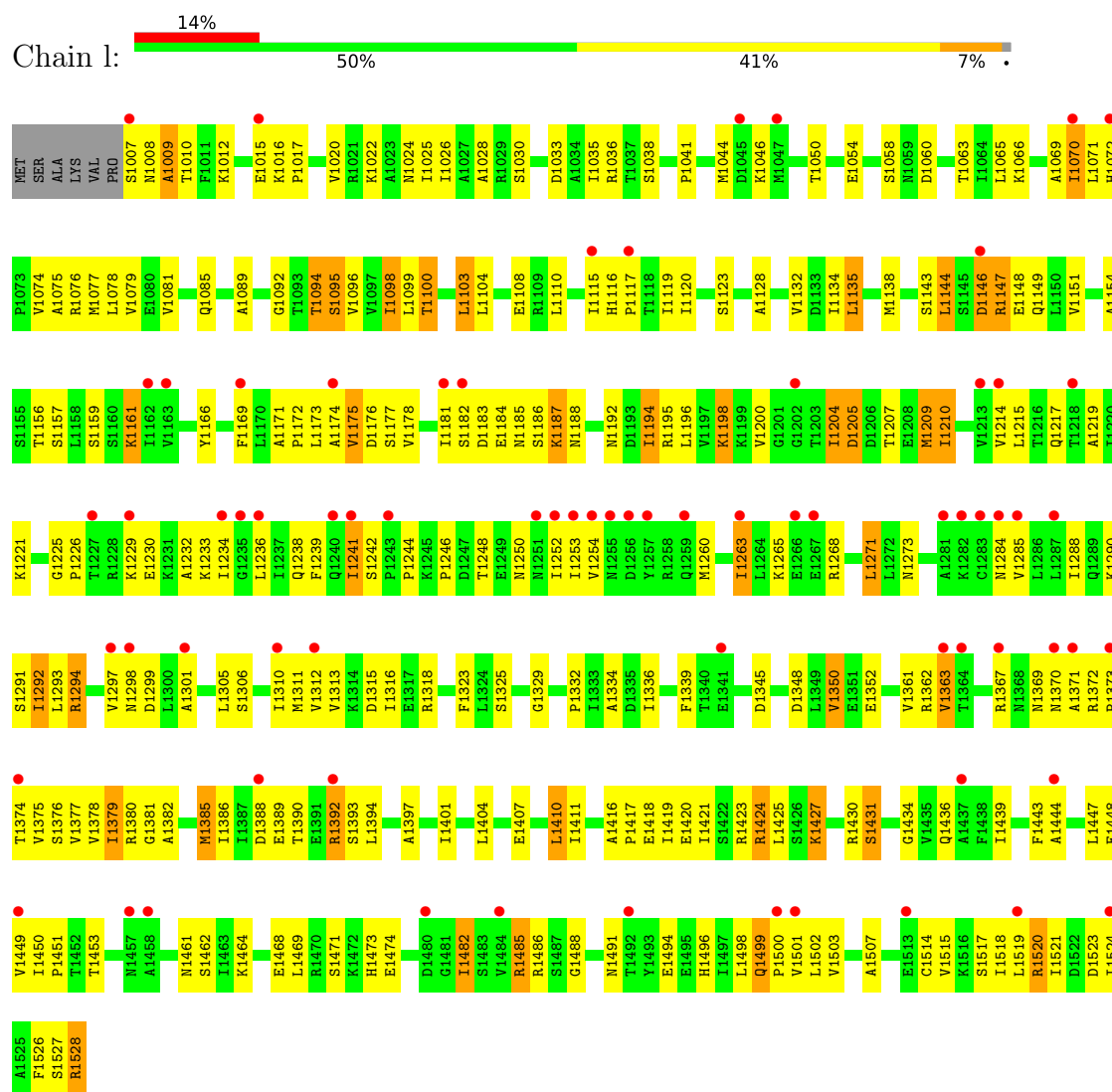




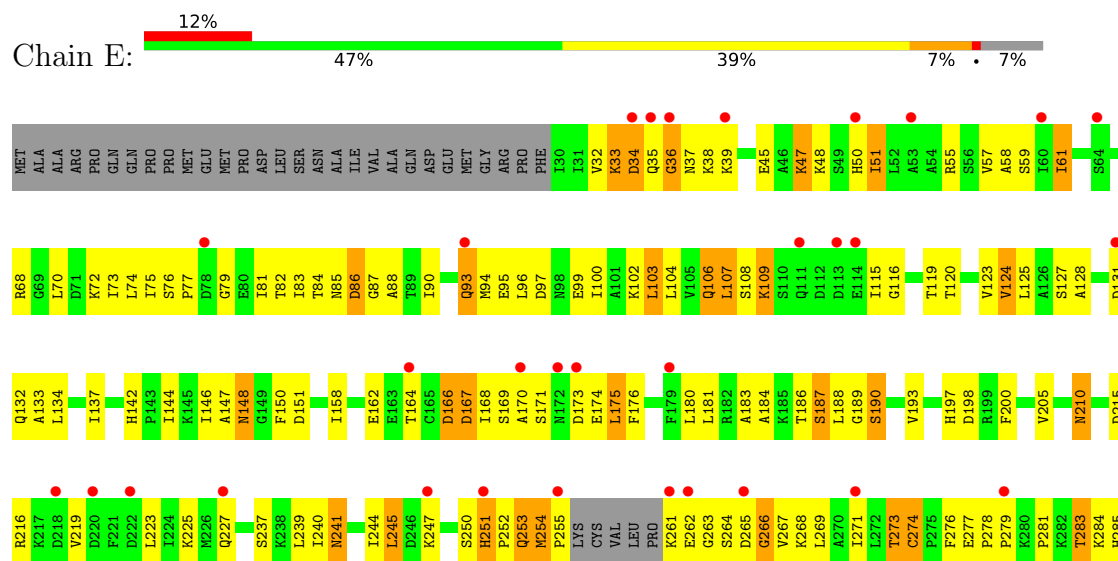
• Molecule 4: T-complex protein 1 subunit delta

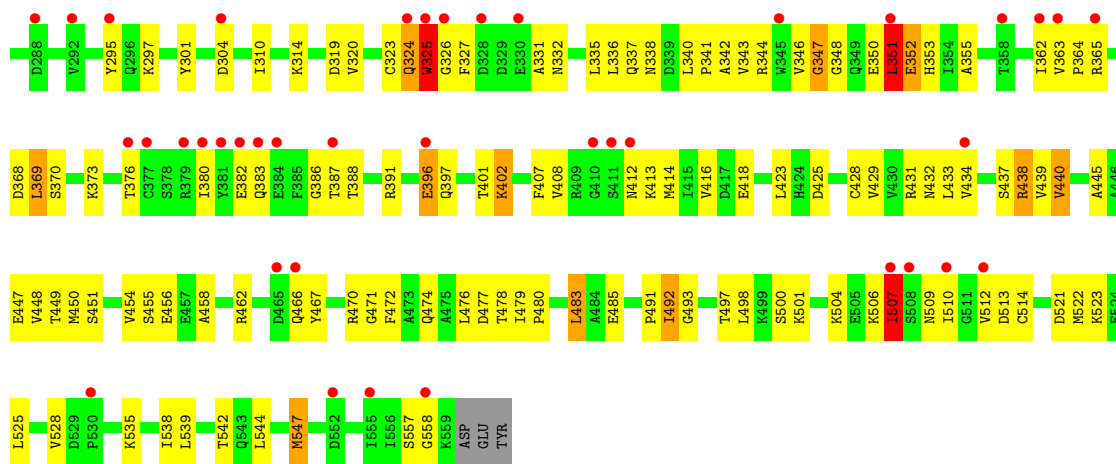


• Molecule 4: T-complex protein 1 subunit delta

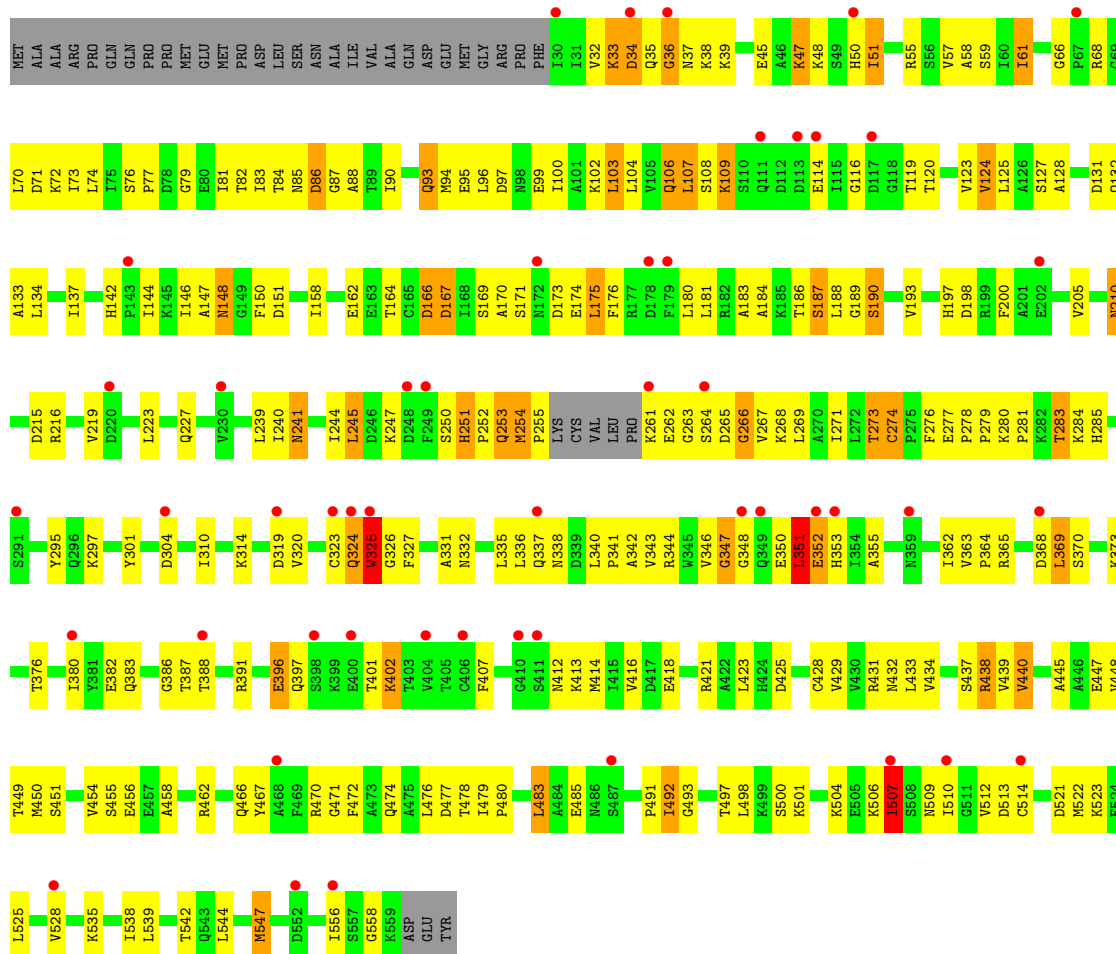


• Molecule 5: T-complex protein 1 subunit epsilon



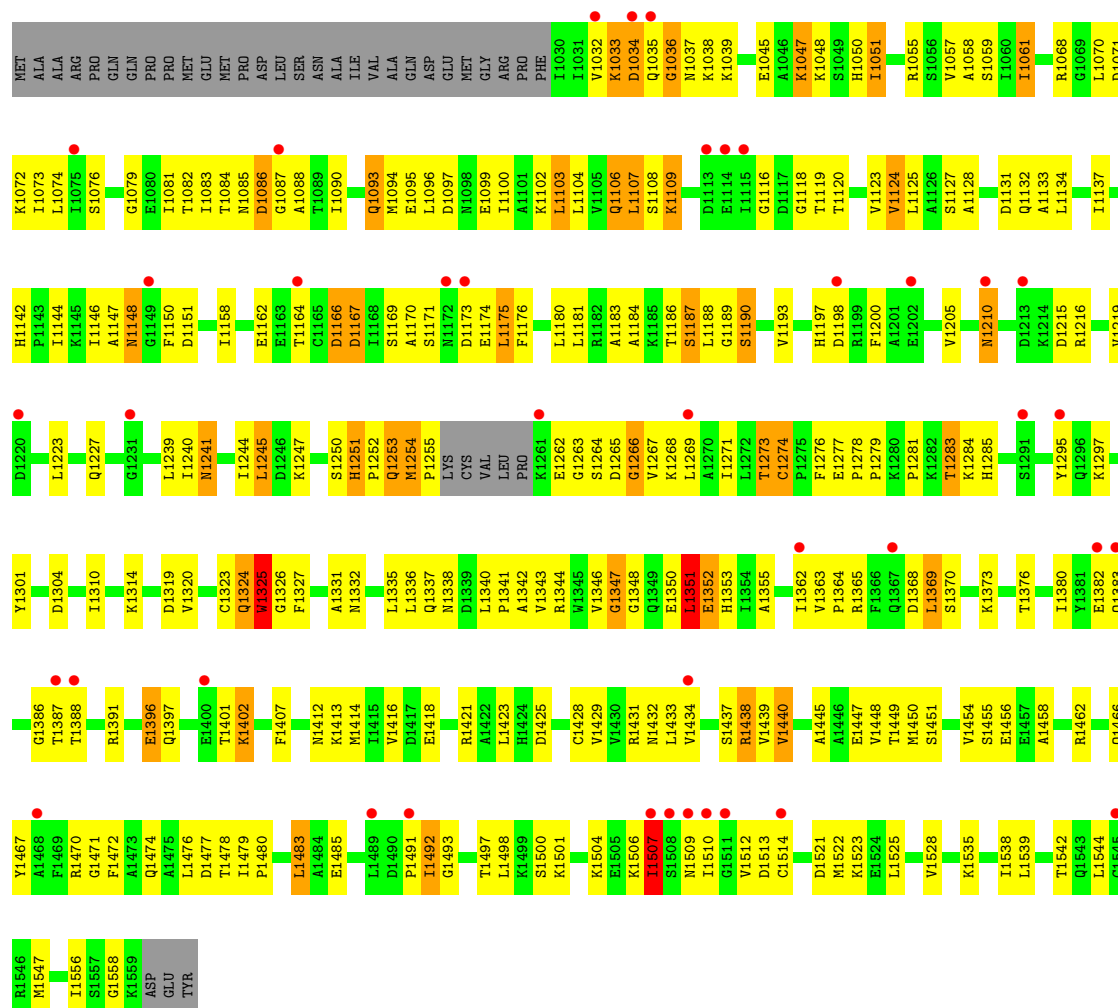


• Molecule 5: T-complex protein 1 subunit epsilon

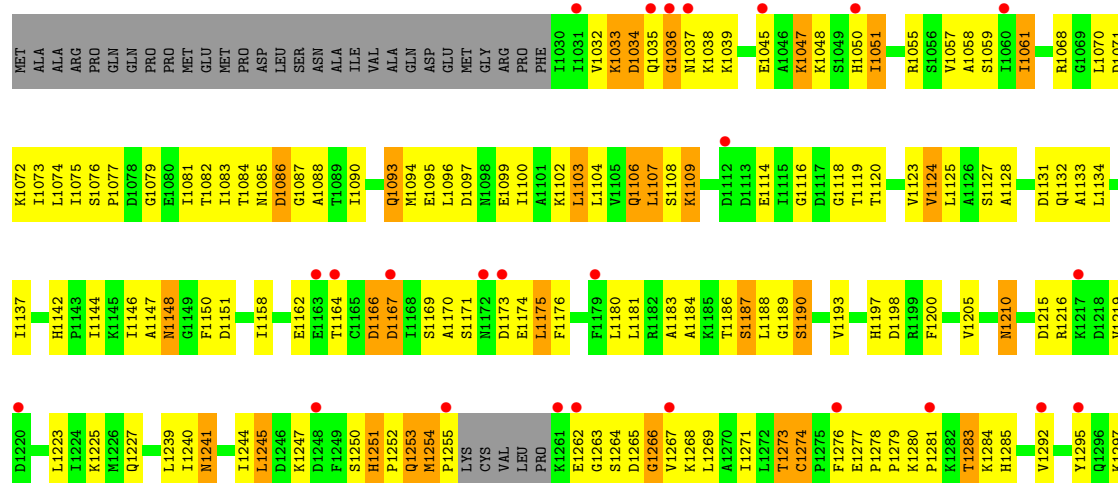


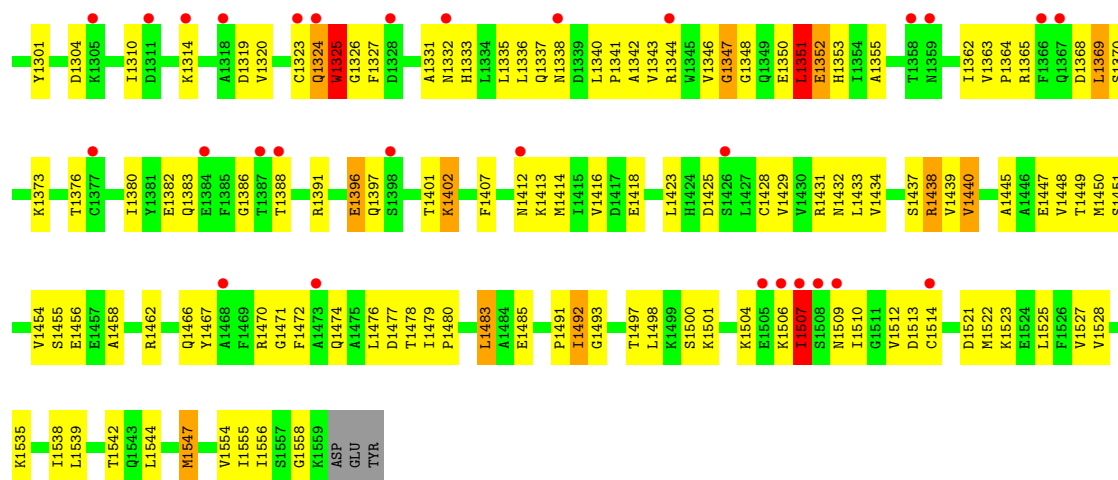
• Molecule 5: T-complex protein 1 subunit epsilon



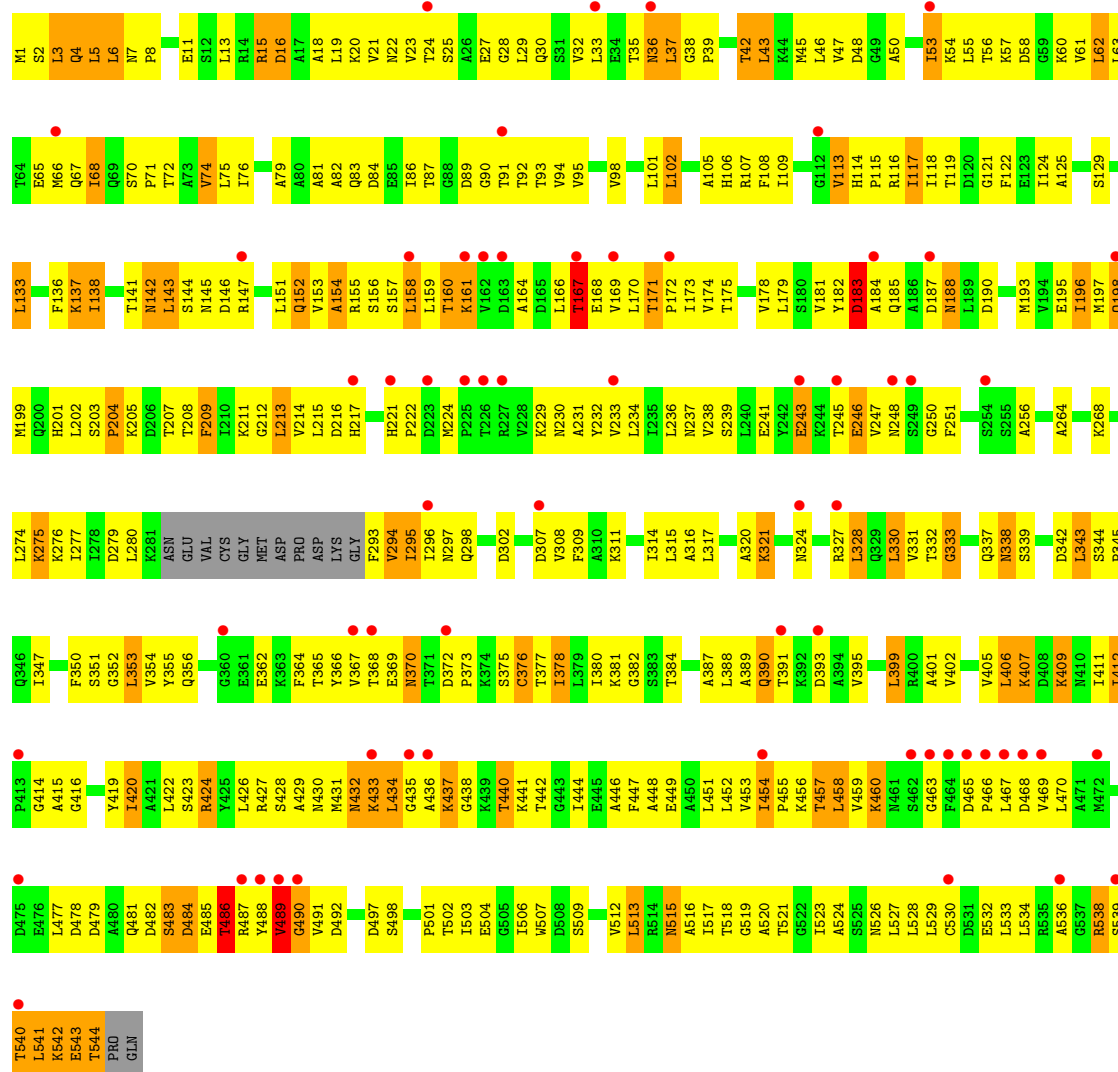


• Molecule 5: T-complex protein 1 subunit epsilon

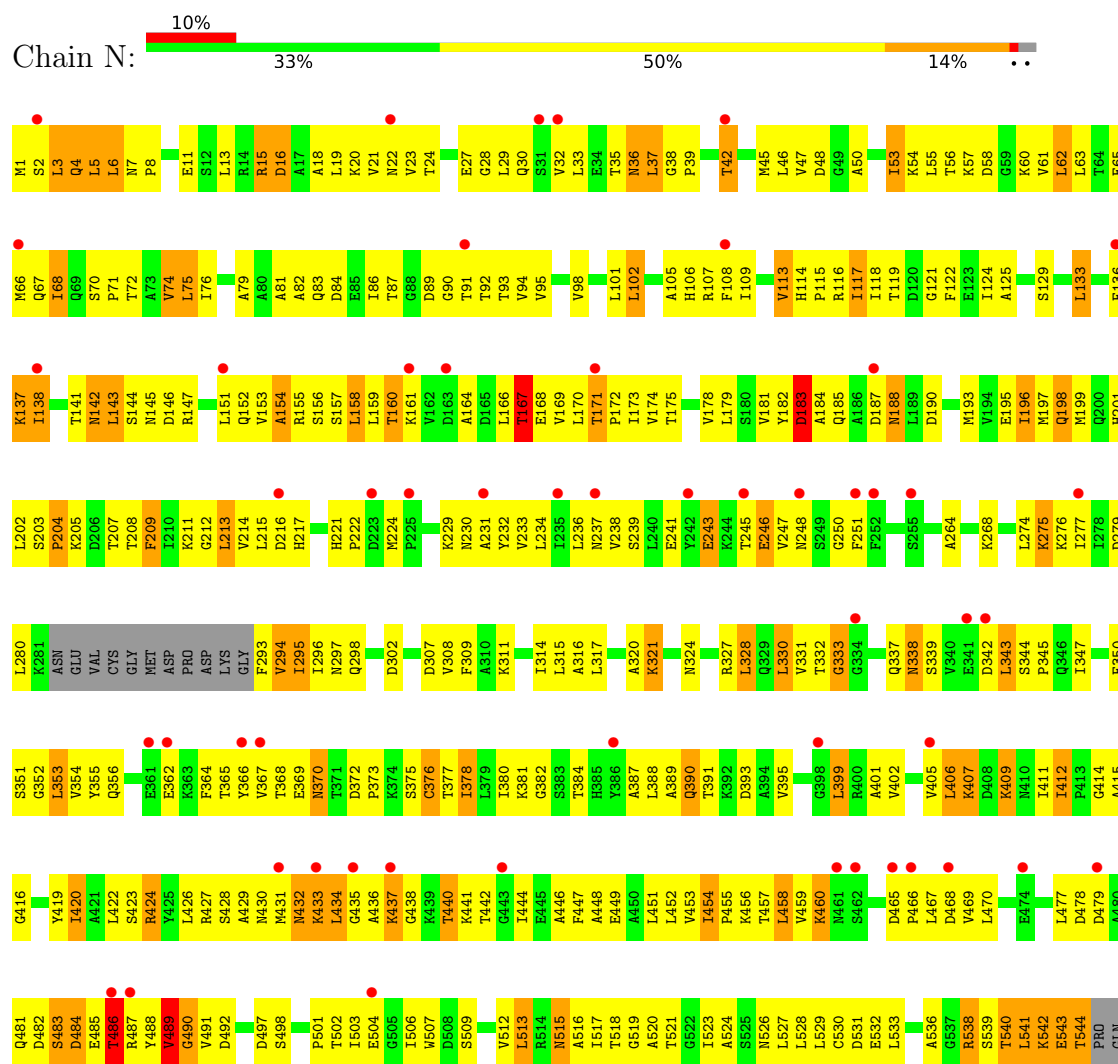




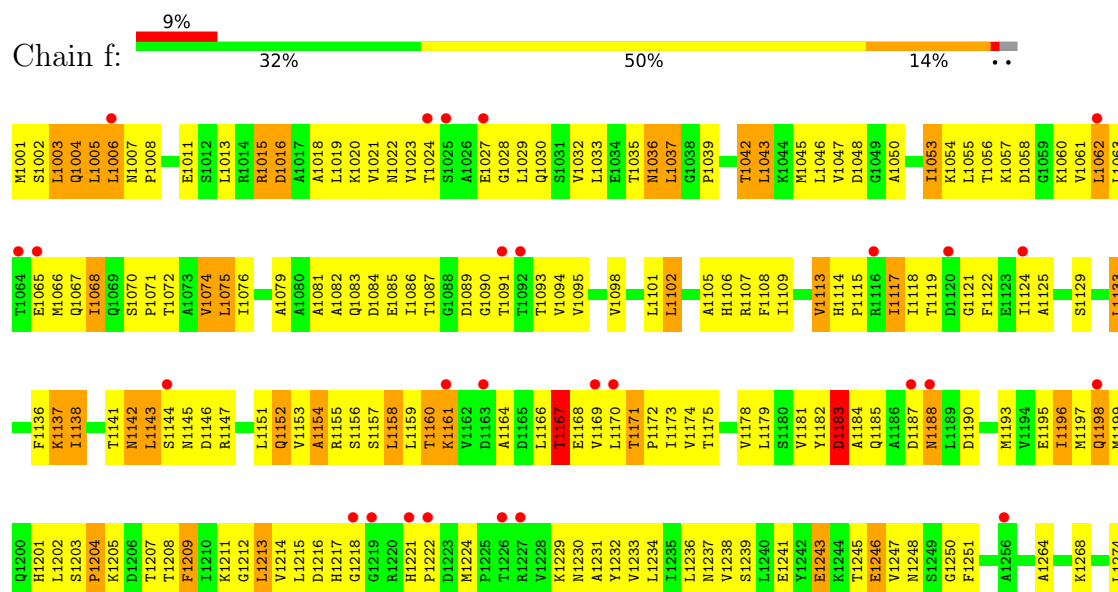
• Molecule 6: T-complex protein 1 subunit zeta

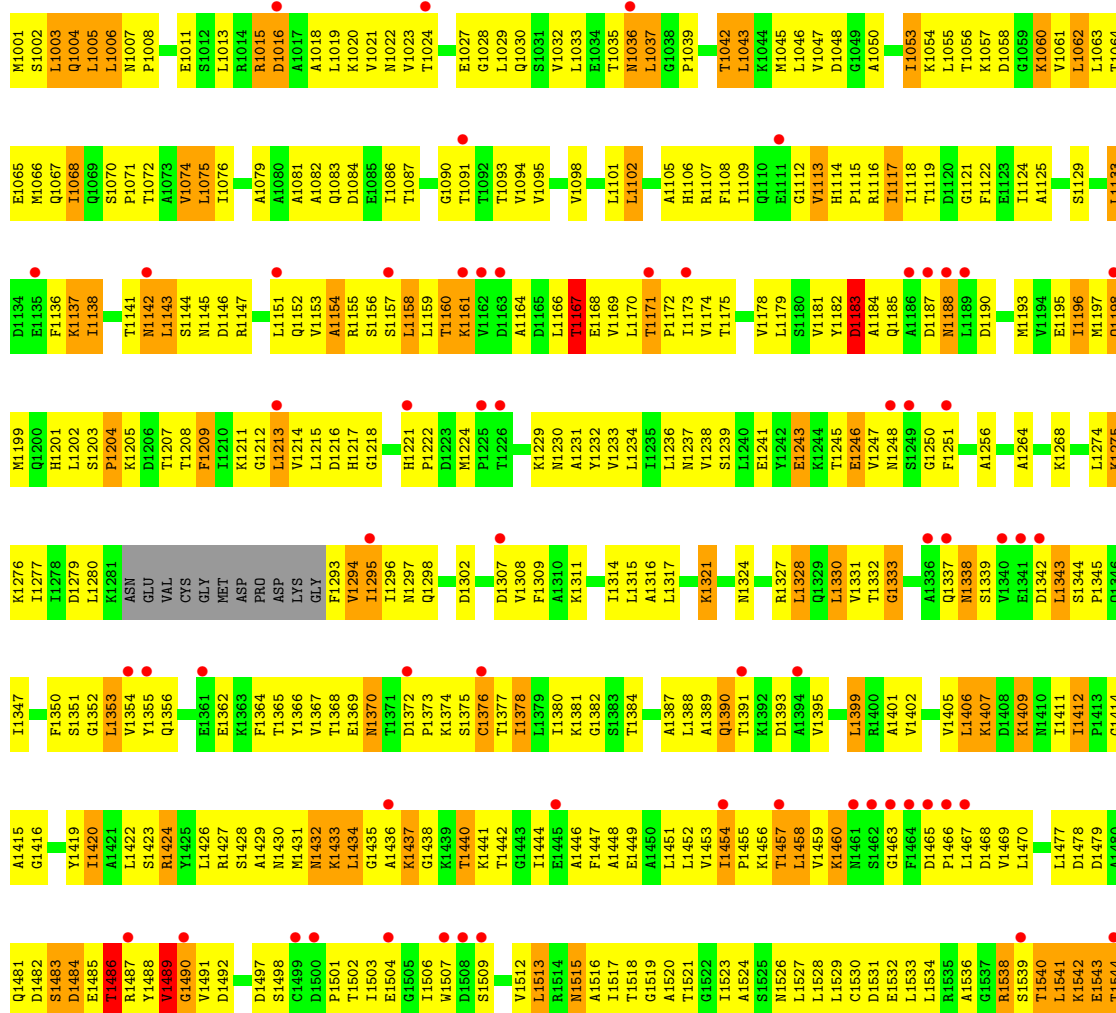
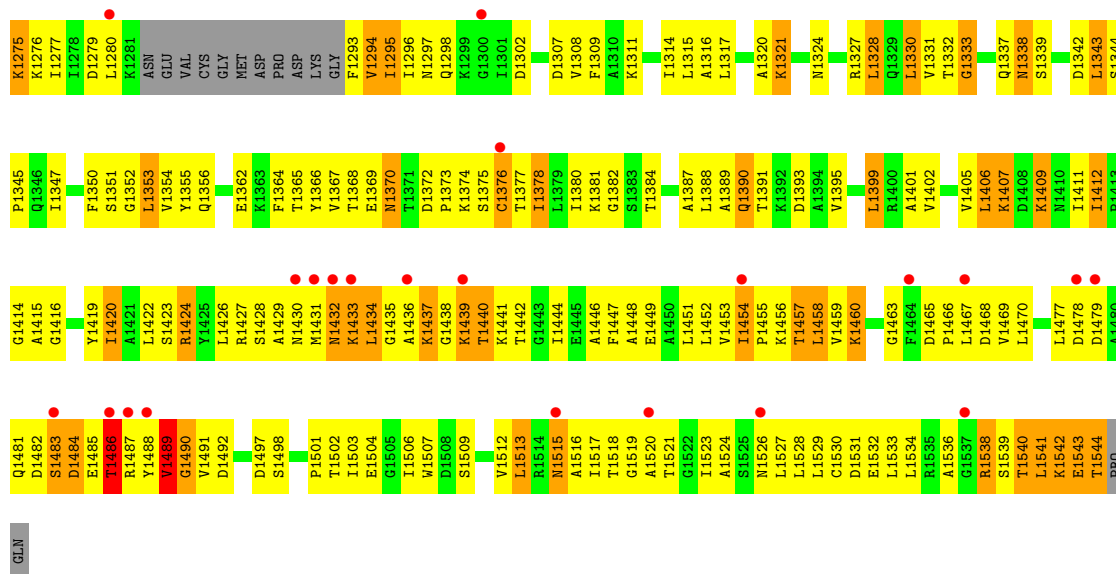


● Molecule 6: T-complex protein 1 subunit zeta



● Molecule 6: T-complex protein 1 subunit zeta

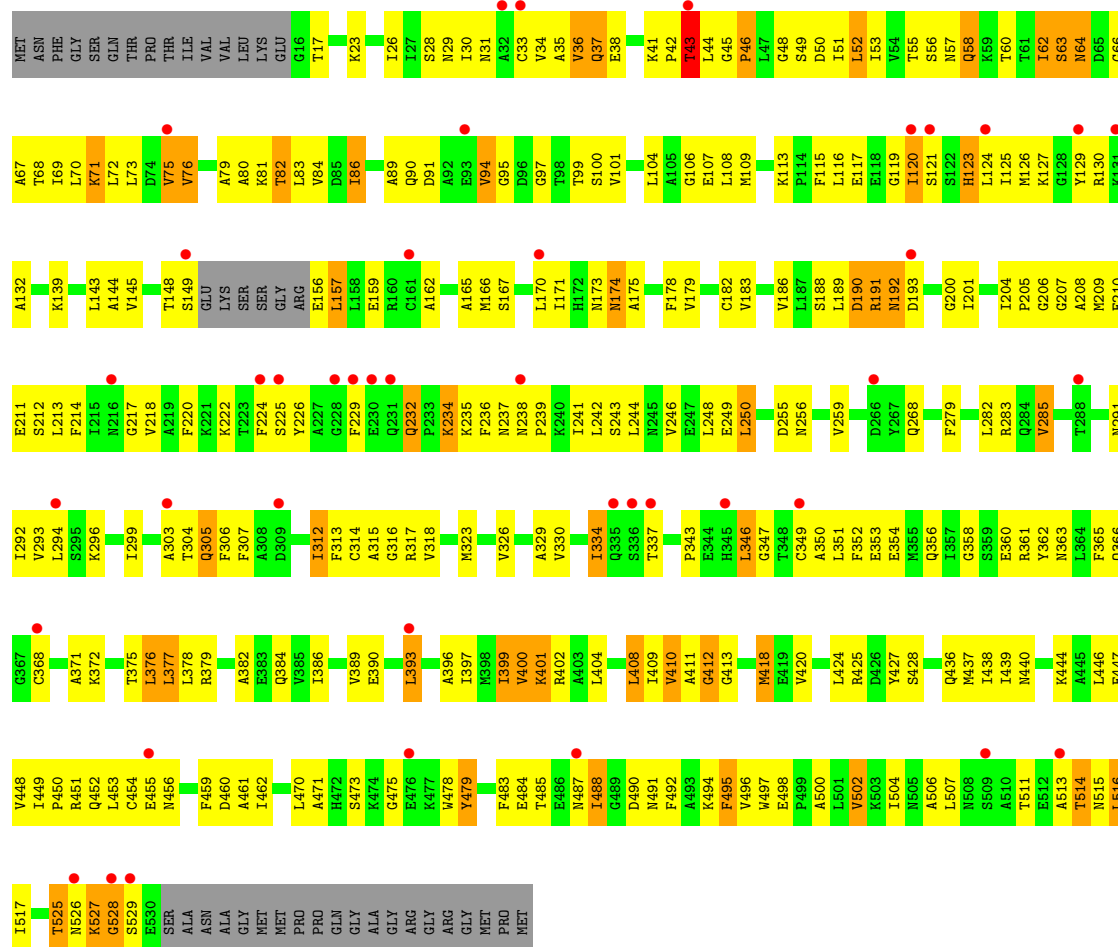




PRO
GLN

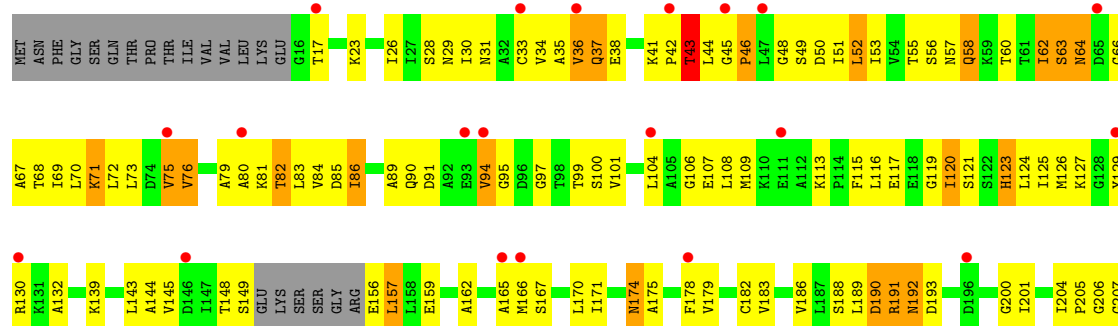
• Molecule 7: T-complex protein 1 subunit eta

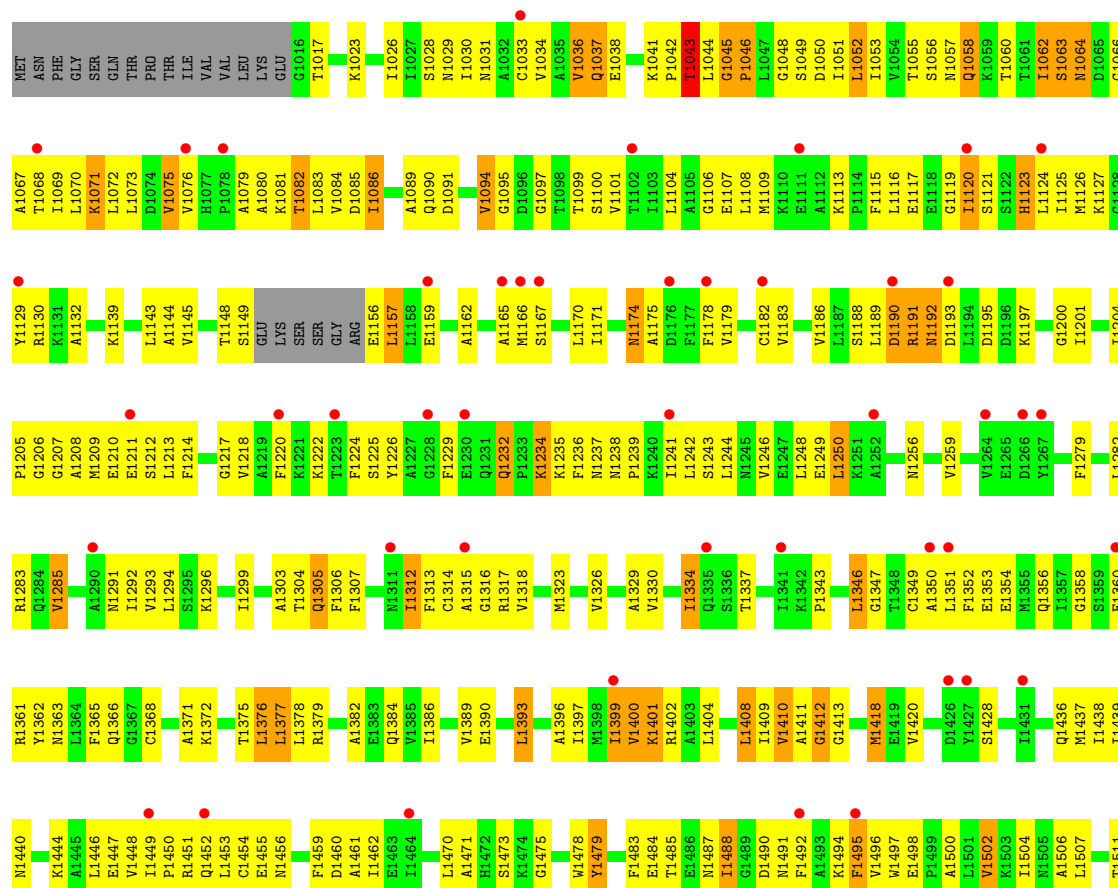
Chain G: 8% 41% 42% 9% 7%

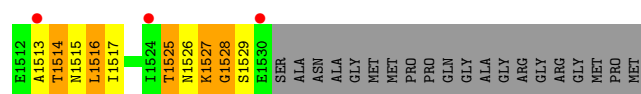


• Molecule 7: T-complex protein 1 subunit eta

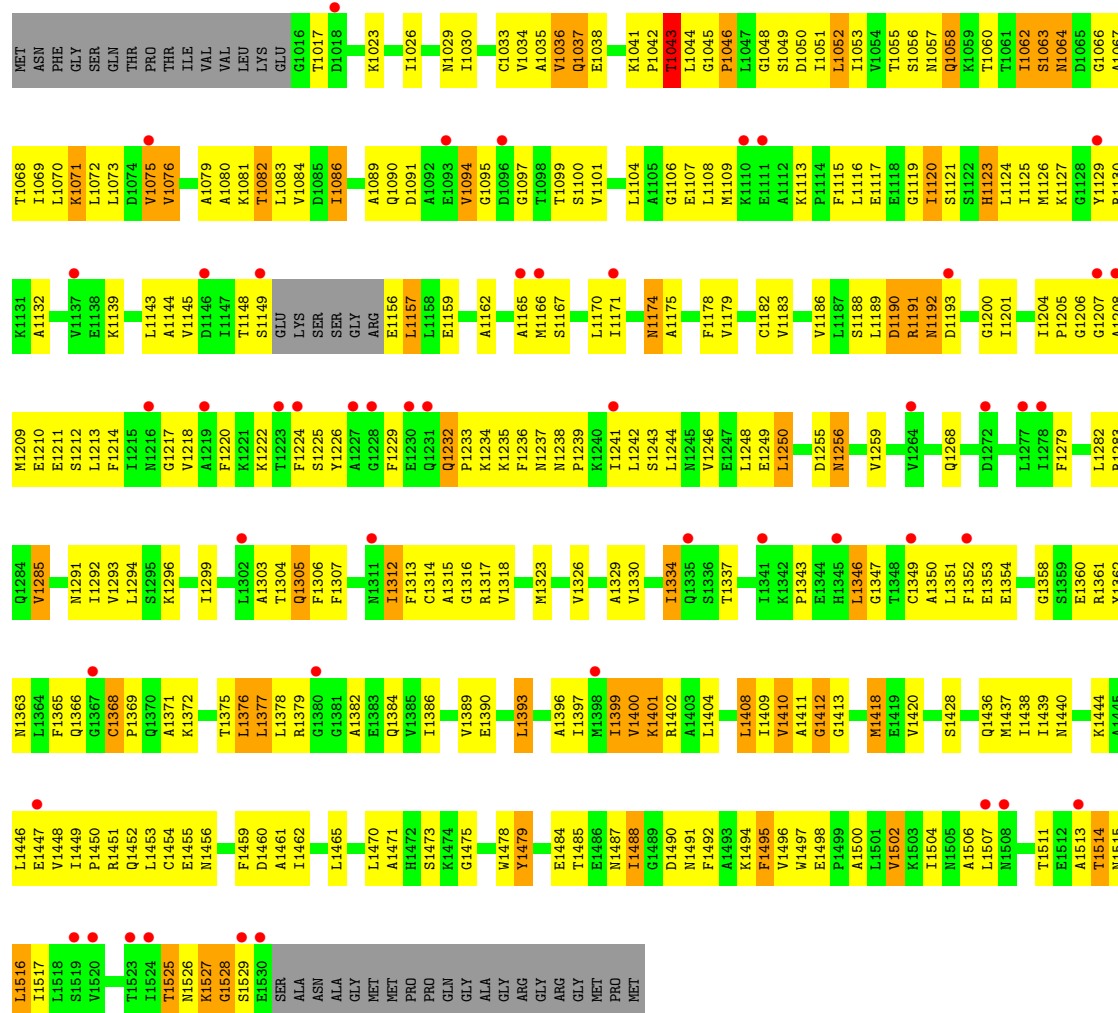
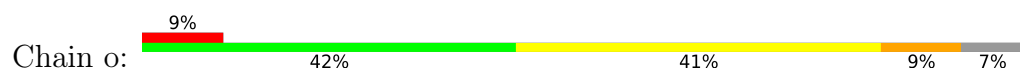
Chain O: 9% 43% 41% 9% 7%



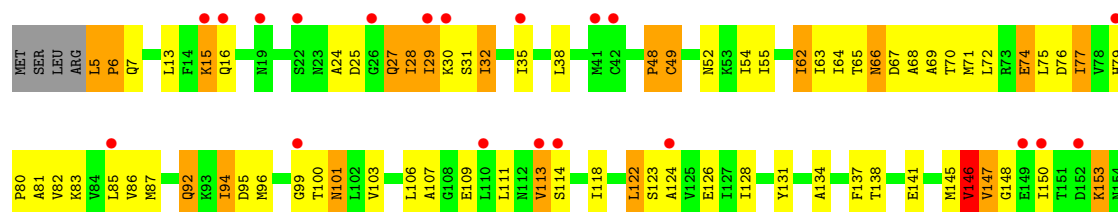
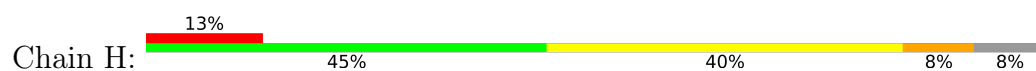


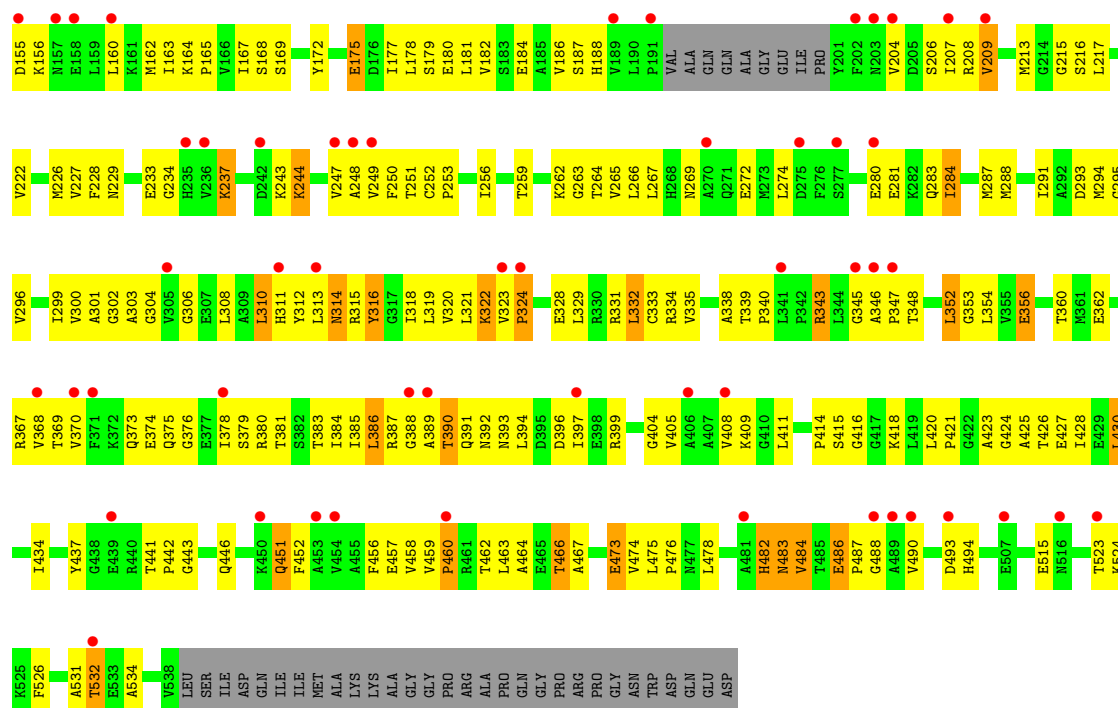


• Molecule 7: T-complex protein 1 subunit eta

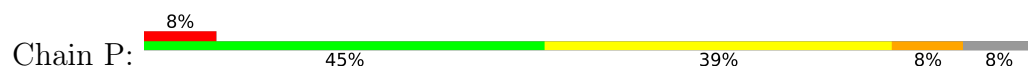


• Molecule 8: T-complex protein 1 subunit theta

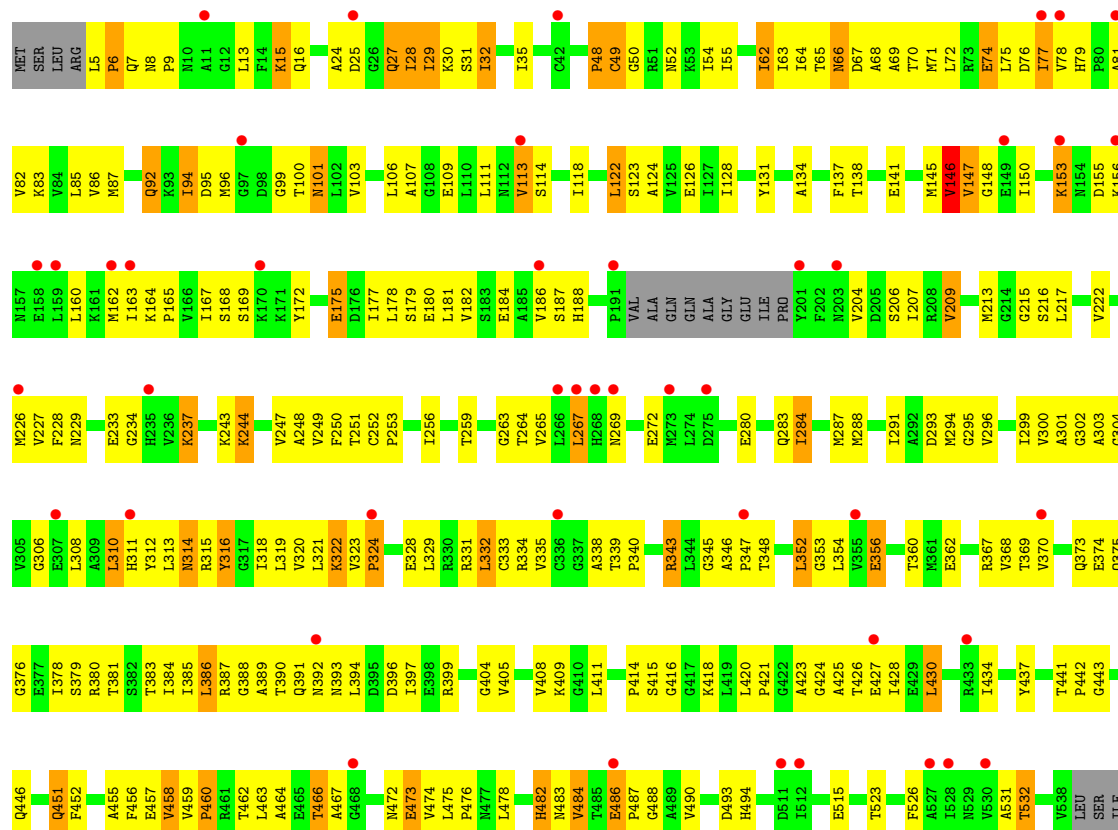




• Molecule 8: T-complex protein 1 subunit theta



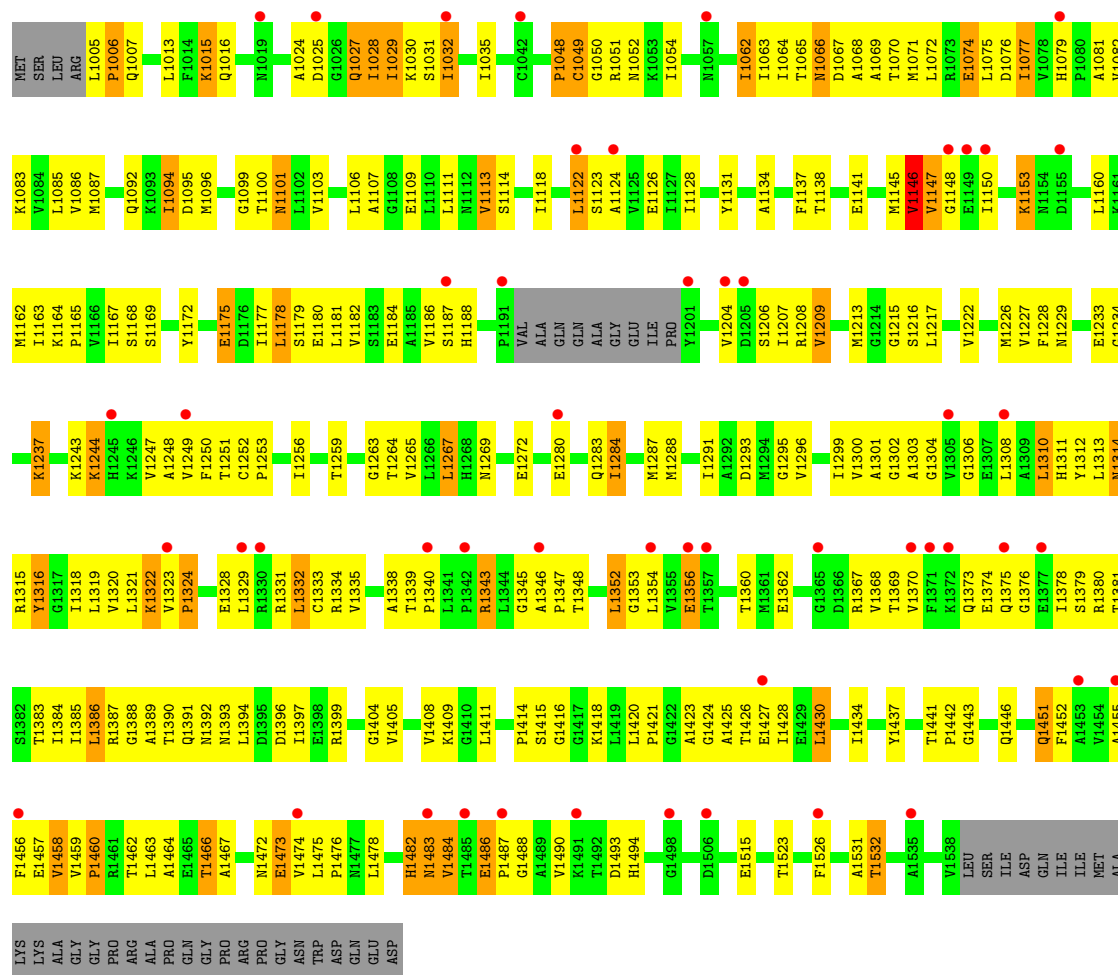
Chain P:



ASP
GLN
ILE
LEU
MET
MET
ALA
LYS
LYS
LYS
ALA
GLY
GLY
PRO
PRO
ARG
ALA
PRO
GLN
GLY
PRO
PRO
ARG
PRO
GLY
ASN
TRP
ASP
ASP
GLN
GLU
ASP

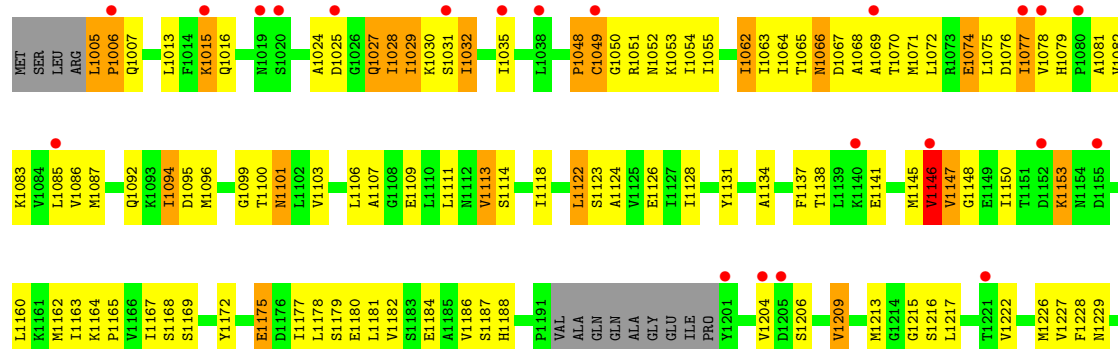
• Molecule 8: T-complex protein 1 subunit theta

Chain h: 9% 46% 38% 8% 8%



• Molecule 8: T-complex protein 1 subunit theta

Chain p: 10% 46% 38% 8% 8%



LYS	E1457	T1383	Y1312	E1233
LYS	V1458	I1384	L1313	G1294
ALA	V1459	I1385	M1314	
GLY	P1460	L1386	R1315	K1237
GLY	R1461	R1387	Y1316	K1243
PRO	T1462	G1388	G1317	K1244
ARG	L1463	A1389	I1318	
ALA	A1464	T1390	L1319	V1247
PRO	E1465	Q1391	V1320	A1248
GLN	T1466	N1392	L1321	V1249
GLY	A1467	N1393	K1322	F1250
PRO		L1394	V1323	T1251
ARG	E1473	D1395	P1324	C1252
PRO	V1474	D1396		
GLY	L1475	I1397	E1328	I1256
ASN	P1476	E1398	L1329	A1257
TRP	N1477	R1399	R1330	N1258
ASP	L1478		R1331	T1259
GLN	Y1479	G1404	L1332	
GLU		V1405	C1333	
ASP			R1334	
	H1482	V1408	V1335	G1263
	N1483	K1409		T1264
	V1484		A1338	V1265
	T1485	G1410	T1339	L1266
	E1486	L1411	P1340	L1267
	P1487			H1268
	G1488	P1414		N1269
	A1489	S1415	R1343	
	V1490	G1416	L1344	E1272
	K1491	G1417	G1345	
	T1492	K1418	A1346	S1277
	D1493	L1419	P1347	
	H1494	L1420	T1348	
		P1421		E1280
	K1497	G1422	L1352	Q1283
	E1507	A1423	G1353	I1284
		G1424	L1354	
	E1515	A1425	V1355	M1287
	N1516	T1426	E1356	M1288
		E1427		
	M1520	I1428	T1360	I1291
		E1429	M1361	A1292
		L1430	E1362	D1293
	T1523			M1294
		I1434		G1295
	F1526		R1367	V1296
		Y1437	V1368	
	A1531		T1369	
	T1532		V1370	I1299
		T1441	F1371	V1300
	V1538	P1442	K1372	A1301
LEU		G1443	Q1373	G1302
SER			E1374	A1303
ILE		Q1446	Q1375	G1304
GLN			G1376	V1305
ASP		Q1451	E1377	G1306
GLN		F1452	I1378	E1307
ILE		A1453	S1379	L1308
ILE		V1454	S1380	A1309
MET		A1455	T1381	L1310
ALA		F1456	S1382	H1311

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	159.10Å 162.54Å 268.10Å 85.23° 81.15° 61.17°	Depositor
Resolution (Å)	89.95 – 3.80 89.95 – 3.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (89.95-3.80) 90.8 (89.95-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.307 , 0.344 0.312 , 0.343	Depositor DCC
R_{free} test set	10483 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	112.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 217.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.024 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	111235	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, SO4, 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	0.34	0/3515	0.86	8/4835 (0.2%)
1	I	0.34	0/3515	0.86	8/4835 (0.2%)
1	a	0.34	0/3515	0.86	8/4835 (0.2%)
1	i	0.34	0/3515	0.86	8/4835 (0.2%)
2	B	0.37	0/3480	0.88	5/4754 (0.1%)
2	J	0.38	0/3480	0.87	5/4754 (0.1%)
2	b	0.38	0/3481	0.88	5/4755 (0.1%)
2	j	0.38	0/3478	0.88	5/4751 (0.1%)
3	C	0.34	0/3421	0.85	7/4689 (0.1%)
3	K	0.34	0/3422	0.85	7/4690 (0.1%)
3	c	0.34	0/3424	0.85	7/4693 (0.1%)
3	k	0.34	0/3424	0.85	7/4693 (0.1%)
4	D	0.34	0/3421	0.85	7/4683 (0.1%)
4	L	0.34	0/3421	0.85	7/4683 (0.1%)
4	d	0.34	0/3421	0.85	7/4683 (0.1%)
4	l	0.34	0/3421	0.85	7/4683 (0.1%)
5	E	0.34	0/3466	0.88	12/4739 (0.3%)
5	M	0.34	0/3466	0.87	12/4739 (0.3%)
5	e	0.34	0/3466	0.87	12/4739 (0.3%)
5	m	0.34	0/3466	0.88	12/4739 (0.3%)
6	F	0.39	0/3663	0.95	16/5008 (0.3%)
6	N	0.39	0/3660	0.95	16/5004 (0.3%)
6	f	0.39	0/3665	0.95	16/5009 (0.3%)
6	n	0.39	0/3661	0.95	16/5005 (0.3%)
7	G	0.34	0/3342	0.88	8/4578 (0.2%)
7	O	0.34	0/3339	0.88	8/4574 (0.2%)
7	g	0.34	0/3339	0.88	8/4574 (0.2%)
7	o	0.34	0/3339	0.88	8/4574 (0.2%)
8	H	0.32	0/3522	0.81	4/4825 (0.1%)
8	P	0.32	0/3522	0.81	4/4825 (0.1%)
8	h	0.32	0/3519	0.80	2/4820 (0.0%)
8	p	0.32	0/3522	0.81	4/4825 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.35	0/111311	0.87	266/152428 (0.2%)

There are no bond length outliers.

The worst 5 of 266 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	375	LYS	N-CA-C	10.89	123.23	111.36
3	c	1375	LYS	N-CA-C	10.88	123.22	111.36
3	K	375	LYS	N-CA-C	10.87	123.20	111.36
3	k	1375	LYS	N-CA-C	10.84	123.17	111.36
7	G	76	VAL	N-CA-C	9.21	120.02	110.72

There are no chirality outliers.

There are no planarity outliers.

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	3492	0	3026	308	0
1	I	3492	0	3026	301	0
1	a	3492	0	3026	304	0
1	i	3492	0	3026	314	0
2	B	3459	0	3146	495	0
2	J	3459	0	3146	505	0
2	b	3460	0	3148	506	0
2	j	3457	0	3139	496	0
3	C	3392	0	3019	313	0
3	K	3393	0	3022	292	0
3	c	3395	0	3029	316	0
3	k	3395	0	3029	331	0
4	D	3398	0	3010	360	0
4	L	3398	0	3010	339	0
4	d	3398	0	3010	315	0
4	l	3398	0	3010	333	0
5	E	3437	0	2943	292	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	3437	0	2943	296	0
5	e	3437	0	2943	295	0
5	m	3437	0	2943	308	0
6	F	3631	0	3330	659	0
6	N	3628	0	3321	653	0
6	f	3633	0	3333	676	0
6	n	3629	0	3322	670	0
7	G	3317	0	2920	395	0
7	O	3314	0	2911	387	0
7	g	3314	0	2911	381	0
7	o	3314	0	2911	383	0
8	H	3487	0	3109	314	0
8	P	3487	0	3109	291	0
8	h	3485	0	3103	286	0
8	p	3487	0	3109	290	0
9	A	27	0	11	3	0
9	B	27	0	11	8	0
9	C	27	0	12	7	0
9	D	27	0	11	8	0
9	E	27	0	11	2	0
9	F	27	0	11	6	0
9	G	27	0	11	5	0
9	H	27	0	12	3	0
9	J	27	0	11	6	0
9	L	27	0	11	7	0
9	M	27	0	11	6	0
9	N	27	0	11	6	0
9	P	27	0	12	5	0
9	a	27	0	11	2	0
9	b	27	0	11	3	0
9	e	27	0	12	3	0
9	f	27	0	11	6	0
9	g	27	0	11	8	0
9	h	27	0	12	5	0
9	k	27	0	11	9	0
9	l	27	0	11	8	0
9	m	27	0	11	4	0
9	n	27	0	11	4	0
9	p	27	0	12	3	0
10	A	4	0	0	0	0
10	B	4	0	0	0	0
10	C	4	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	4	0	0	0	0
10	E	4	0	0	0	0
10	F	4	0	0	2	0
10	G	4	0	0	0	0
10	H	4	0	0	0	0
10	J	4	0	0	0	0
10	L	4	0	0	1	0
10	M	4	0	0	0	0
10	N	4	0	0	3	0
10	P	4	0	0	0	0
10	a	4	0	0	0	0
10	b	4	0	0	0	0
10	e	4	0	0	0	0
10	f	4	0	0	0	0
10	g	4	0	0	0	0
10	h	4	0	0	1	0
10	k	4	0	0	0	0
10	l	4	0	0	0	0
10	m	4	0	0	0	0
10	n	4	0	0	0	0
10	p	4	0	0	0	0
11	I	5	0	0	0	0
11	K	5	0	0	0	0
11	O	5	0	0	0	0
11	c	5	0	0	0	0
11	d	5	0	0	0	0
11	i	5	0	0	0	0
11	j	5	0	0	1	0
11	o	5	0	0	0	0
12	B	1	0	0	0	0
12	E	1	0	0	0	0
12	G	1	0	0	0	0
12	M	1	0	0	0	0
12	e	1	0	0	0	0
12	g	1	0	0	0	0
12	m	1	0	0	0	0
All	All	111235	0	98253	11582	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 55.

The worst 5 of 11582 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:k:1301:VAL:CG2	3:k:1305:ALA:HB1	1.28	1.61
3:c:1301:VAL:CG2	3:c:1305:ALA:HB1	1.28	1.60
3:k:1301:VAL:HG22	3:k:1305:ALA:CB	1.25	1.60
3:c:1301:VAL:HG22	3:c:1305:ALA:CB	1.25	1.56
2:b:1348:LEU:HG	6:f:1085:GLU:C	1.31	1.54

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	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	3	23
1	I	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	3	23
1	a	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	3	23
1	i	538/559 (96%)	441 (82%)	78 (14%)	19 (4%)	3	23
2	B	509/527 (97%)	417 (82%)	67 (13%)	25 (5%)	1	17
2	J	509/527 (97%)	417 (82%)	67 (13%)	25 (5%)	1	17
2	b	509/527 (97%)	417 (82%)	68 (13%)	24 (5%)	2	18
2	j	509/527 (97%)	417 (82%)	67 (13%)	25 (5%)	1	17
3	C	508/590 (86%)	420 (83%)	68 (13%)	20 (4%)	2	20
3	K	508/590 (86%)	421 (83%)	67 (13%)	20 (4%)	2	20
3	c	508/590 (86%)	419 (82%)	70 (14%)	19 (4%)	2	21
3	k	508/590 (86%)	420 (83%)	68 (13%)	20 (4%)	2	20
4	D	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	5	30
4	L	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	5	30
4	d	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	5	30
4	l	520/528 (98%)	429 (82%)	79 (15%)	12 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	521/562 (93%)	443 (85%)	59 (11%)	19 (4%)	2	22
5	M	521/562 (93%)	443 (85%)	59 (11%)	19 (4%)	2	22
5	e	521/562 (93%)	442 (85%)	60 (12%)	19 (4%)	2	22
5	m	521/562 (93%)	443 (85%)	59 (11%)	19 (4%)	2	22
6	F	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	3	23
6	N	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	3	23
6	f	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	3	23
6	n	529/546 (97%)	429 (81%)	82 (16%)	18 (3%)	3	23
7	G	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	2	19
7	O	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	2	19
7	g	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	2	19
7	o	505/550 (92%)	424 (84%)	60 (12%)	21 (4%)	2	19
8	H	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	2	18
8	P	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	2	18
8	h	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	2	18
8	p	521/568 (92%)	439 (84%)	58 (11%)	24 (5%)	2	18
All	All	16604/17720 (94%)	13767 (83%)	2207 (13%)	630 (4%)	2	21

5 of 630 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5	ILE
2	B	165	ILE
2	B	184	LEU
2	B	185	LYS
2	B	307	GLU

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	301/471 (64%)	272 (90%)	29 (10%)	8	29
1	I	301/471 (64%)	272 (90%)	29 (10%)	8	29
1	a	301/471 (64%)	272 (90%)	29 (10%)	8	29
1	i	301/471 (64%)	272 (90%)	29 (10%)	8	29
2	B	320/441 (73%)	264 (82%)	56 (18%)	2	12
2	J	320/441 (73%)	264 (82%)	56 (18%)	2	12
2	b	320/441 (73%)	263 (82%)	57 (18%)	2	12
2	j	319/441 (72%)	263 (82%)	56 (18%)	2	12
3	C	295/497 (59%)	267 (90%)	28 (10%)	8	30
3	K	296/497 (60%)	268 (90%)	28 (10%)	8	30
3	c	297/497 (60%)	269 (91%)	28 (9%)	8	30
3	k	297/497 (60%)	269 (91%)	28 (9%)	8	30
4	D	290/454 (64%)	257 (89%)	33 (11%)	5	23
4	L	290/454 (64%)	257 (89%)	33 (11%)	5	23
4	d	290/454 (64%)	258 (89%)	32 (11%)	6	24
4	l	290/454 (64%)	257 (89%)	33 (11%)	5	23
5	E	293/483 (61%)	262 (89%)	31 (11%)	6	26
5	M	293/483 (61%)	262 (89%)	31 (11%)	6	26
5	e	293/483 (61%)	262 (89%)	31 (11%)	6	26
5	m	293/483 (61%)	262 (89%)	31 (11%)	6	26
6	F	334/463 (72%)	261 (78%)	73 (22%)	1	6
6	N	333/463 (72%)	260 (78%)	73 (22%)	1	6
6	f	334/463 (72%)	259 (78%)	75 (22%)	1	5
6	n	333/463 (72%)	259 (78%)	74 (22%)	1	5
7	G	275/454 (61%)	238 (86%)	37 (14%)	4	19
7	O	274/454 (60%)	237 (86%)	37 (14%)	4	19
7	g	274/454 (60%)	237 (86%)	37 (14%)	4	19
7	o	274/454 (60%)	237 (86%)	37 (14%)	4	19
8	H	307/473 (65%)	270 (88%)	37 (12%)	5	21
8	P	307/473 (65%)	270 (88%)	37 (12%)	5	21
8	h	306/473 (65%)	269 (88%)	37 (12%)	5	21
8	p	307/473 (65%)	270 (88%)	37 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9658/14944 (65%)	8359 (87%)	1299 (13%)	4 19

5 of 1299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	g	1399	ILE
5	m	1440	VAL
8	h	1175	GLU
7	g	1393	LEU
2	j	1379	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 303 such sidechains are listed below:

Mol	Chain	Res	Type
1	i	1090	GLN
6	n	1494	ASN
1	i	1363	GLN
3	k	1439	GLN
8	p	1373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

56 ligands are modelled in this entry.

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
10	BEF	H	602	-	0,3,3	-	-	-		
10	BEF	p	1602	9	0,3,3	-	-	-		
9	ADP	f	1601	-	28,29,29	2.30	8 (28%)	43,45,45	2.17	16 (37%)
10	BEF	G	602	-	0,3,3	-	-	-		
11	SO4	I	600	-	4,4,4	0.26	0	6,6,6	0.17	0
9	ADP	H	601	-	28,29,29	2.28	9 (32%)	43,45,45	2.06	14 (32%)
9	ADP	g	1601	-	28,29,29	2.32	9 (32%)	43,45,45	2.13	16 (37%)
10	BEF	b	1602	9	0,3,3	-	-	-		
10	BEF	J	602	9	0,3,3	-	-	-		
9	ADP	D	601	-	28,29,29	2.33	9 (32%)	43,45,45	2.16	14 (32%)
10	BEF	l	1602	9	0,3,3	-	-	-		
9	ADP	F	601	-	28,29,29	2.36	9 (32%)	43,45,45	2.15	16 (37%)
10	BEF	h	1602	9	0,3,3	-	-	-		
9	ADP	k	2101	10	28,29,29	2.32	9 (32%)	43,45,45	2.14	16 (37%)
10	BEF	k	2102	9	0,3,3	-	-	-		
9	ADP	a	1601	-	28,29,29	2.28	9 (32%)	43,45,45	2.16	14 (32%)
9	ADP	N	601	10	28,29,29	2.27	9 (32%)	43,45,45	2.17	17 (39%)
10	BEF	N	602	9	0,3,3	-	-	-		
9	ADP	L	601	-	28,29,29	2.31	9 (32%)	43,45,45	2.13	15 (34%)
11	SO4	O	600	-	4,4,4	0.27	0	6,6,6	0.14	0
11	SO4	i	1600	-	4,4,4	0.22	0	6,6,6	0.30	0
10	BEF	e	1602	-	0,3,3	-	-	-		
10	BEF	m	1602	-	0,3,3	-	-	-		
10	BEF	F	602	-	0,3,3	-	-	-		
10	BEF	B	602	9	0,3,3	-	-	-		
10	BEF	f	1602	-	0,3,3	-	-	-		
9	ADP	J	601	10	28,29,29	2.27	9 (32%)	43,45,45	2.20	13 (30%)
10	BEF	P	602	-	0,3,3	-	-	-		
9	ADP	C	1101	-	28,29,29	2.25	9 (32%)	43,45,45	2.05	16 (37%)
9	ADP	e	1601	-	28,29,29	2.25	9 (32%)	43,45,45	2.06	14 (32%)
10	BEF	A	602	9	0,3,3	-	-	-		
9	ADP	b	1601	10	28,29,29	2.27	9 (32%)	43,45,45	2.08	15 (34%)
11	SO4	o	1600	-	4,4,4	0.23	0	6,6,6	0.10	0
11	SO4	d	1600	-	4,4,4	0.23	0	6,6,6	0.15	0
10	BEF	n	1602	-	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ADP	n	1601	-	28,29,29	2.28	8 (28%)	43,45,45	2.11	16 (37%)
10	BEF	M	602	-	0,3,3	-	-	-	-	-
9	ADP	G	601	-	28,29,29	2.24	9 (32%)	43,45,45	2.17	16 (37%)
10	BEF	g	1602	-	0,3,3	-	-	-	-	-
9	ADP	E	601	10	28,29,29	2.30	9 (32%)	43,45,45	2.16	15 (34%)
9	ADP	h	1601	10	28,29,29	2.29	9 (32%)	43,45,45	1.99	16 (37%)
11	SO4	K	1101	-	4,4,4	0.24	0	6,6,6	0.21	0
9	ADP	B	601	10	28,29,29	2.26	10 (35%)	43,45,45	2.18	14 (32%)
10	BEF	D	602	-	0,3,3	-	-	-	-	-
10	BEF	a	1602	-	0,3,3	-	-	-	-	-
9	ADP	M	601	-	28,29,29	2.26	10 (35%)	43,45,45	2.11	15 (34%)
9	ADP	P	601	-	28,29,29	2.27	9 (32%)	43,45,45	2.04	15 (34%)
9	ADP	l	1601	10	28,29,29	2.35	9 (32%)	43,45,45	2.21	16 (37%)
11	SO4	j	1600	-	4,4,4	0.20	0	6,6,6	0.15	0
9	ADP	m	1601	-	28,29,29	2.29	9 (32%)	43,45,45	2.11	15 (34%)
10	BEF	C	1102	-	0,3,3	-	-	-	-	-
10	BEF	L	602	-	0,3,3	-	-	-	-	-
9	ADP	A	601	10	28,29,29	2.27	9 (32%)	43,45,45	2.18	16 (37%)
11	SO4	c	2101	-	4,4,4	0.28	0	6,6,6	0.16	0
10	BEF	E	602	9	0,3,3	-	-	-	-	-
9	ADP	p	1601	10	28,29,29	2.28	9 (32%)	43,45,45	2.09	14 (32%)

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
9	ADP	f	1601	-	2/2/6/6	6/16/32/32	0/3/3/3
9	ADP	H	601	-	1/1/6/6	7/16/32/32	0/3/3/3
9	ADP	g	1601	-	1/1/6/6	4/16/32/32	0/3/3/3
9	ADP	D	601	-	2/2/6/6	3/16/32/32	0/3/3/3
9	ADP	F	601	-	-	10/16/32/32	0/3/3/3
9	ADP	k	2101	10	2/2/6/6	4/16/32/32	0/3/3/3
9	ADP	a	1601	-	2/2/6/6	7/16/32/32	0/3/3/3
9	ADP	N	601	10	2/2/6/6	7/16/32/32	0/3/3/3
9	ADP	L	601	-	-	5/16/32/32	0/3/3/3
9	ADP	J	601	10	2/2/6/6	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	C	1101	-	2/2/6/6	5/16/32/32	0/3/3/3
9	ADP	e	1601	-	2/2/6/6	5/16/32/32	0/3/3/3
9	ADP	b	1601	10	2/2/6/6	8/16/32/32	0/3/3/3
9	ADP	n	1601	-	1/1/6/6	4/16/32/32	0/3/3/3
9	ADP	G	601	-	1/1/6/6	6/16/32/32	0/3/3/3
9	ADP	E	601	10	1/1/6/6	5/16/32/32	0/3/3/3
9	ADP	h	1601	10	1/1/6/6	3/16/32/32	0/3/3/3
9	ADP	B	601	10	2/2/6/6	4/16/32/32	0/3/3/3
9	ADP	M	601	-	2/2/6/6	7/16/32/32	0/3/3/3
9	ADP	P	601	-	1/1/6/6	3/16/32/32	0/3/3/3
9	ADP	l	1601	10	-	3/16/32/32	0/3/3/3
9	ADP	m	1601	-	2/2/6/6	5/16/32/32	0/3/3/3
9	ADP	A	601	10	2/2/6/6	7/16/32/32	0/3/3/3
9	ADP	p	1601	10	1/1/6/6	5/16/32/32	0/3/3/3

The worst 5 of 216 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	601	ADP	PA-O3A	5.87	1.65	1.59
9	F	601	ADP	PA-O3A	5.46	1.65	1.59
9	l	1601	ADP	PA-O3A	5.40	1.65	1.59
9	k	2101	ADP	PA-O3A	5.33	1.65	1.59
9	L	601	ADP	PA-O3A	5.21	1.65	1.59

The worst 5 of 364 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	601	ADP	N3-C2-N1	-6.09	119.36	128.58
9	H	601	ADP	N3-C2-N1	-5.95	119.58	128.58
9	l	1601	ADP	N3-C2-N1	-5.83	119.76	128.58
9	a	1601	ADP	N3-C2-N1	-5.77	119.86	128.58
9	P	601	ADP	N3-C2-N1	-5.70	119.96	128.58

5 of 34 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	601	ADP	C4'
9	A	601	ADP	C3'
9	B	601	ADP	C4'

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Mol	Chain	Res	Type	Atom
9	B	601	ADP	C3'
9	C	1101	ADP	C4'

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	601	ADP	C5'-O5'-PA-O3A
9	B	601	ADP	PB-O3A-PA-O5'
9	C	1101	ADP	C5'-O5'-PA-O1A
9	C	1101	ADP	C5'-O5'-PA-O3A
9	D	601	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

30 monomers are involved in 136 short contacts:

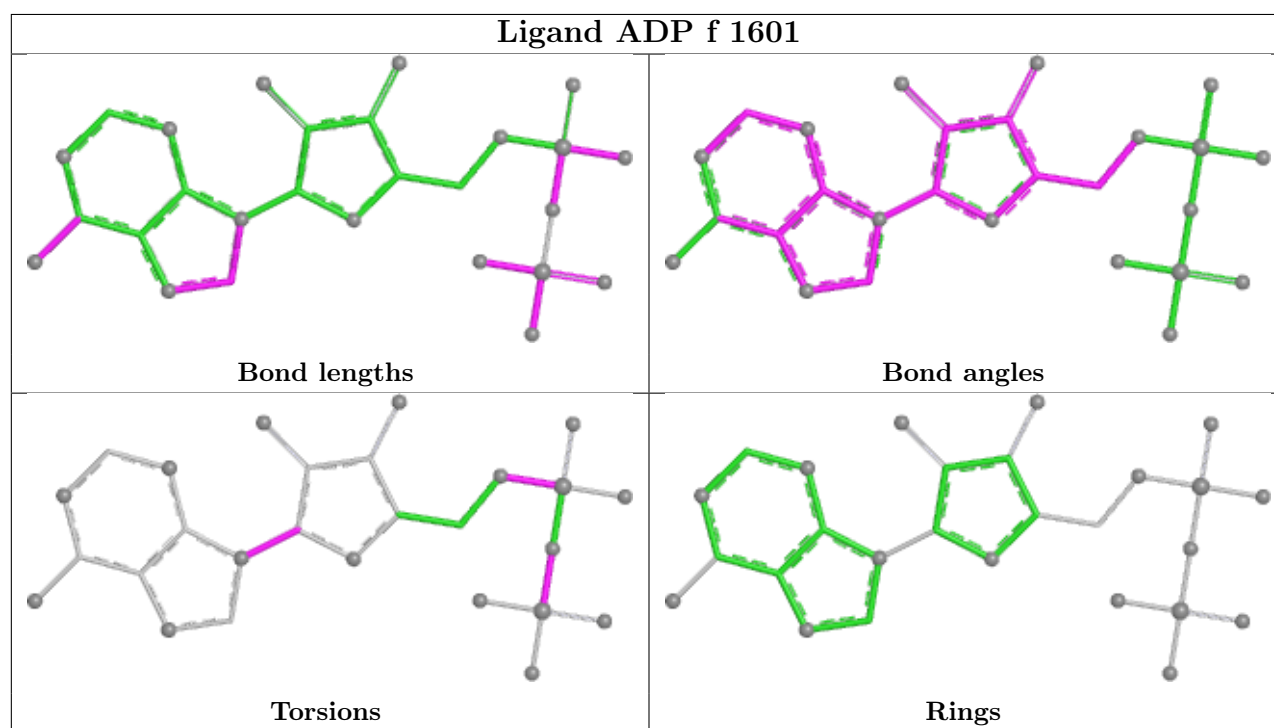
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	f	1601	ADP	6	0
9	H	601	ADP	3	0
9	g	1601	ADP	8	0
9	D	601	ADP	8	0
9	F	601	ADP	6	0
10	h	1602	BEF	1	0
9	k	2101	ADP	9	0
9	a	1601	ADP	2	0
9	N	601	ADP	6	0
10	N	602	BEF	3	0
9	L	601	ADP	7	0
10	F	602	BEF	2	0
9	J	601	ADP	6	0
9	C	1101	ADP	7	0
9	e	1601	ADP	3	0
9	b	1601	ADP	3	0
9	n	1601	ADP	4	0
9	G	601	ADP	5	0
9	E	601	ADP	2	0
9	h	1601	ADP	5	0
9	B	601	ADP	8	0
9	M	601	ADP	6	0
9	P	601	ADP	5	0
9	l	1601	ADP	8	0
11	j	1600	SO4	1	0
9	m	1601	ADP	4	0

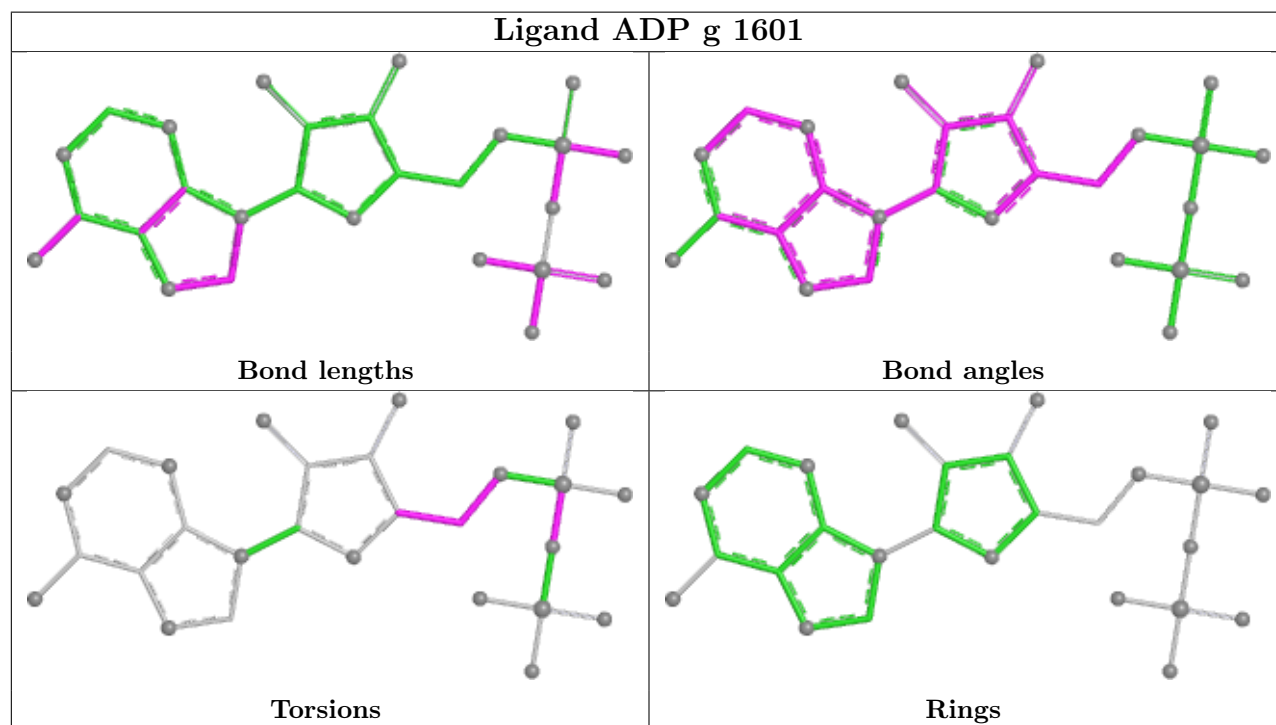
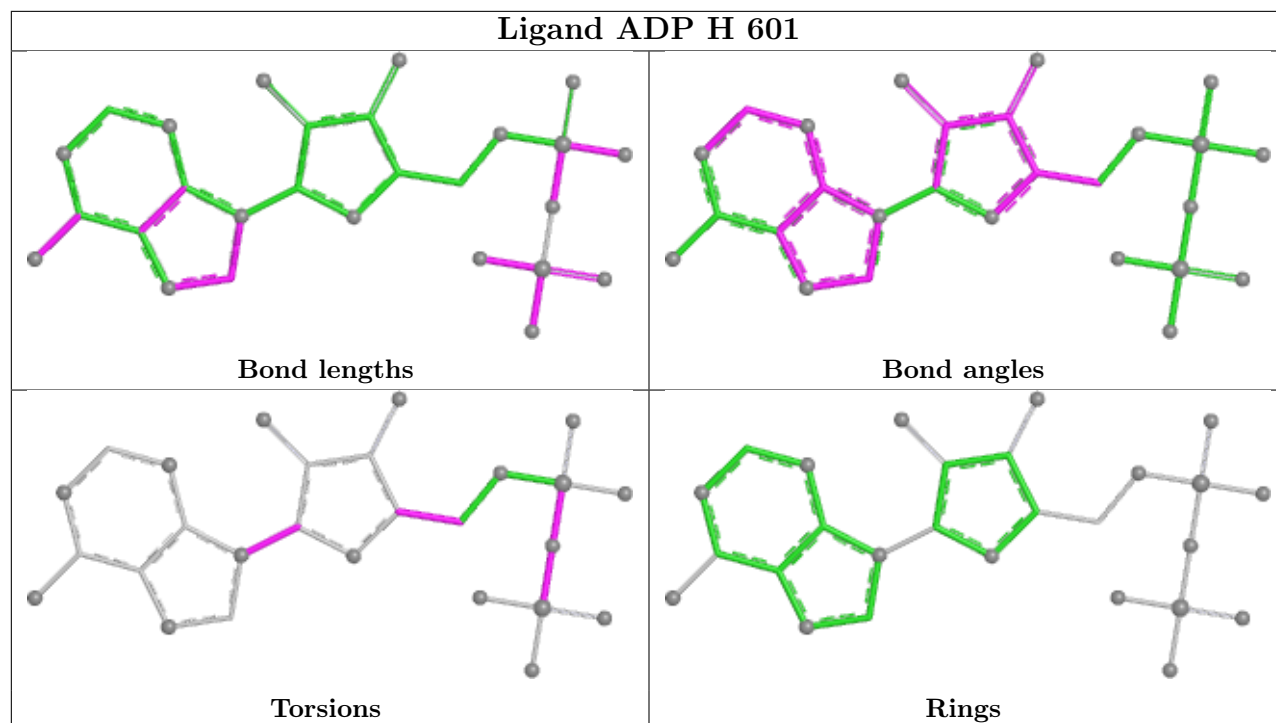
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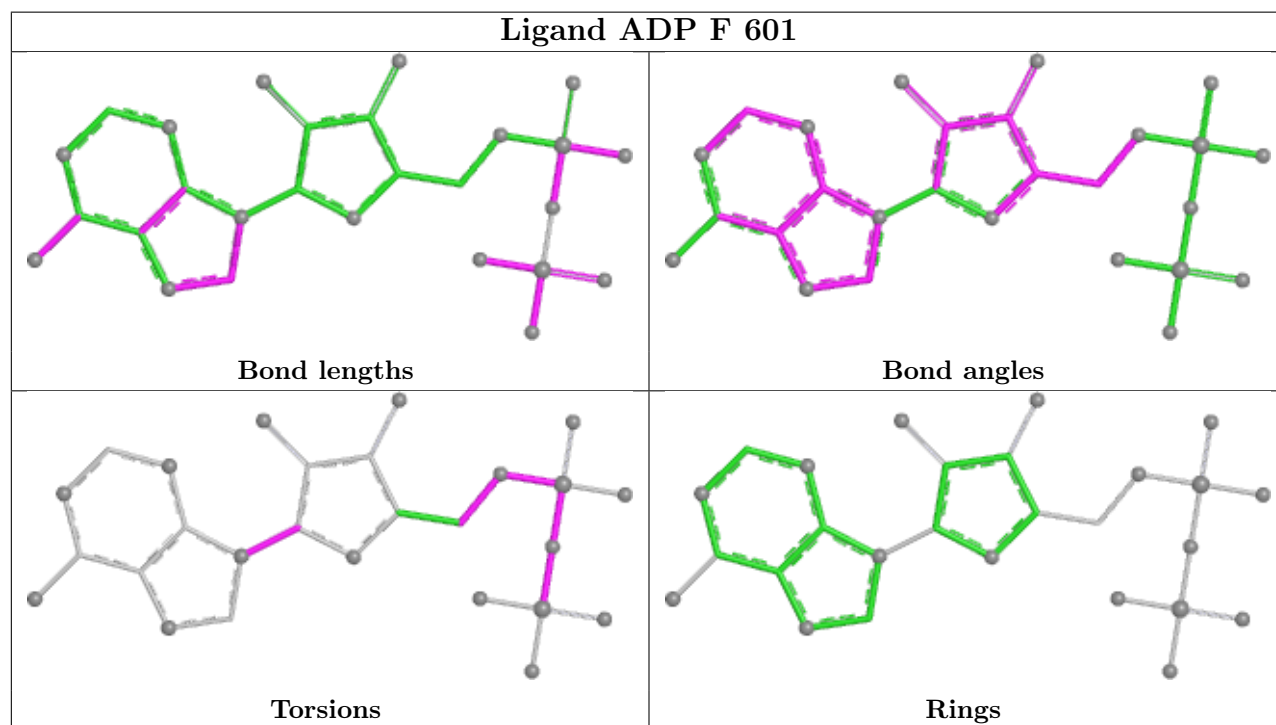
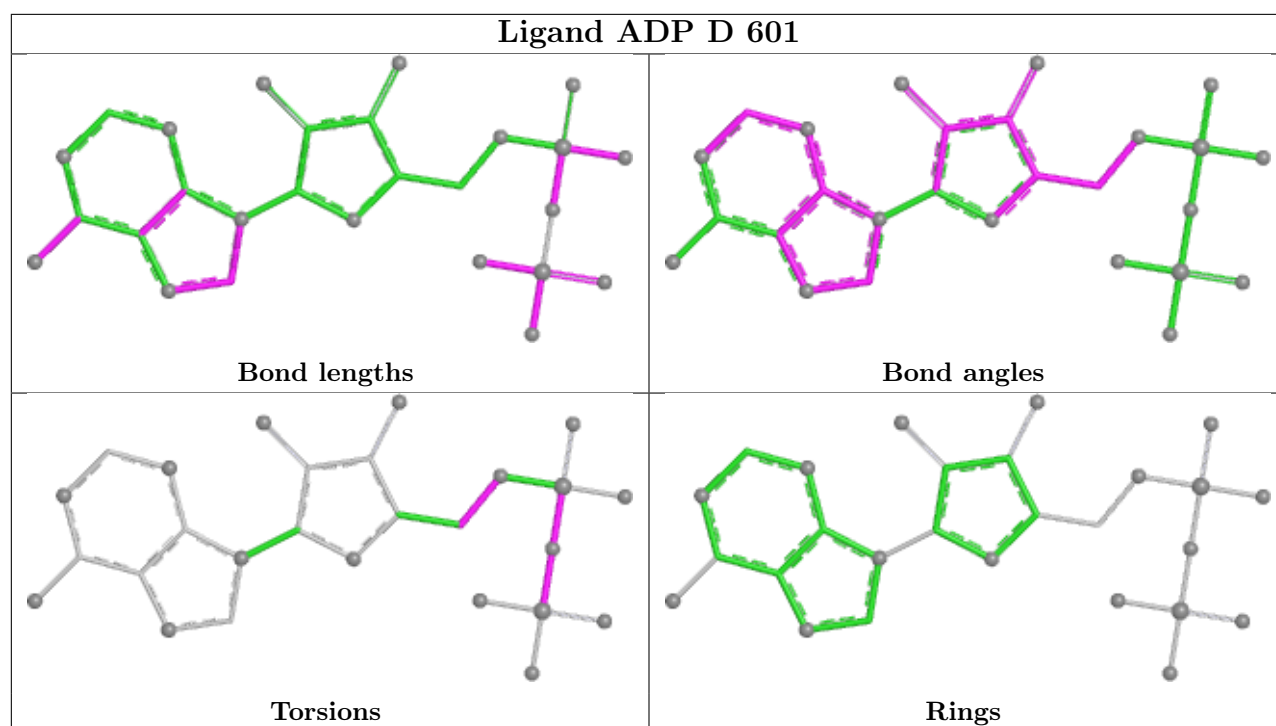
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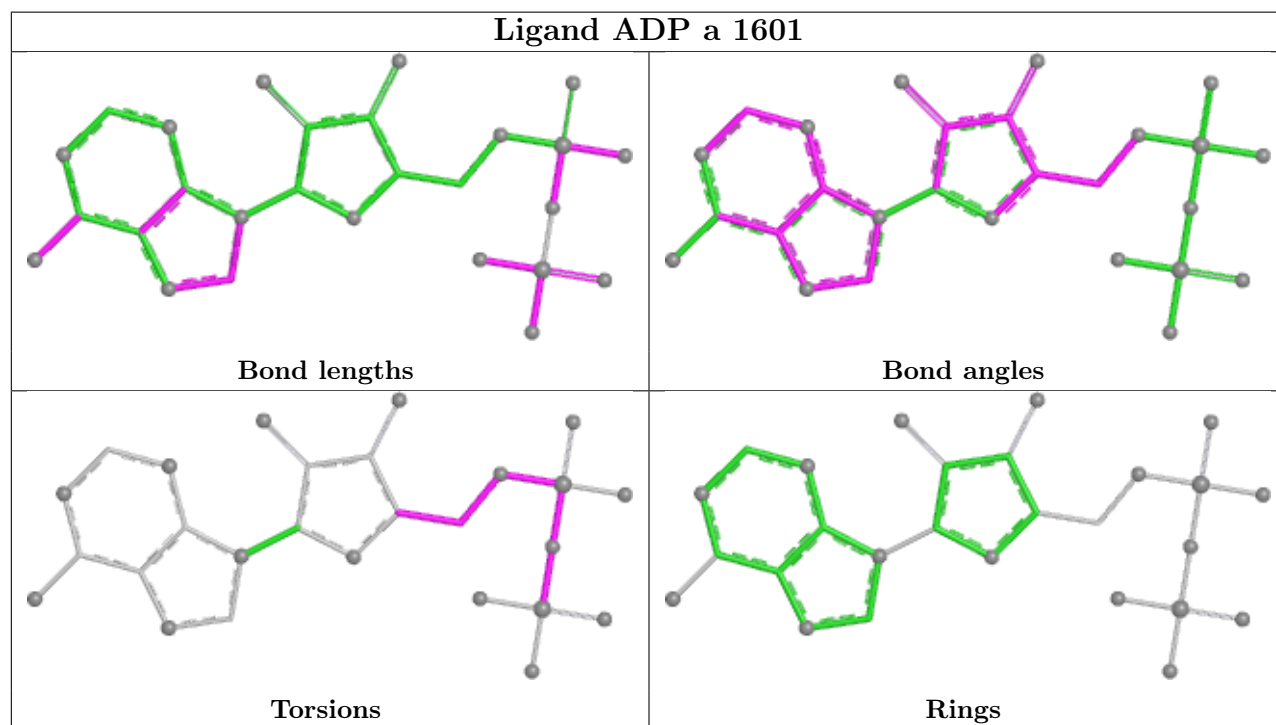
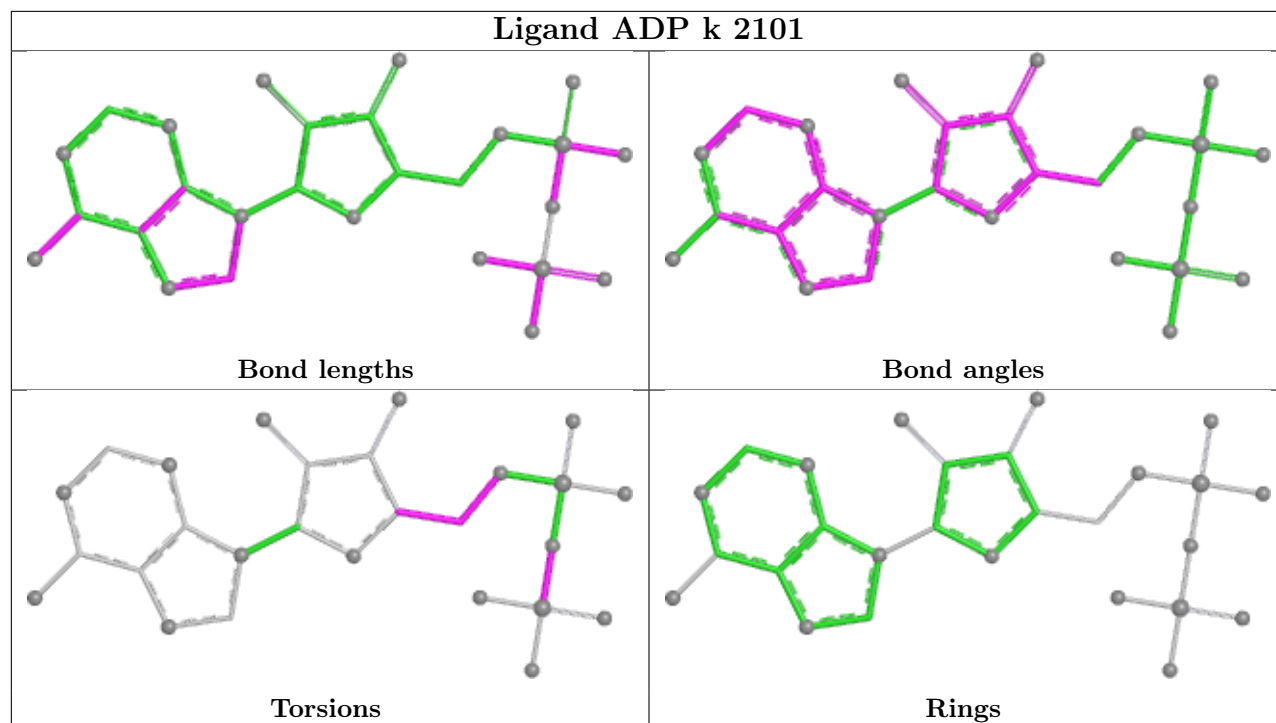
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1102	BEF	3	0
10	L	602	BEF	1	0
9	A	601	ADP	3	0
9	p	1601	ADP	3	0

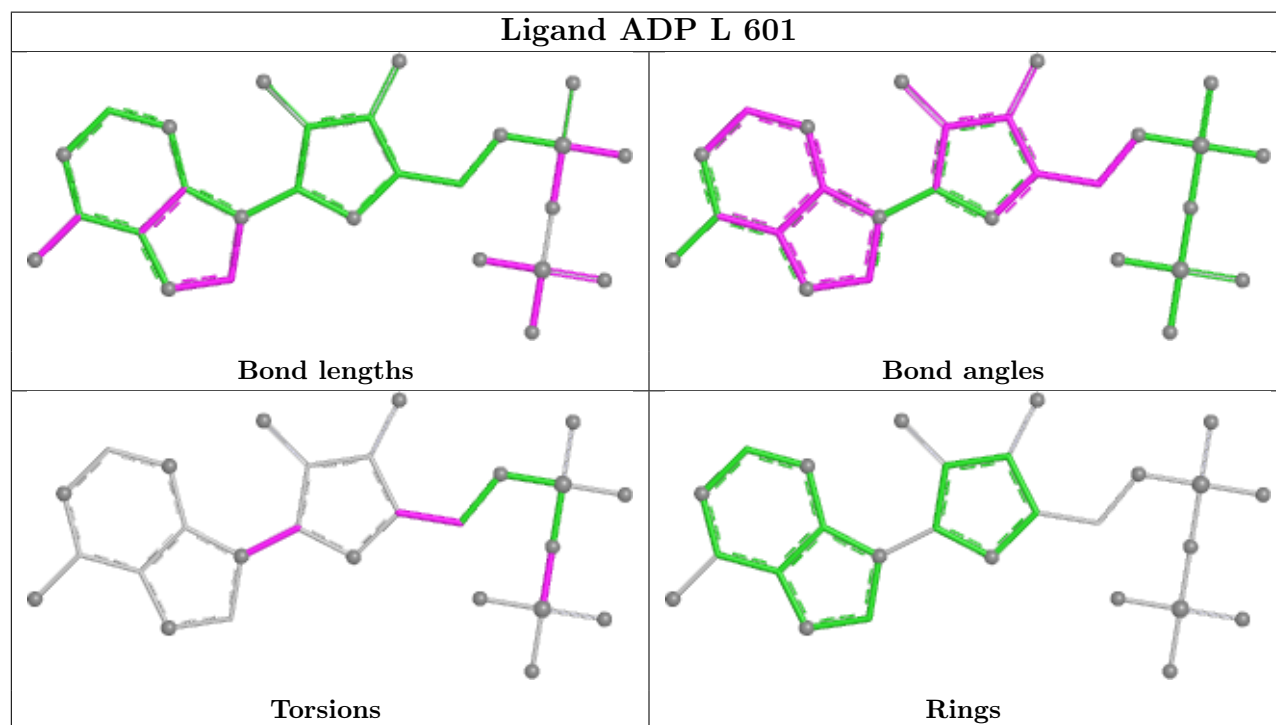
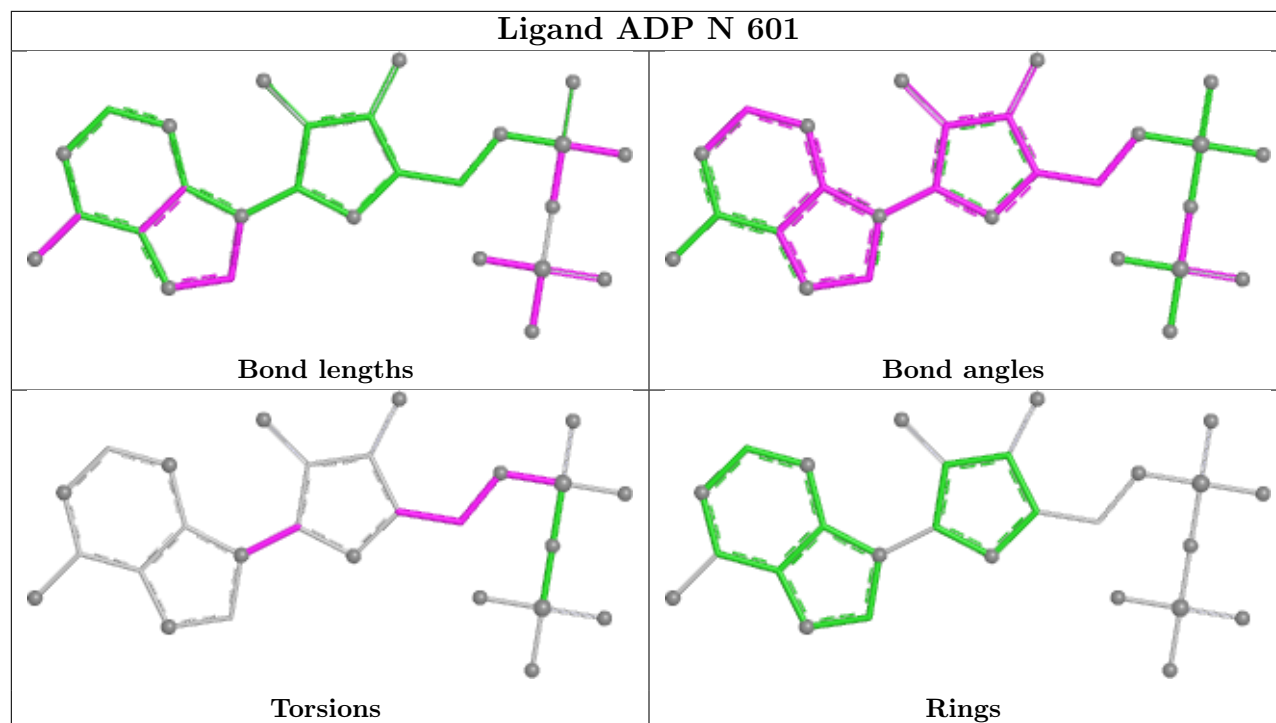
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



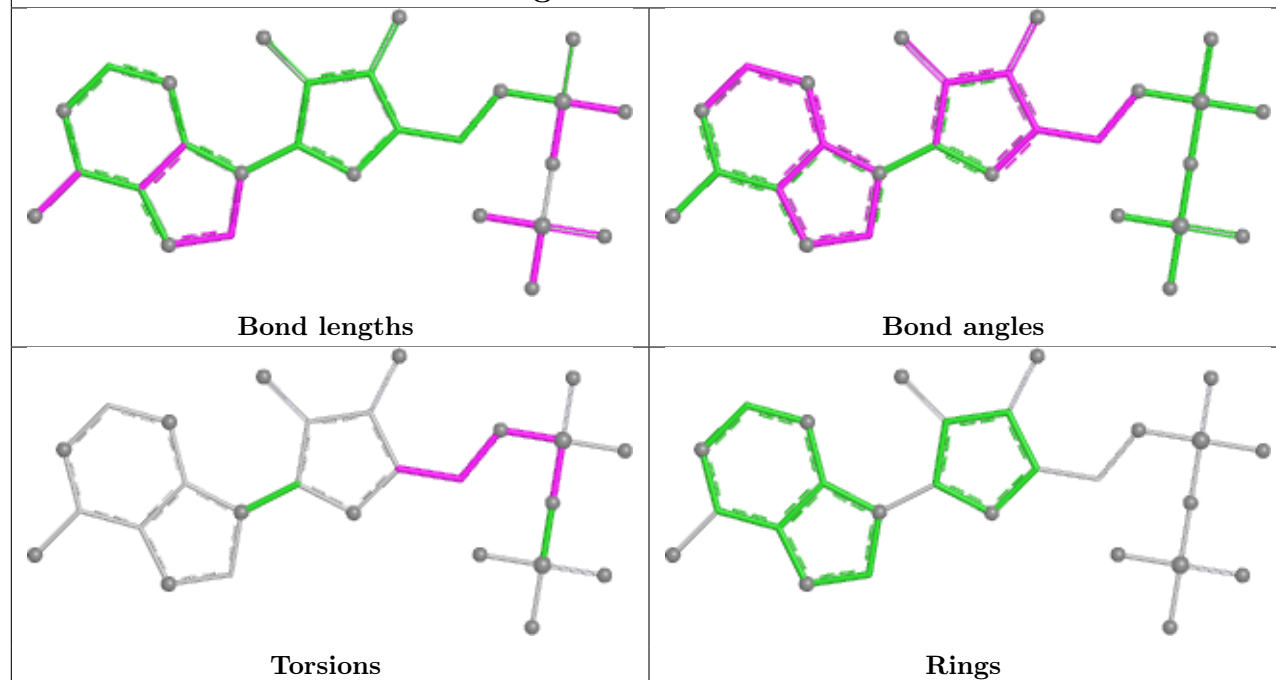




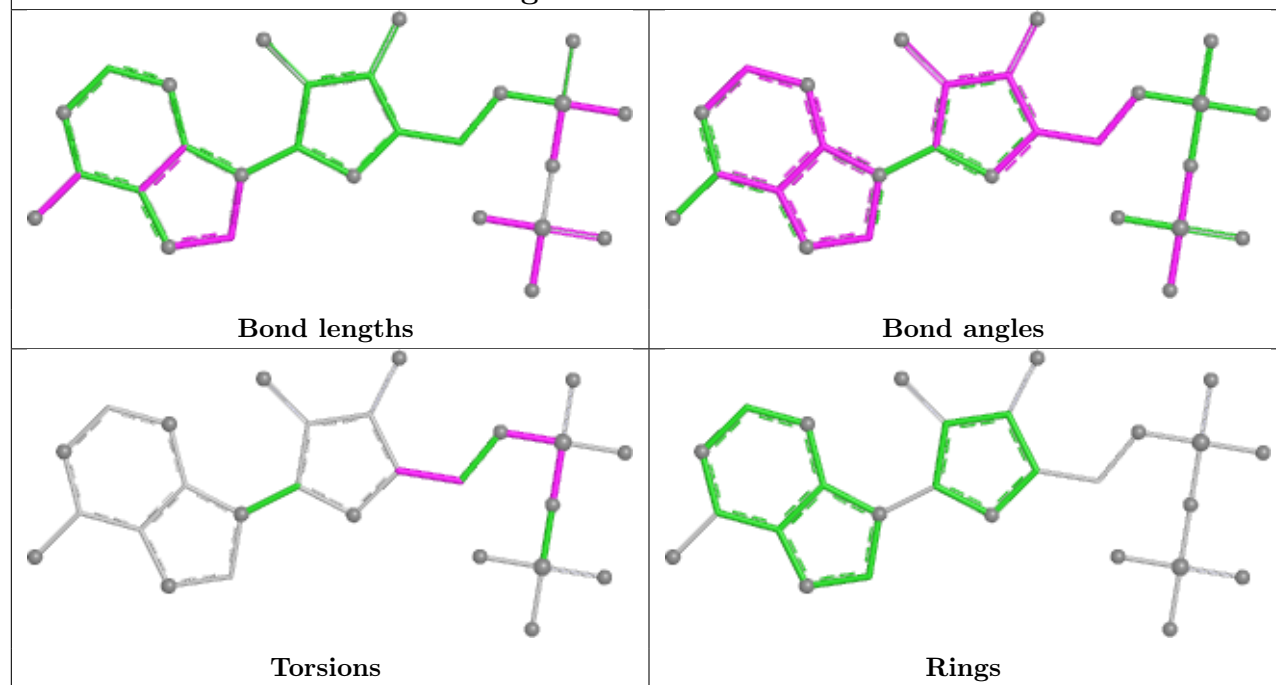


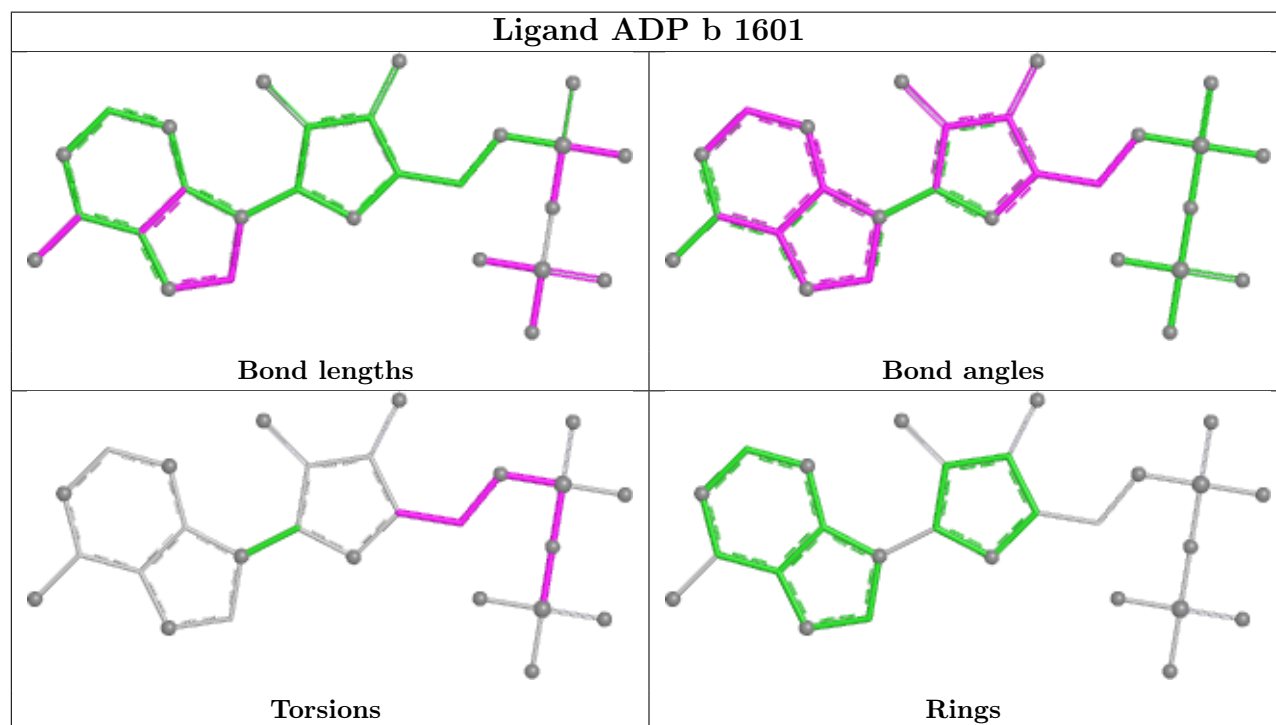
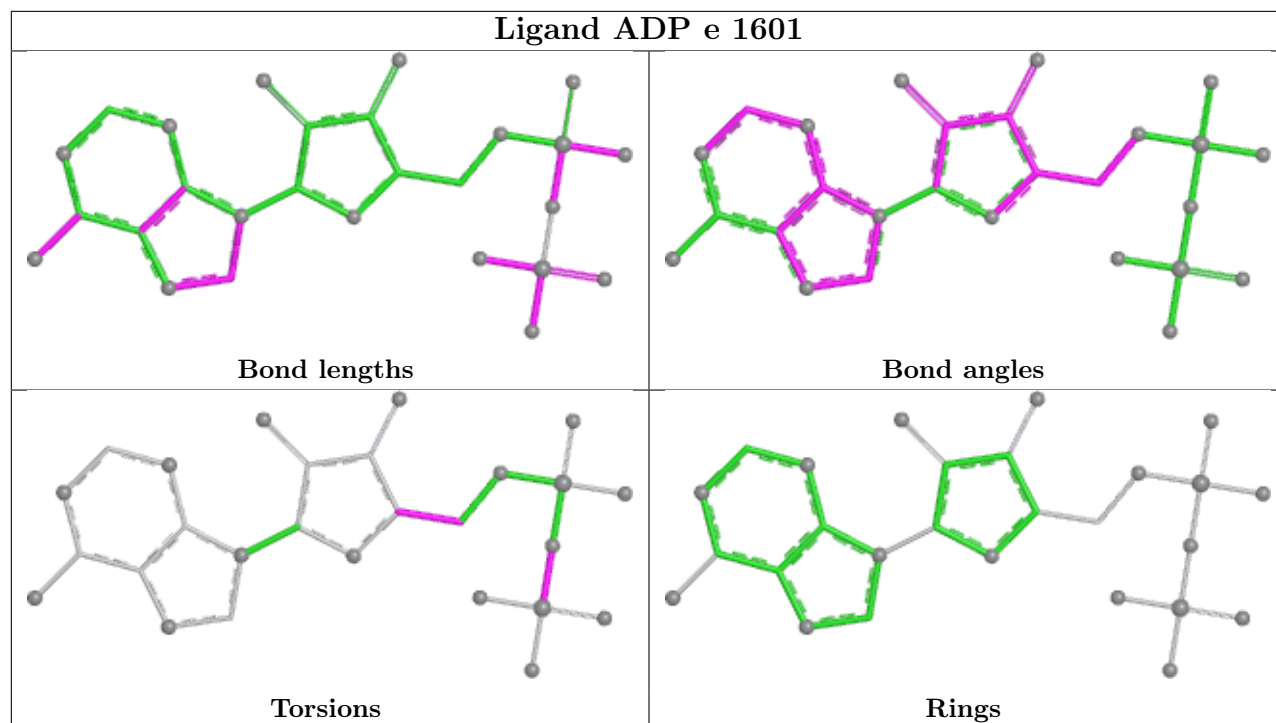


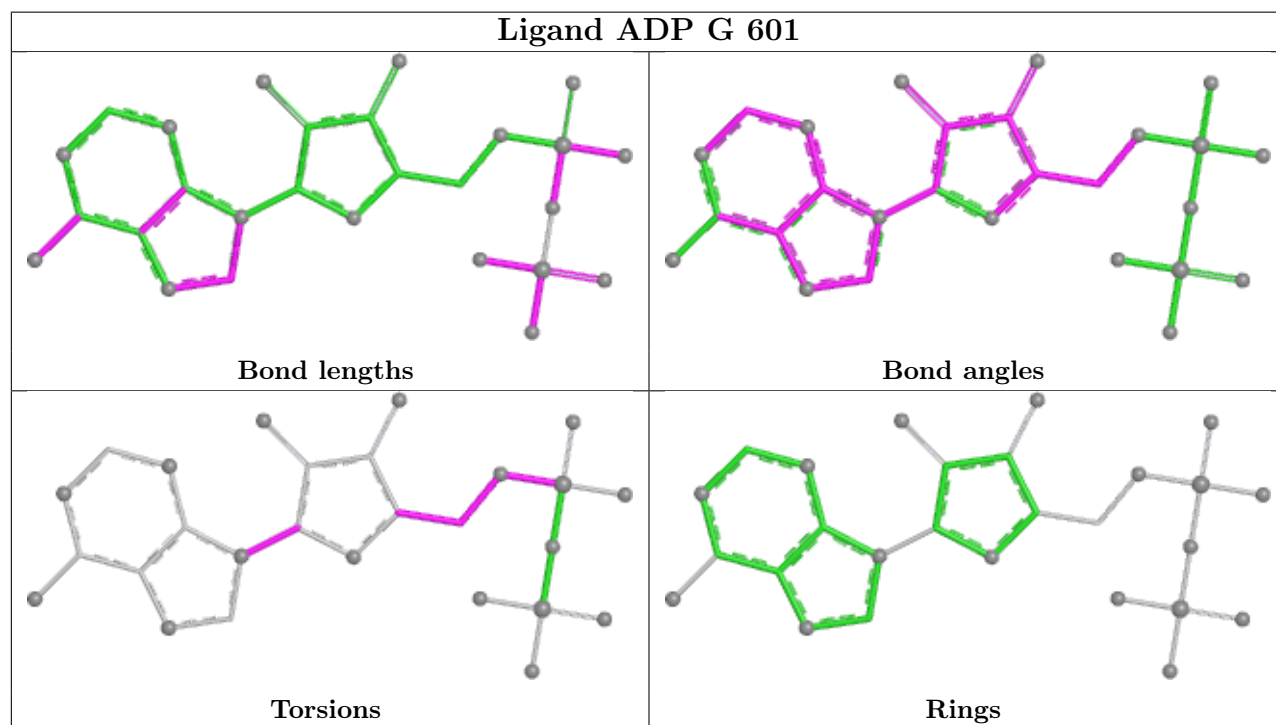
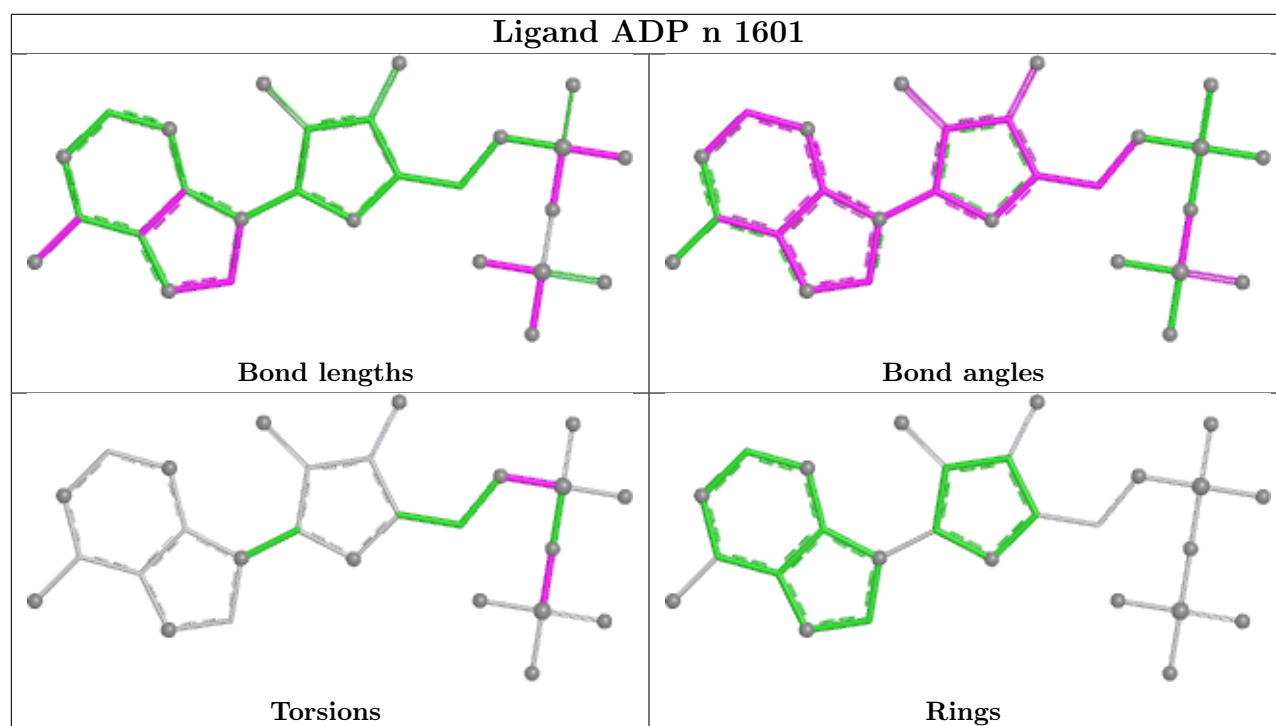
Ligand ADP J 601

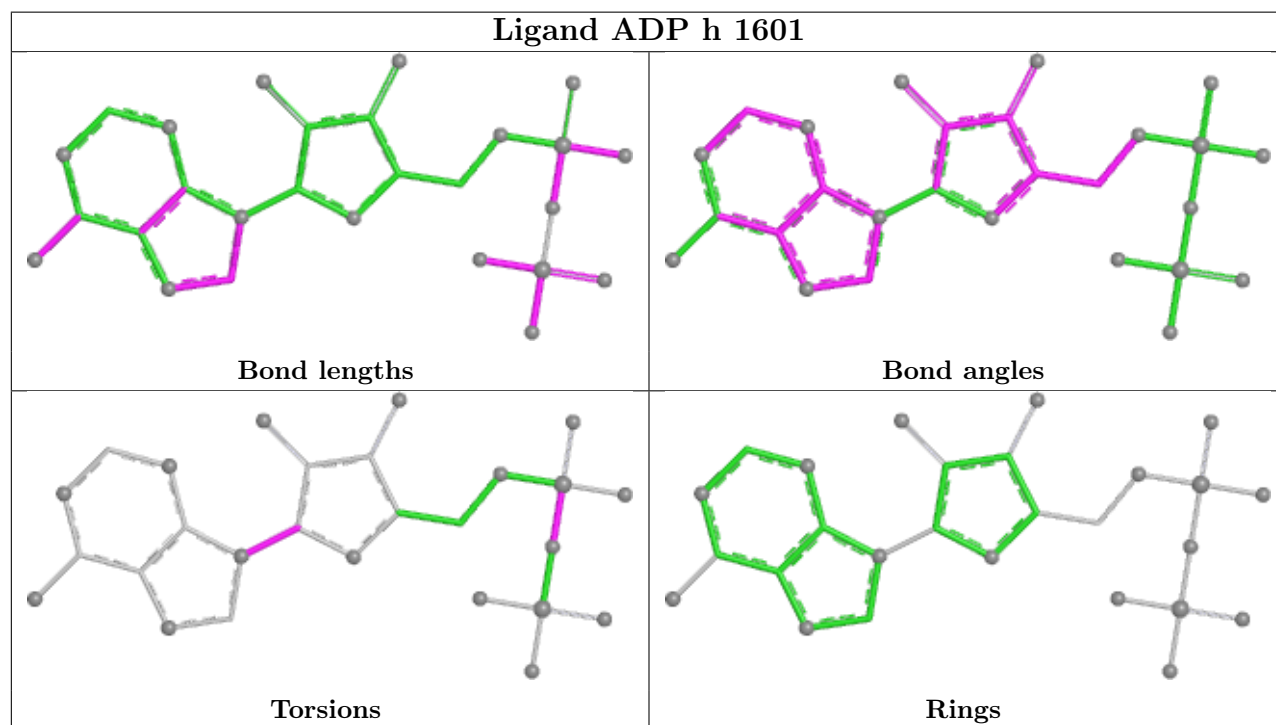
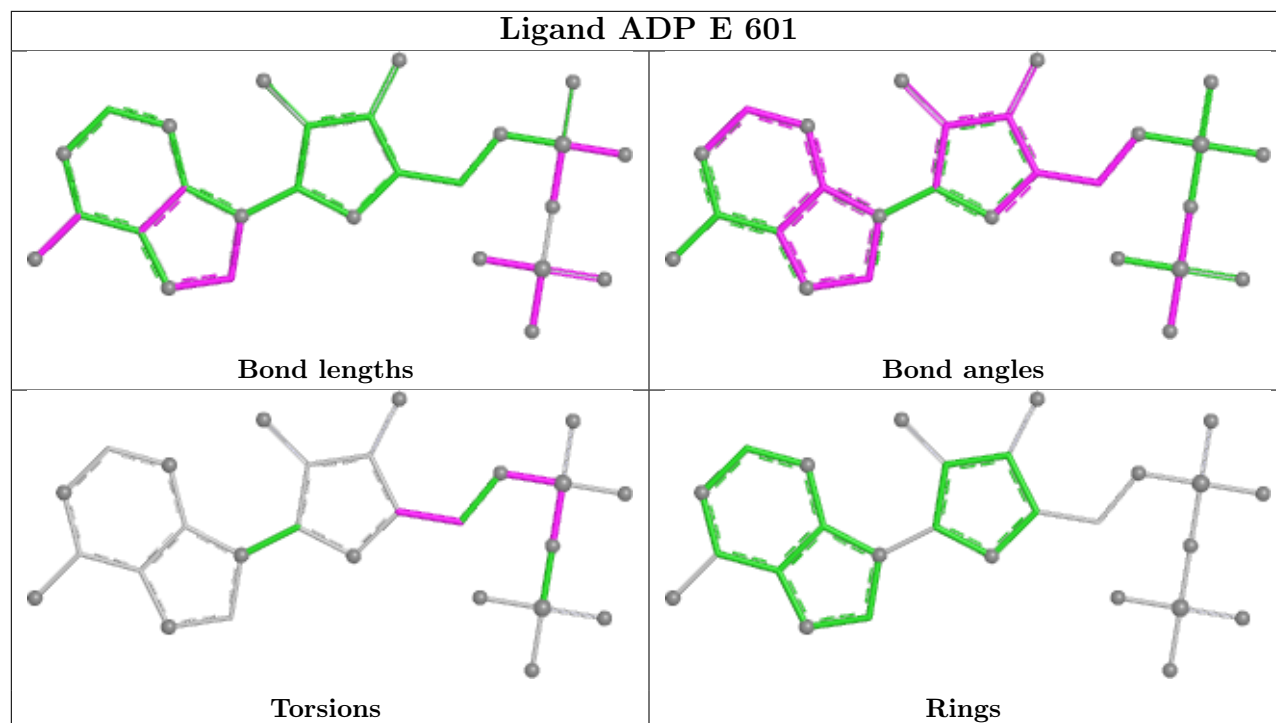


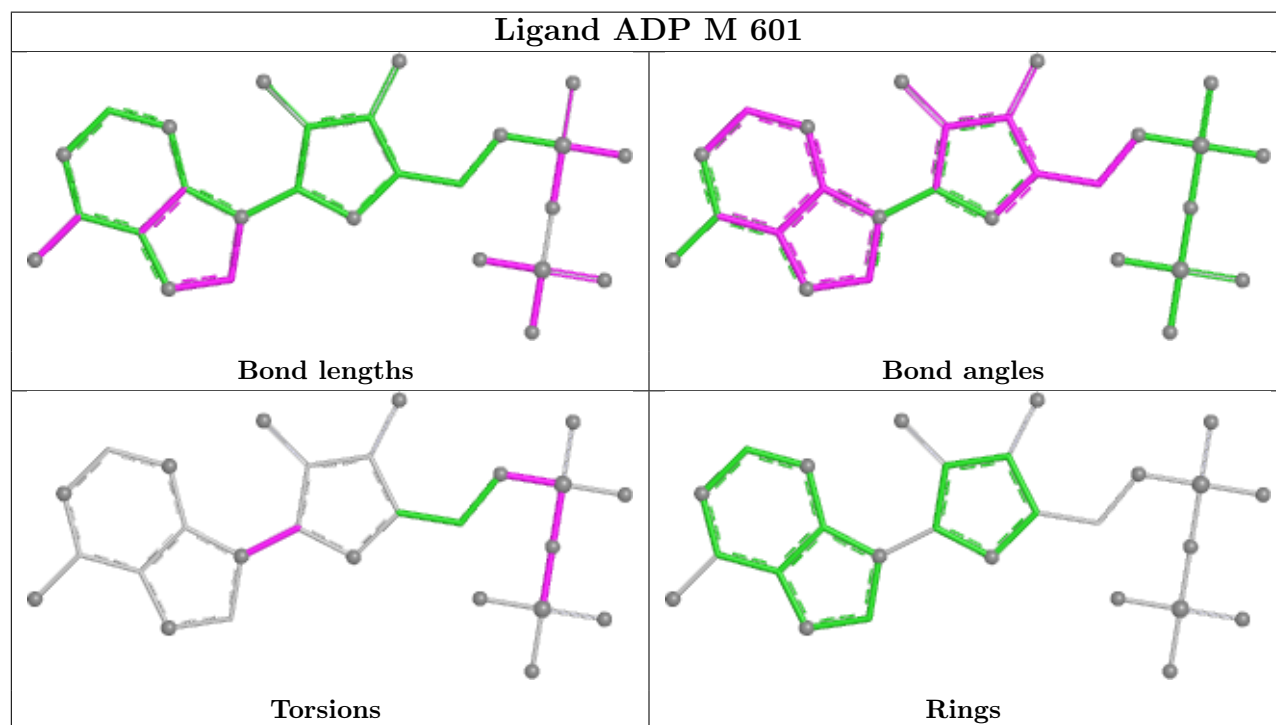
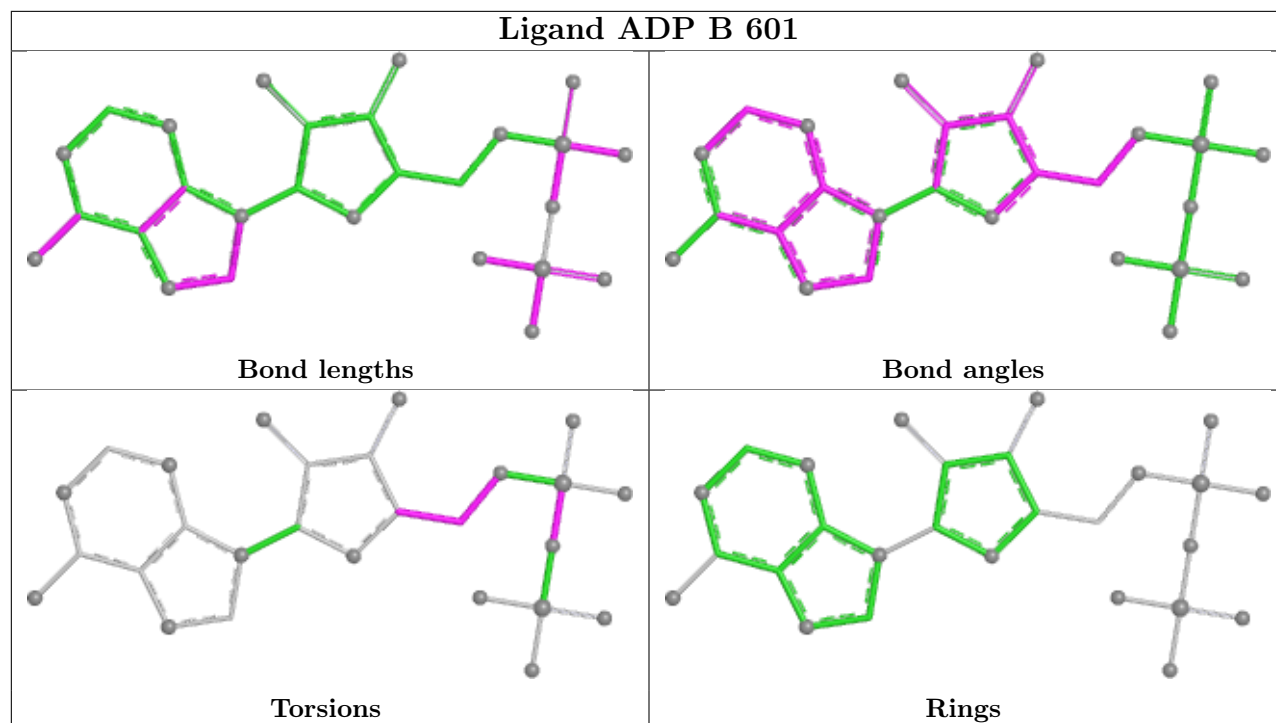
Ligand ADP C 1101

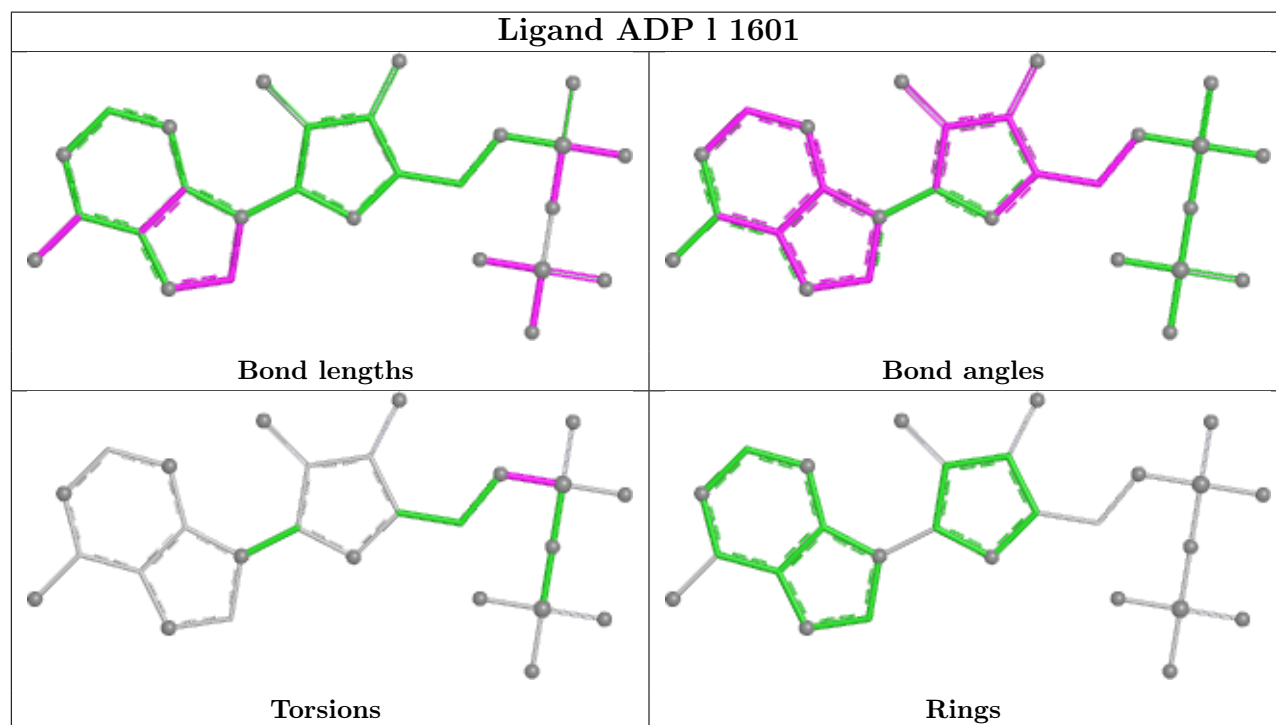
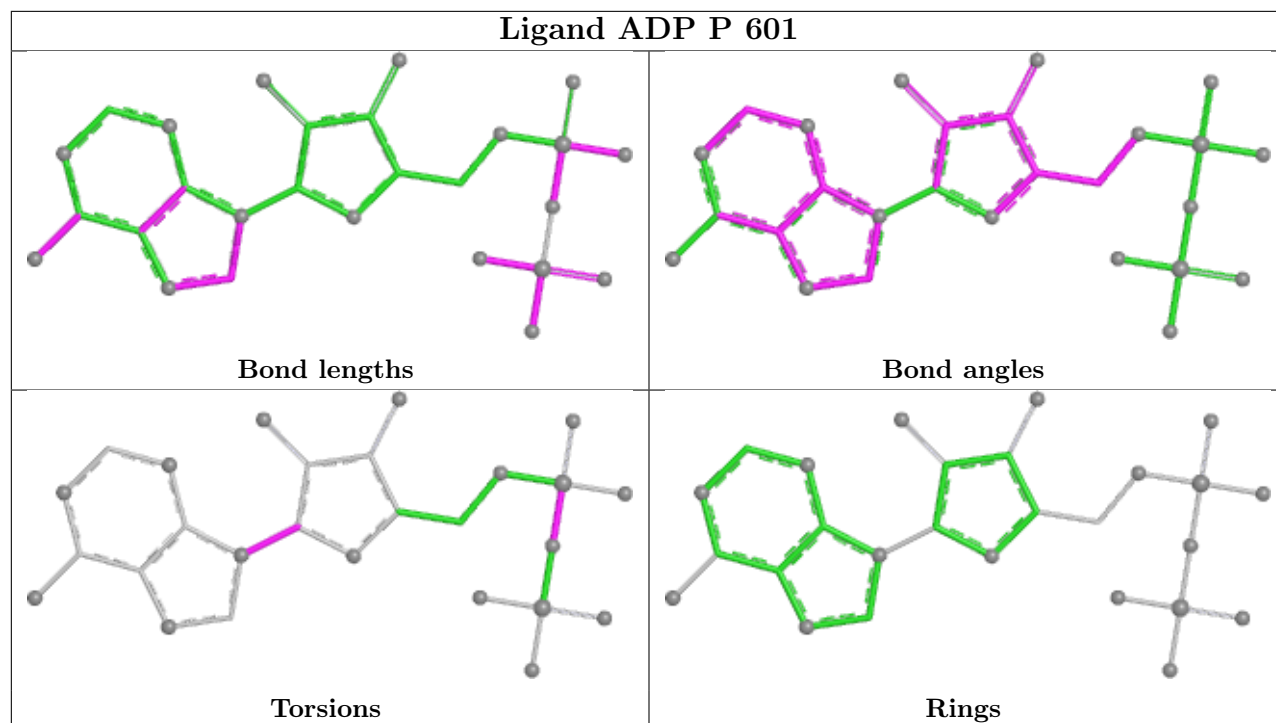




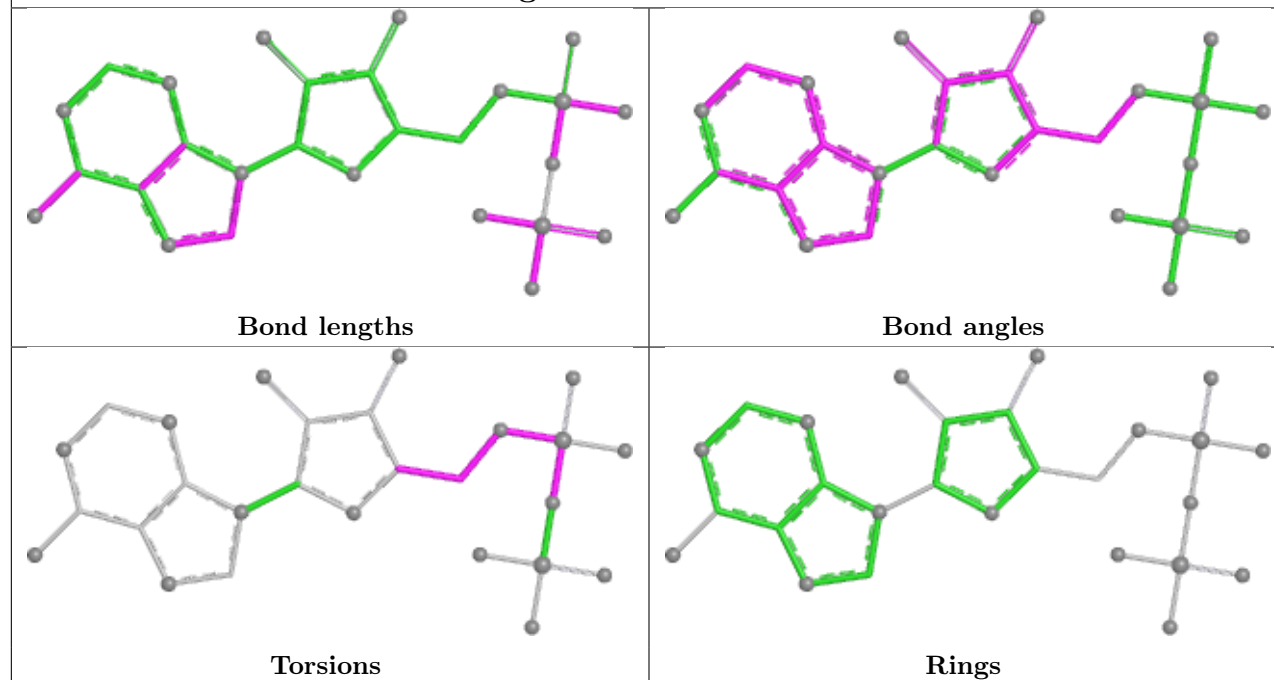




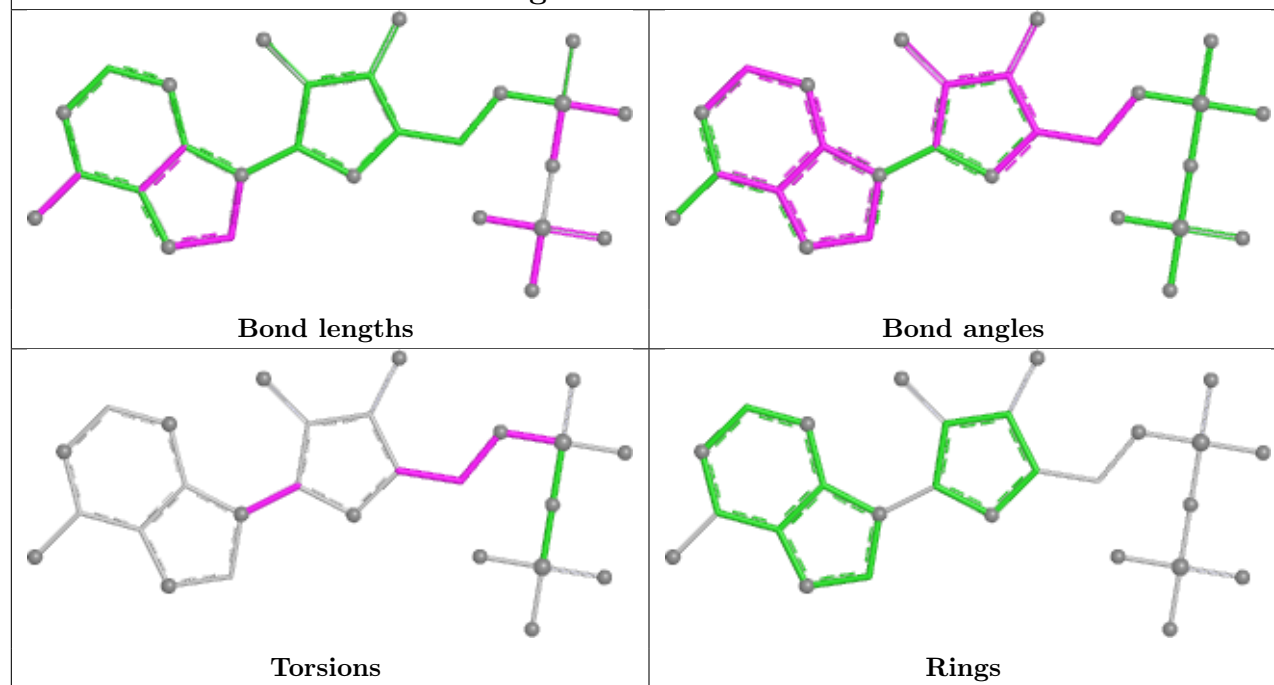


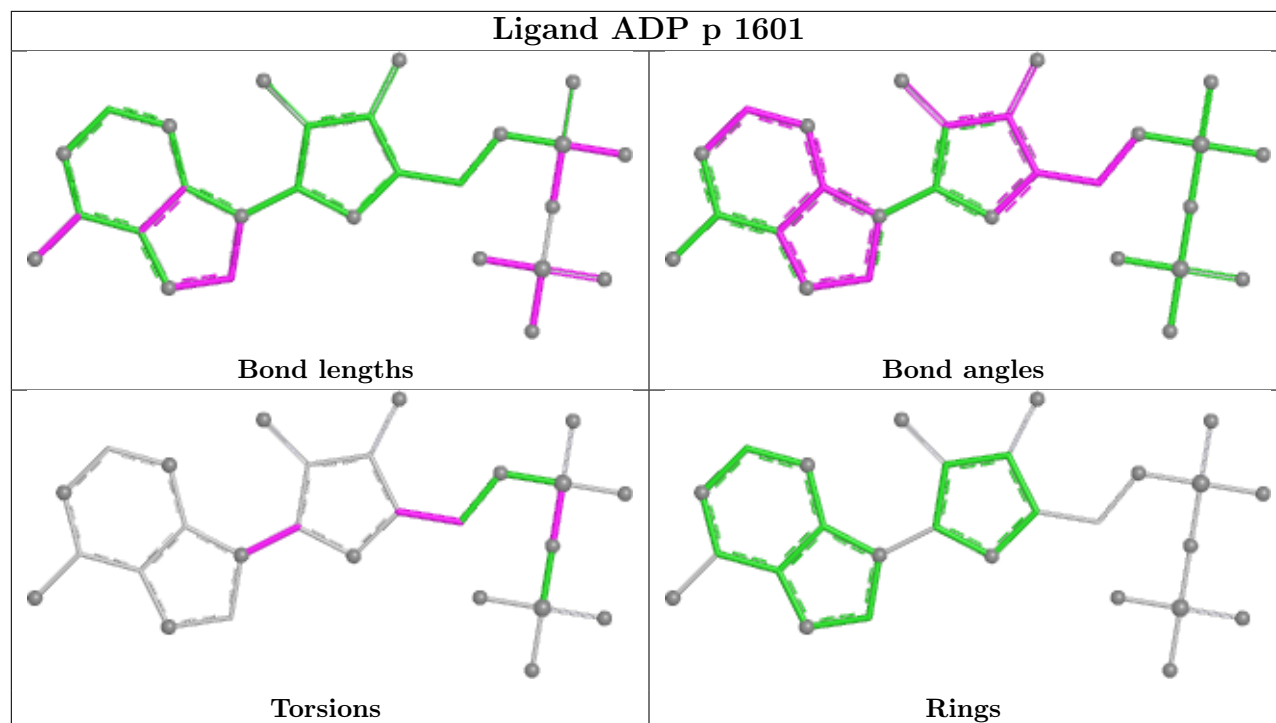


Ligand ADP m 1601



Ligand ADP A 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	544/559 (97%)	0.75	42 (7%)	19	18	72, 134, 206, 254	0
1	I	544/559 (97%)	0.84	55 (10%)	12	14	72, 134, 206, 254	0
1	a	544/559 (97%)	0.58	22 (4%)	42	30	72, 134, 206, 254	0
1	i	544/559 (97%)	0.69	37 (6%)	23	20	72, 134, 206, 254	0
2	B	513/527 (97%)	0.80	42 (8%)	17	17	47, 120, 192, 236	0
2	J	513/527 (97%)	0.87	52 (10%)	12	14	47, 120, 192, 236	0
2	b	513/527 (97%)	0.78	48 (9%)	14	16	47, 120, 192, 236	0
2	j	513/527 (97%)	0.77	48 (9%)	14	16	47, 120, 192, 236	0
3	C	514/590 (87%)	1.10	71 (13%)	6	10	73, 141, 205, 295	0
3	K	514/590 (87%)	0.90	54 (10%)	11	14	73, 141, 205, 295	0
3	c	514/590 (87%)	0.77	42 (8%)	17	17	73, 141, 205, 295	0
3	k	514/590 (87%)	0.85	45 (8%)	15	16	73, 141, 205, 295	0
4	D	522/528 (98%)	1.18	90 (17%)	4	6	70, 149, 232, 297	0
4	L	522/528 (98%)	0.95	63 (12%)	8	12	70, 149, 232, 297	0
4	d	522/528 (98%)	0.85	49 (9%)	14	16	70, 149, 232, 297	0
4	l	522/528 (98%)	0.99	72 (13%)	6	10	70, 149, 232, 297	0
5	E	525/562 (93%)	0.96	70 (13%)	7	10	56, 138, 238, 297	0
5	M	525/562 (93%)	0.84	49 (9%)	14	16	56, 138, 238, 297	0
5	e	525/562 (93%)	0.74	40 (7%)	20	18	56, 138, 238, 297	0
5	m	525/562 (93%)	0.81	54 (10%)	12	14	56, 138, 238, 297	0
6	F	533/546 (97%)	0.89	63 (11%)	9	12	42, 116, 214, 301	0
6	N	533/546 (97%)	0.85	53 (9%)	13	15	42, 116, 214, 301	0
6	f	533/546 (97%)	0.84	49 (9%)	14	16	42, 116, 214, 301	0
6	n	533/546 (97%)	0.88	61 (11%)	10	13	42, 116, 214, 301	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	G	509/550 (92%)	0.88	42 (8%) 17 17	65, 136, 207, 264	0
7	O	509/550 (92%)	0.91	52 (10%) 12 14	65, 136, 207, 264	0
7	g	509/550 (92%)	0.85	48 (9%) 14 16	65, 136, 207, 264	0
7	o	509/550 (92%)	0.84	49 (9%) 13 15	65, 136, 207, 264	0
8	H	525/568 (92%)	1.00	73 (13%) 6 9	70, 148, 236, 294	0
8	P	525/568 (92%)	0.85	45 (8%) 16 16	70, 148, 236, 294	0
8	h	525/568 (92%)	0.87	50 (9%) 14 15	70, 148, 236, 294	0
8	p	525/568 (92%)	0.87	55 (10%) 11 14	70, 148, 236, 294	0
All	All	16740/17720 (94%)	0.86	1685 (10%) 12 14	42, 136, 217, 301	0

The worst 5 of 1685 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	364	THR	8.8
4	l	1283	CYS	7.4
5	e	1034	ASP	7.2
8	p	1006	PRO	6.8
4	D	283	CYS	6.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	BEF	J	602	4/4	0.53	0.20	235,236,240,246	0
10	BEF	N	602	4/4	0.60	0.29	112,120,121,122	0

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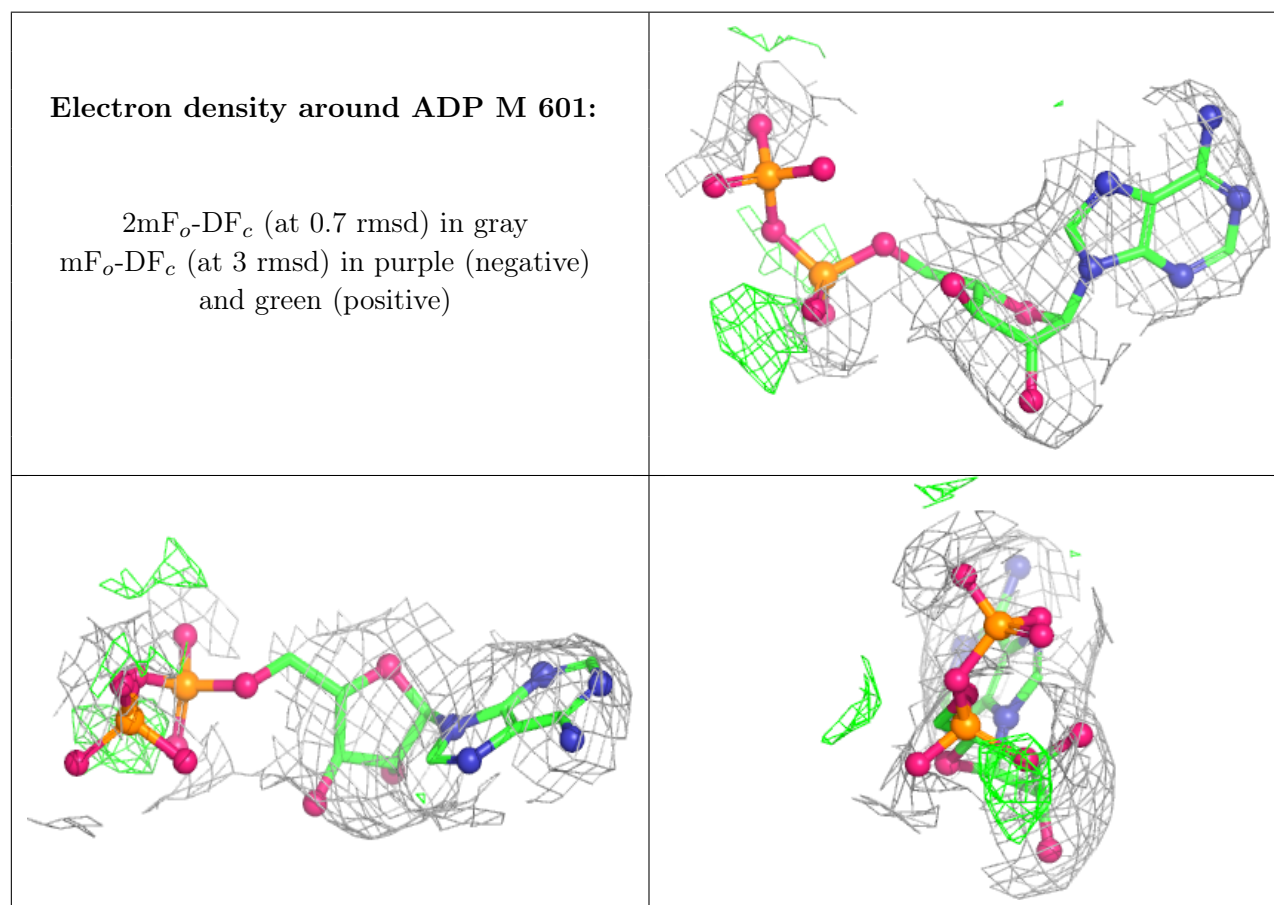
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	BEF	A	602	4/4	0.66	0.18	246,247,249,251	0
10	BEF	E	602	4/4	0.68	0.29	240,241,242,244	0
10	BEF	n	1602	4/4	0.68	0.42	163,167,167,173	0
10	BEF	f	1602	4/4	0.69	0.26	167,170,171,173	0
10	BEF	F	602	4/4	0.71	0.37	157,163,163,171	0
10	BEF	G	602	4/4	0.71	0.20	236,237,238,239	0
10	BEF	g	1602	4/4	0.75	0.20	162,165,165,166	0
11	SO4	K	1101	5/5	0.75	0.18	84,89,97,102	0
10	BEF	B	602	4/4	0.76	0.24	210,215,215,215	0
10	BEF	M	602	4/4	0.78	0.12	152,158,161,170	0
11	SO4	O	600	5/5	0.78	0.14	78,79,92,100	0
11	SO4	c	2101	5/5	0.78	0.18	82,98,107,111	0
11	SO4	d	1600	5/5	0.78	0.15	106,109,115,118	0
10	BEF	L	602	4/4	0.80	0.13	172,177,177,180	0
10	BEF	a	1602	4/4	0.81	0.17	235,239,240,241	0
11	SO4	j	1600	5/5	0.81	0.18	79,96,98,100	0
11	SO4	I	600	5/5	0.82	0.17	98,103,110,113	0
11	SO4	o	1600	5/5	0.82	0.17	107,107,115,117	0
9	ADP	M	601	27/27	0.83	0.12	43,113,256,333	0
11	SO4	i	1600	5/5	0.85	0.14	91,94,103,116	0
9	ADP	l	1601	27/27	0.85	0.13	62,105,189,226	0
10	BEF	m	1602	4/4	0.85	0.14	185,193,195,196	0
9	ADP	k	2101	27/27	0.86	0.12	80,131,164,321	0
10	BEF	P	602	4/4	0.86	0.11	158,158,158,162	0
9	ADP	L	601	27/27	0.86	0.13	102,157,212,241	0
10	BEF	b	1602	4/4	0.86	0.12	154,158,161,163	0
9	ADP	n	1601	27/27	0.87	0.17	27,94,337,491	0
9	ADP	f	1601	27/27	0.88	0.20	13,50,316,499	0
10	BEF	p	1602	4/4	0.88	0.10	84,99,102,108	0
10	BEF	e	1602	4/4	0.90	0.11	201,205,207,207	0
9	ADP	D	601	27/27	0.90	0.11	41,92,238,264	0
9	ADP	J	601	27/27	0.91	0.13	74,85,241,279	0
9	ADP	B	601	27/27	0.91	0.13	62,105,202,218	0
9	ADP	A	601	27/27	0.91	0.15	46,110,243,330	0
9	ADP	E	601	27/27	0.91	0.12	11,102,242,288	0
9	ADP	g	1601	27/27	0.91	0.13	26,159,211,215	0
10	BEF	C	1102	4/4	0.91	0.10	104,105,105,120	0
9	ADP	a	1601	27/27	0.92	0.12	50,112,239,328	0
9	ADP	e	1601	27/27	0.92	0.09	30,116,232,274	0
9	ADP	H	601	27/27	0.92	0.10	11,112,145,153	0
9	ADP	m	1601	27/27	0.92	0.11	13,87,195,273	0
9	ADP	F	601	27/27	0.93	0.19	11,105,323,481	0

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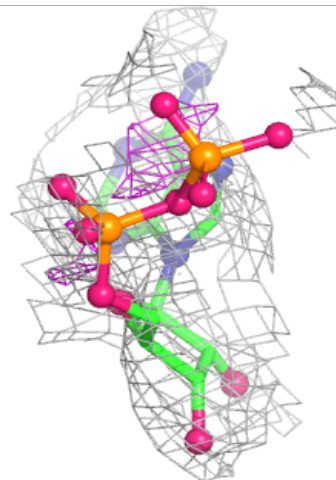
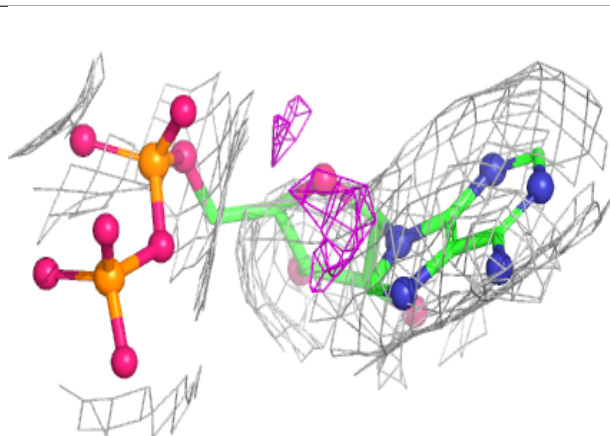
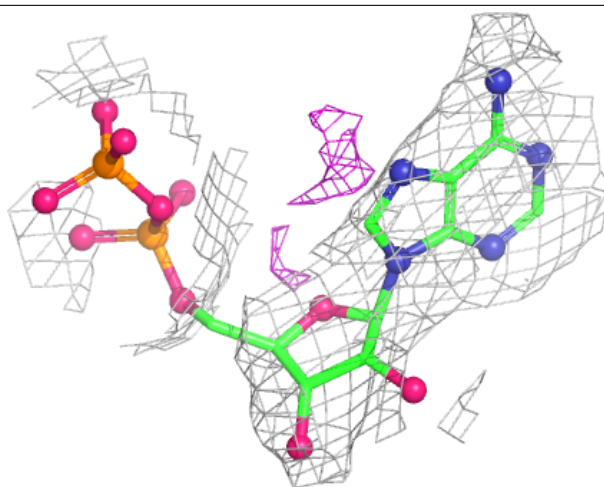
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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9	ADP	C	1101	27/27	0.93	0.14	38,135,163,237	0
9	ADP	h	1601	27/27	0.93	0.11	40,139,153,188	0
9	ADP	b	1601	27/27	0.93	0.11	44,69,220,243	0
9	ADP	N	601	27/27	0.94	0.13	11,88,232,484	0
9	ADP	G	601	27/27	0.94	0.12	12,133,240,248	0
9	ADP	p	1601	27/27	0.94	0.10	11,114,136,239	0
10	BEF	h	1602	4/4	0.96	0.07	85,93,93,106	0
10	BEF	H	602	4/4	0.96	0.04	101,103,104,110	0
10	BEF	l	1602	4/4	0.97	0.06	28,61,73,75	0
10	BEF	D	602	4/4	0.97	0.06	81,84,91,92	0
10	BEF	k	2102	4/4	0.97	0.05	68,69,80,82	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



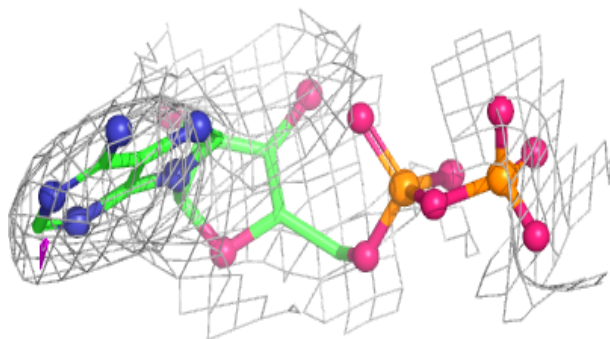
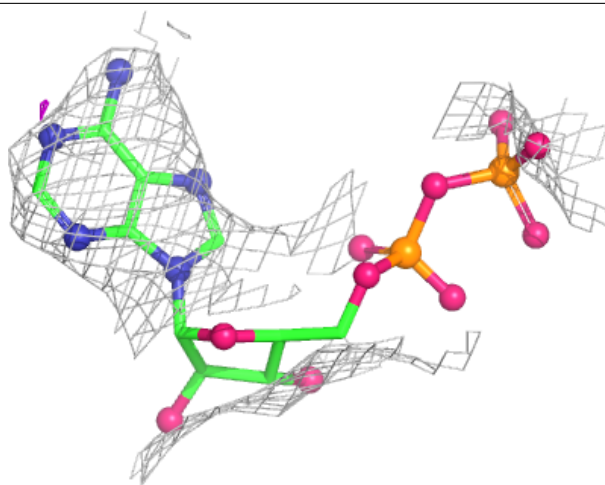
Electron density around ADP 1 1601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



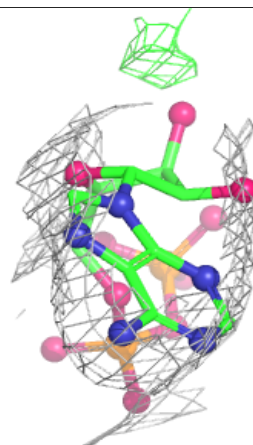
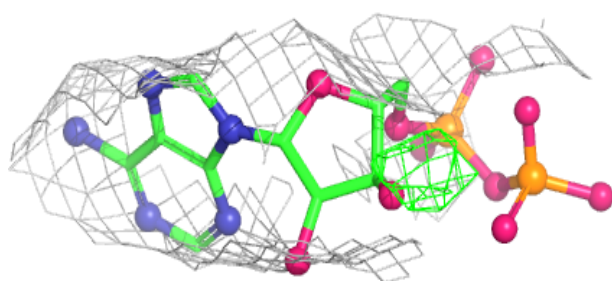
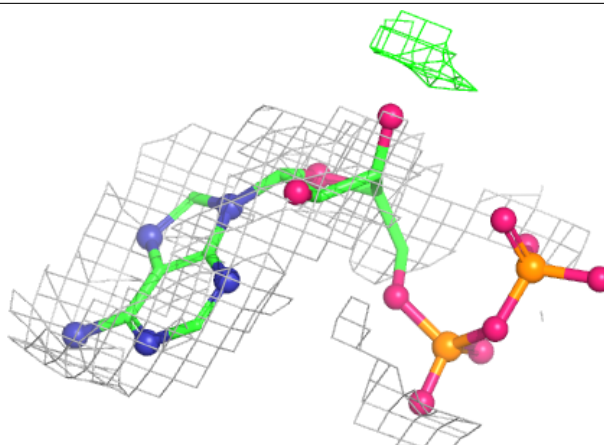
Electron density around ADP k 2101:

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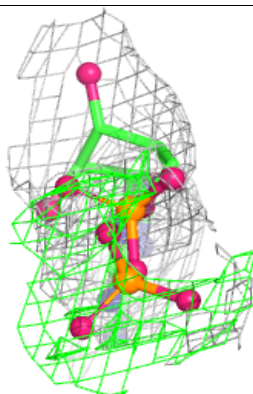
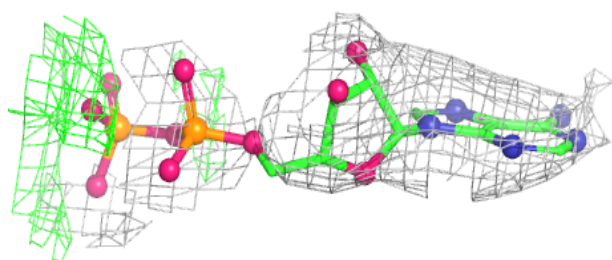
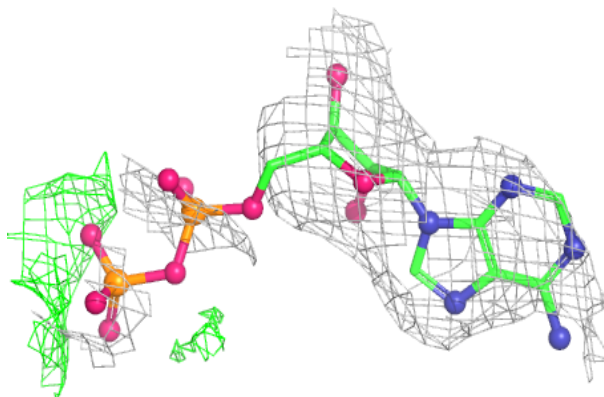


Electron density around ADP L 601:

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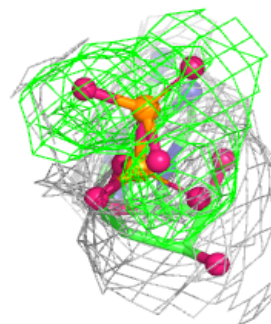
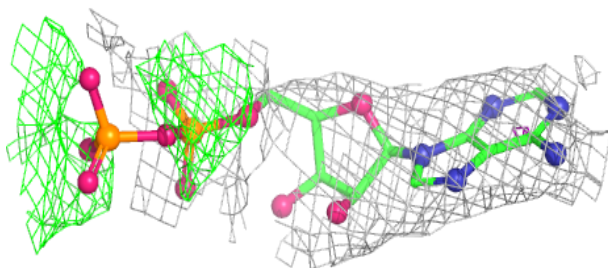
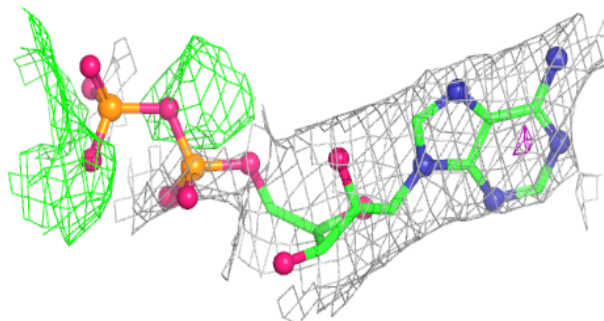
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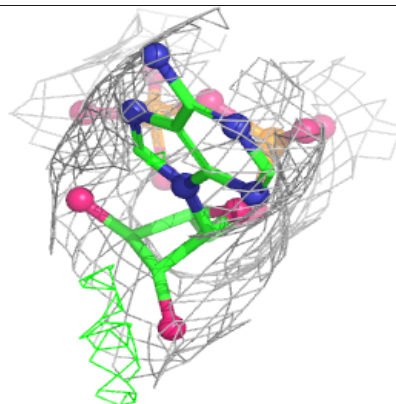
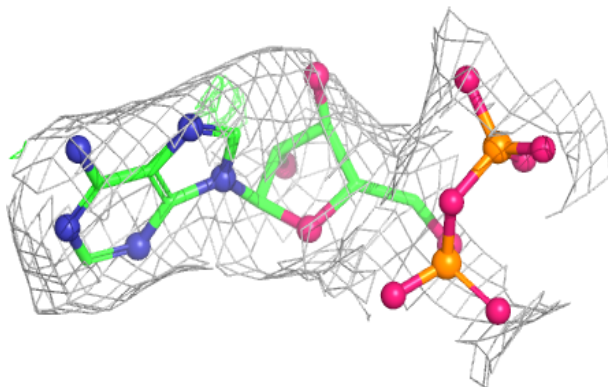
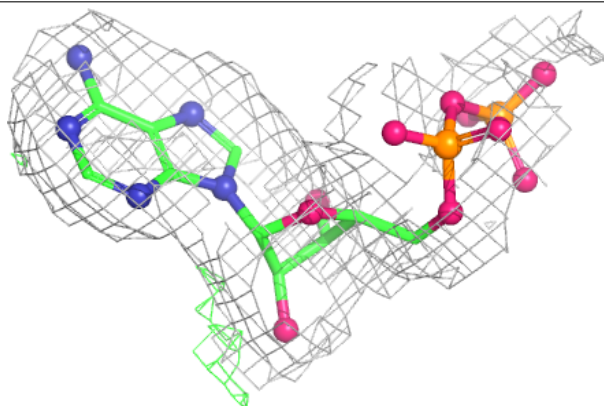


Electron density around ADP f 1601:

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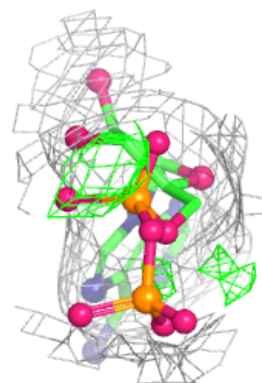
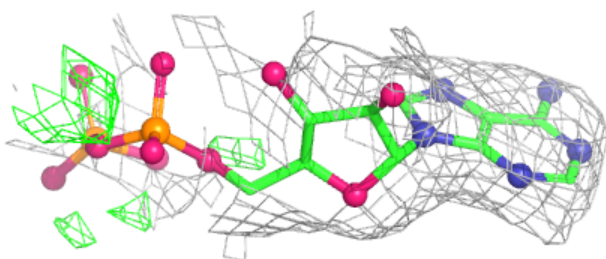
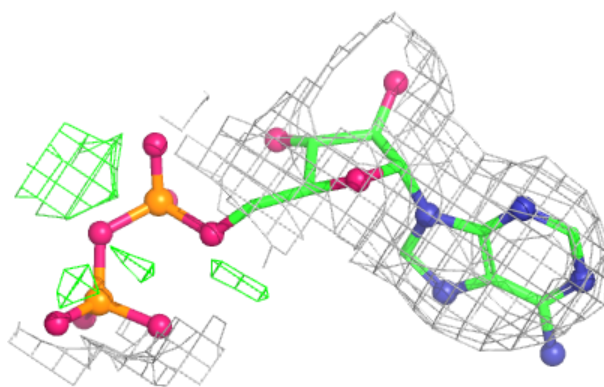
**Electron density around ADP D 601:**

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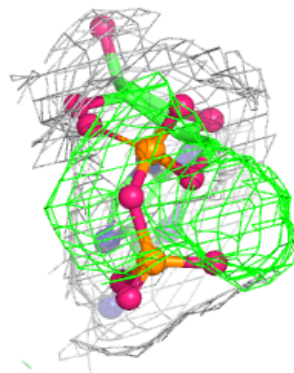
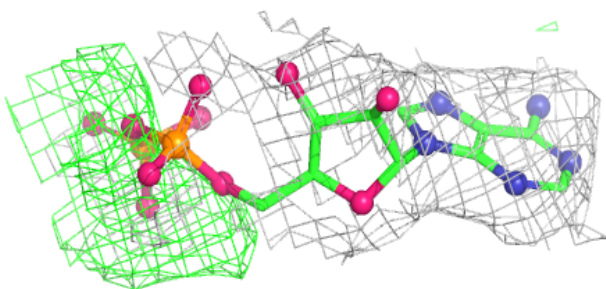
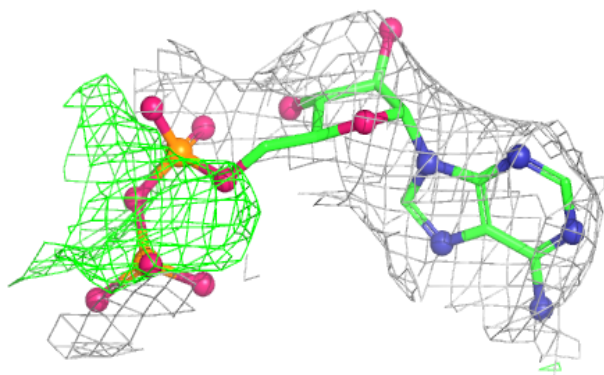


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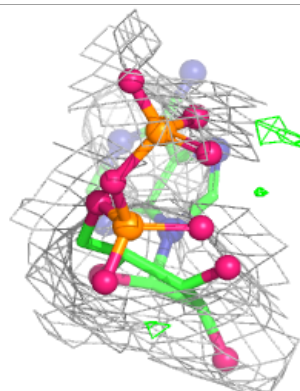
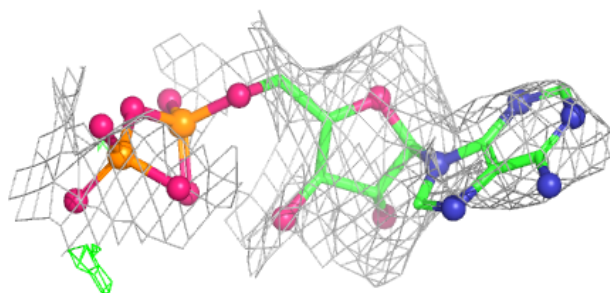
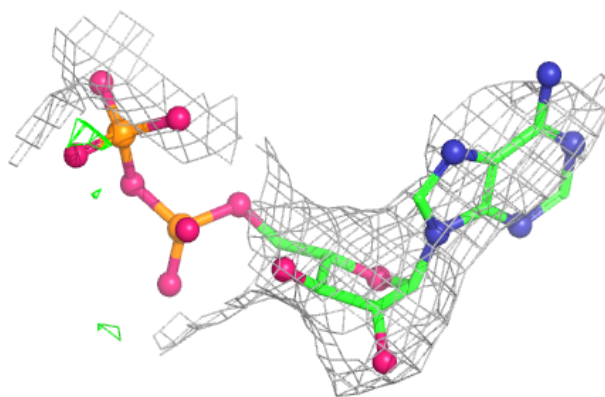
**Electron density around ADP B 601:**

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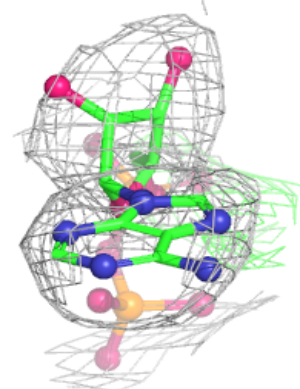
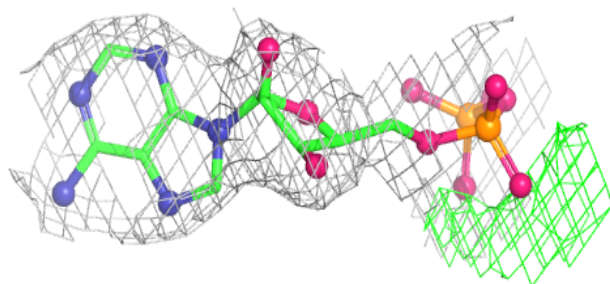
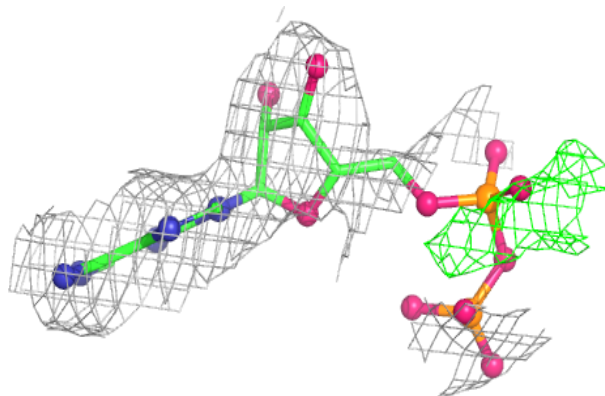


Electron density around ADP A 601:

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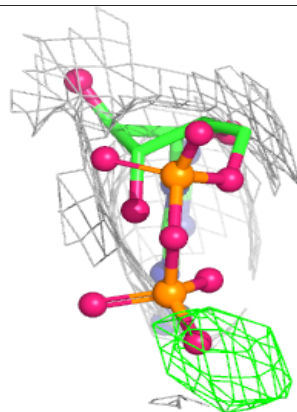
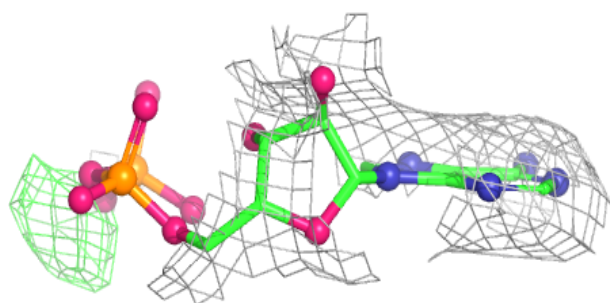
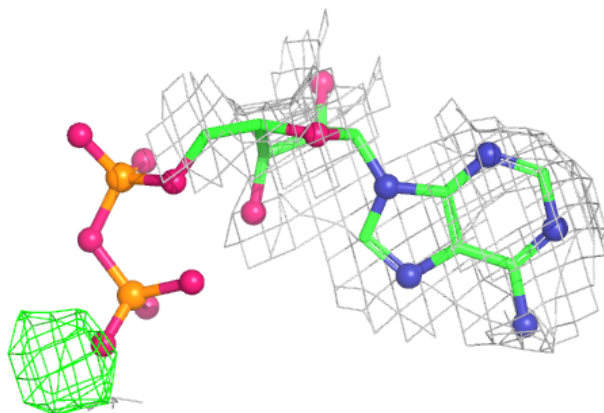
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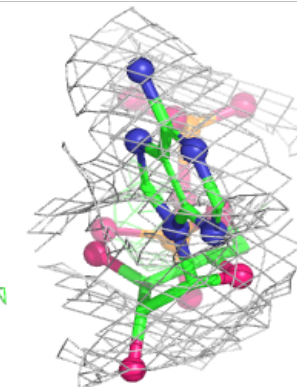
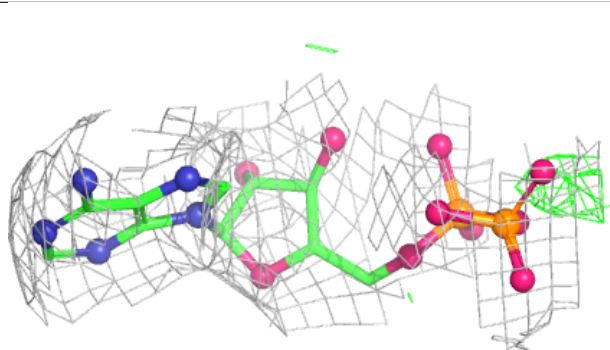
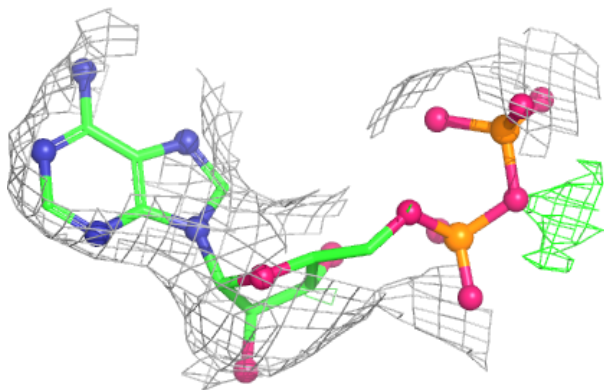


Electron density around ADP g 1601:

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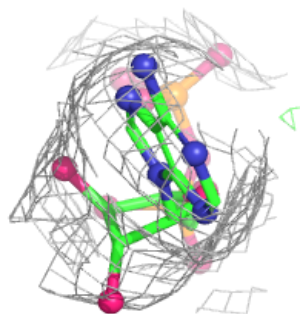
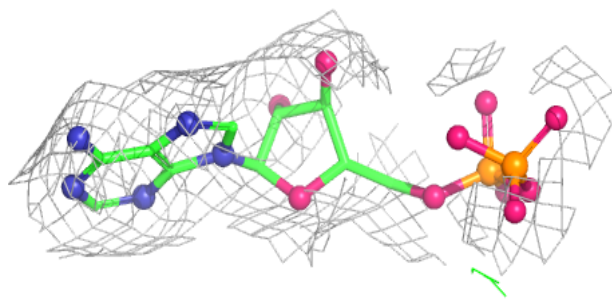
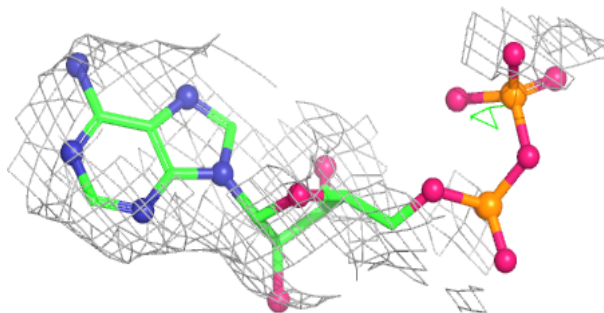
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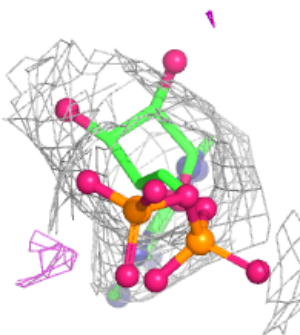
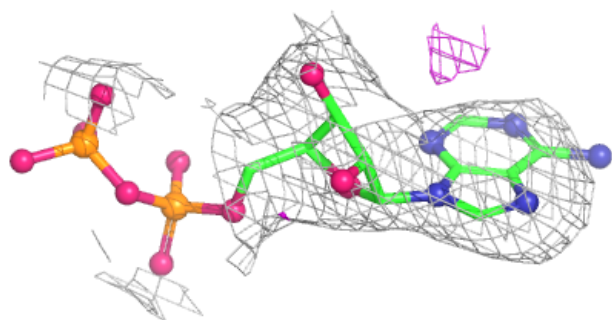
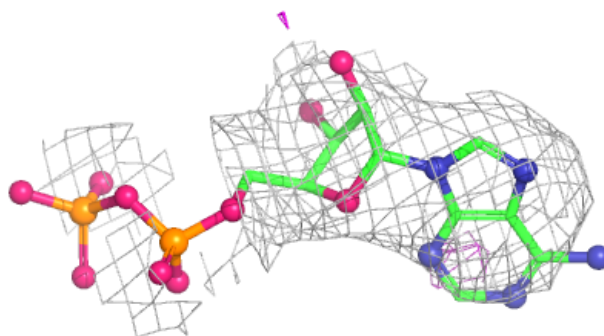


Electron density around ADP e 1601:

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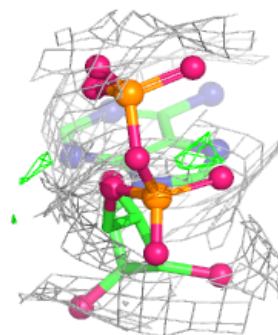
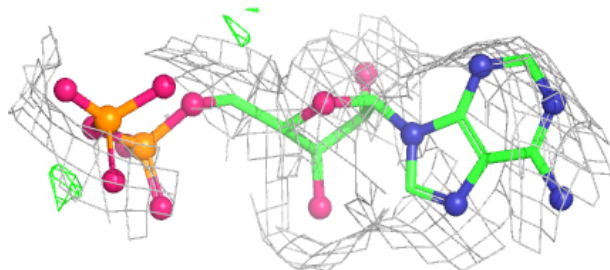
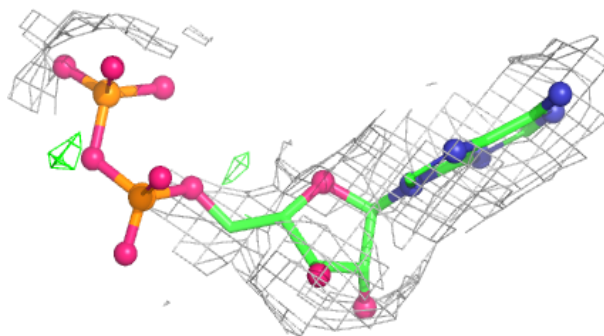
**Electron density around ADP H 601:**

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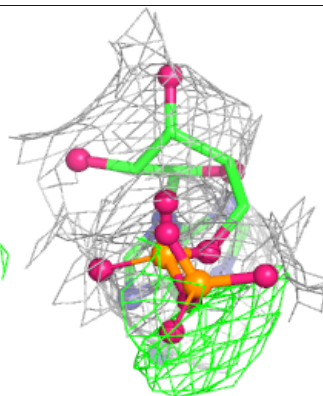
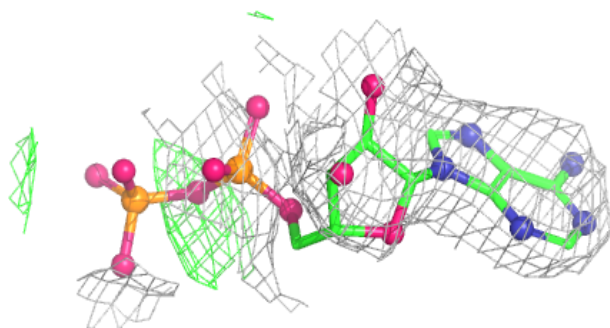
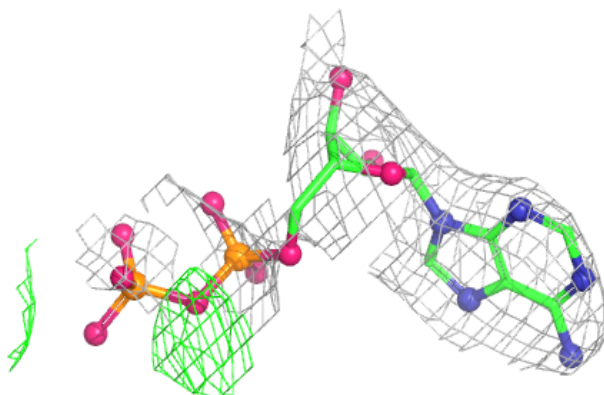


Electron density around ADP m 1601:

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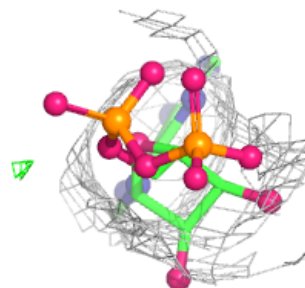
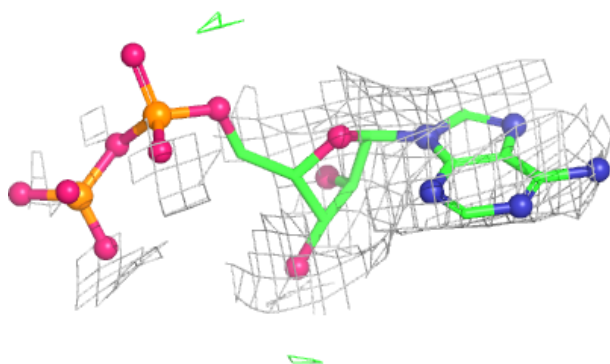
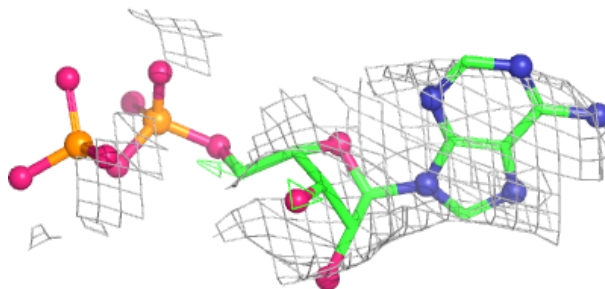
**Electron density around ADP F 601:**

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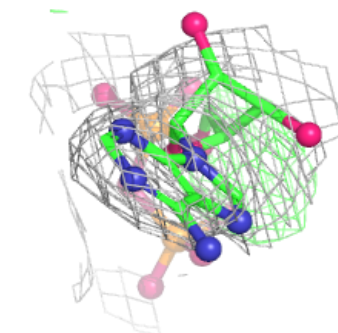
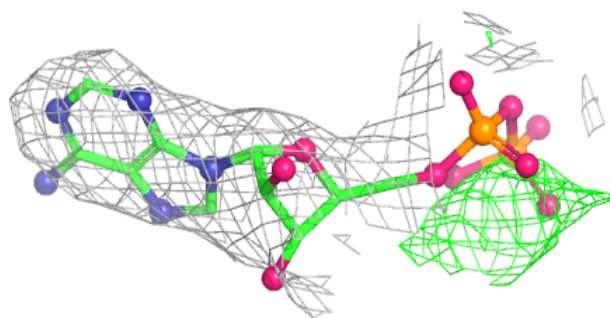
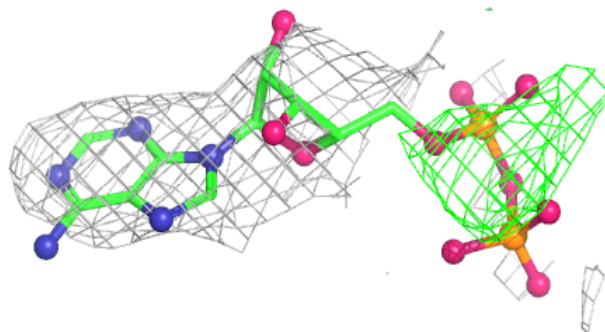


Electron density around ADP P 601:

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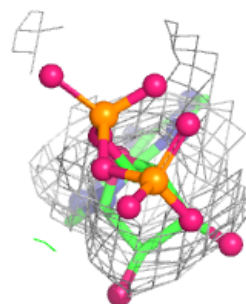
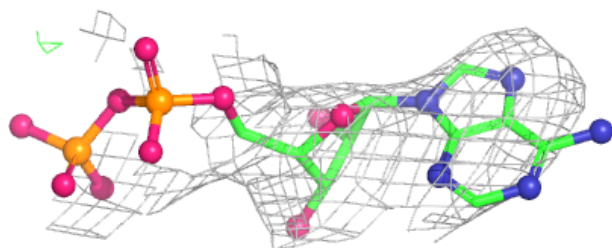
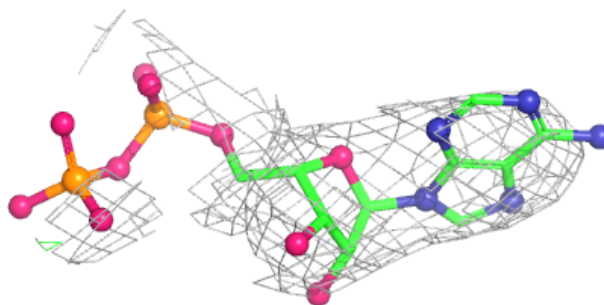
**Electron density around ADP C 1101:**

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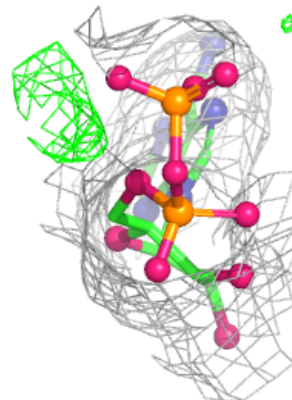
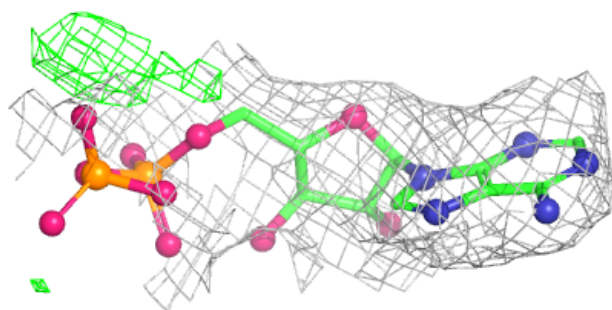
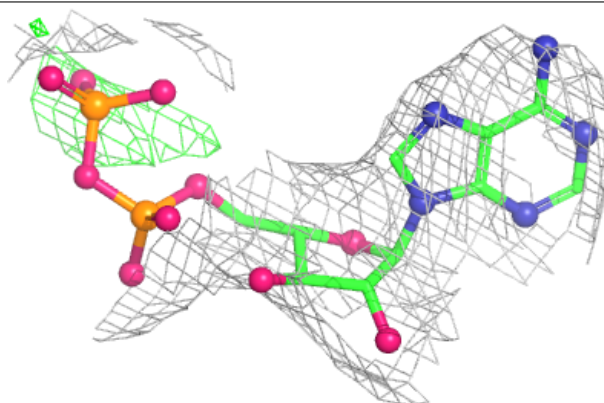


Electron density around ADP h 1601:

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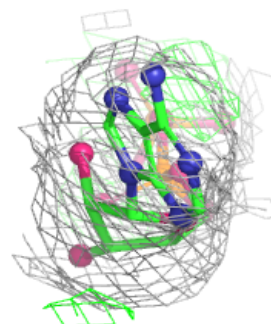
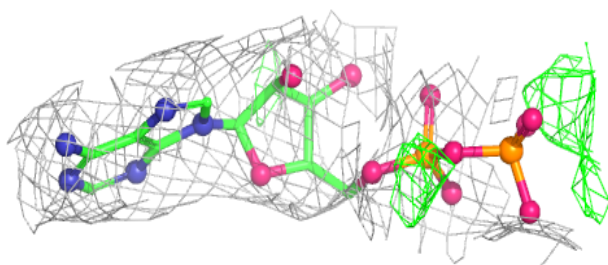
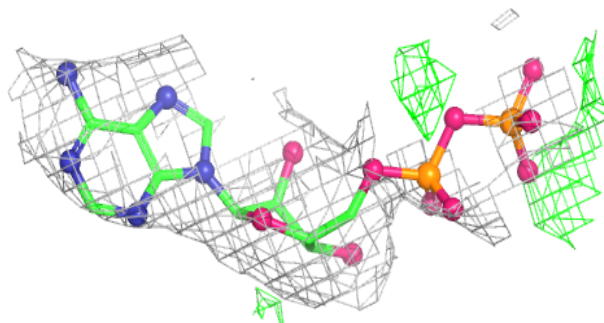
**Electron density around ADP b 1601:**

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and green (positive)



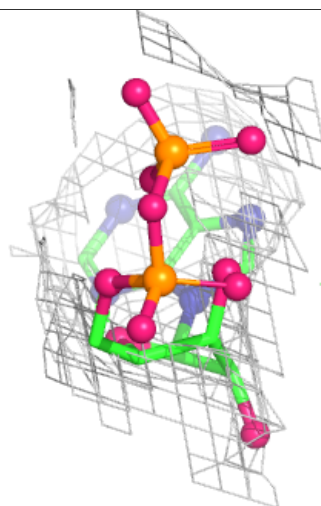
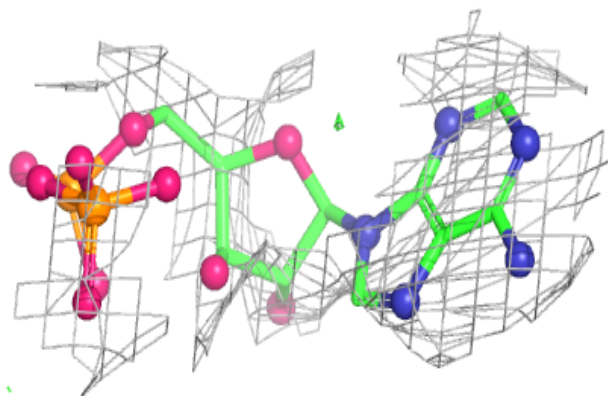
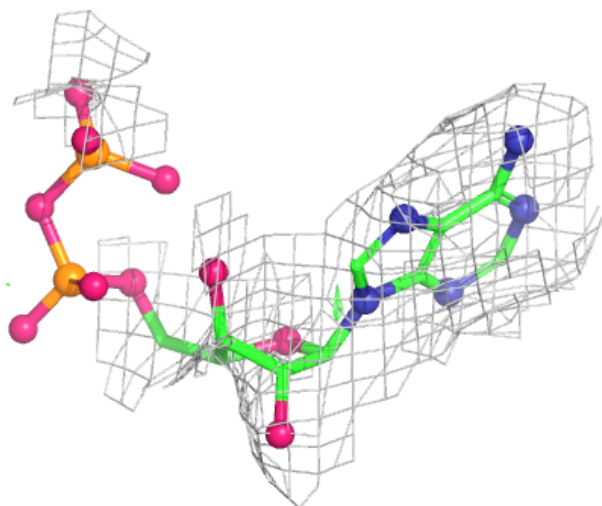
Electron density around ADP N 601:

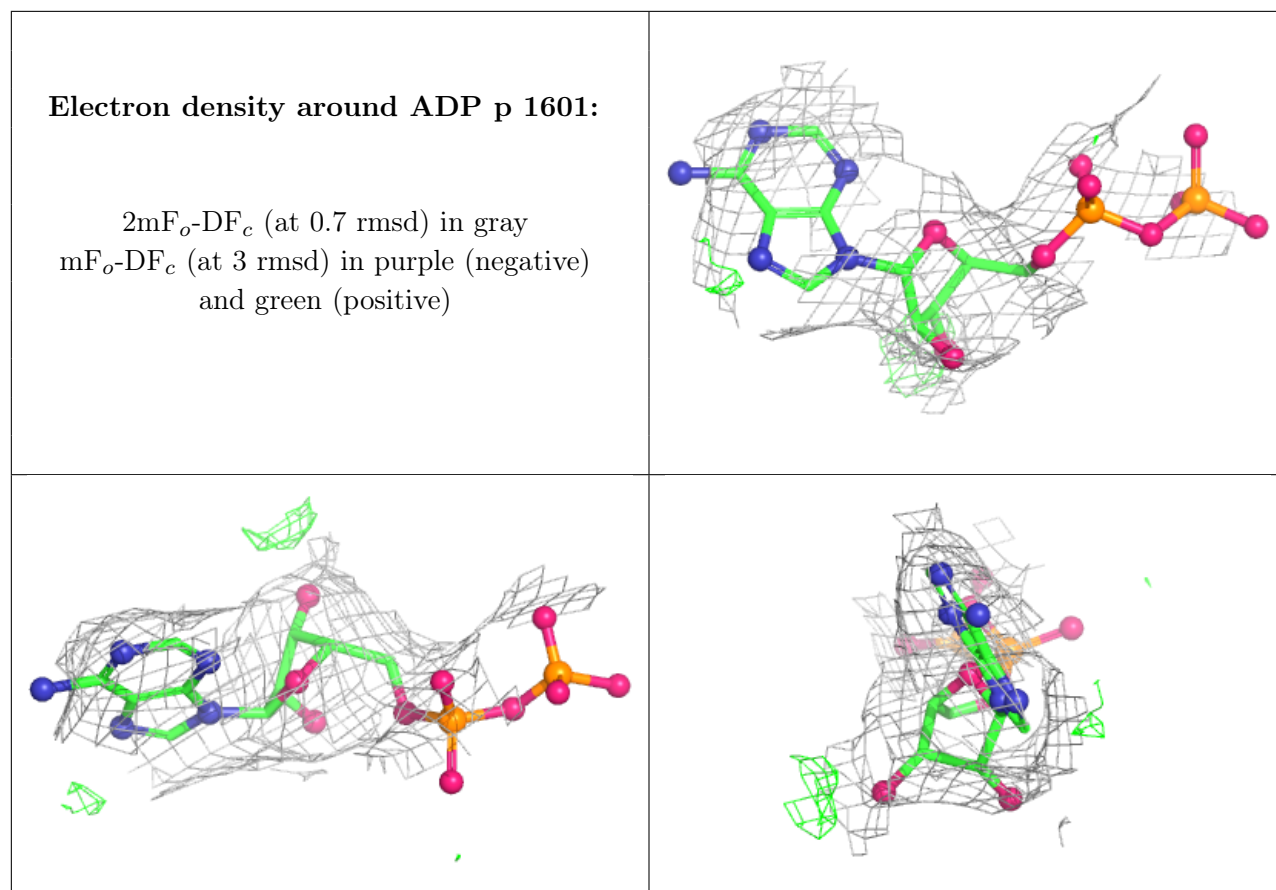
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP G 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.