wwPDB X-ray Structure Validation Summary Report (i)

Aug 4, 2026 – 09:55 PM EDT

PDB ID	:	4V94 / pdb_00004v94
Title	:	Molecular architecture of the eukaryotic chaperonin TRiC/CCT derived by a combination of chemical crosslinking and mass-spectrometry, XL-MS
Authors	:	Leitner, A.; Joachimiak, L.A.; Bracher, A.; Walzthoeni, T.; Chen, B.; Monkemeyer, L.; Pechmann, S.; Holmes, S.; Cong, Y.; Ma, B.; Ludtke, S.; Chiu, W.; Hartl, F.U.; Aebersold, R.; Frydman, J.
Deposited on	:	2012-01-11
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 (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:

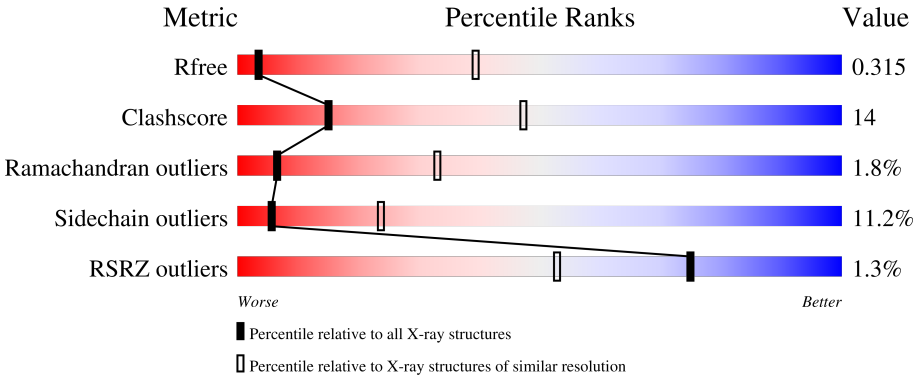
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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 <=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	F	546	66% 28% 5%
1	N	546	72% 24%
1	f	546	73% 23%
1	n	546	73% 23%
2	H	568	63% 25% 8%

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Mol	Chain	Length	Quality of chain
2	P	568	2% 69% 19% 8%
2	h	568	3% 68% 21% 8%
2	p	568	% 64% 24% 8%
3	G	550	% 61% 29% 5%
3	O	550	3% 63% 27% 5%
3	g	550	% 66% 25%
3	o	550	% 65% 26% 5%
4	E	562	64% 27% 5%
4	M	562	3% 70% 22% 5%
4	e	562	% 68% 23% 5%
4	m	562	66% 25% 5%
5	B	527	61% 30% 7%
5	J	527	2% 67% 28%
5	b	527	68% 27%
5	j	527	% 65% 29%
6	D	528	62% 33%
6	L	528	6% 69% 27%
6	d	528	2% 68% 28%
6	l	528	% 65% 30%
7	A	559	% 63% 27% 6%
7	I	559	3% 67% 25%
7	a	559	68% 25%
7	i	559	% 66% 26%
8	C	590	53% 29% 13%
8	K	590	% 58% 26% 13%

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Mol	Chain	Length	Quality of chain
8	c	590	% 59% 24% 13%
8	k	590	% 60% 23% 13%

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
11	BEF	b	603	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 120080 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 zeta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			
1	N	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			
1	f	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			
1	n	538	Total	C	N	O	S	0	0	0
			3836	2417	640	765	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			
2	P	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			
2	h	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			
2	p	521	Total	C	N	O	S	0	0	0
			3619	2286	602	708	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			
3	O	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			
3	g	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			
3	o	526	Total	C	N	O	S	0	0	0
			3752	2372	631	730	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			
4	M	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			
4	e	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			
4	m	535	Total	C	N	O	S	0	0	0
			3798	2391	634	752	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			
5	J	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			
5	b	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			
5	j	518	Total	C	N	O	S	0	0	0
			3689	2306	623	747	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			
6	L	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			
6	d	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			
6	l	523	Total	C	N	O	S	0	0	0
			3685	2306	631	731	17			

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	345	ASP	GLY	engineered mutation	UNP P39078
l	345	ASP	GLY	engineered mutation	UNP P39078

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			
7	I	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			
7	a	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			
7	i	539	Total	C	N	O	S	0	0	0
			3770	2369	638	746	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			
8	K	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			
8	c	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			
8	k	513	Total	C	N	O	S	0	0	0
			3615	2270	620	699	26			

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

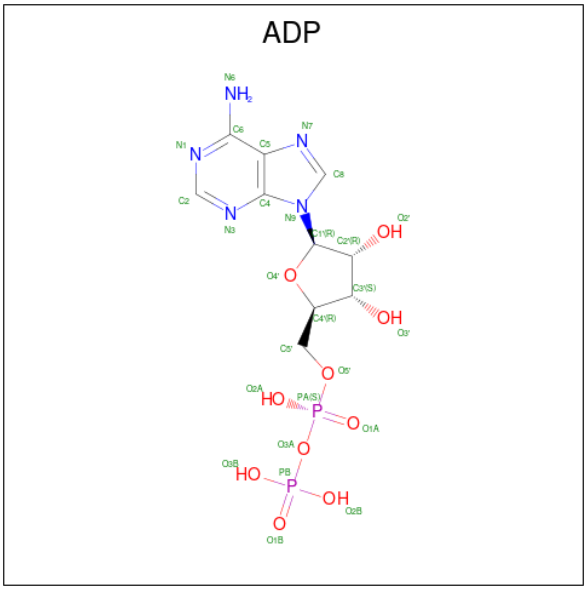
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total Mg 1 1	0	0
9	H	1	Total Mg 1 1	0	0
9	G	1	Total Mg 1 1	0	0
9	E	1	Total Mg 1 1	0	0
9	B	1	Total Mg 1 1	0	0
9	D	1	Total Mg 1 1	0	0
9	A	1	Total Mg 1 1	0	0
9	C	1	Total Mg 1 1	0	0
9	N	1	Total Mg 1 1	0	0
9	P	1	Total Mg 1 1	0	0
9	O	1	Total Mg 1 1	0	0
9	M	1	Total Mg 1 1	0	0
9	J	1	Total Mg 1 1	0	0
9	L	1	Total Mg 1 1	0	0
9	I	1	Total Mg 1 1	0	0
9	K	1	Total Mg 1 1	0	0
9	f	1	Total Mg 1 1	0	0
9	h	1	Total Mg 1 1	0	0
9	g	1	Total Mg 1 1	0	0
9	e	1	Total Mg 1 1	0	0
9	b	1	Total Mg 1 1	0	0
9	d	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	a	1	Total Mg 1 1	0	0
9	c	1	Total Mg 1 1	0	0
9	n	1	Total Mg 1 1	0	0
9	p	1	Total Mg 1 1	0	0
9	o	1	Total Mg 1 1	0	0
9	m	1	Total Mg 1 1	0	0
9	j	1	Total Mg 1 1	0	0
9	l	1	Total Mg 1 1	0	0
9	i	1	Total Mg 1 1	0	0
9	k	1	Total Mg 1 1	0	0

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	1	Total C N O P 27 10 5 10 2	0	0

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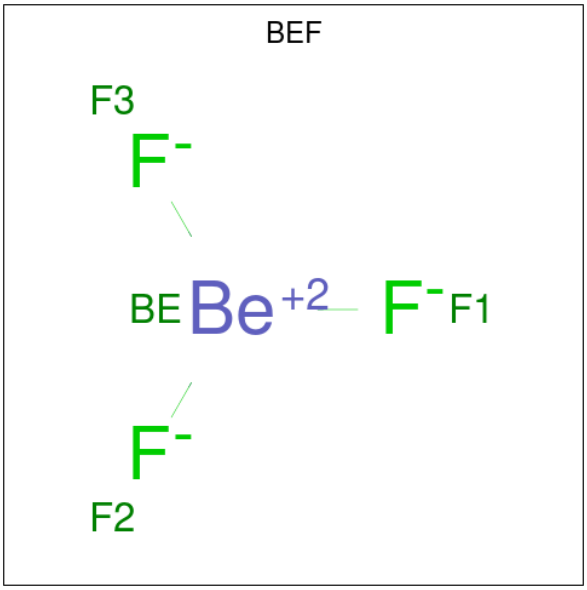
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	P	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	f	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	h	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	g	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	e	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	b	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	d	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	a	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	c	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	n	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	p	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	o	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	m	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	j	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	l	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	i	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
10	k	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 11 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	1	Total Be F 4 1 3	0	0
11	G	1	Total Be F 4 1 3	0	0
11	E	1	Total Be F 4 1 3	0	0
11	B	1	Total Be F 4 1 3	0	0
11	D	1	Total Be F 4 1 3	0	0
11	A	1	Total Be F 4 1 3	0	0
11	C	1	Total Be F 4 1 3	0	0
11	N	1	Total Be F 4 1 3	0	0
11	P	1	Total Be F 4 1 3	0	0
11	O	1	Total Be F 4 1 3	0	0
11	M	1	Total Be F 4 1 3	0	0
11	J	1	Total Be F 4 1 3	0	0
11	L	1	Total Be F 4 1 3	0	0
11	I	1	Total Be F 4 1 3	0	0
11	K	1	Total Be F 4 1 3	0	0
11	f	1	Total Be F 4 1 3	0	0
11	h	1	Total Be F 4 1 3	0	0
11	g	1	Total Be F 4 1 3	0	0
11	e	1	Total Be F 4 1 3	0	0
11	b	1	Total Be F 4 1 3	0	0
11	d	1	Total Be F 4 1 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	a	1	Total Be F 4 1 3	0	0
11	c	1	Total Be F 4 1 3	0	0
11	n	1	Total Be F 4 1 3	0	0
11	p	1	Total Be F 4 1 3	0	0
11	o	1	Total Be F 4 1 3	0	0
11	m	1	Total Be F 4 1 3	0	0
11	j	1	Total Be F 4 1 3	0	0
11	l	1	Total Be F 4 1 3	0	0
11	i	1	Total Be F 4 1 3	0	0
11	k	1	Total Be F 4 1 3	0	0

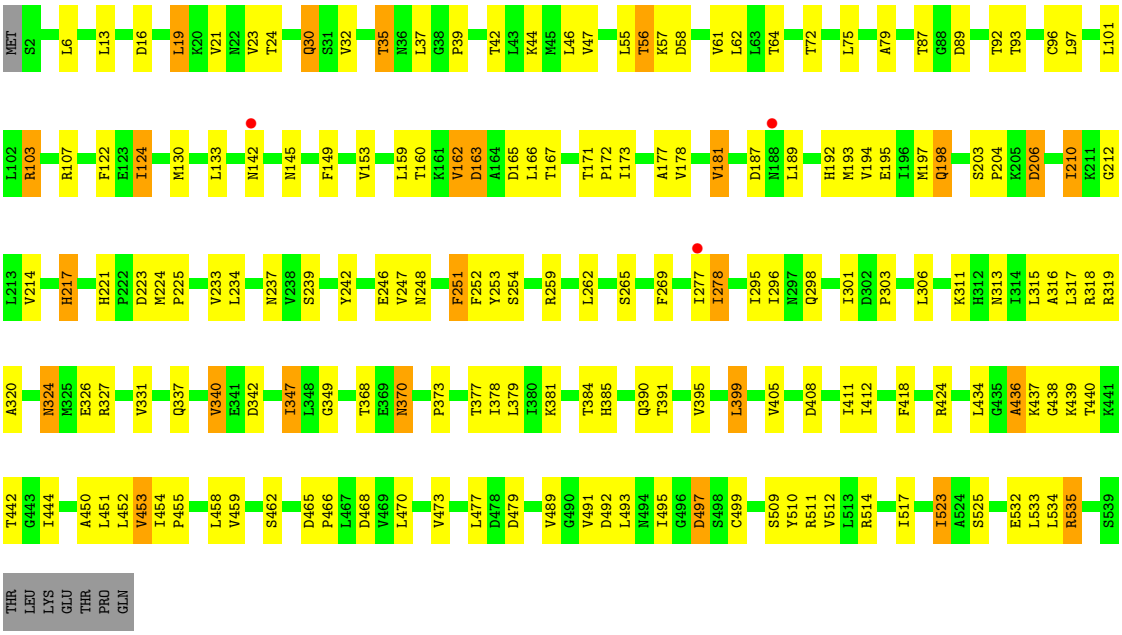
3 Residue-property plots (i)

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 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 zeta

Chain F:

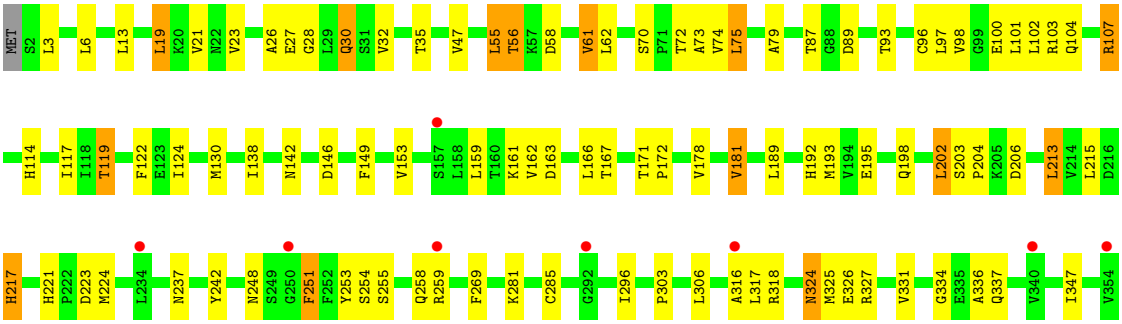


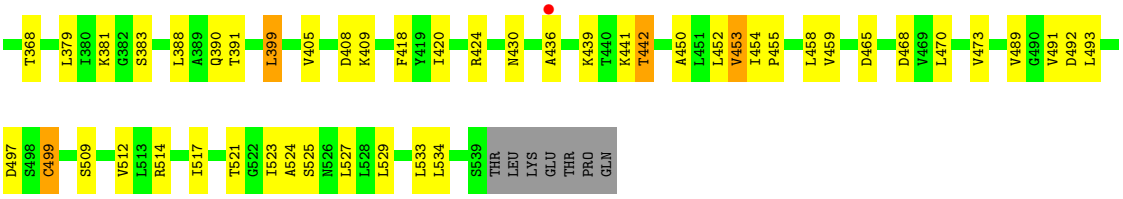


• Molecule 1: T-complex protein 1 subunit zeta

Chain N:

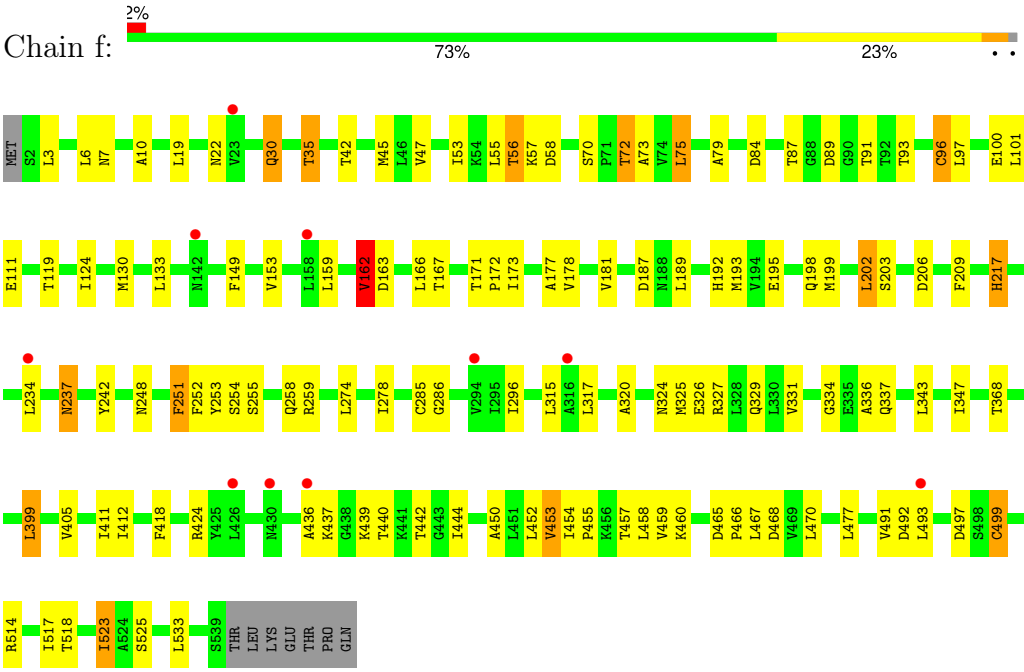






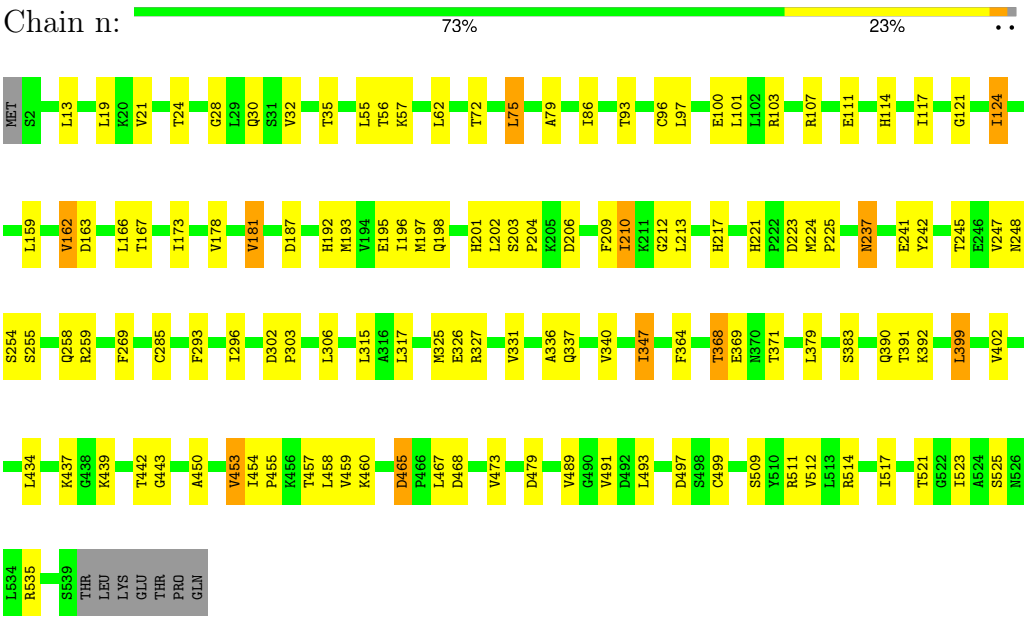
• Molecule 1: T-complex protein 1 subunit zeta

Chain f:



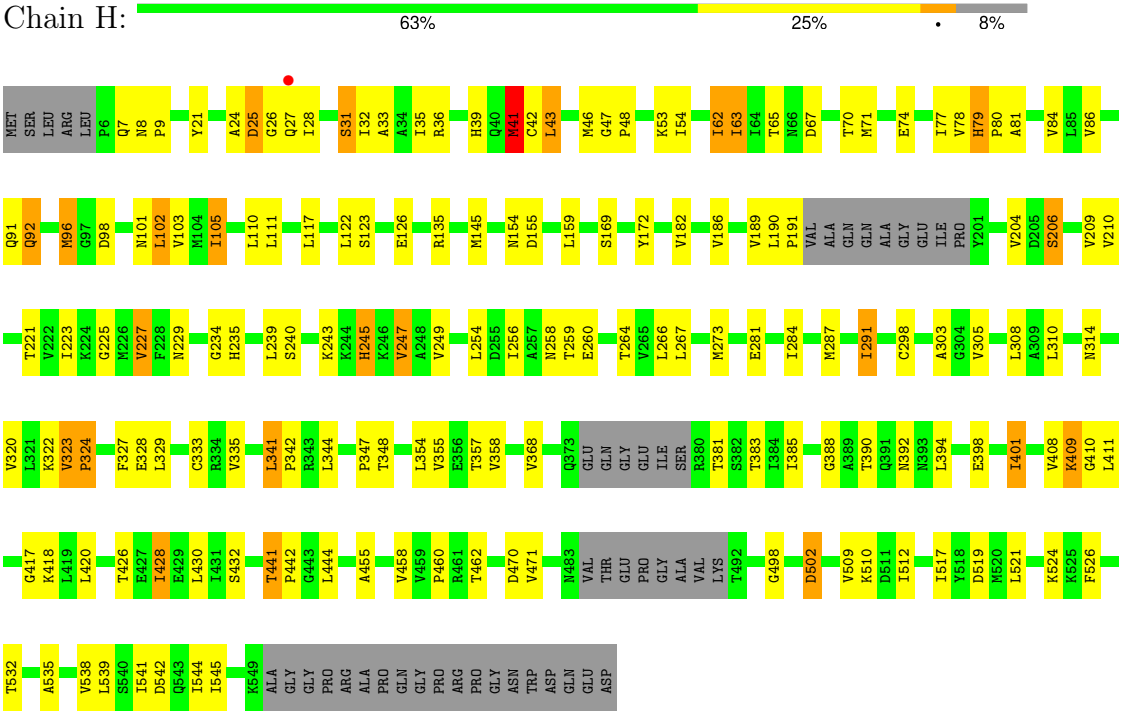
• Molecule 1: T-complex protein 1 subunit zeta

Chain n:



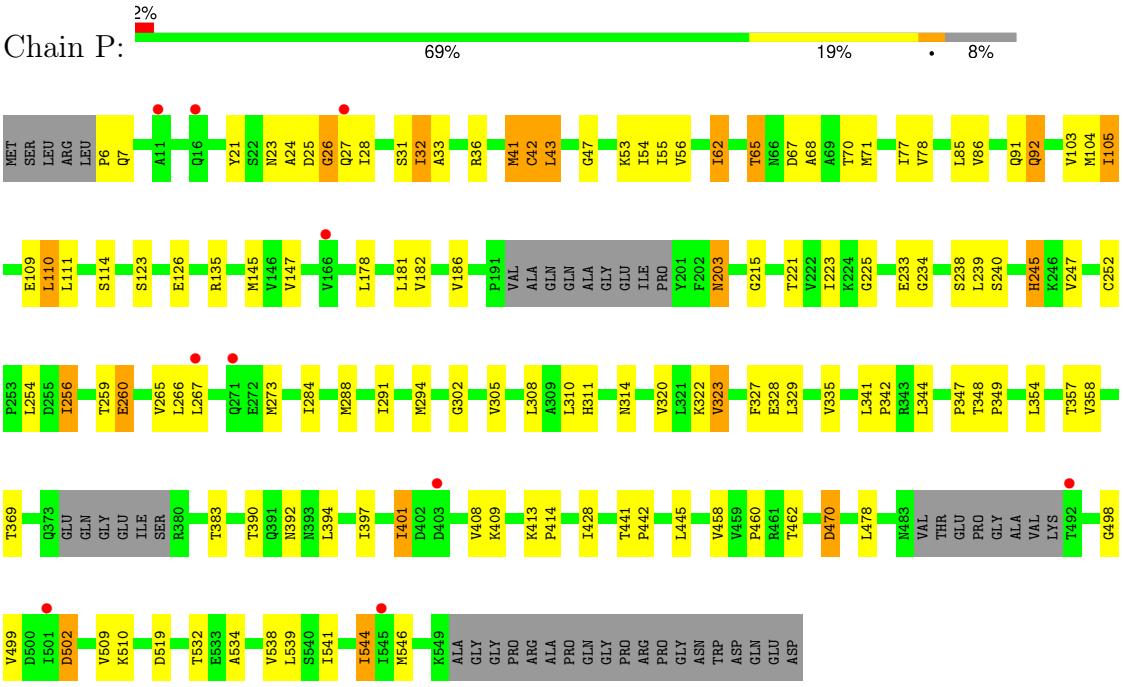
• Molecule 2: T-complex protein 1 subunit theta

Chain H:



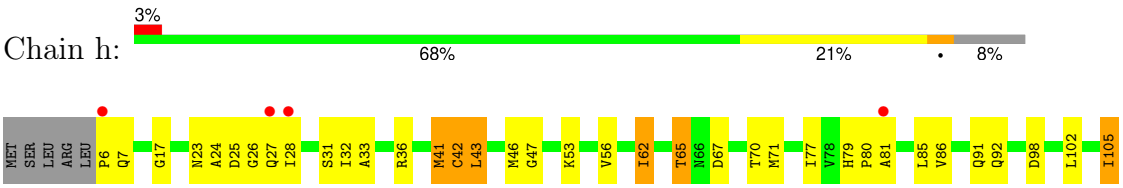
• Molecule 2: T-complex protein 1 subunit theta

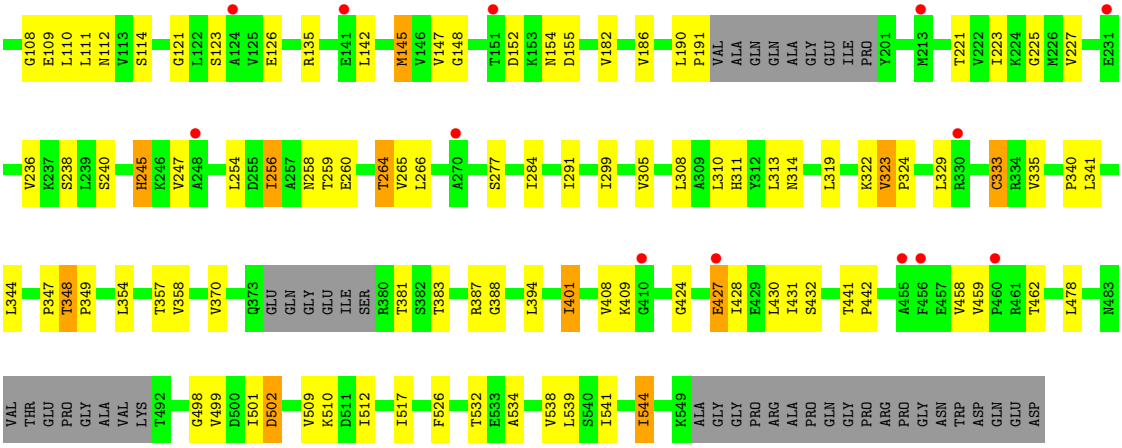
Chain P:



• Molecule 2: T-complex protein 1 subunit theta

Chain h:



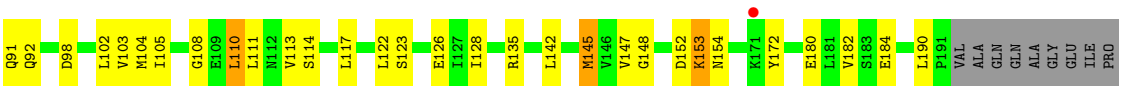


• Molecule 2: T-complex protein 1 subunit theta

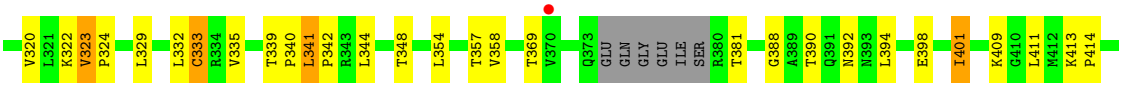
Chain p:



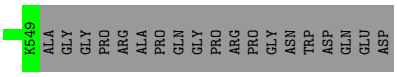








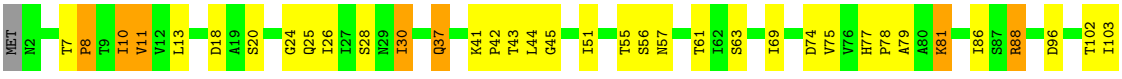


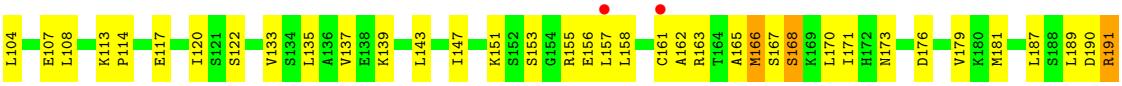


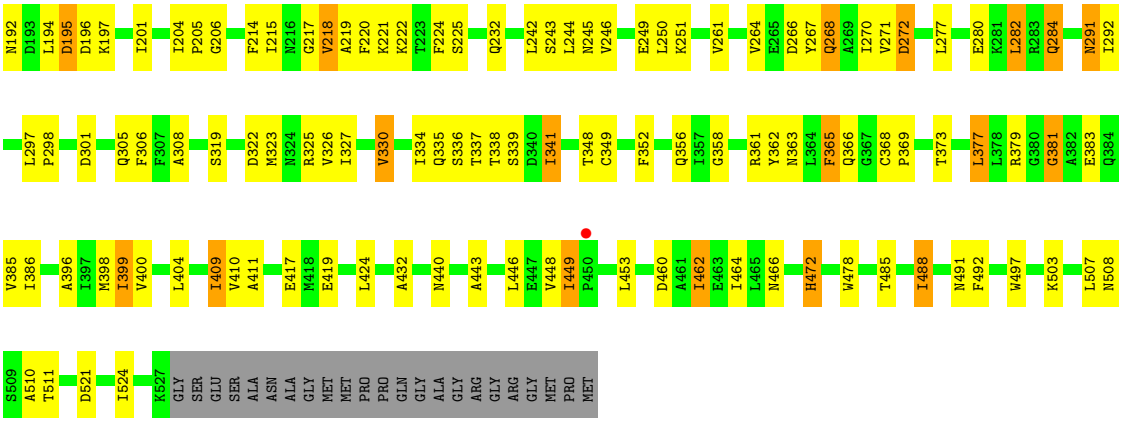
• Molecule 3: T-complex protein 1 subunit eta

Chain G:





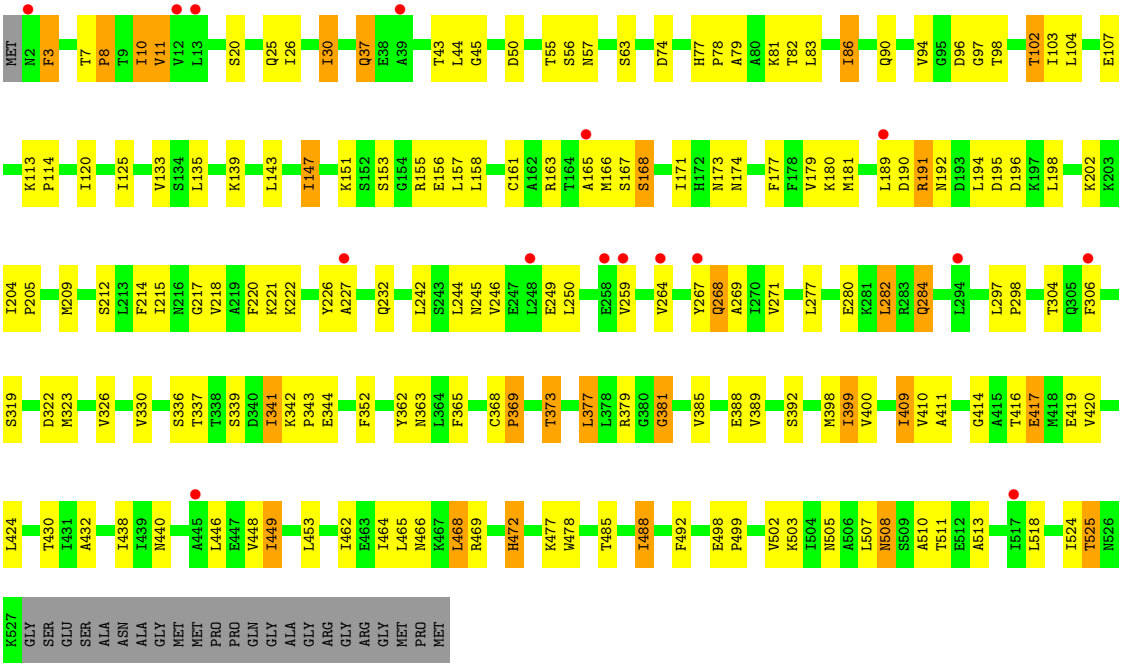




• Molecule 3: T-complex protein 1 subunit eta

Chain O:

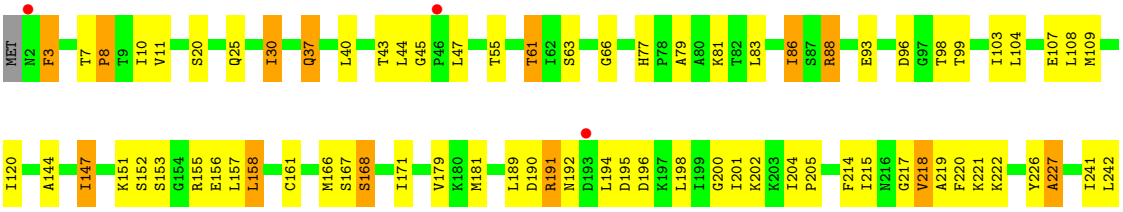


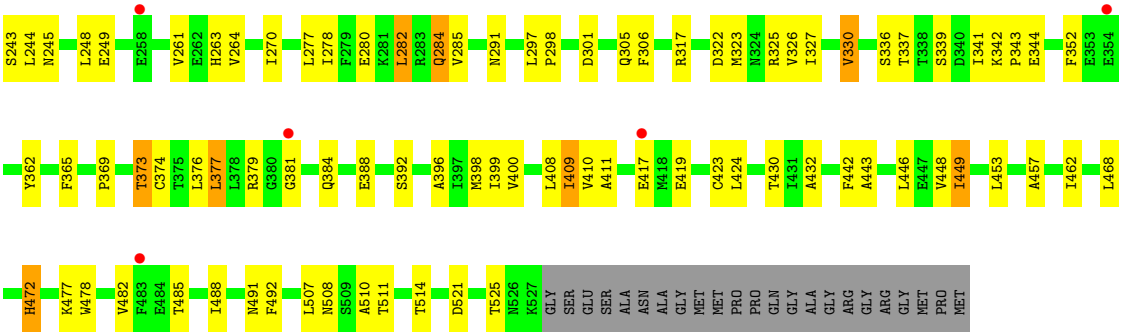


• Molecule 3: T-complex protein 1 subunit eta

Chain g:



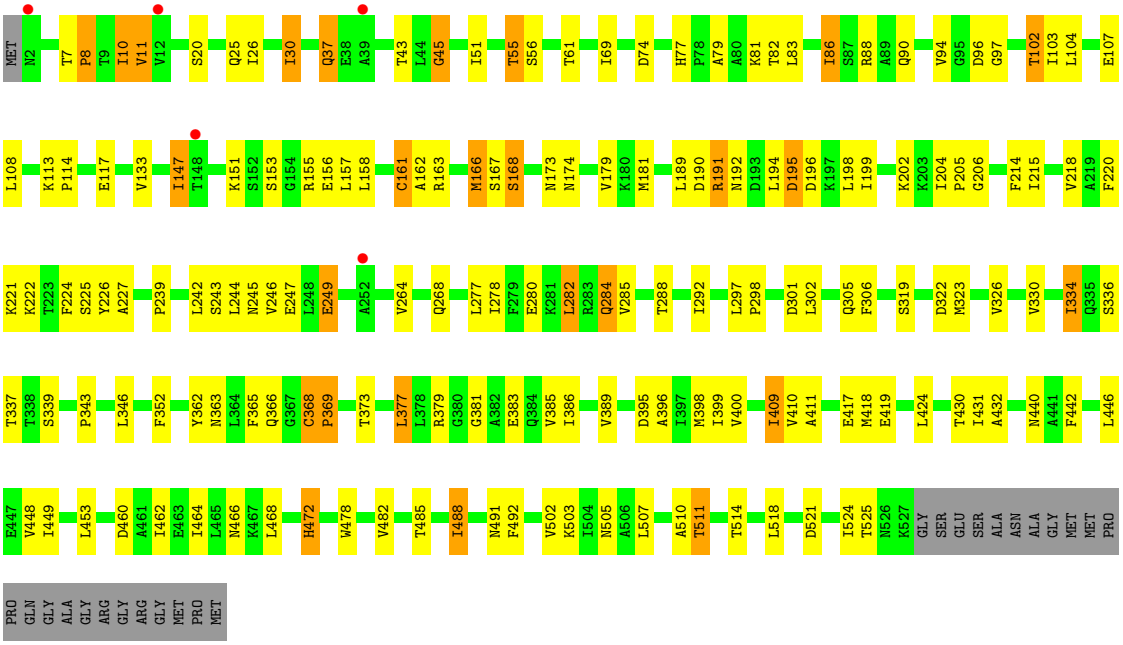




• Molecule 3: T-complex protein 1 subunit eta

Chain o:

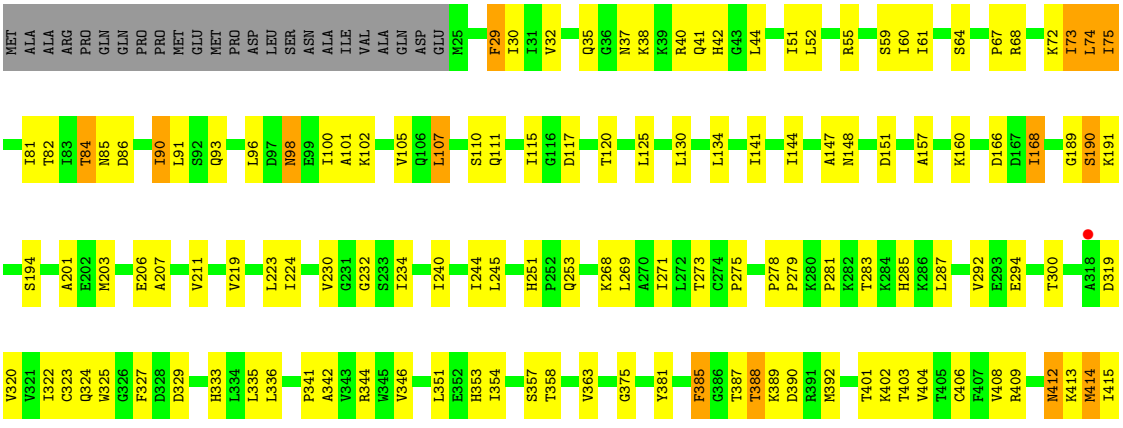


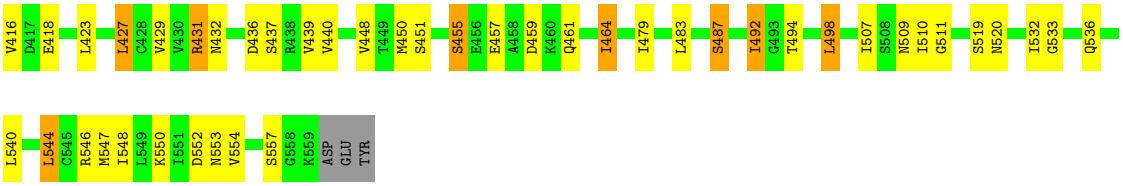


• Molecule 4: T-complex protein 1 subunit epsilon

Chain E:

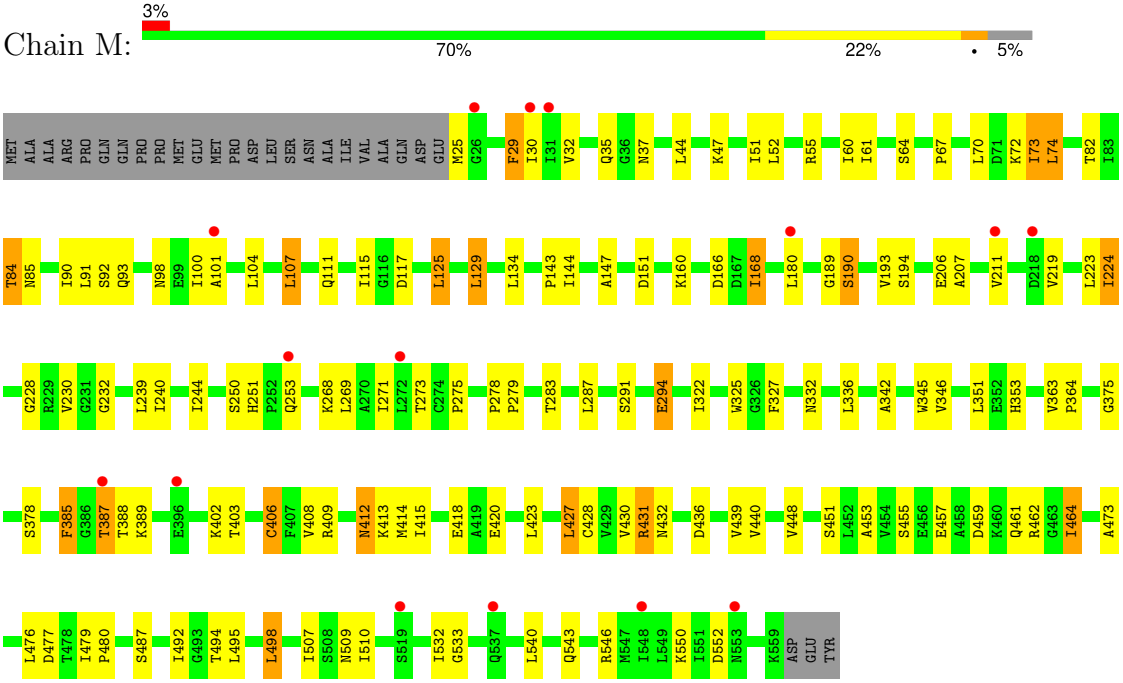






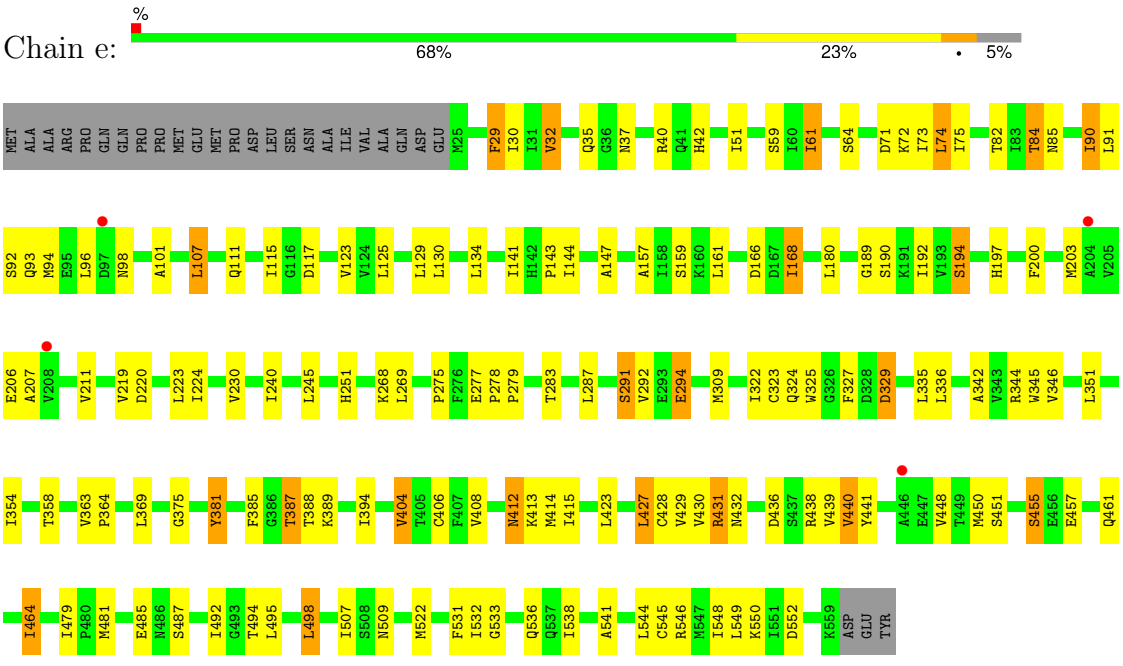
• Molecule 4: T-complex protein 1 subunit epsilon

Chain M:



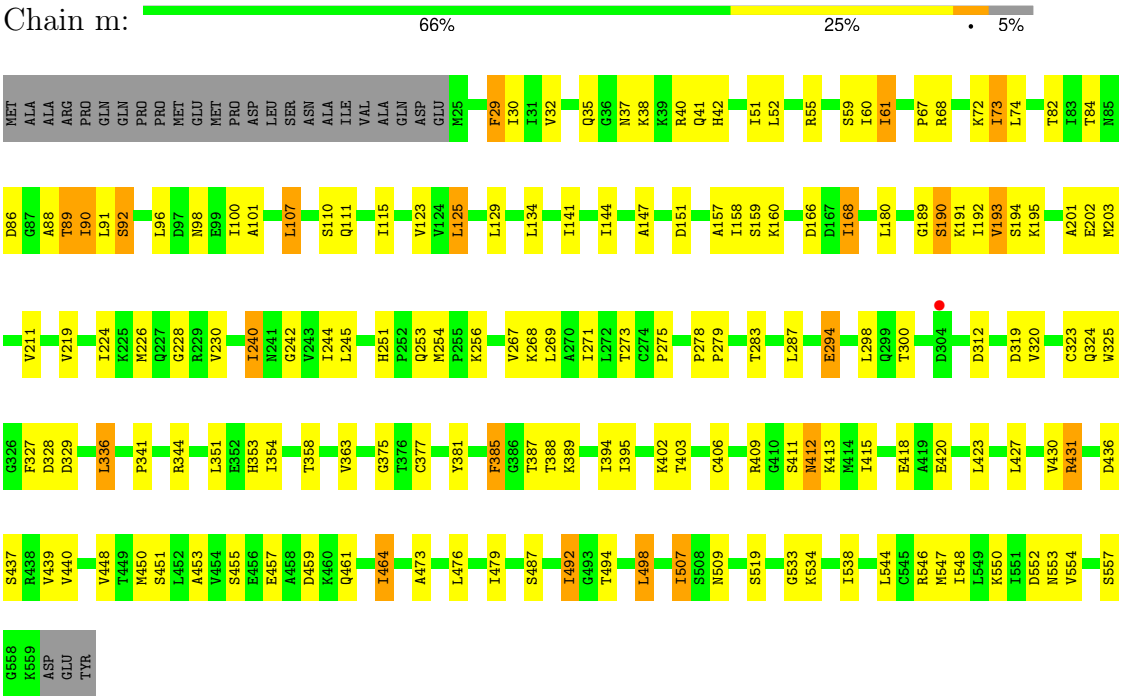
• Molecule 4: T-complex protein 1 subunit epsilon

Chain e:



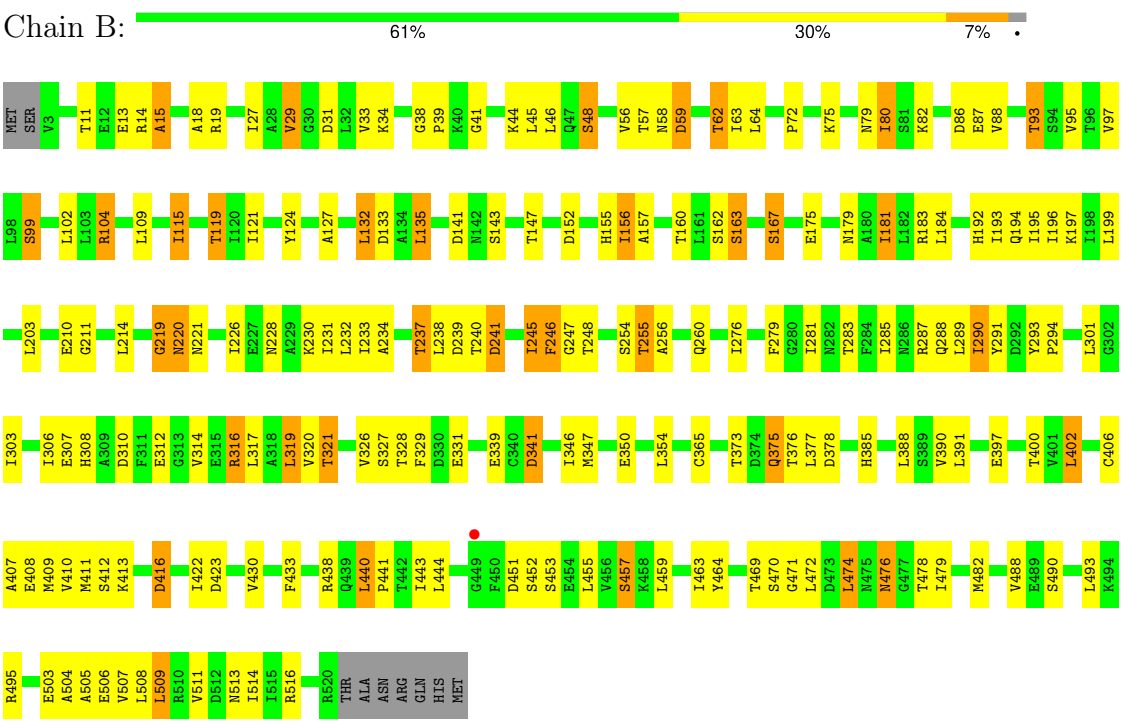
• Molecule 4: T-complex protein 1 subunit epsilon

Chain m:



• Molecule 5: T-complex protein 1 subunit beta

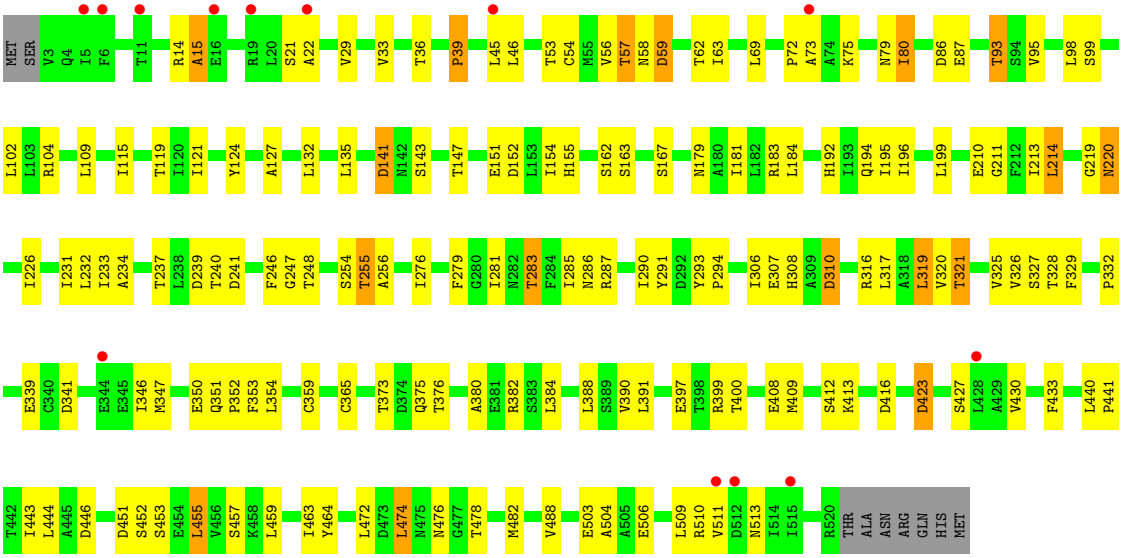
Chain B:



• Molecule 5: T-complex protein 1 subunit beta

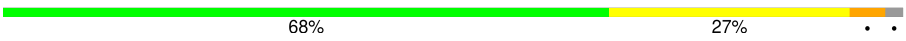
Chain J:

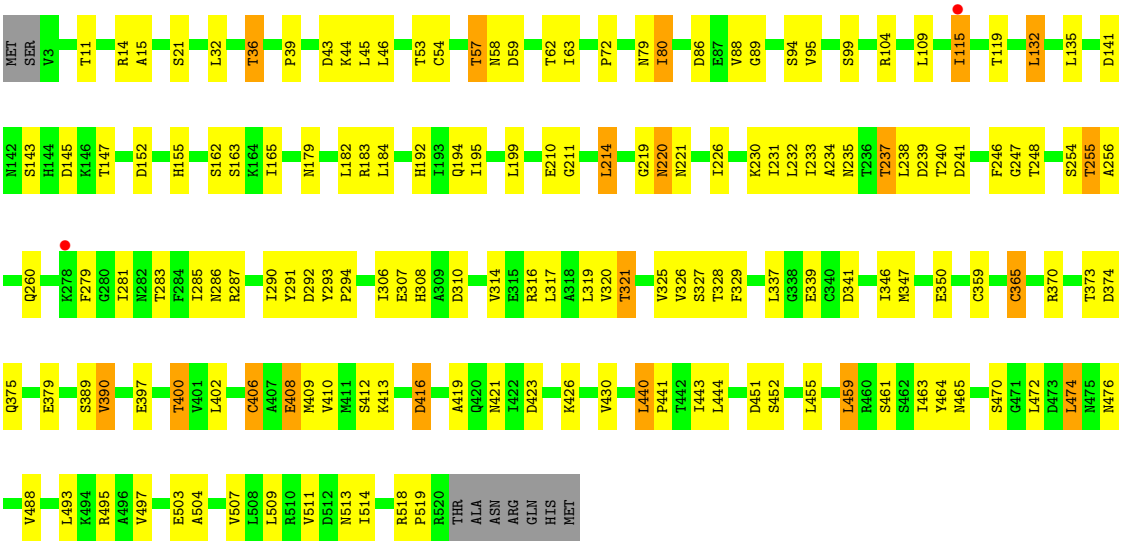




• Molecule 5: T-complex protein 1 subunit beta

Chain b:

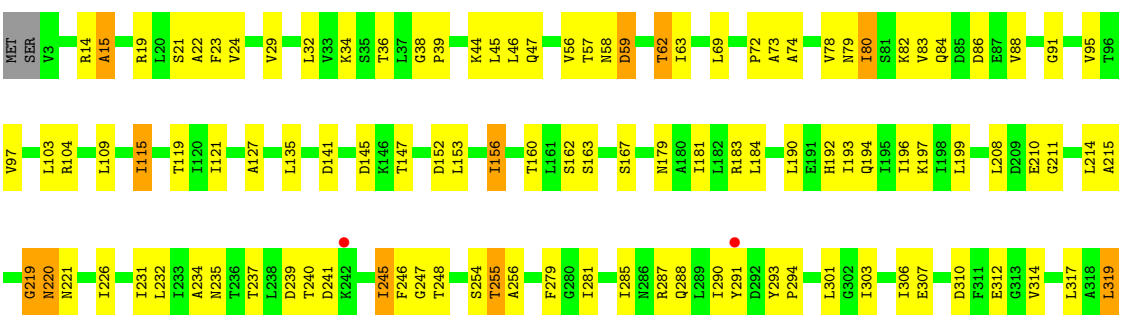


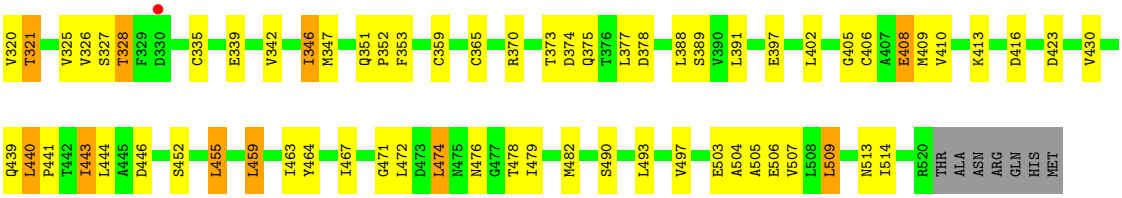


• Molecule 5: T-complex protein 1 subunit beta

Chain j:



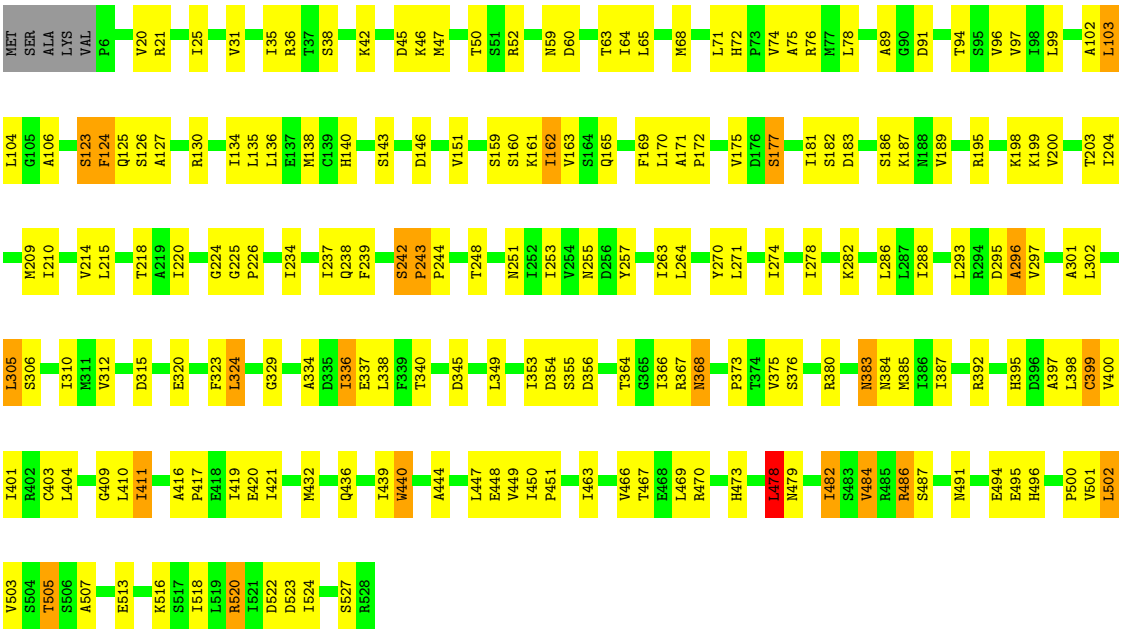




• Molecule 6: T-complex protein 1 subunit delta

Chain D:

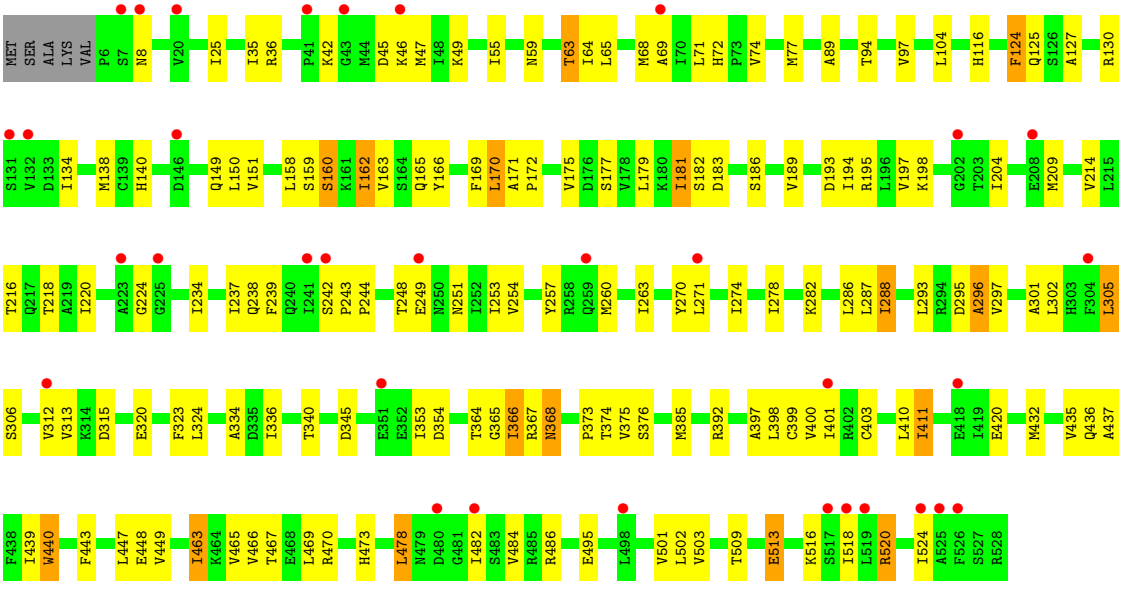




• Molecule 6: T-complex protein 1 subunit delta

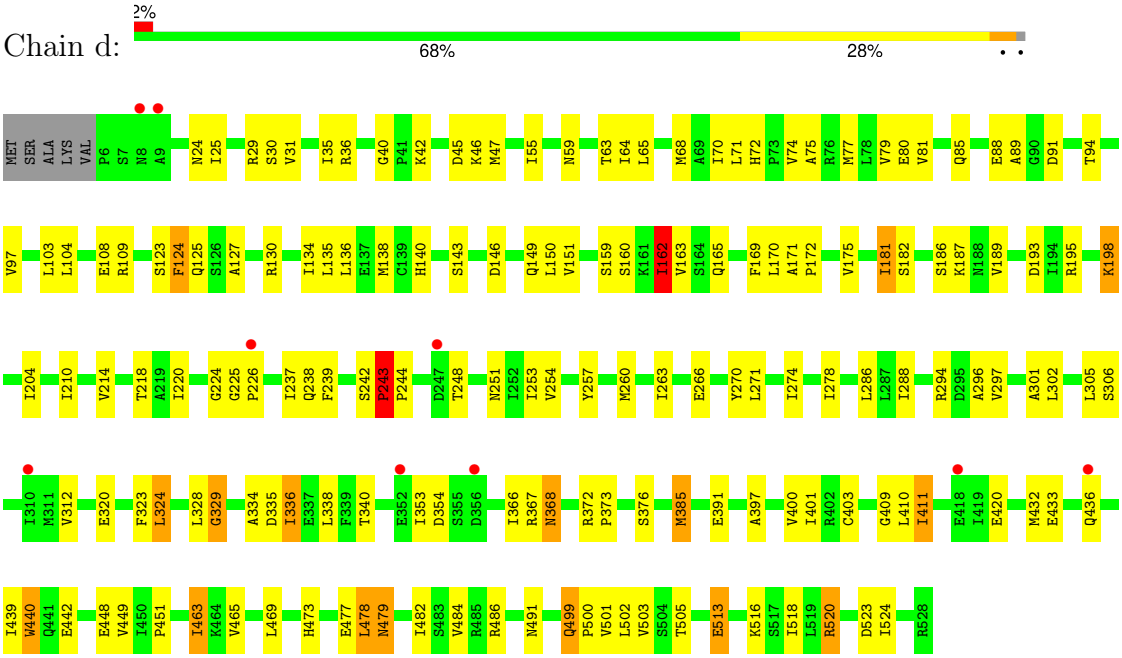
Chain L:





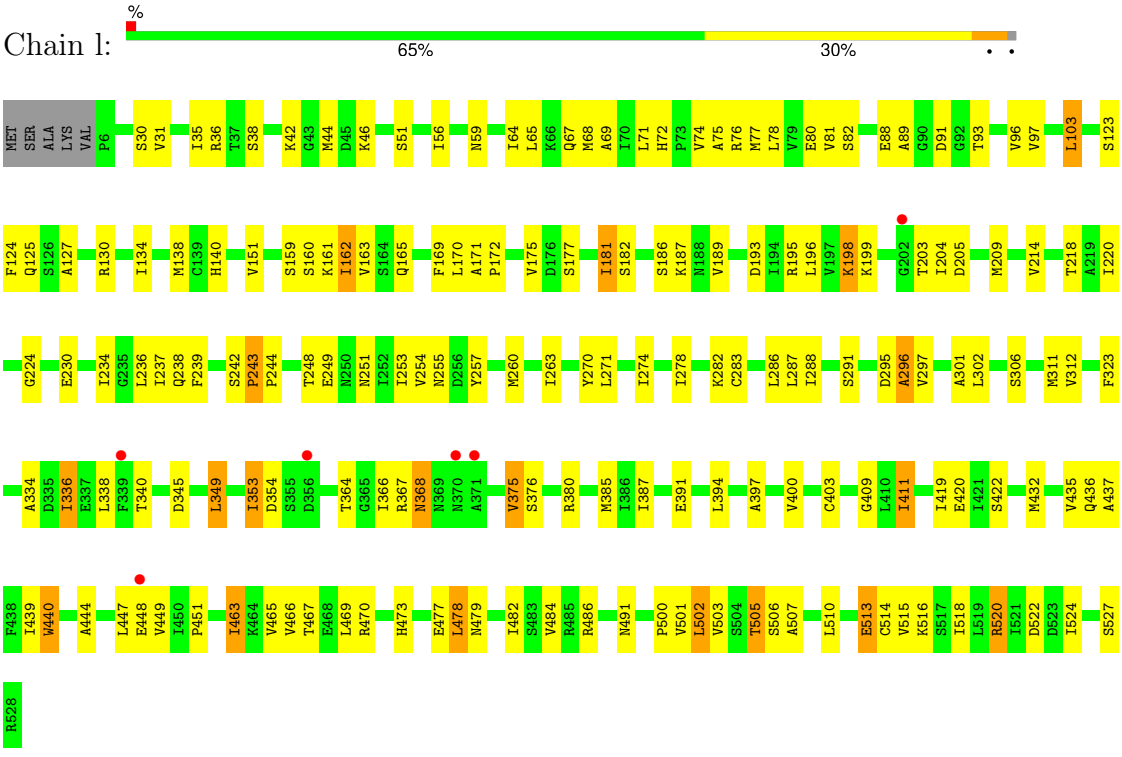
• Molecule 6: T-complex protein 1 subunit delta

Chain d:



• Molecule 6: T-complex protein 1 subunit delta

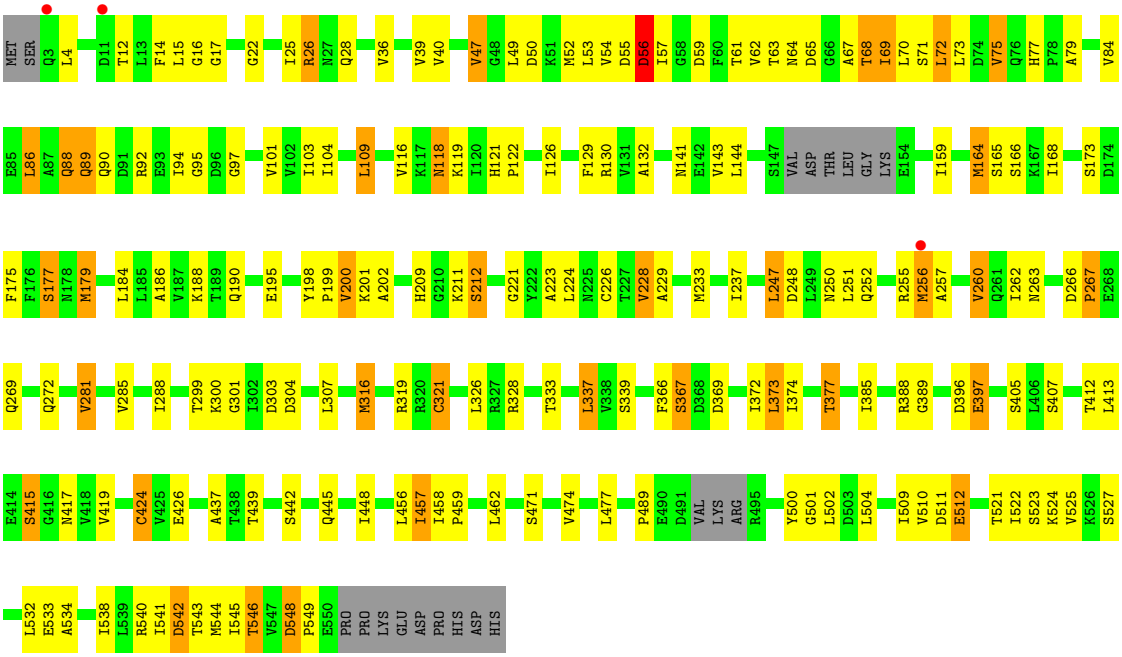
Chain l:



• Molecule 7: T-complex protein 1 subunit alpha

Chain A:

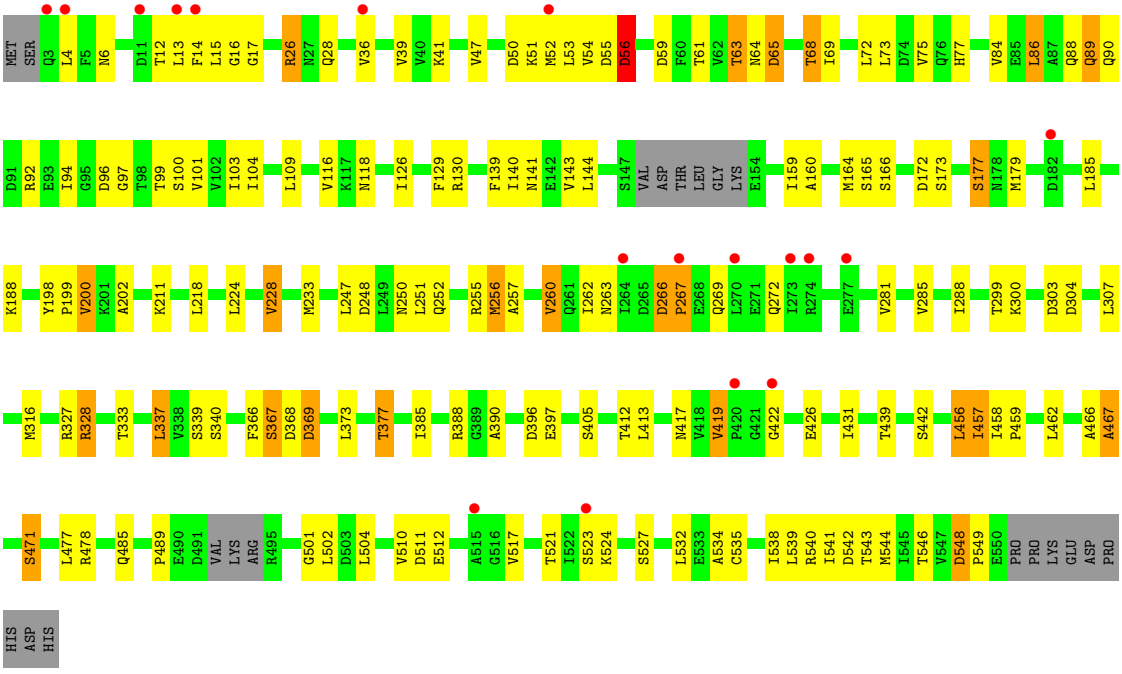




• Molecule 7: T-complex protein 1 subunit alpha

Chain I:

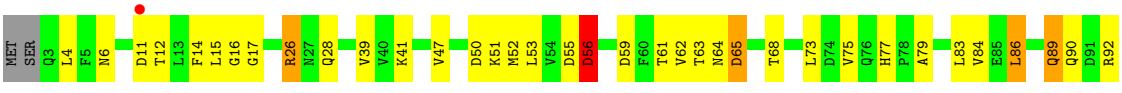


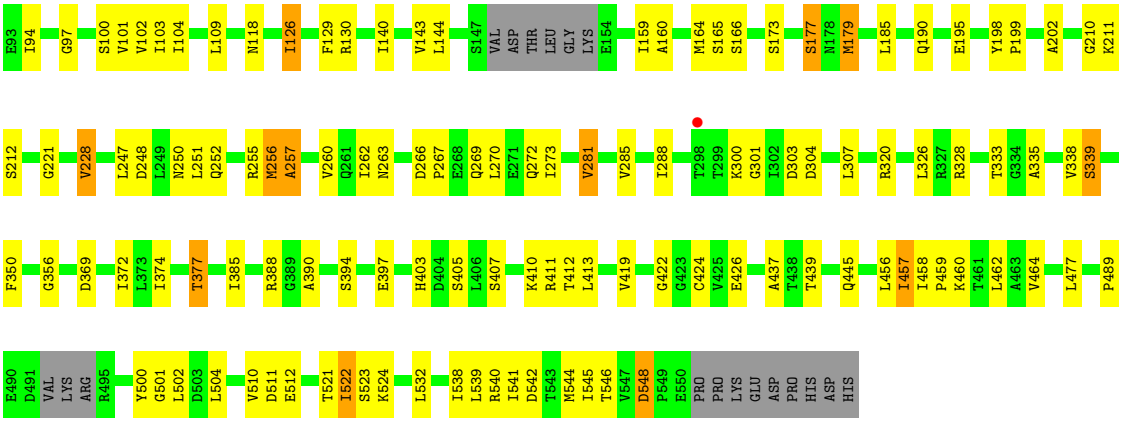


• Molecule 7: T-complex protein 1 subunit alpha

Chain a:



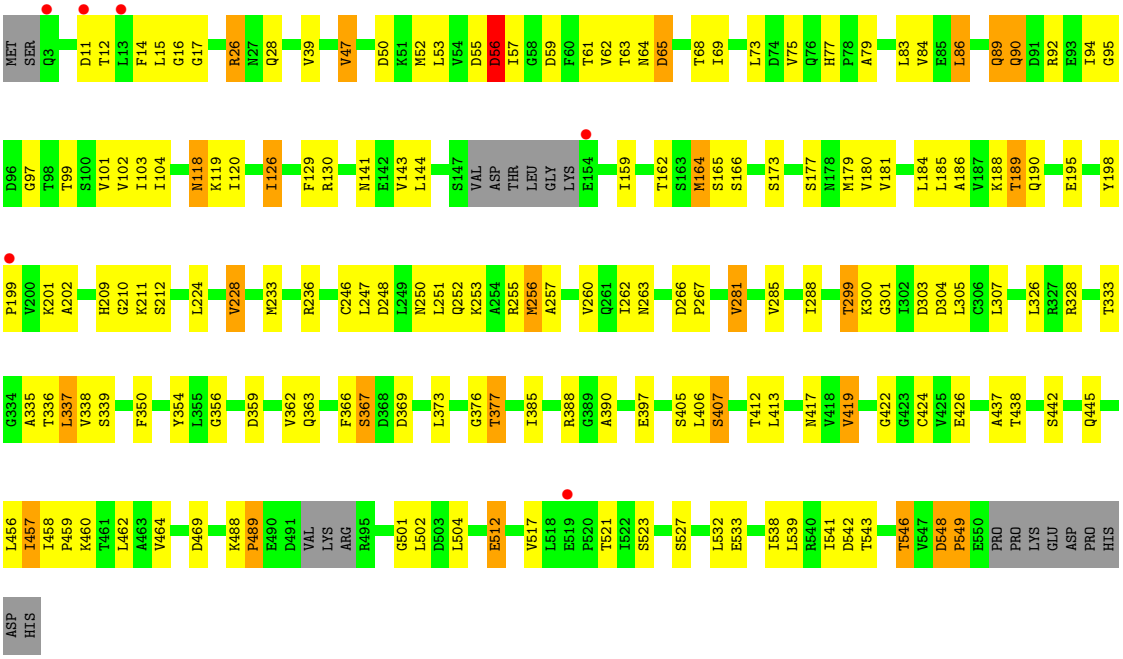




• Molecule 7: T-complex protein 1 subunit alpha

Chain i:

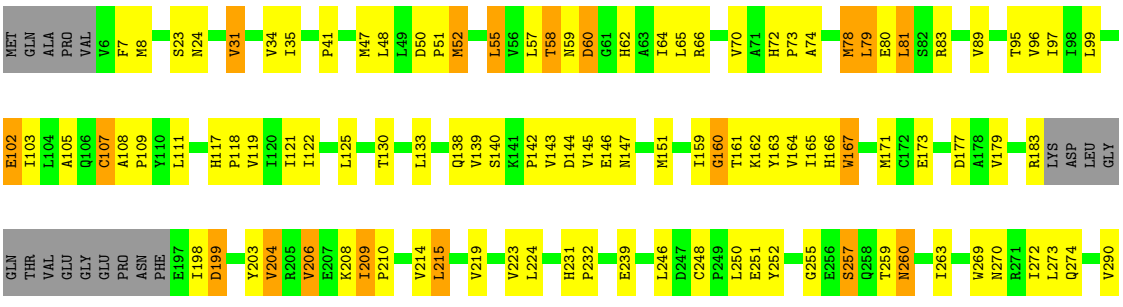


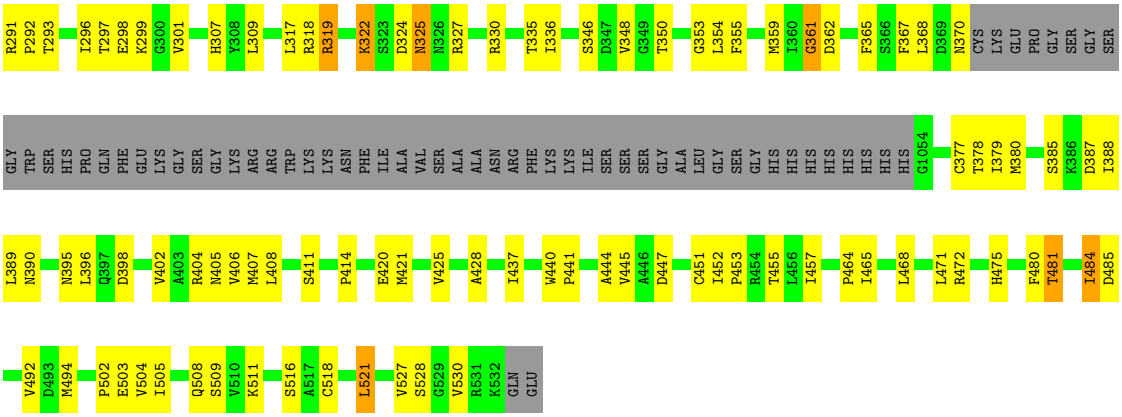


• Molecule 8: T-complex protein 1 subunit gamma

Chain C:



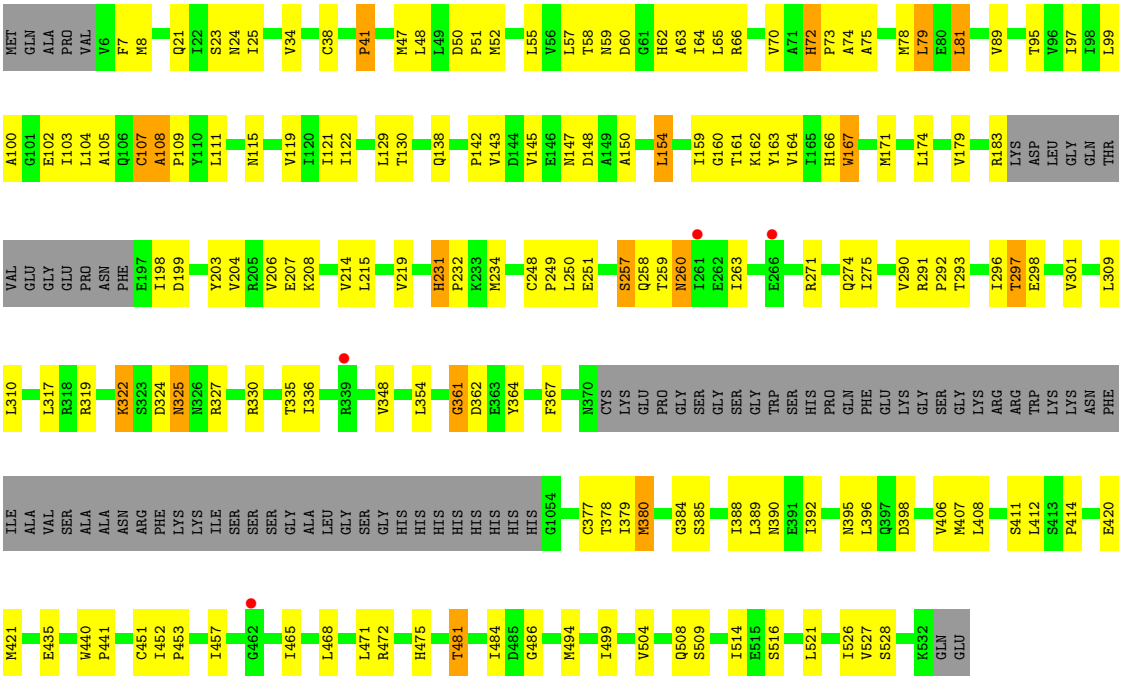




• Molecule 8: T-complex protein 1 subunit gamma

Chain K:

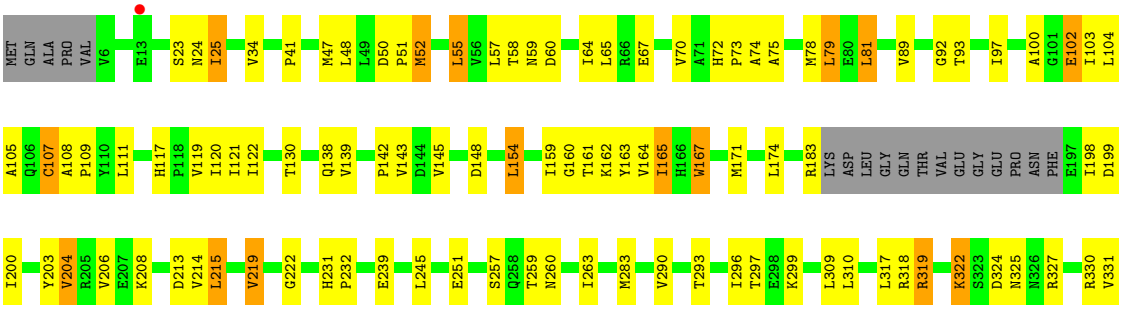


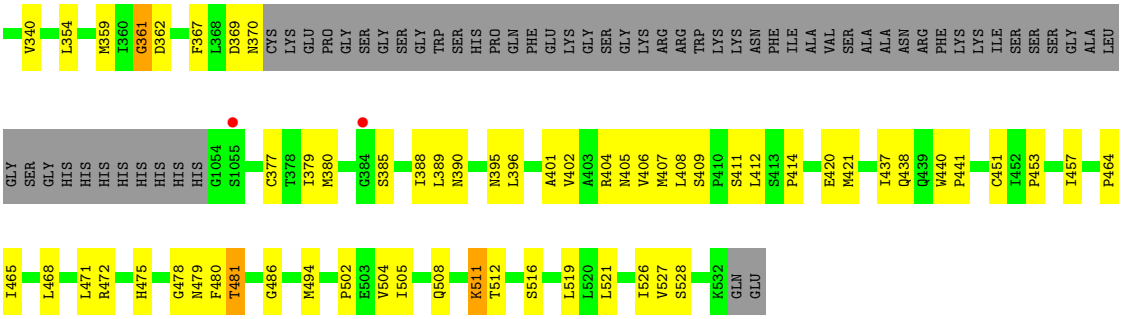


• Molecule 8: T-complex protein 1 subunit gamma

Chain c:



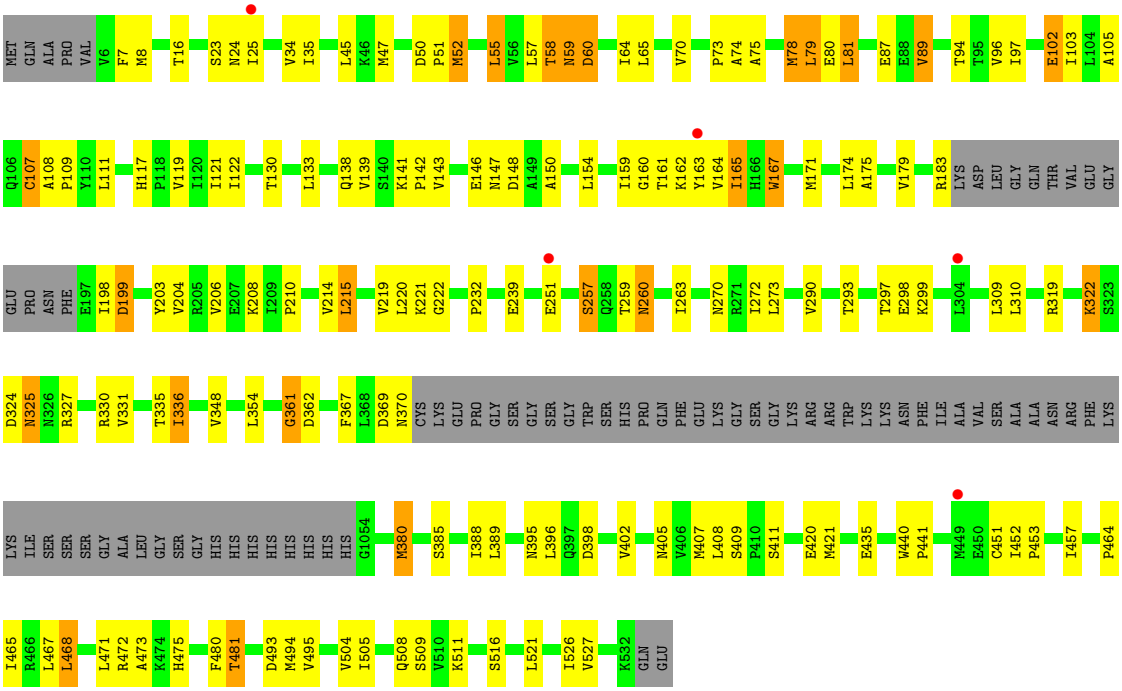




• Molecule 8: T-complex protein 1 subunit gamma

Chain k:





4 Data and refinement statistics (i)

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)	30.00 – 3.80 30.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (30.00-3.80) 91.4 (30.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 3.75Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.257 , 0.305 0.278 , 0.315	Depositor DCC
R_{free} test set	10463 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å^2)	116.0	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 119.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.024 for -h,-h+k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	120080	wwPDB-VP
Average B, all atoms (Å^2)	138.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	F	0.49	0/3886	0.88	1/5318 (0.0%)
1	N	0.49	0/3886	0.86	0/5318
1	f	0.48	0/3886	0.85	1/5318 (0.0%)
1	n	0.50	1/3886 (0.0%)	0.87	3/5318 (0.1%)
2	H	0.53	0/3661	0.91	5/5005 (0.1%)
2	P	0.53	0/3661	0.89	3/5005 (0.1%)
2	h	0.53	1/3661 (0.0%)	0.88	2/5005 (0.0%)
2	p	0.53	0/3661	0.88	2/5005 (0.0%)
3	G	0.51	1/3803 (0.0%)	0.89	5/5194 (0.1%)
3	O	0.48	1/3803 (0.0%)	0.89	6/5194 (0.1%)
3	g	0.51	1/3803 (0.0%)	0.90	3/5194 (0.1%)
3	o	0.50	0/3803	0.89	5/5194 (0.1%)
4	E	0.46	0/3849	0.86	2/5252 (0.0%)
4	M	0.47	1/3849 (0.0%)	0.88	3/5252 (0.1%)
4	e	0.49	0/3849	0.88	1/5252 (0.0%)
4	m	0.48	0/3849	0.88	1/5252 (0.0%)
5	B	0.50	0/3726	0.92	5/5077 (0.1%)
5	J	0.49	0/3726	0.87	0/5077
5	b	0.48	0/3726	0.89	0/5077
5	j	0.52	1/3726 (0.0%)	0.90	3/5077 (0.1%)
6	D	0.51	0/3723	0.91	1/5089 (0.0%)
6	L	0.49	0/3723	0.88	3/5089 (0.1%)
6	d	0.50	0/3723	0.89	6/5089 (0.1%)
6	l	0.51	0/3723	0.89	1/5089 (0.0%)
7	A	0.51	0/3805	0.93	9/5196 (0.2%)
7	I	0.49	0/3805	0.89	4/5196 (0.1%)
7	a	0.49	0/3805	0.89	4/5196 (0.1%)
7	i	0.50	0/3805	0.90	5/5196 (0.1%)
8	C	0.54	0/3657	0.92	5/5003 (0.1%)
8	K	0.51	0/3657	0.89	5/5003 (0.1%)
8	c	0.51	0/3657	0.91	7/5003 (0.1%)
8	k	0.50	0/3657	0.91	4/5003 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.50	7/120440 (0.0%)	0.89	105/164536 (0.1%)

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
1	F	0	1
6	d	0	1
6	l	0	1
All	All	0	3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	449	ILE	CA-CB	7.91	1.58	1.54
2	h	459	VAL	CA-CB	6.64	1.57	1.54
1	n	454	ILE	CA-CB	5.86	1.57	1.54
3	O	449	ILE	CA-CB	5.36	1.56	1.54
4	M	479	ILE	CA-CB	5.30	1.57	1.54

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	548	ASP	CA-C-N	7.51	129.22	119.84
7	I	548	ASP	C-N-CA	7.51	129.22	119.84
7	A	548	ASP	CA-C-N	7.21	128.85	119.84
7	A	548	ASP	C-N-CA	7.21	128.85	119.84
8	C	231	HIS	CA-C-N	6.71	126.22	119.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	194	VAL	Peptide
6	d	243	PRO	Peptide
6	l	243	PRO	Peptide

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	F	3836	0	3618	124	0
1	N	3836	0	3618	104	0
1	f	3836	0	3618	98	0
1	n	3836	0	3618	87	0
2	H	3619	0	3425	109	0
2	P	3619	0	3425	85	0
2	h	3619	0	3425	82	0
2	p	3619	0	3425	108	0
3	G	3752	0	3581	129	0
3	O	3752	0	3581	117	0
3	g	3752	0	3581	103	0
3	o	3752	0	3581	113	0
4	E	3798	0	3576	107	0
4	M	3798	0	3576	86	0
4	e	3798	0	3576	94	0
4	m	3798	0	3576	100	0
5	B	3689	0	3546	136	0
5	J	3689	0	3546	113	0
5	b	3689	0	3546	104	0
5	j	3689	0	3546	123	0
6	D	3685	0	3540	134	0
6	L	3685	0	3540	102	0
6	d	3685	0	3540	116	0
6	l	3685	0	3540	115	0
7	A	3770	0	3626	132	0
7	I	3770	0	3626	114	0
7	a	3770	0	3626	113	0
7	i	3770	0	3626	121	0
8	C	3615	0	3455	141	0
8	K	3615	0	3455	100	0
8	c	3615	0	3455	101	0
8	k	3615	0	3455	101	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
9	M	1	0	0	0	0
9	N	1	0	0	0	0
9	O	1	0	0	0	0
9	P	1	0	0	0	0
9	a	1	0	0	0	0
9	b	1	0	0	0	0
9	c	1	0	0	0	0
9	d	1	0	0	0	0
9	e	1	0	0	0	0
9	f	1	0	0	0	0
9	g	1	0	0	0	0
9	h	1	0	0	0	0
9	i	1	0	0	0	0
9	j	1	0	0	0	0
9	k	1	0	0	0	0
9	l	1	0	0	0	0
9	m	1	0	0	0	0
9	n	1	0	0	0	0
9	o	1	0	0	0	0
9	p	1	0	0	0	0
10	A	27	0	12	0	0
10	B	27	0	12	1	0
10	C	27	0	12	1	0
10	D	27	0	12	1	0
10	E	27	0	12	1	0
10	F	27	0	12	0	0
10	G	27	0	12	0	0
10	H	27	0	12	0	0
10	I	27	0	12	1	0
10	J	27	0	12	1	0
10	K	27	0	12	1	0
10	L	27	0	12	0	0
10	M	27	0	12	1	0
10	N	27	0	12	0	0
10	O	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	P	27	0	12	0	0
10	a	27	0	12	1	0
10	b	27	0	12	3	0
10	c	27	0	12	4	0
10	d	27	0	12	1	0
10	e	27	0	12	0	0
10	f	27	0	12	0	0
10	g	27	0	12	0	0
10	h	27	0	12	0	0
10	i	27	0	12	0	0
10	j	27	0	12	1	0
10	k	27	0	12	1	0
10	l	27	0	12	0	0
10	m	27	0	12	0	0
10	n	27	0	12	0	0
10	o	27	0	12	0	0
10	p	27	0	12	0	0
11	A	4	0	0	0	0
11	B	4	0	0	0	0
11	C	4	0	0	1	0
11	D	4	0	0	1	0
11	E	4	0	0	1	0
11	F	4	0	0	0	0
11	G	4	0	0	0	0
11	H	4	0	0	0	0
11	I	4	0	0	0	0
11	J	4	0	0	1	0
11	K	4	0	0	1	0
11	L	4	0	0	0	0
11	M	4	0	0	1	0
11	N	4	0	0	0	0
11	O	4	0	0	0	0
11	P	4	0	0	0	0
11	a	4	0	0	0	0
11	b	4	0	0	2	0
11	c	4	0	0	1	0
11	d	4	0	0	1	0
11	e	4	0	0	0	0
11	f	4	0	0	0	0
11	g	4	0	0	1	0
11	h	4	0	0	0	0
11	i	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	j	4	0	0	0	0
11	k	4	0	0	1	0
11	l	4	0	0	0	0
11	m	4	0	0	0	0
11	n	4	0	0	0	0
11	o	4	0	0	1	0
11	p	4	0	0	0	0
All	All	120080	0	113852	3203	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 14.

The worst 5 of 3203 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)
2:H:27:GLN:HE21	2:H:544:ILE:HD11	1.02	1.15
3:G:107:GLU:HG2	3:G:448:VAL:HG21	1.24	1.11
3:g:147:ILE:HD11	3:g:409:ILE:HB	1.28	1.11
7:i:26:ARG:HG3	7:i:26:ARG:HH11	1.13	1.09
6:d:520:ARG:HH21	6:d:520:ARG:HG3	1.18	1.08

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	F	536/546 (98%)	477 (89%)	56 (10%)	3 (1%)	21 54
1	N	536/546 (98%)	483 (90%)	51 (10%)	2 (0%)	30 62
1	f	536/546 (98%)	484 (90%)	49 (9%)	3 (1%)	21 54
1	n	536/546 (98%)	486 (91%)	48 (9%)	2 (0%)	30 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	513/568 (90%)	445 (87%)	57 (11%)	11 (2%)	5	31
2	P	513/568 (90%)	458 (89%)	47 (9%)	8 (2%)	7	35
2	h	513/568 (90%)	460 (90%)	46 (9%)	7 (1%)	9	37
2	p	513/568 (90%)	450 (88%)	53 (10%)	10 (2%)	6	32
3	G	524/550 (95%)	467 (89%)	48 (9%)	9 (2%)	7	34
3	O	524/550 (95%)	479 (91%)	36 (7%)	9 (2%)	7	34
3	g	524/550 (95%)	477 (91%)	38 (7%)	9 (2%)	7	34
3	o	524/550 (95%)	472 (90%)	41 (8%)	11 (2%)	5	31
4	E	533/562 (95%)	482 (90%)	45 (8%)	6 (1%)	11	41
4	M	533/562 (95%)	494 (93%)	31 (6%)	8 (2%)	8	36
4	e	533/562 (95%)	500 (94%)	27 (5%)	6 (1%)	11	41
4	m	533/562 (95%)	492 (92%)	33 (6%)	8 (2%)	8	36
5	B	516/527 (98%)	452 (88%)	48 (9%)	16 (3%)	3	25
5	J	516/527 (98%)	460 (89%)	42 (8%)	14 (3%)	4	27
5	b	516/527 (98%)	461 (89%)	41 (8%)	14 (3%)	4	27
5	j	516/527 (98%)	459 (89%)	47 (9%)	10 (2%)	6	32
6	D	521/528 (99%)	457 (88%)	46 (9%)	18 (4%)	3	23
6	L	521/528 (99%)	474 (91%)	33 (6%)	14 (3%)	4	27
6	d	521/528 (99%)	473 (91%)	34 (6%)	14 (3%)	4	27
6	l	521/528 (99%)	469 (90%)	41 (8%)	11 (2%)	5	31
7	A	533/559 (95%)	470 (88%)	50 (9%)	13 (2%)	4	29
7	I	533/559 (95%)	483 (91%)	36 (7%)	14 (3%)	4	27
7	a	533/559 (95%)	482 (90%)	43 (8%)	8 (2%)	8	36
7	i	533/559 (95%)	484 (91%)	37 (7%)	12 (2%)	5	30
8	C	507/590 (86%)	445 (88%)	54 (11%)	8 (2%)	7	35
8	K	507/590 (86%)	454 (90%)	43 (8%)	10 (2%)	6	32
8	c	507/590 (86%)	456 (90%)	44 (9%)	7 (1%)	9	37
8	k	507/590 (86%)	448 (88%)	50 (10%)	9 (2%)	6	33
All	All	16732/17720 (94%)	15033 (90%)	1395 (8%)	304 (2%)	6	33

5 of 304 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	323	VAL
2	H	442	PRO
2	H	502	ASP
3	G	8	PRO
4	E	389	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	380/463 (82%)	337 (89%)	43 (11%)	5 23
1	N	380/463 (82%)	348 (92%)	32 (8%)	10 34
1	f	380/463 (82%)	355 (93%)	25 (7%)	15 41
1	n	380/463 (82%)	348 (92%)	32 (8%)	10 34
2	H	352/473 (74%)	306 (87%)	46 (13%)	4 20
2	P	352/473 (74%)	315 (90%)	37 (10%)	6 26
2	h	352/473 (74%)	312 (89%)	40 (11%)	5 23
2	p	352/473 (74%)	307 (87%)	45 (13%)	4 21
3	G	373/454 (82%)	323 (87%)	50 (13%)	4 19
3	O	373/454 (82%)	333 (89%)	40 (11%)	6 25
3	g	373/454 (82%)	330 (88%)	43 (12%)	5 23
3	o	373/454 (82%)	333 (89%)	40 (11%)	6 25
4	E	382/483 (79%)	328 (86%)	54 (14%)	3 18
4	M	382/483 (79%)	340 (89%)	42 (11%)	6 24
4	e	382/483 (79%)	332 (87%)	50 (13%)	4 20
4	m	382/483 (79%)	339 (89%)	43 (11%)	5 23
5	B	374/441 (85%)	316 (84%)	58 (16%)	2 15
5	J	374/441 (85%)	338 (90%)	36 (10%)	8 29
5	b	374/441 (85%)	330 (88%)	44 (12%)	5 22
5	j	374/441 (85%)	334 (89%)	40 (11%)	6 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	D	374/454 (82%)	332 (89%)	42 (11%)	6 24
6	L	374/454 (82%)	341 (91%)	33 (9%)	9 33
6	d	374/454 (82%)	340 (91%)	34 (9%)	9 32
6	l	374/454 (82%)	335 (90%)	39 (10%)	7 26
7	A	375/471 (80%)	324 (86%)	51 (14%)	3 18
7	I	375/471 (80%)	335 (89%)	40 (11%)	6 25
7	a	375/471 (80%)	345 (92%)	30 (8%)	11 36
7	i	375/471 (80%)	341 (91%)	34 (9%)	9 32
8	C	359/497 (72%)	308 (86%)	51 (14%)	3 17
8	K	359/497 (72%)	314 (88%)	45 (12%)	4 21
8	c	359/497 (72%)	315 (88%)	44 (12%)	4 21
8	k	359/497 (72%)	313 (87%)	46 (13%)	4 21
All	All	11876/14944 (80%)	10547 (89%)	1329 (11%)	6 24

5 of 1329 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	d	411	ILE
4	m	240	ILE
7	a	281	VAL
6	d	385	MET
1	n	499	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 305 such sidechains are listed below:

Mol	Chain	Res	Type
1	n	248	ASN
7	i	29	ASN
2	p	79	HIS
4	m	227	GLN
8	k	138	GLN

5.3.3 RNA

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)

Of 96 ligands modelled in this entry, 32 are monoatomic - leaving 64 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	$\#\|Z\| > 2$
10	ADP	J	602	11,9	28,29,29	1.50	5 (17%)	43,45,45	1.90	9 (20%)
10	ADP	K	1102	11,9	28,29,29	1.44	5 (17%)	43,45,45	1.78	9 (20%)
11	BEF	m	603	10	0,3,3	-	-	-		
11	BEF	F	603	10	0,3,3	-	-	-		
10	ADP	h	602	9	28,29,29	1.45	5 (17%)	43,45,45	1.86	9 (20%)
11	BEF	H	603	-	0,3,3	-	-	-		
10	ADP	p	602	9	28,29,29	1.44	5 (17%)	43,45,45	1.93	10 (23%)
11	BEF	I	603	10	0,3,3	-	-	-		
10	ADP	A	602	11,9	28,29,29	1.49	4 (14%)	43,45,45	1.88	9 (20%)
10	ADP	g	602	9	28,29,29	1.50	5 (17%)	43,45,45	1.83	7 (16%)
11	BEF	n	603	10	0,3,3	-	-	-		
11	BEF	j	603	10	0,3,3	-	-	-		
10	ADP	I	602	11,9	28,29,29	1.42	4 (14%)	43,45,45	1.83	8 (18%)
11	BEF	B	603	10	0,3,3	-	-	-		
11	BEF	K	1103	10	0,3,3	-	-	-		
10	ADP	E	602	11,9	28,29,29	1.41	4 (14%)	43,45,45	1.88	10 (23%)
11	BEF	O	603	-	0,3,3	-	-	-		
11	BEF	f	603	10	0,3,3	-	-	-		
11	BEF	g	603	-	0,3,3	-	-	-		
11	BEF	a	603	10	0,3,3	-	-	-		
11	BEF	e	603	10	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	ADP	a	602	11,9	28,29,29	1.48	5 (17%)	43,45,45	1.86	8 (18%)
11	BEF	h	603	-	0,3,3	-	-	-		
11	BEF	J	603	10	0,3,3	-	-	-		
10	ADP	j	602	11,9	28,29,29	1.59	6 (21%)	43,45,45	1.79	7 (16%)
10	ADP	C	1102	11,9	28,29,29	1.44	4 (14%)	43,45,45	1.80	9 (20%)
11	BEF	A	603	10	0,3,3	-	-	-		
11	BEF	b	603	10	0,3,3	-	-	-		
10	ADP	L	602	11,9	28,29,29	1.46	4 (14%)	43,45,45	1.86	9 (20%)
10	ADP	O	602	9	28,29,29	1.51	5 (17%)	43,45,45	1.88	9 (20%)
10	ADP	D	602	11,9	28,29,29	1.43	4 (14%)	43,45,45	1.89	9 (20%)
10	ADP	l	602	11,9	28,29,29	1.47	4 (14%)	43,45,45	1.85	9 (20%)
10	ADP	e	602	11,9	28,29,29	1.43	4 (14%)	43,45,45	1.86	9 (20%)
10	ADP	i	602	11,9	28,29,29	1.45	4 (14%)	43,45,45	1.87	8 (18%)
11	BEF	E	603	10	0,3,3	-	-	-		
10	ADP	B	602	11,9	28,29,29	1.48	5 (17%)	43,45,45	1.80	9 (20%)
10	ADP	F	602	11,9	28,29,29	1.51	5 (17%)	43,45,45	1.75	8 (18%)
10	ADP	N	602	11,9	28,29,29	1.48	5 (17%)	43,45,45	1.82	8 (18%)
10	ADP	P	602	9	28,29,29	1.45	5 (17%)	43,45,45	1.88	10 (23%)
10	ADP	c	1102	11,9	28,29,29	1.43	4 (14%)	43,45,45	1.76	7 (16%)
11	BEF	G	603	-	0,3,3	-	-	-		
10	ADP	M	602	11,9	28,29,29	1.45	5 (17%)	43,45,45	1.87	10 (23%)
11	BEF	P	603	-	0,3,3	-	-	-		
11	BEF	L	603	10	0,3,3	-	-	-		
10	ADP	o	602	9	28,29,29	1.51	5 (17%)	43,45,45	1.90	10 (23%)
10	ADP	k	1102	11,9	28,29,29	1.45	4 (14%)	43,45,45	1.83	8 (18%)
10	ADP	H	602	9	28,29,29	1.45	5 (17%)	43,45,45	1.81	9 (20%)
11	BEF	M	603	10	0,3,3	-	-	-		
11	BEF	c	1103	10	0,3,3	-	-	-		
11	BEF	d	603	10	0,3,3	-	-	-		
11	BEF	i	603	10	0,3,3	-	-	-		
10	ADP	d	602	11,9	28,29,29	1.44	6 (21%)	43,45,45	1.82	9 (20%)
10	ADP	m	602	11,9	28,29,29	1.54	5 (17%)	43,45,45	1.91	9 (20%)
10	ADP	b	602	11,9	28,29,29	1.54	5 (17%)	43,45,45	1.76	8 (18%)
11	BEF	o	603	-	0,3,3	-	-	-		
10	ADP	n	602	11,9	28,29,29	1.54	5 (17%)	43,45,45	1.81	8 (18%)
11	BEF	D	603	10	0,3,3	-	-	-		
11	BEF	C	1103	10	0,3,3	-	-	-		
11	BEF	l	603	10	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	BEF	N	603	10	0,3,3	-	-	-		
11	BEF	p	603	-	0,3,3	-	-	-		
10	ADP	G	602	9	28,29,29	1.44	4 (14%)	43,45,45	1.93	10 (23%)
11	BEF	k	1103	10	0,3,3	-	-	-		
10	ADP	f	602	11,9	28,29,29	1.53	5 (17%)	43,45,45	1.87	9 (20%)

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
10	ADP	J	602	11,9	-	2/16/32/32	0/3/3/3
10	ADP	K	1102	11,9	-	1/16/32/32	0/3/3/3
10	ADP	h	602	9	-	1/16/32/32	0/3/3/3
10	ADP	p	602	9	-	1/16/32/32	0/3/3/3
10	ADP	A	602	11,9	-	5/16/32/32	0/3/3/3
10	ADP	g	602	9	-	5/16/32/32	0/3/3/3
10	ADP	I	602	11,9	-	5/16/32/32	0/3/3/3
10	ADP	E	602	11,9	-	7/16/32/32	0/3/3/3
10	ADP	a	602	11,9	-	5/16/32/32	0/3/3/3
10	ADP	j	602	11,9	-	2/16/32/32	0/3/3/3
10	ADP	C	1102	11,9	-	2/16/32/32	0/3/3/3
10	ADP	L	602	11,9	-	7/16/32/32	0/3/3/3
10	ADP	O	602	9	-	4/16/32/32	0/3/3/3
10	ADP	D	602	11,9	-	6/16/32/32	0/3/3/3
10	ADP	l	602	11,9	-	6/16/32/32	0/3/3/3
10	ADP	e	602	11,9	-	8/16/32/32	0/3/3/3
10	ADP	i	602	11,9	-	6/16/32/32	0/3/3/3
10	ADP	B	602	11,9	-	3/16/32/32	0/3/3/3
10	ADP	F	602	11,9	-	8/16/32/32	0/3/3/3
10	ADP	N	602	11,9	-	8/16/32/32	0/3/3/3
10	ADP	P	602	9	-	1/16/32/32	0/3/3/3
10	ADP	c	1102	11,9	-	2/16/32/32	0/3/3/3
10	ADP	M	602	11,9	-	8/16/32/32	0/3/3/3
10	ADP	o	602	9	-	5/16/32/32	0/3/3/3
10	ADP	k	1102	11,9	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	H	602	9	-	1/16/32/32	0/3/3/3
10	ADP	d	602	11,9	-	6/16/32/32	0/3/3/3
10	ADP	m	602	11,9	-	7/16/32/32	0/3/3/3
10	ADP	b	602	11,9	-	2/16/32/32	0/3/3/3
10	ADP	n	602	11,9	-	8/16/32/32	0/3/3/3
10	ADP	G	602	9	-	5/16/32/32	0/3/3/3
10	ADP	f	602	11,9	-	7/16/32/32	0/3/3/3

The worst 5 of 150 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	f	602	ADP	C5-C4	5.11	1.48	1.39
10	m	602	ADP	C5-C4	5.07	1.48	1.39
10	n	602	ADP	C5-C4	5.06	1.48	1.39
10	b	602	ADP	C5-C4	5.00	1.48	1.39
10	k	1102	ADP	C5-C4	4.97	1.47	1.39

The worst 5 of 280 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	i	602	ADP	C5-C4-N3	-6.35	117.97	126.72
10	f	602	ADP	C5-C4-N3	-6.31	118.03	126.72
10	p	602	ADP	C5-C4-N3	-6.29	118.05	126.72
10	m	602	ADP	C5-C4-N3	-6.29	118.06	126.72
10	J	602	ADP	C5-C4-N3	-6.28	118.07	126.72

There are no chirality outliers.

5 of 146 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	F	602	ADP	C5'-O5'-PA-O1A
10	F	602	ADP	C5'-O5'-PA-O2A
10	F	602	ADP	C5'-O5'-PA-O3A
10	G	602	ADP	C5'-O5'-PA-O1A
10	E	602	ADP	C5'-O5'-PA-O3A

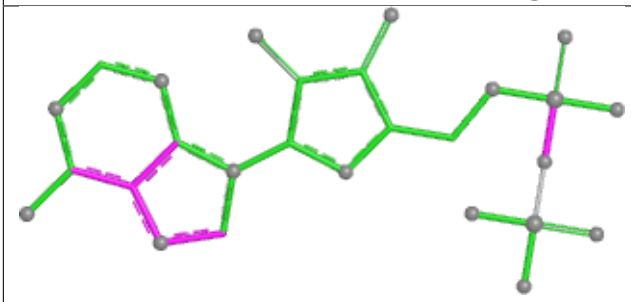
There are no ring outliers.

26 monomers are involved in 22 short contacts:

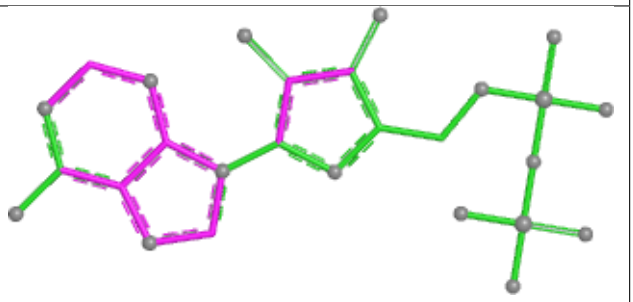
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	602	ADP	1	0
10	K	1102	ADP	1	0
10	I	602	ADP	1	0
11	K	1103	BEF	1	0
10	E	602	ADP	1	0
11	g	603	BEF	1	0
10	a	602	ADP	1	0
11	J	603	BEF	1	0
10	j	602	ADP	1	0
10	C	1102	ADP	1	0
11	b	603	BEF	2	0
10	D	602	ADP	1	0
11	E	603	BEF	1	0
10	B	602	ADP	1	0
10	c	1102	ADP	4	0
10	M	602	ADP	1	0
10	k	1102	ADP	1	0
11	M	603	BEF	1	0
11	c	1103	BEF	1	0
11	d	603	BEF	1	0
10	d	602	ADP	1	0
10	b	602	ADP	3	0
11	o	603	BEF	1	0
11	D	603	BEF	1	0
11	C	1103	BEF	1	0
11	k	1103	BEF	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.

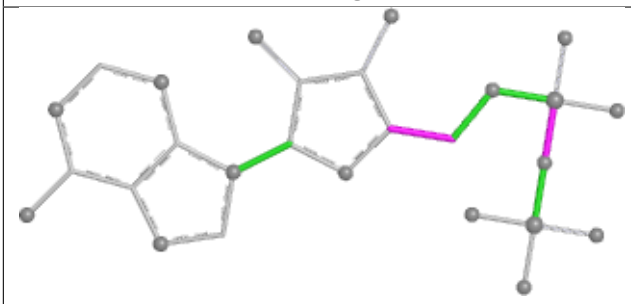
Ligand ADP J 602



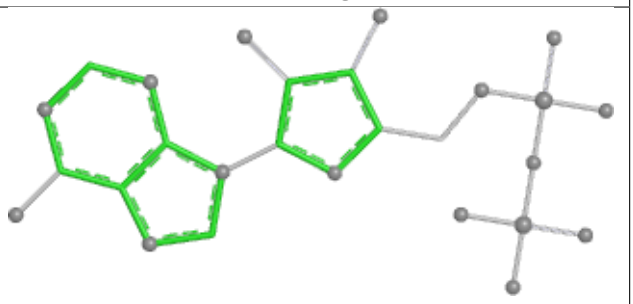
Bond lengths



Bond angles

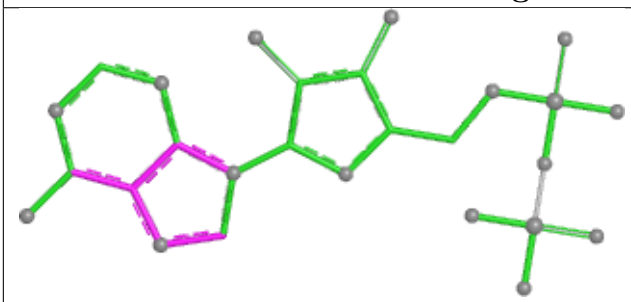


Torsions

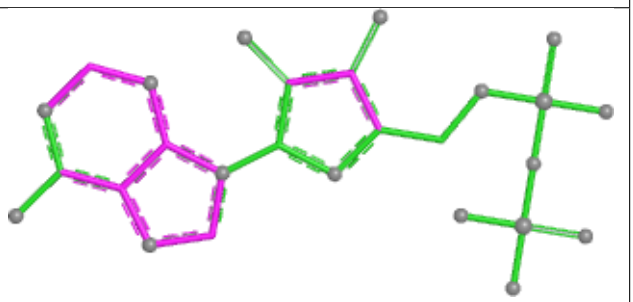


Rings

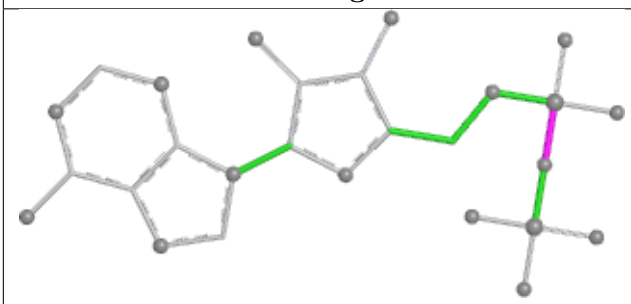
Ligand ADP K 1102



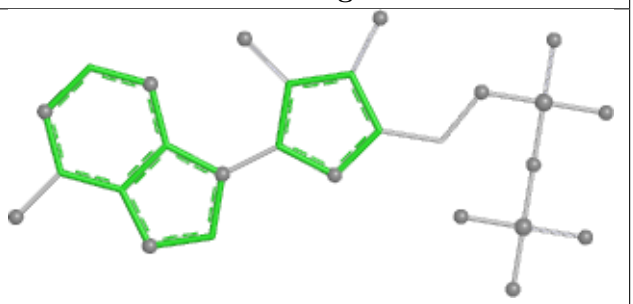
Bond lengths



Bond angles

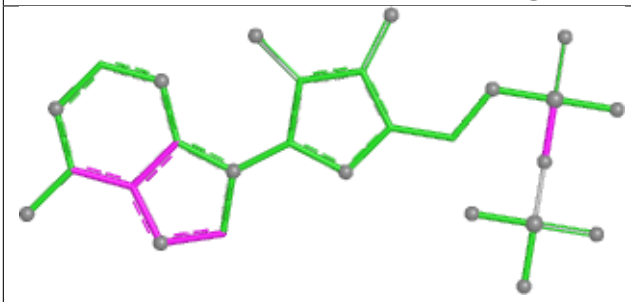


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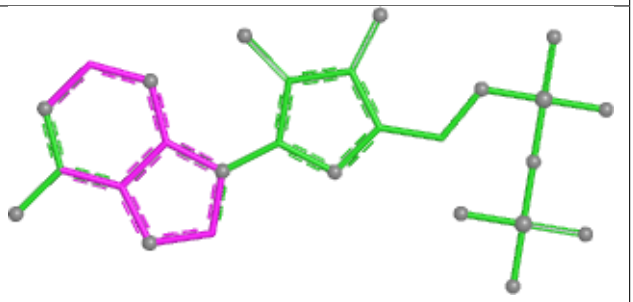


Rings

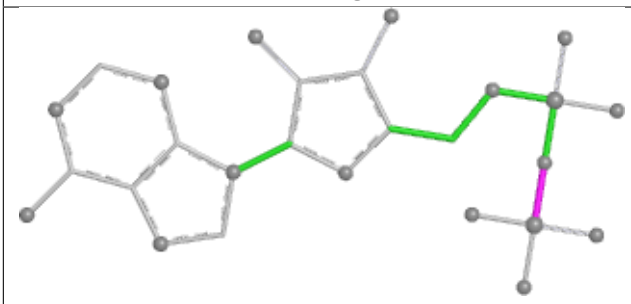
Ligand ADP h 602



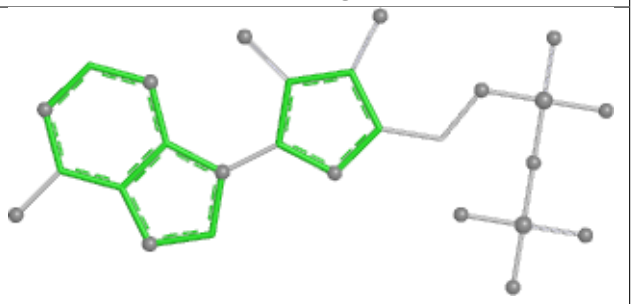
Bond lengths



Bond angles

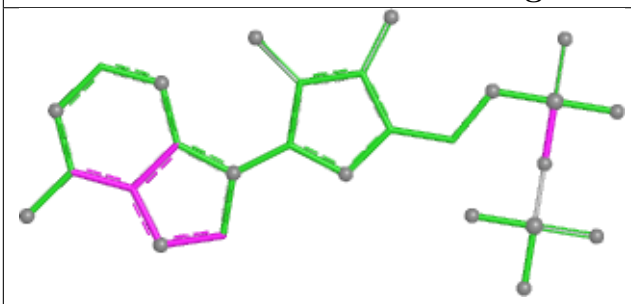


Torsions

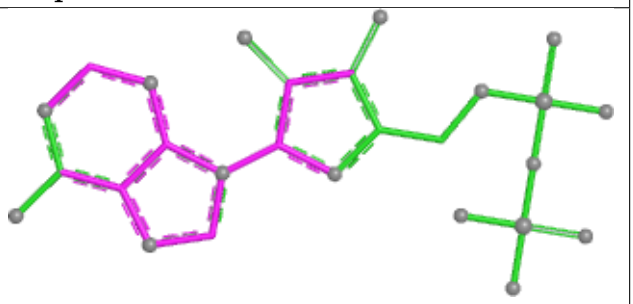


Rings

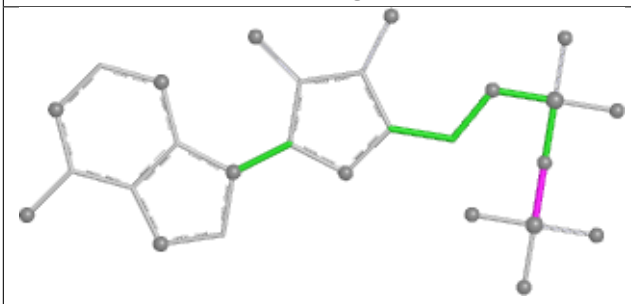
Ligand ADP p 602



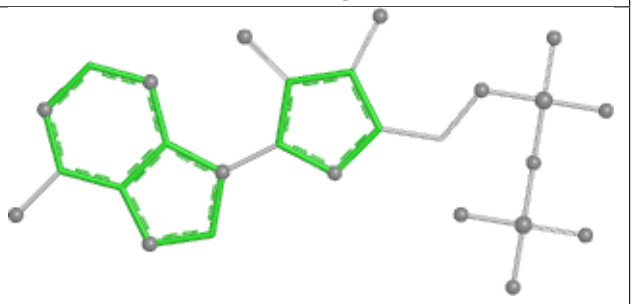
Bond lengths



Bond angles

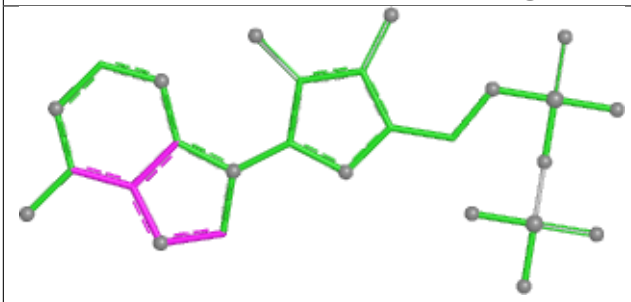


Torsions

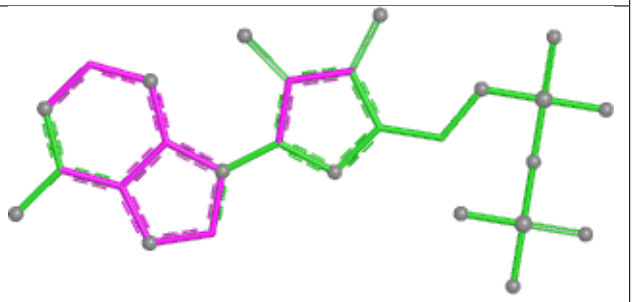


Rings

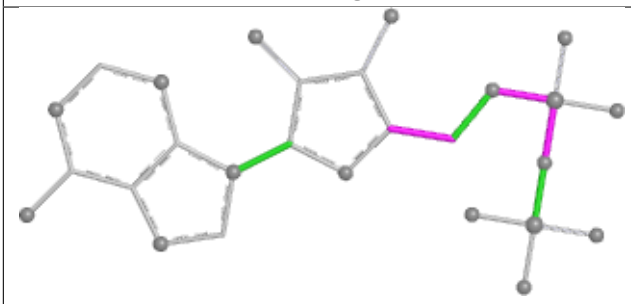
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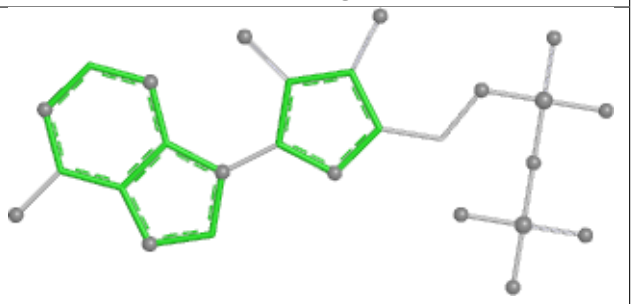
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Bond angles

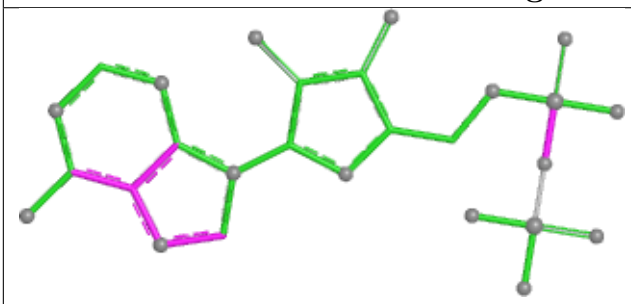


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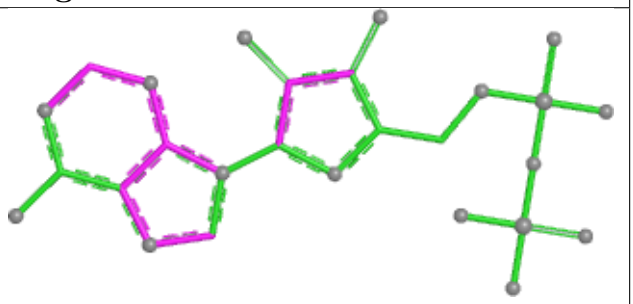


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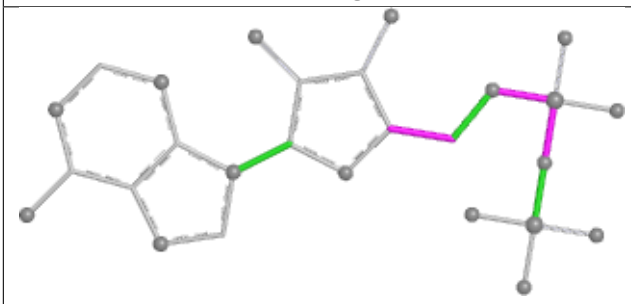
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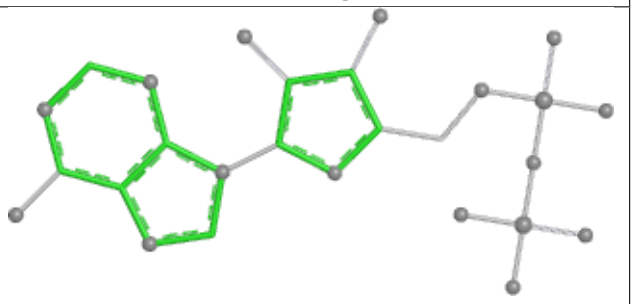
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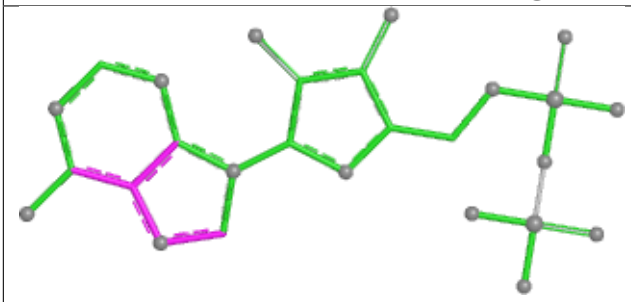


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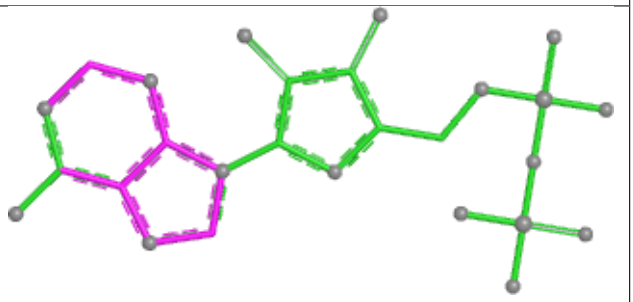


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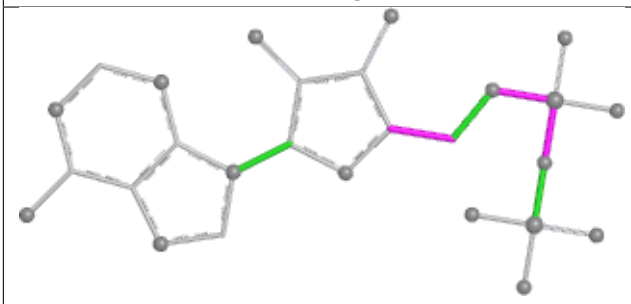
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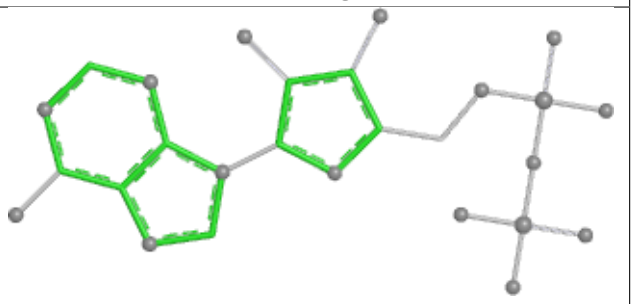
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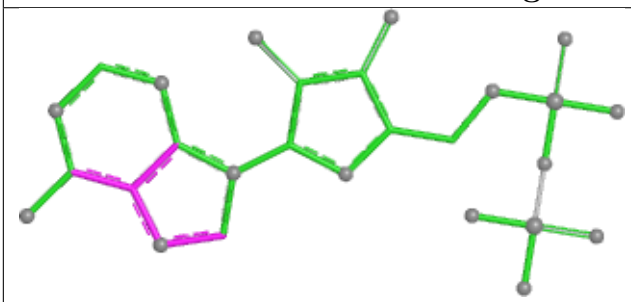


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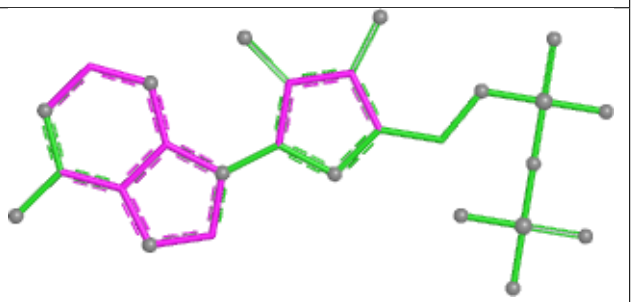


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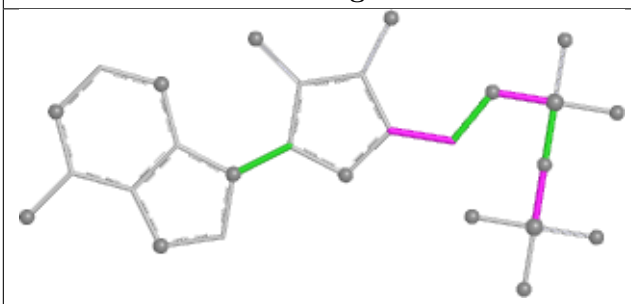
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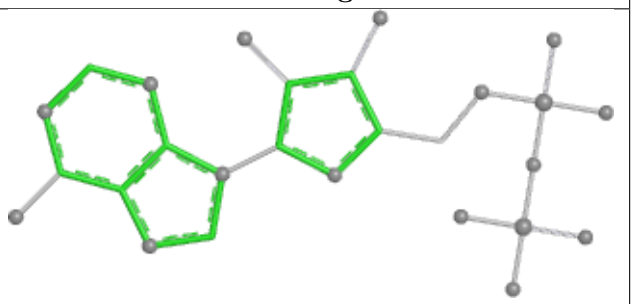
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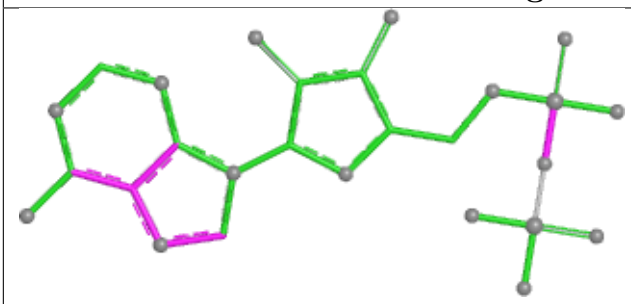


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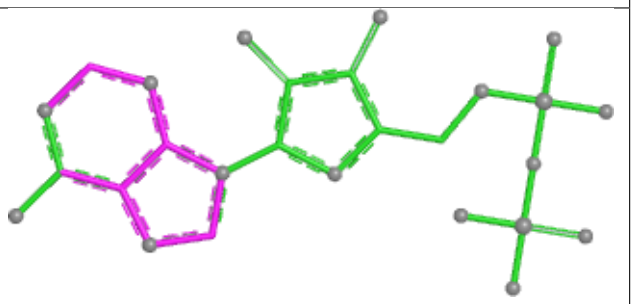


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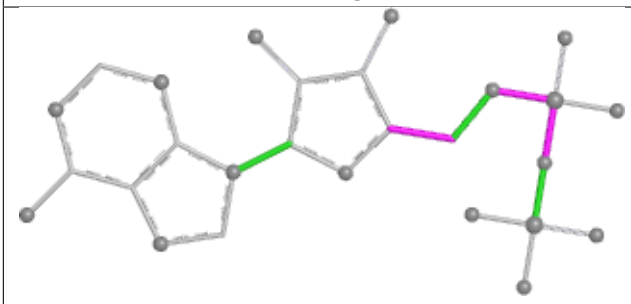
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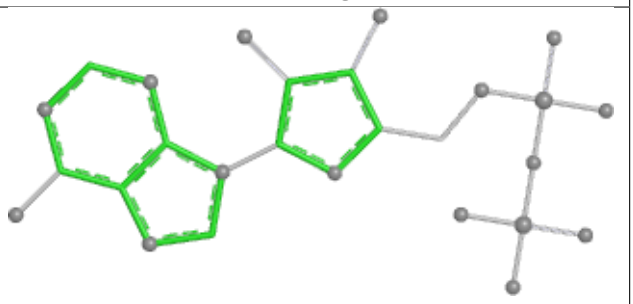
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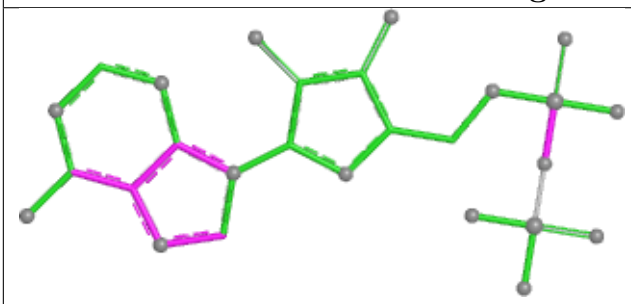


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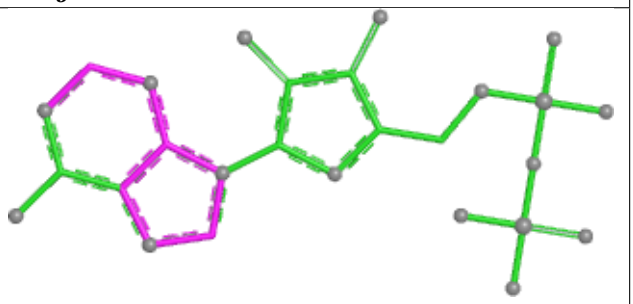


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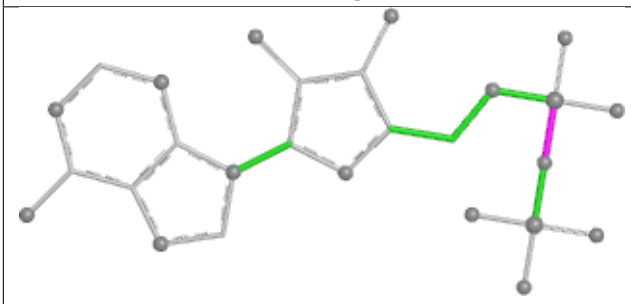
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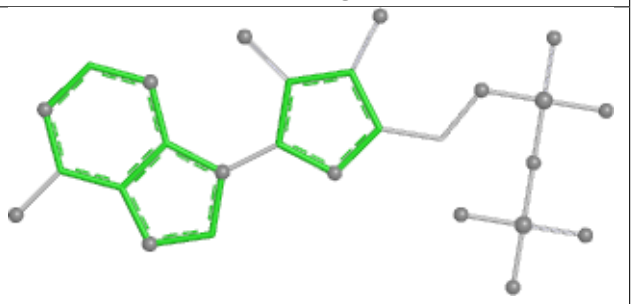
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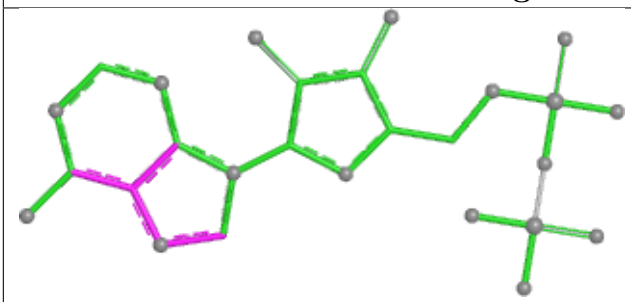


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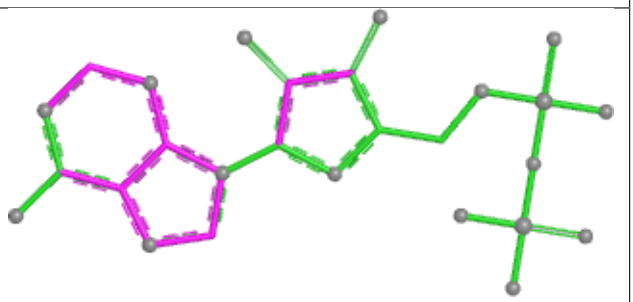


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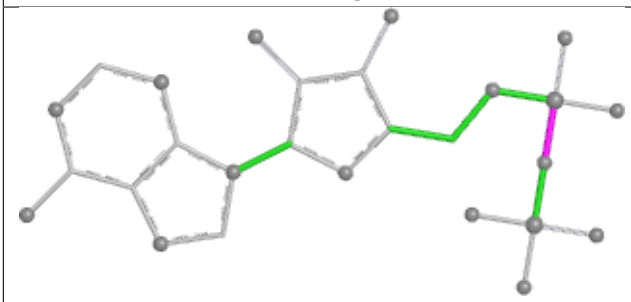
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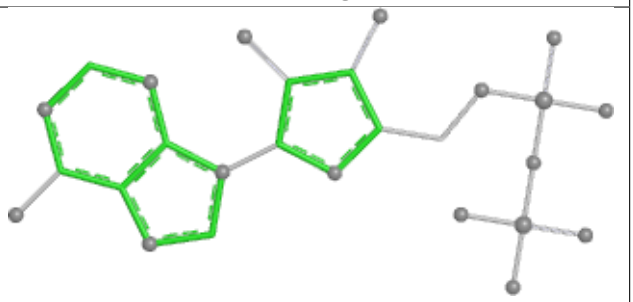
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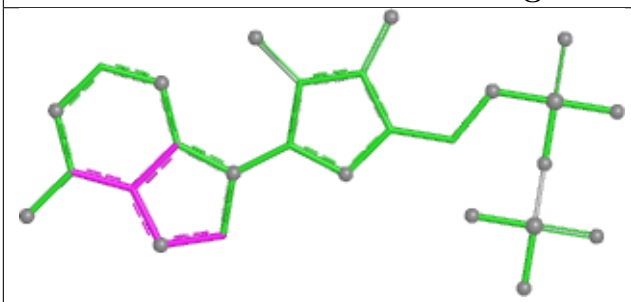


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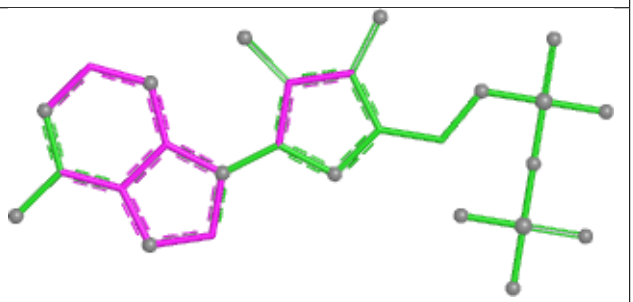


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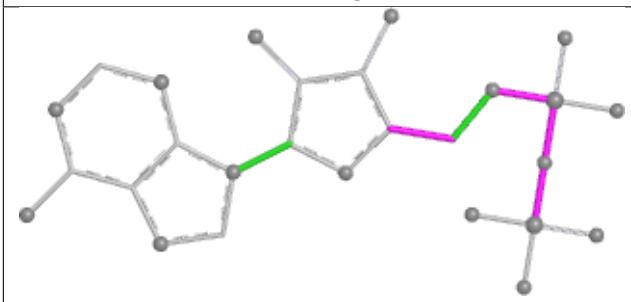
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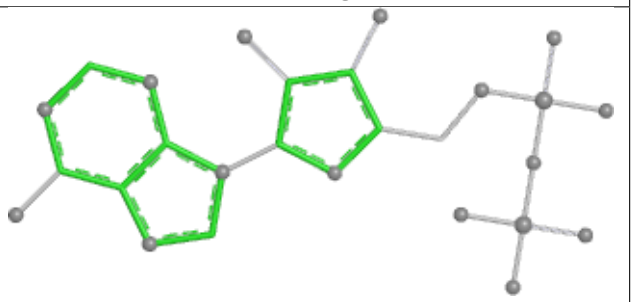
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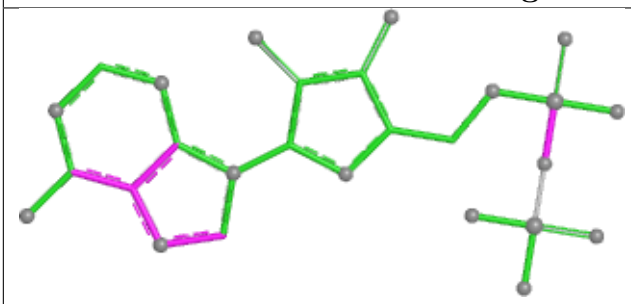


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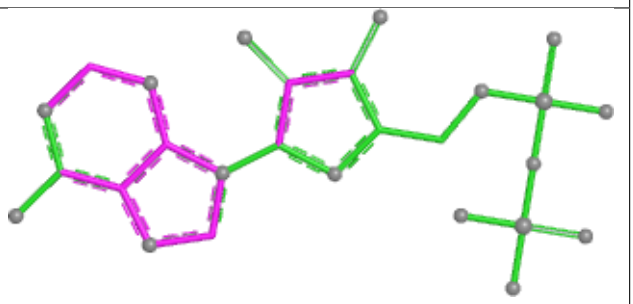


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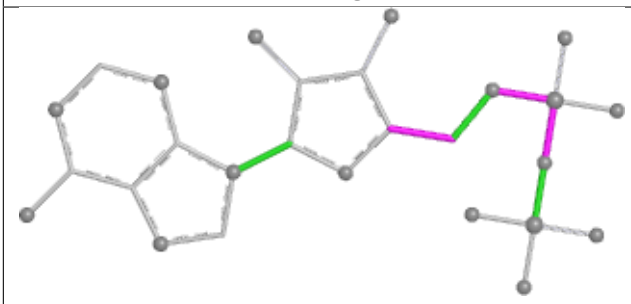
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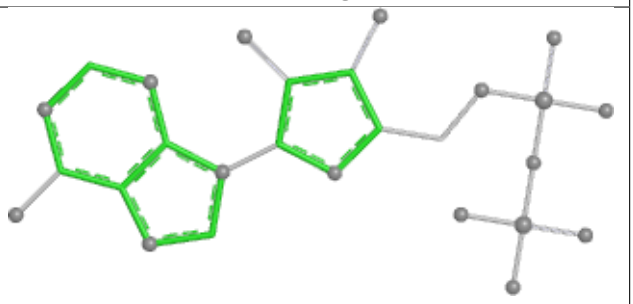
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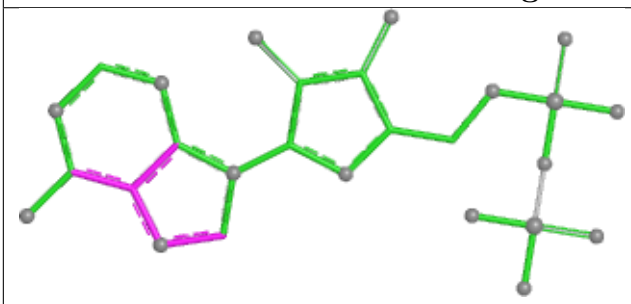


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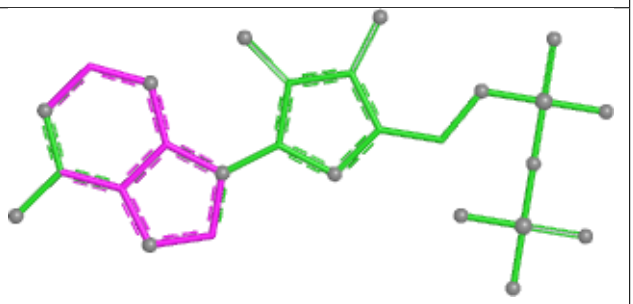


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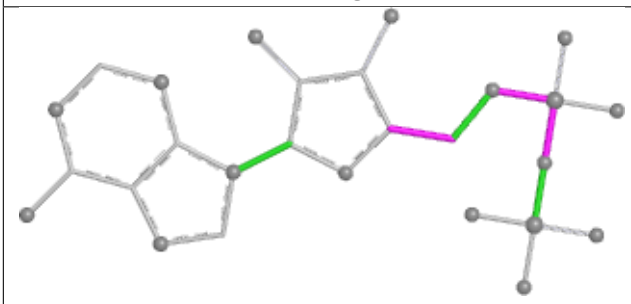
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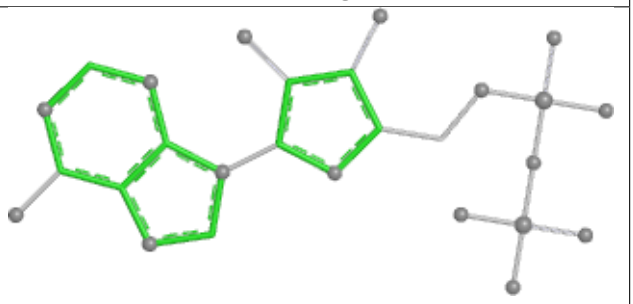
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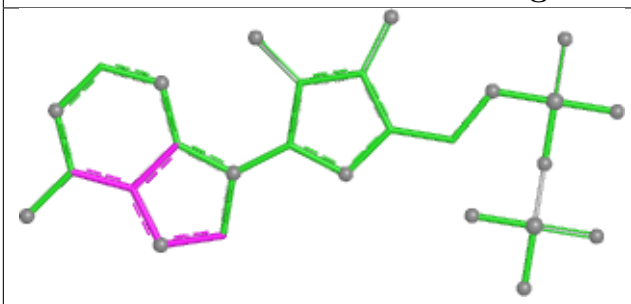


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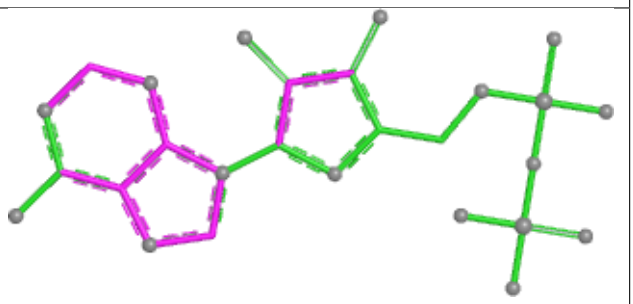


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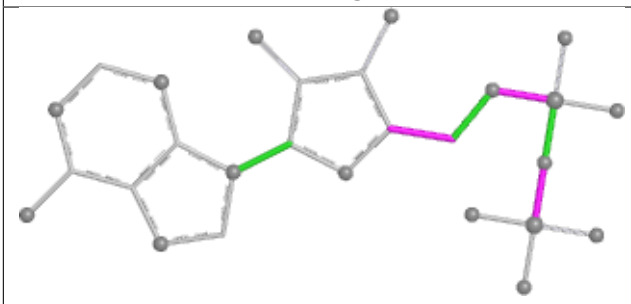
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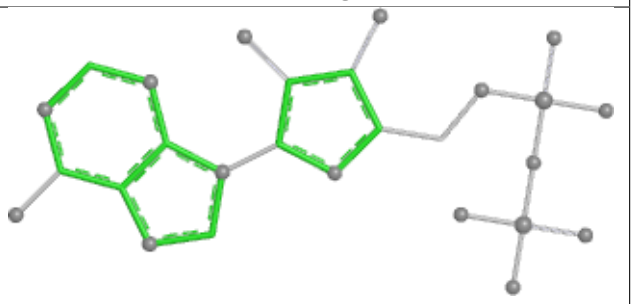
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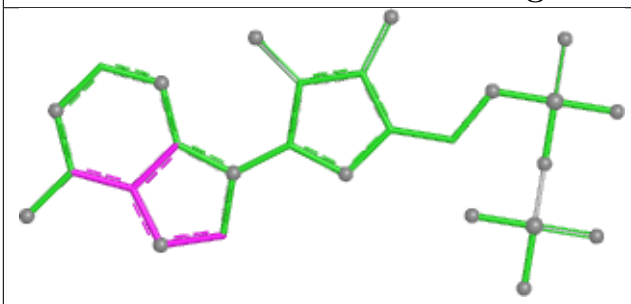


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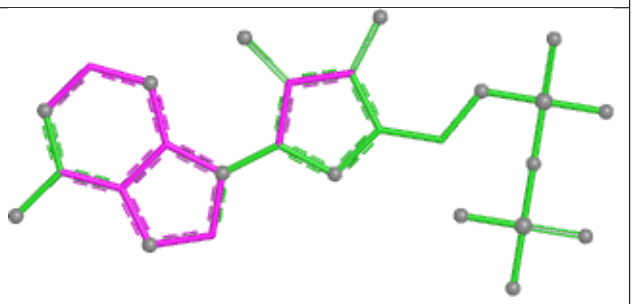


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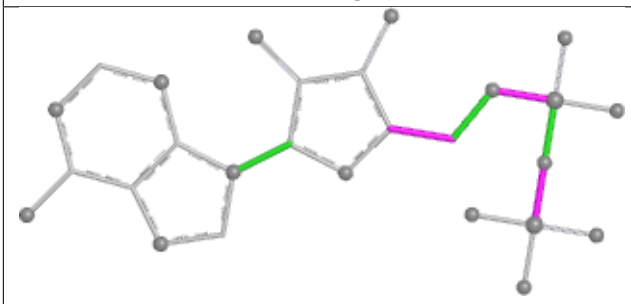
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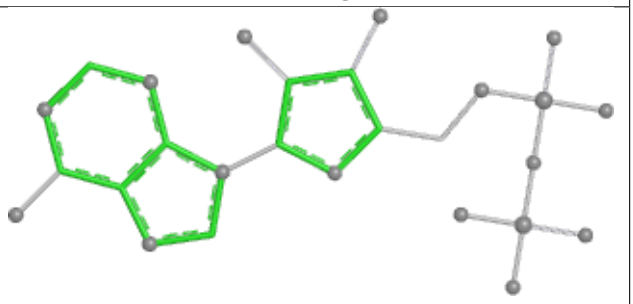
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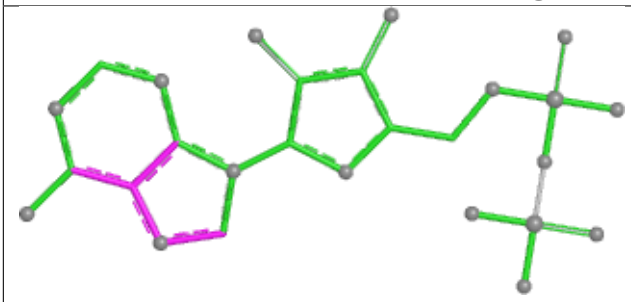


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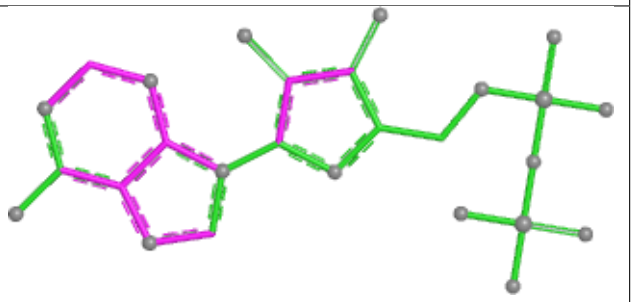


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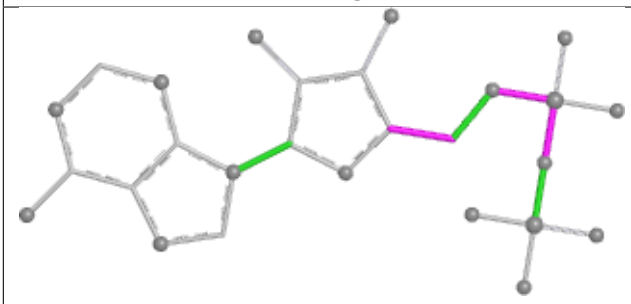
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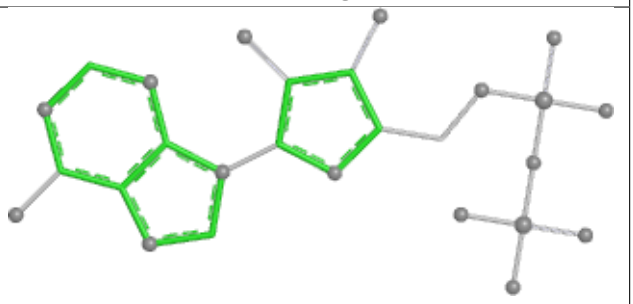
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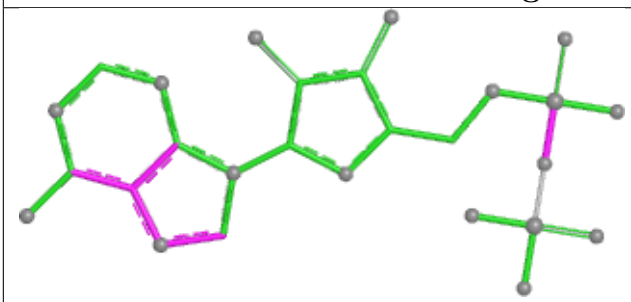


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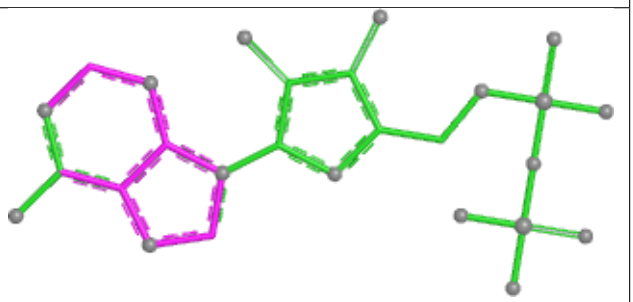


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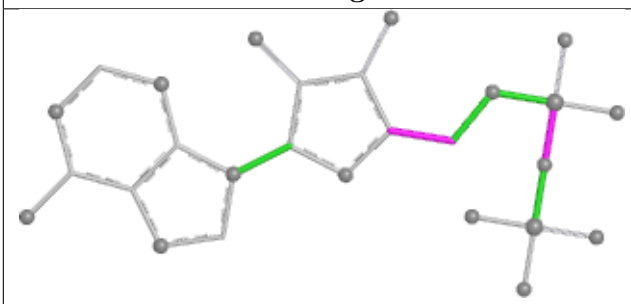
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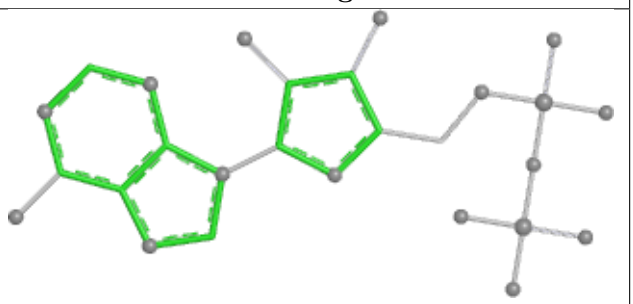
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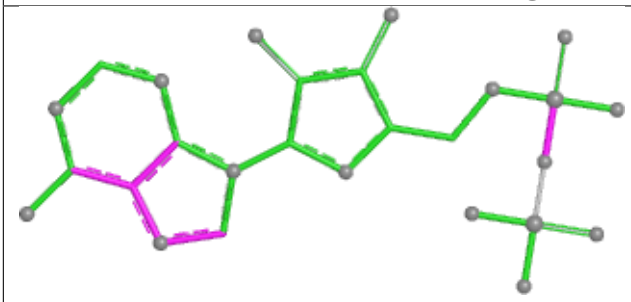


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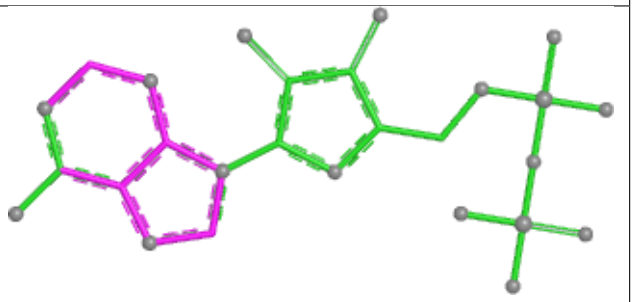


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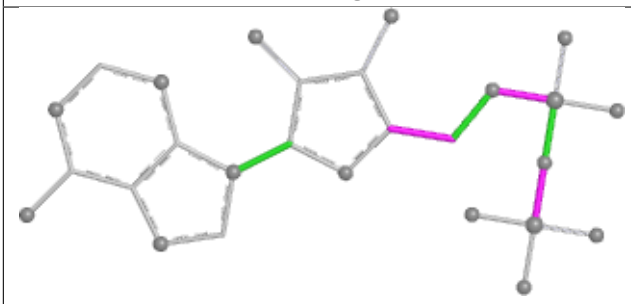
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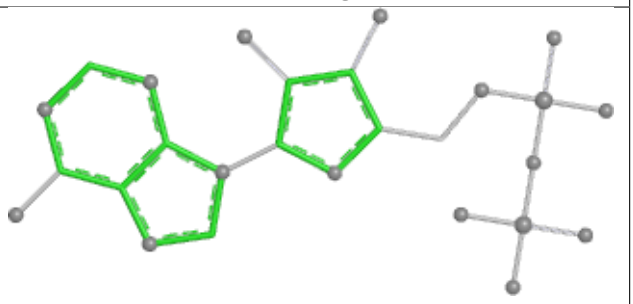
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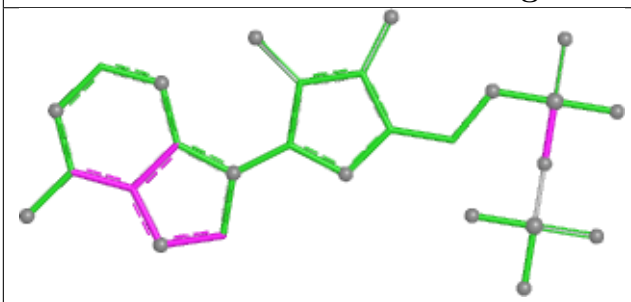


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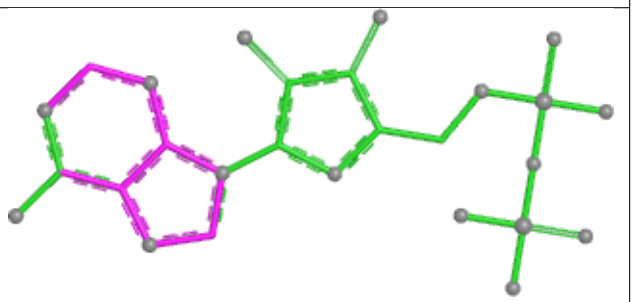


Rings

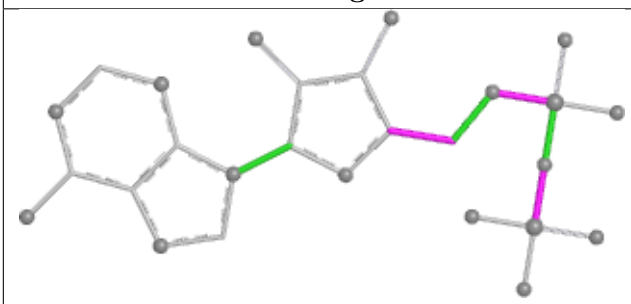
Ligand ADP N 602



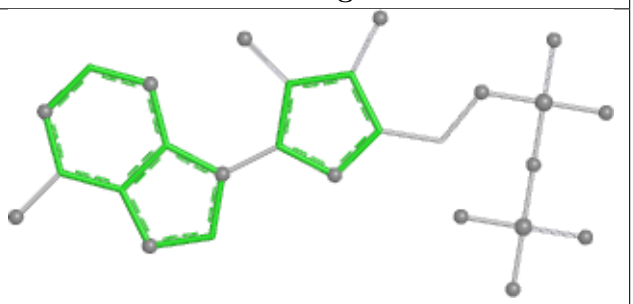
Bond lengths



Bond angles

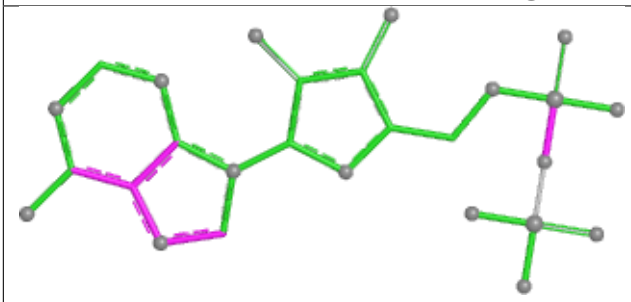


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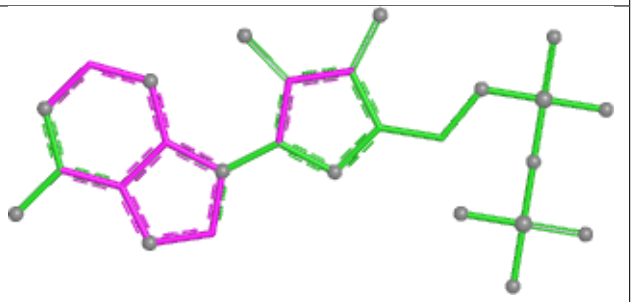


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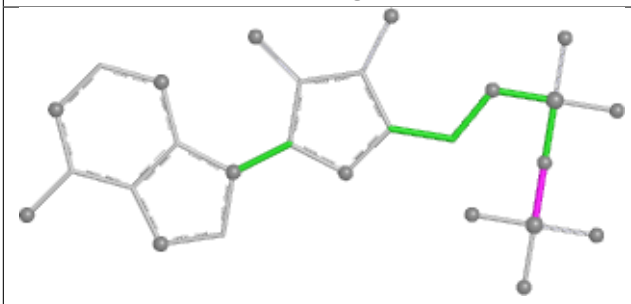
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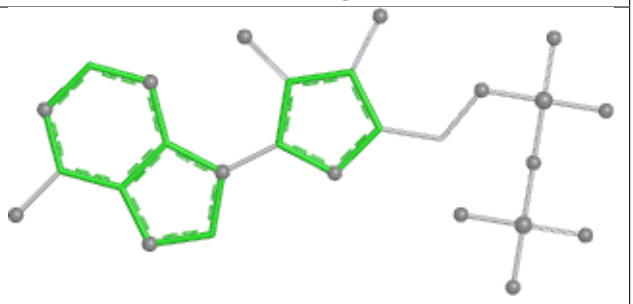
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Bond angles

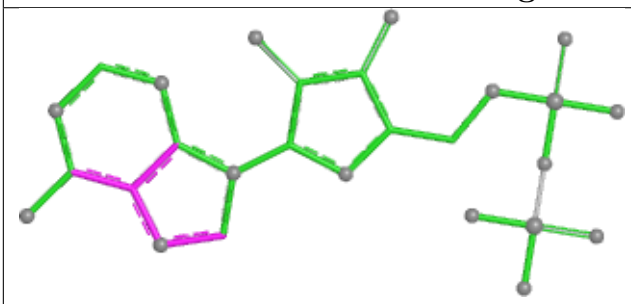


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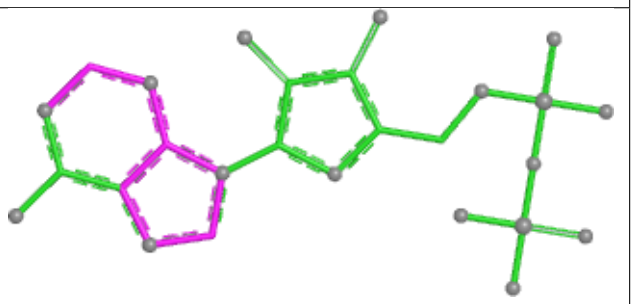


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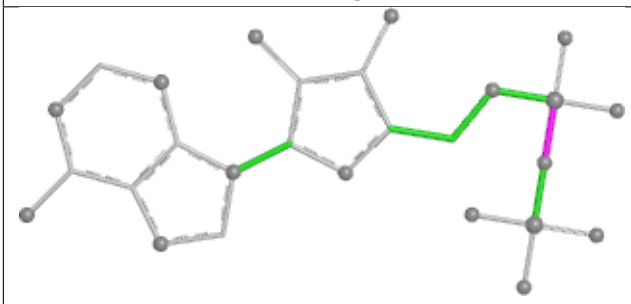
Ligand ADP c 1102



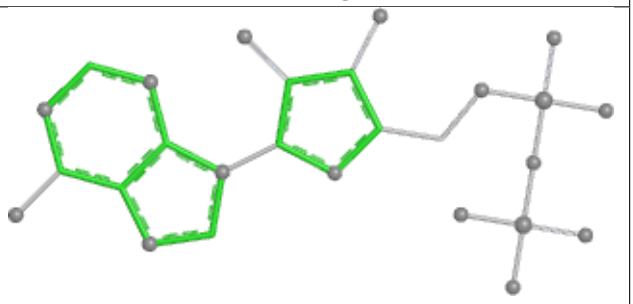
Bond lengths



Bond angles

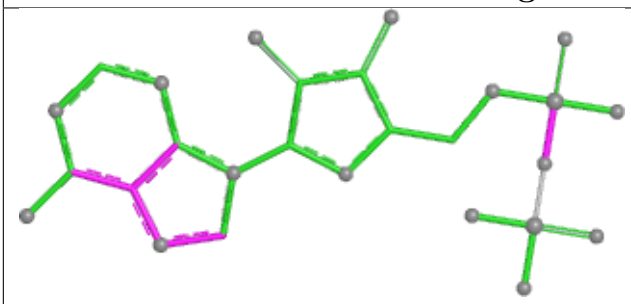


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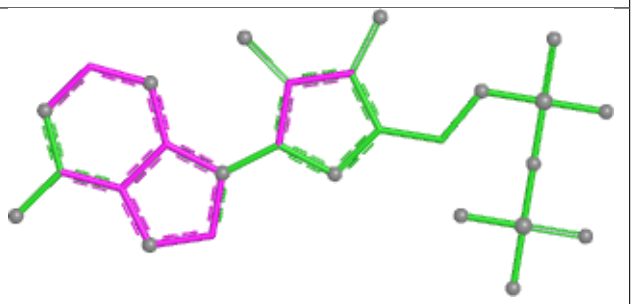


Rings

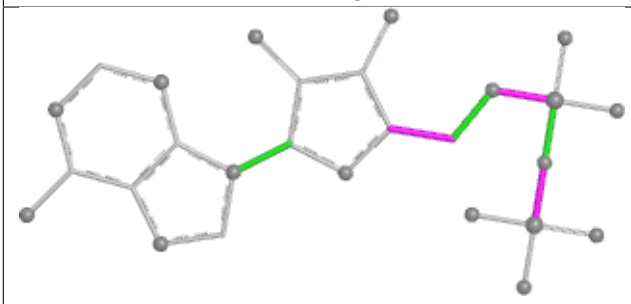
Ligand ADP M 602



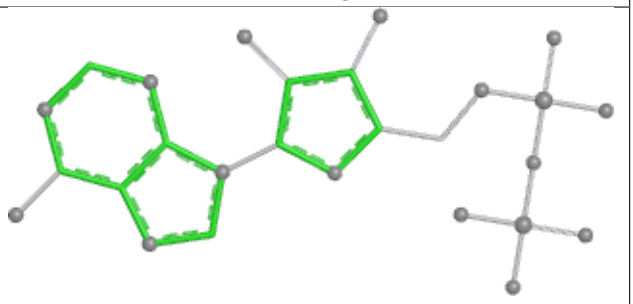
Bond lengths



Bond angles

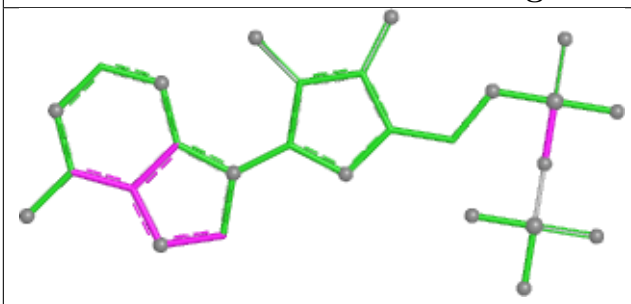


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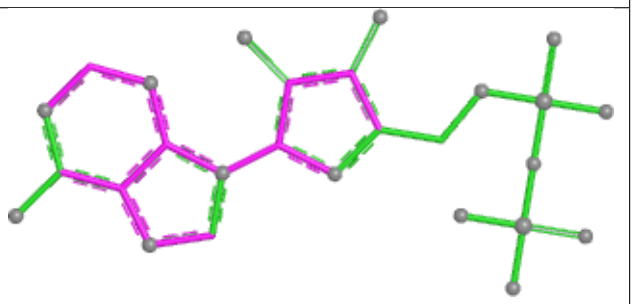


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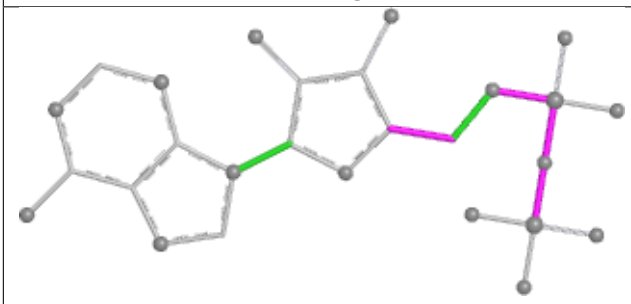
Ligand ADP o 602



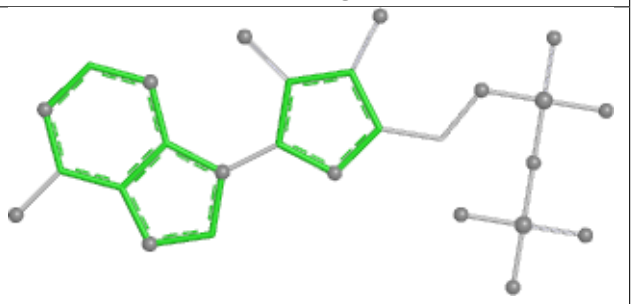
Bond lengths



Bond angles

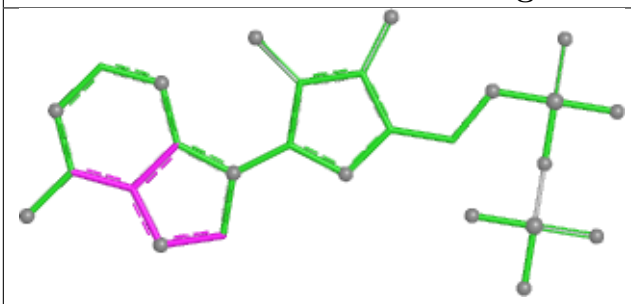


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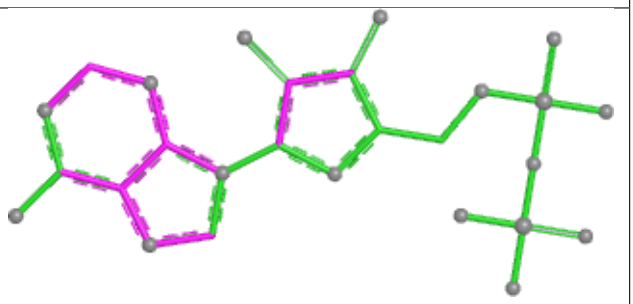


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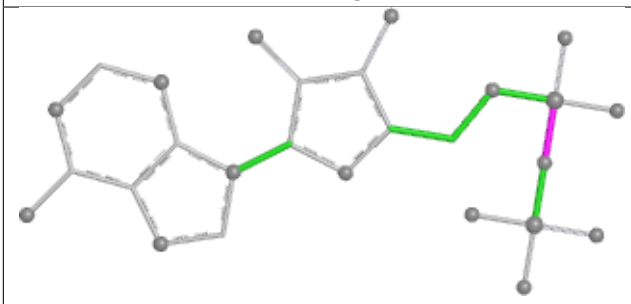
Ligand ADP k 1102



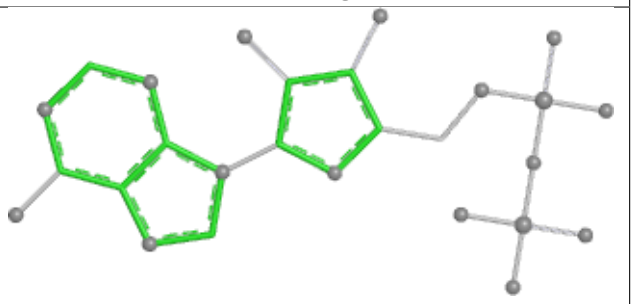
Bond lengths



Bond angles

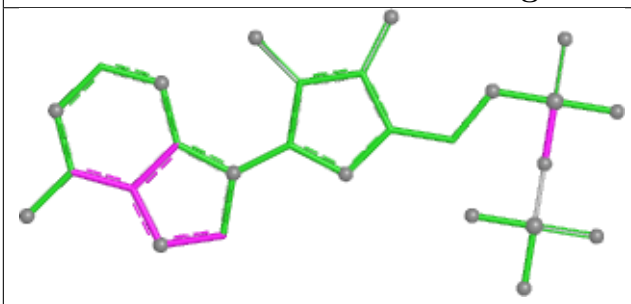


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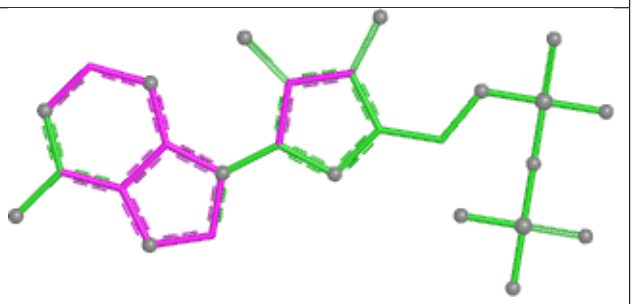


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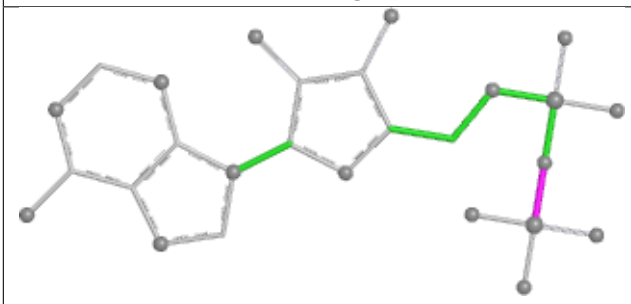
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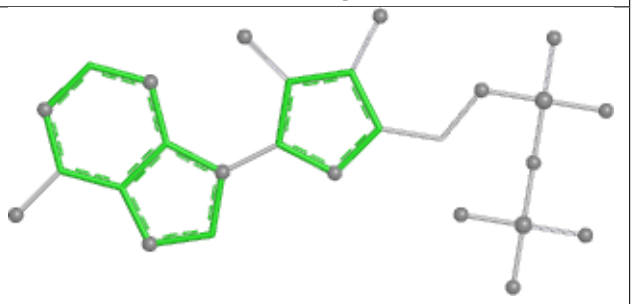
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Bond angles

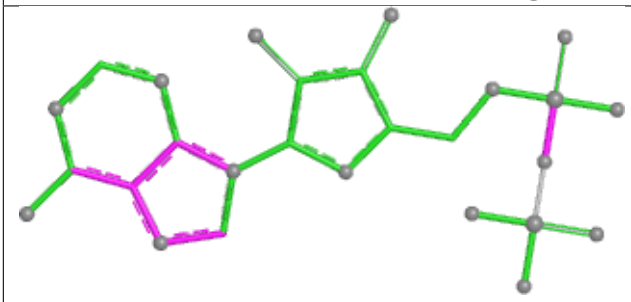


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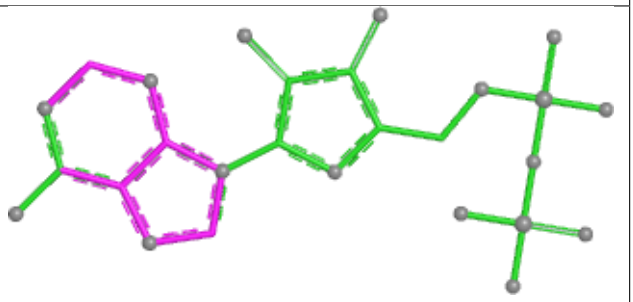


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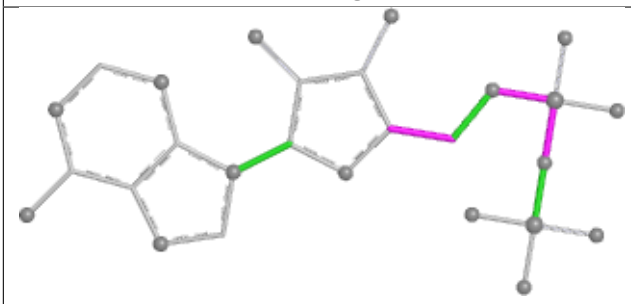
Ligand ADP d 602



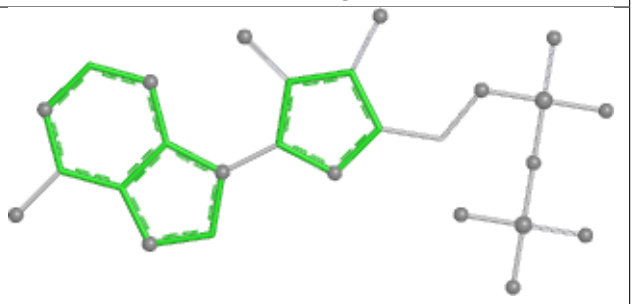
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Bond angles

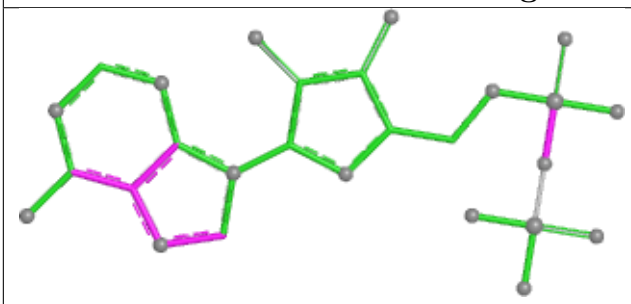


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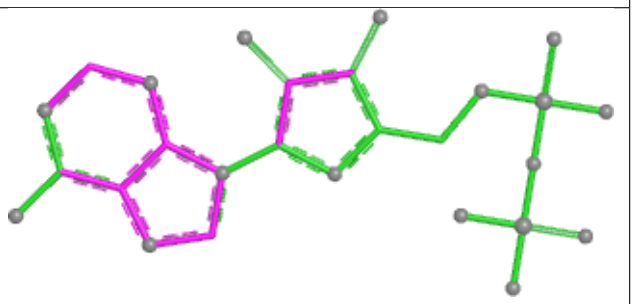


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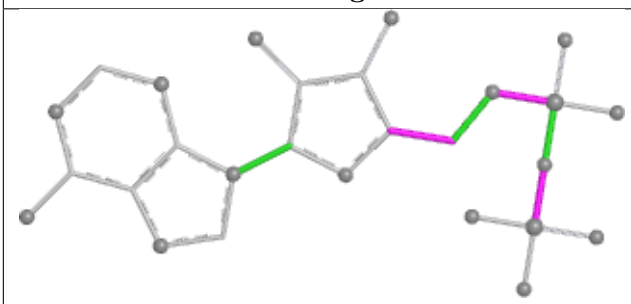
Ligand ADP m 602



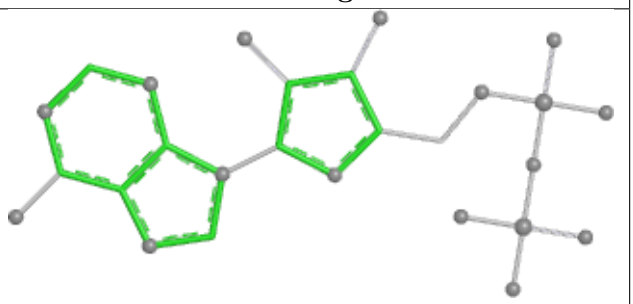
Bond lengths



Bond angles

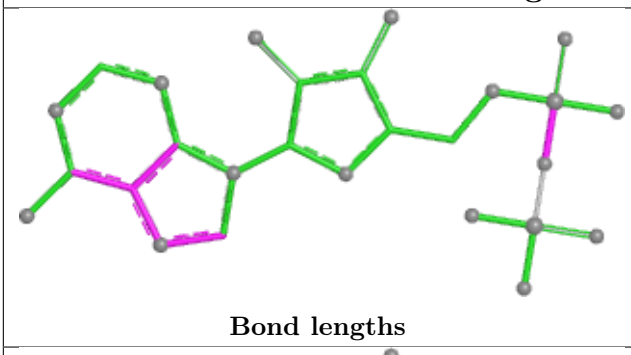


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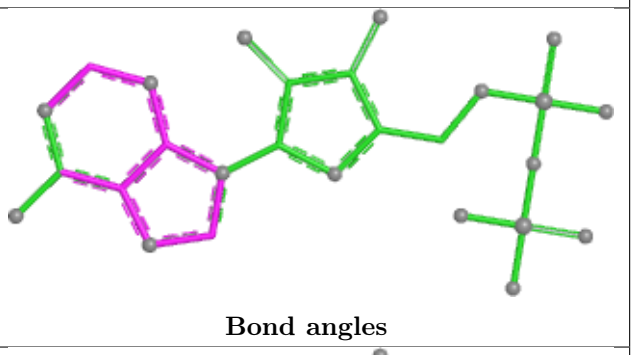


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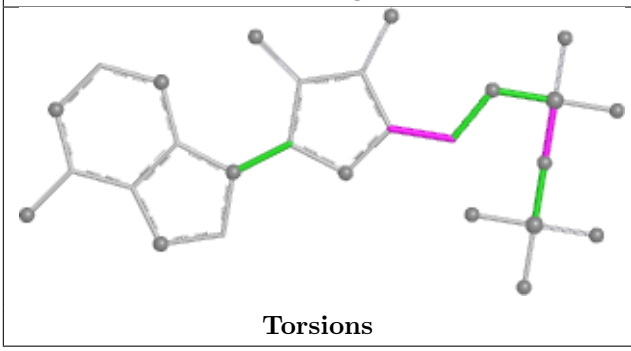
Ligand ADP b 602



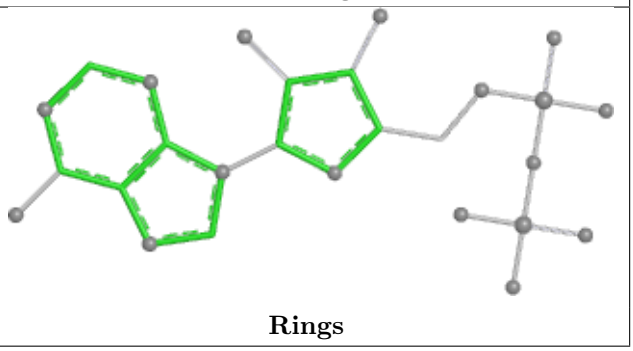
Bond lengths



Bond angles

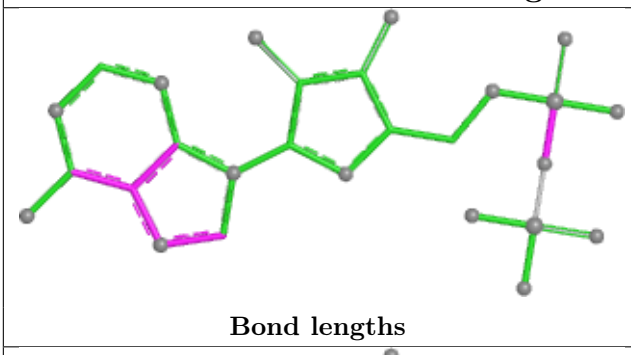


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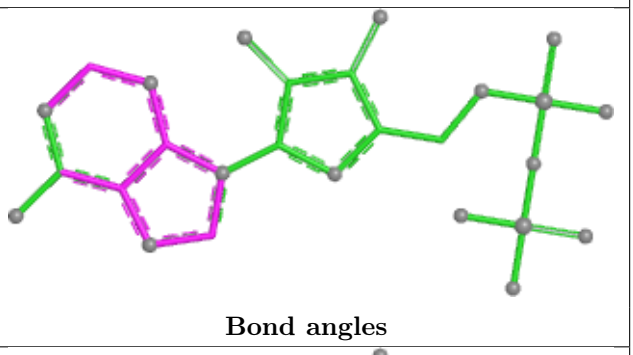


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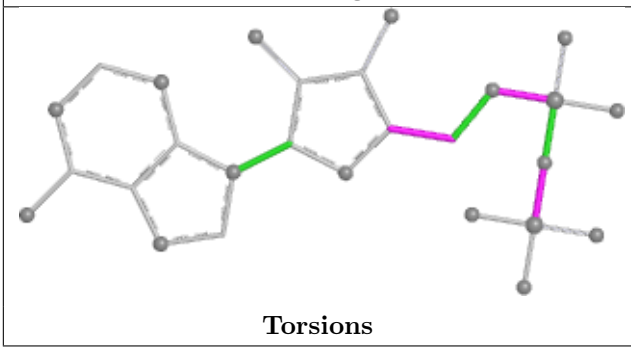
Ligand ADP n 602



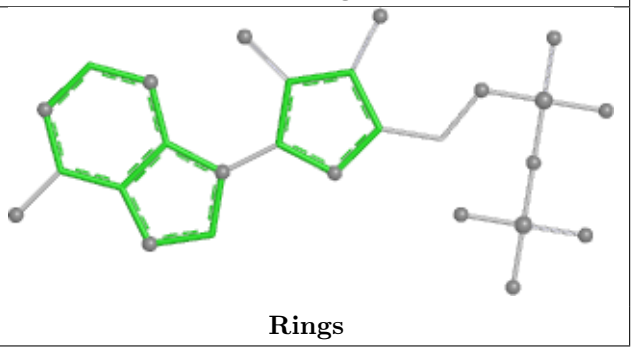
Bond lengths



Bond angles

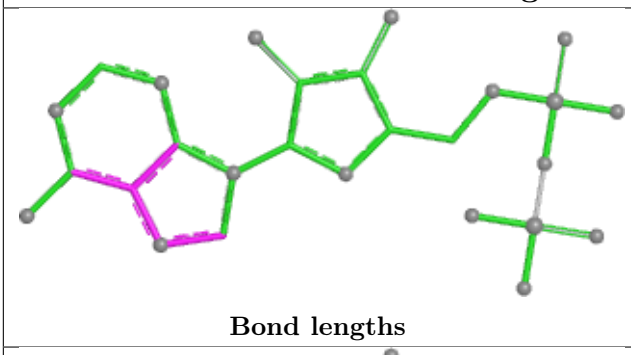


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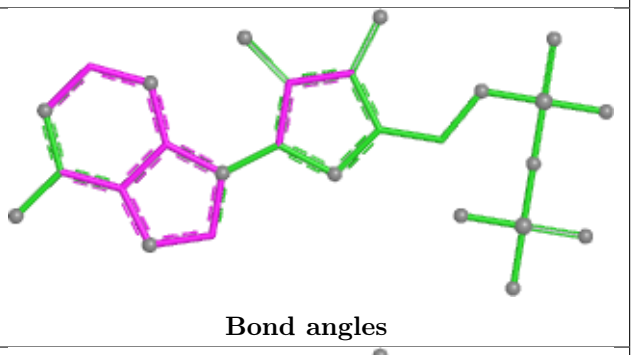


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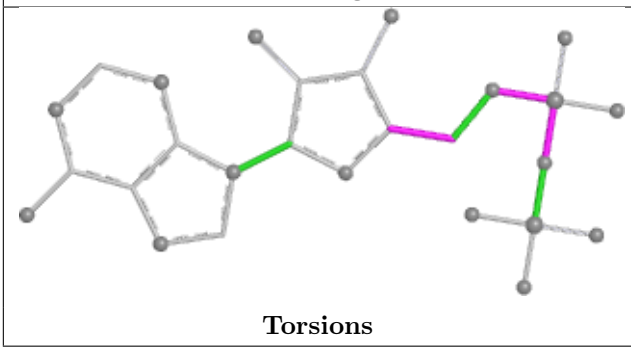
Ligand ADP G 602



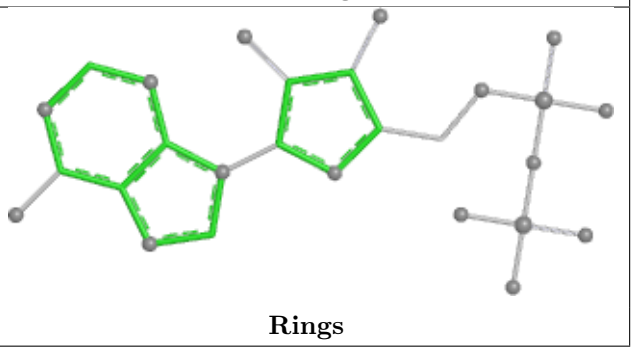
Bond lengths



Bond angles

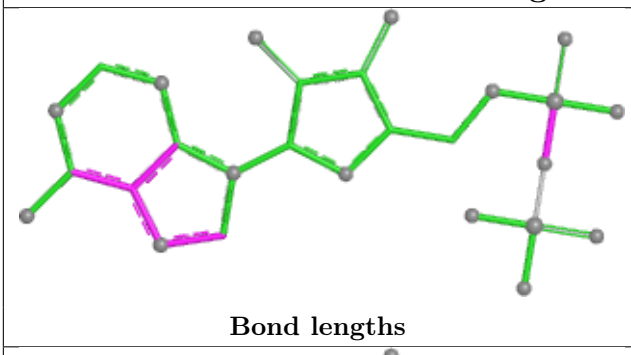


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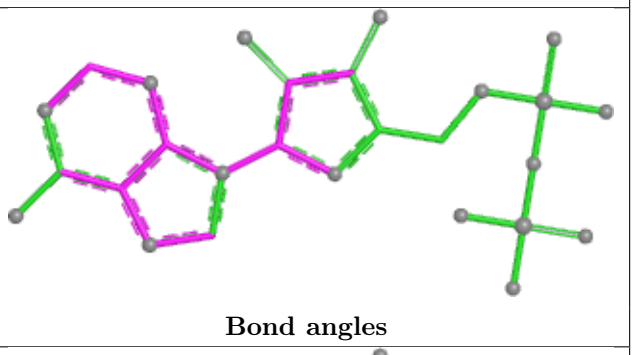


Rings

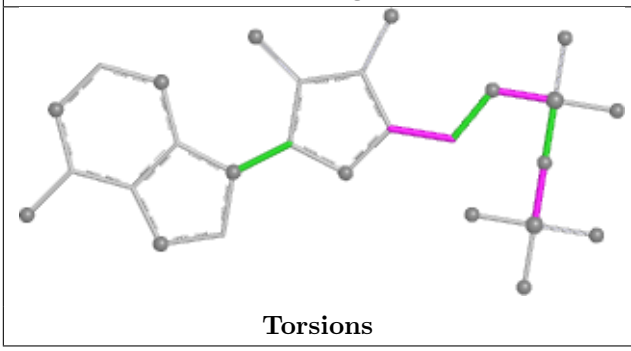
Ligand ADP f 602



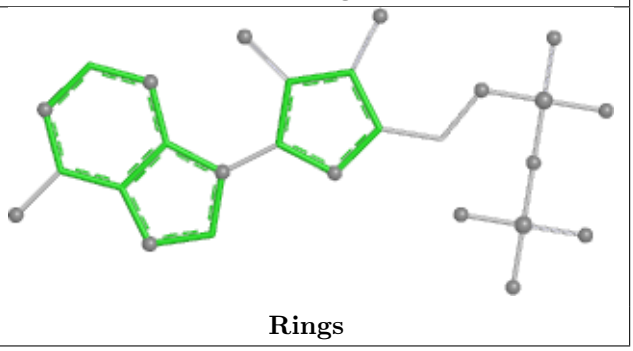
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	F	538/546 (98%)	-0.22	3 (0%) 85 68	94, 122, 163, 189	0
1	N	538/546 (98%)	0.17	9 (1%) 69 47	111, 164, 220, 255	0
1	f	538/546 (98%)	0.24	11 (2%) 65 44	132, 160, 198, 229	0
1	n	538/546 (98%)	0.04	2 (0%) 88 74	112, 129, 161, 201	0
2	H	521/568 (91%)	-0.13	1 (0%) 91 81	94, 131, 172, 189	0
2	P	521/568 (91%)	0.27	10 (1%) 66 45	119, 171, 234, 265	0
2	h	521/568 (91%)	0.36	17 (3%) 49 34	133, 160, 194, 273	0
2	p	521/568 (91%)	0.15	3 (0%) 85 68	101, 140, 177, 203	0
3	G	526/550 (95%)	-0.09	3 (0%) 85 68	95, 137, 174, 196	0
3	O	526/550 (95%)	0.48	16 (3%) 52 36	106, 157, 253, 338	0
3	g	526/550 (95%)	0.27	8 (1%) 72 50	115, 141, 180, 238	0
3	o	526/550 (95%)	0.07	5 (0%) 79 58	99, 128, 174, 247	0
4	E	535/562 (95%)	-0.15	1 (0%) 91 81	88, 130, 172, 188	0
4	M	535/562 (95%)	0.43	15 (2%) 55 38	106, 140, 233, 319	0
4	e	535/562 (95%)	0.15	4 (0%) 84 65	100, 124, 173, 249	0
4	m	535/562 (95%)	0.02	1 (0%) 91 81	94, 113, 161, 235	0
5	B	518/527 (98%)	-0.28	1 (0%) 91 81	75, 100, 146, 172	0
5	J	518/527 (98%)	0.30	13 (2%) 58 40	101, 127, 198, 249	0
5	b	518/527 (98%)	0.04	2 (0%) 88 74	100, 116, 141, 176	0
5	j	518/527 (98%)	-0.06	3 (0%) 85 68	90, 110, 131, 155	0
6	D	523/528 (99%)	-0.22	0 100 100	78, 119, 153, 183	0
6	L	523/528 (99%)	0.65	33 (6%) 26 21	118, 160, 239, 313	0
6	d	523/528 (99%)	0.10	9 (1%) 69 47	112, 136, 166, 182	0
6	l	523/528 (99%)	0.07	6 (1%) 78 56	103, 129, 170, 196	0

Continued on next page...

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
7	A	539/559 (96%)	-0.22	3 (0%) 85 68	88, 120, 160, 203	0
7	I	539/559 (96%)	0.32	18 (3%) 49 34	107, 144, 223, 317	0
7	a	539/559 (96%)	0.06	2 (0%) 88 74	112, 135, 177, 208	0
7	i	539/559 (96%)	0.11	6 (1%) 78 56	101, 132, 185, 212	0
8	C	513/590 (86%)	-0.19	0 100 100	91, 121, 154, 181	0
8	K	513/590 (86%)	0.11	4 (0%) 82 62	103, 150, 238, 312	0
8	c	513/590 (86%)	0.23	3 (0%) 85 68	121, 143, 186, 223	0
8	k	513/590 (86%)	0.10	5 (0%) 79 58	114, 131, 176, 246	0
All	All	16852/17720 (95%)	0.10	217 (1%) 75 53	75, 134, 194, 338	0

The worst 5 of 217 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	267	TYR	5.6
1	f	142	ASN	5.3
6	L	351	GLU	4.8
4	e	204	ALA	4.5
2	h	455	ALA	4.1

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

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

6.3 Carbohydrates (i)

There are no 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
9	MG	L	601	1/1	0.68	0.15	124,124,124,124	0
9	MG	c	1101	1/1	0.71	0.09	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	BEF	N	603	4/4	0.77	0.12	132,135,135,137	0
11	BEF	h	603	4/4	0.81	0.15	55,55,55,55	0
11	BEF	k	1103	4/4	0.85	0.09	110,111,111,112	0
11	BEF	p	603	4/4	0.86	0.09	130,132,133,133	0
9	MG	d	601	1/1	0.87	0.12	115,115,115,115	0
10	ADP	N	602	27/27	0.87	0.11	133,145,153,154	0
9	MG	h	601	1/1	0.88	0.08	151,151,151,151	0
11	BEF	f	603	4/4	0.89	0.08	152,152,154,156	0
10	ADP	f	602	27/27	0.89	0.11	149,154,159,160	0
9	MG	o	601	1/1	0.89	0.09	115,115,115,115	0
11	BEF	o	603	4/4	0.89	0.07	116,118,119,119	0
11	BEF	L	603	4/4	0.89	0.08	135,138,138,141	0
11	BEF	J	603	4/4	0.90	0.10	110,112,113,114	0
9	MG	N	601	1/1	0.90	0.12	132,132,132,132	0
10	ADP	p	602	27/27	0.90	0.11	133,145,154,156	0
11	BEF	G	603	4/4	0.90	0.10	110,110,112,116	0
11	BEF	c	1103	4/4	0.90	0.07	126,127,127,129	0
11	BEF	D	603	4/4	0.90	0.09	89,89,91,94	0
10	ADP	L	602	27/27	0.90	0.10	135,138,144,147	0
11	BEF	O	603	4/4	0.90	0.08	117,118,119,120	0
9	MG	a	601	1/1	0.91	0.12	126,126,126,126	0
11	BEF	n	603	4/4	0.91	0.06	115,115,116,118	0
11	BEF	K	1103	4/4	0.91	0.06	118,120,120,123	0
10	ADP	c	1102	27/27	0.91	0.09	134,138,142,143	0
10	ADP	n	602	27/27	0.91	0.09	112,116,123,124	0
10	ADP	O	602	27/27	0.92	0.11	109,115,120,121	0
10	ADP	m	602	27/27	0.92	0.11	102,106,108,109	0
10	ADP	i	602	27/27	0.92	0.10	113,121,126,127	0
10	ADP	h	602	27/27	0.92	0.14	152,159,166,167	0
11	BEF	e	603	4/4	0.92	0.11	114,114,116,118	0
10	ADP	P	602	27/27	0.93	0.09	136,143,148,149	0
9	MG	l	601	1/1	0.93	0.12	107,107,107,107	0
10	ADP	o	602	27/27	0.93	0.09	119,128,133,134	0
9	MG	k	1101	1/1	0.93	0.11	111,111,111,111	0
10	ADP	F	602	27/27	0.93	0.07	97,105,112,113	0
11	BEF	g	603	4/4	0.93	0.07	128,132,132,134	0
10	ADP	k	1102	27/27	0.93	0.10	115,117,120,121	0
11	BEF	d	603	4/4	0.93	0.07	116,120,121,121	0
11	BEF	a	603	4/4	0.93	0.09	118,120,121,121	0
10	ADP	A	602	27/27	0.93	0.10	98,113,126,127	0
11	BEF	B	603	4/4	0.93	0.10	76,77,77,78	0
10	ADP	g	602	27/27	0.93	0.10	132,141,149,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	ADP	d	602	27/27	0.93	0.10	125,135,149,151	0
11	BEF	i	603	4/4	0.93	0.07	104,105,105,106	0
9	MG	j	601	1/1	0.93	0.13	88,88,88,88	0
11	BEF	b	603	4/4	0.94	0.07	103,105,105,107	0
11	BEF	l	603	4/4	0.94	0.09	107,110,111,111	0
11	BEF	C	1103	4/4	0.94	0.09	91,92,93,94	0
10	ADP	M	602	27/27	0.94	0.09	104,111,114,115	0
10	ADP	b	602	27/27	0.95	0.10	104,109,115,115	0
11	BEF	E	603	4/4	0.95	0.09	98,98,100,102	0
10	ADP	H	602	27/27	0.95	0.07	106,117,128,130	0
10	ADP	a	602	27/27	0.95	0.09	126,139,146,148	0
10	ADP	B	602	27/27	0.95	0.08	78,83,86,87	0
10	ADP	D	602	27/27	0.95	0.09	95,106,120,123	0
10	ADP	I	602	27/27	0.95	0.09	121,126,133,135	0
10	ADP	K	1102	27/27	0.95	0.08	122,131,144,147	0
9	MG	I	601	1/1	0.95	0.11	121,121,121,121	0
10	ADP	j	602	27/27	0.95	0.12	94,100,106,107	0
9	MG	m	601	1/1	0.95	0.06	84,84,84,84	0
9	MG	n	601	1/1	0.95	0.07	108,108,108,108	0
9	MG	K	1101	1/1	0.96	0.07	126,126,126,126	0
10	ADP	l	602	27/27	0.96	0.08	117,129,144,145	0
11	BEF	P	603	4/4	0.96	0.04	140,141,142,145	0
10	ADP	G	602	27/27	0.96	0.09	111,127,140,142	0
11	BEF	M	603	4/4	0.96	0.06	111,113,114,116	0
9	MG	O	601	1/1	0.96	0.06	113,113,113,113	0
11	BEF	H	603	4/4	0.96	0.05	105,106,106,108	0
9	MG	C	1101	1/1	0.96	0.08	99,99,99,99	0
11	BEF	m	603	4/4	0.96	0.08	99,100,101,103	0
10	ADP	J	602	27/27	0.96	0.08	104,108,113,113	0
10	ADP	e	602	27/27	0.96	0.09	117,124,127,128	0
9	MG	D	601	1/1	0.96	0.09	89,89,89,89	0
11	BEF	A	603	4/4	0.97	0.06	91,91,92,95	0
9	MG	A	601	1/1	0.97	0.13	102,102,102,102	0
10	ADP	E	602	27/27	0.97	0.07	102,115,123,124	0
9	MG	E	601	1/1	0.97	0.07	91,91,91,91	0
9	MG	g	601	1/1	0.97	0.08	129,129,129,129	0
9	MG	e	601	1/1	0.97	0.07	102,102,102,102	0
10	ADP	C	1102	27/27	0.97	0.06	100,111,118,119	0
9	MG	G	601	1/1	0.97	0.09	113,113,113,113	0
11	BEF	F	603	4/4	0.98	0.04	99,101,101,102	0
9	MG	f	601	1/1	0.98	0.05	143,143,143,143	0
9	MG	b	601	1/1	0.98	0.12	97,97,97,97	0

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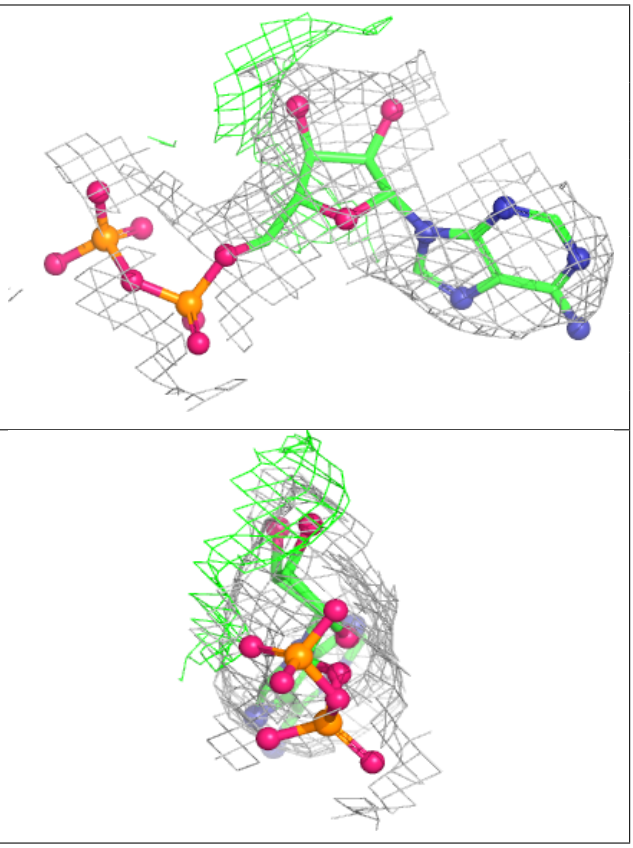
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	MG	i	601	1/1	0.98	0.06	111,111,111,111	0
9	MG	p	601	1/1	0.98	0.05	131,131,131,131	0
11	BEF	j	603	4/4	0.98	0.11	93,94,94,96	0
9	MG	F	601	1/1	0.98	0.03	94,94,94,94	0
9	MG	P	601	1/1	0.98	0.04	140,140,140,140	0
11	BEF	I	603	4/4	0.98	0.05	119,119,120,122	0
9	MG	J	601	1/1	0.99	0.06	101,101,101,101	0
9	MG	H	601	1/1	0.99	0.02	109,109,109,109	0
9	MG	B	601	1/1	0.99	0.04	70,70,70,70	0
9	MG	M	601	1/1	0.99	0.07	96,96,96,96	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.

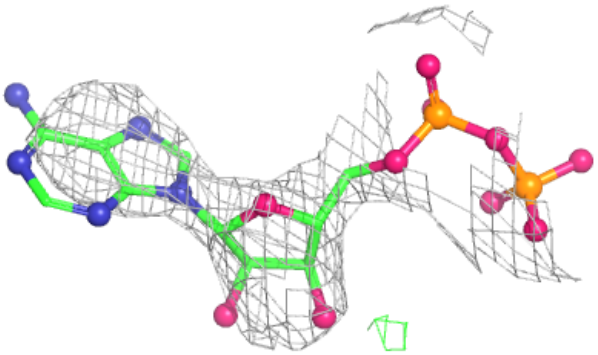
Electron density around ADP N 602:

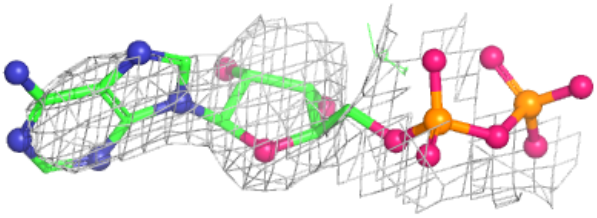
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

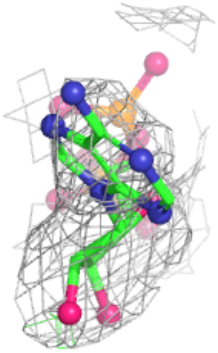


Electron density around ADP f 602:

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

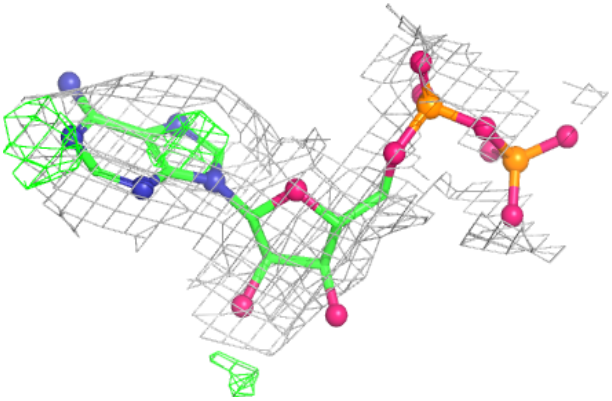


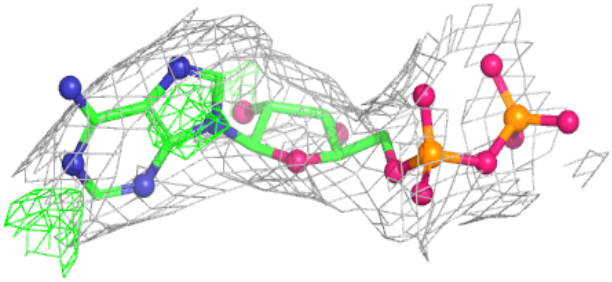


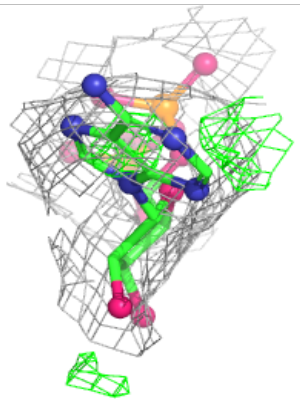


Electron density around ADP p 602:

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

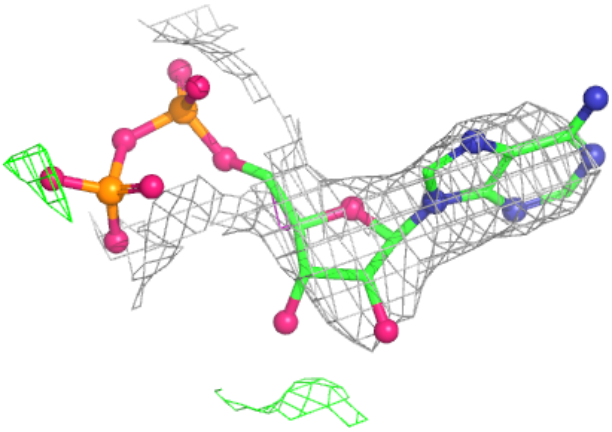


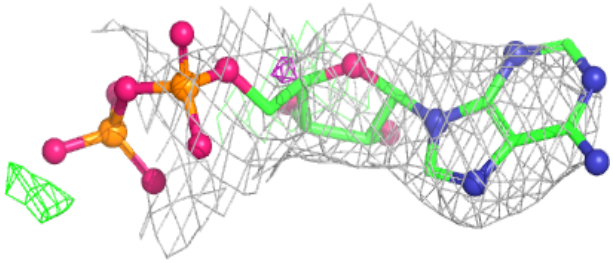


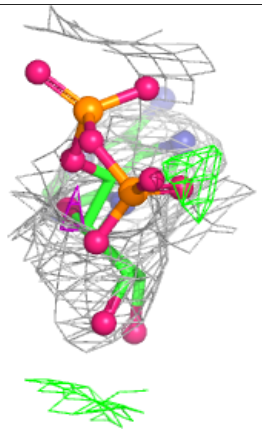


Electron density around ADP L 602:

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

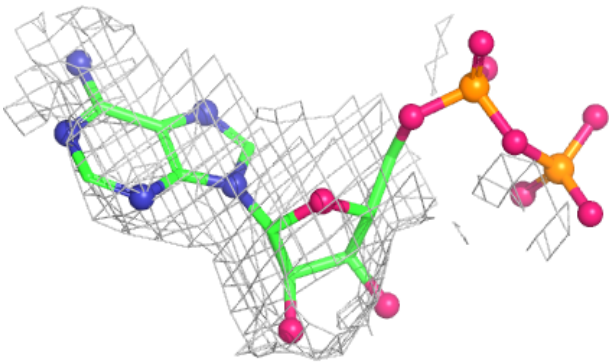


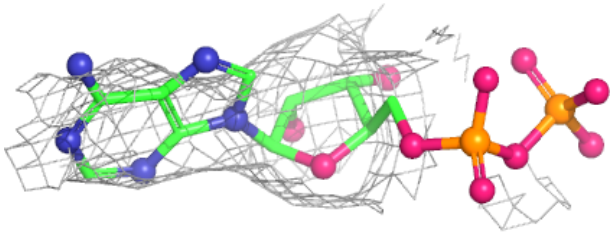


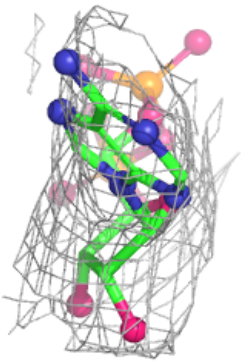


Electron density around ADP c 1102:

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

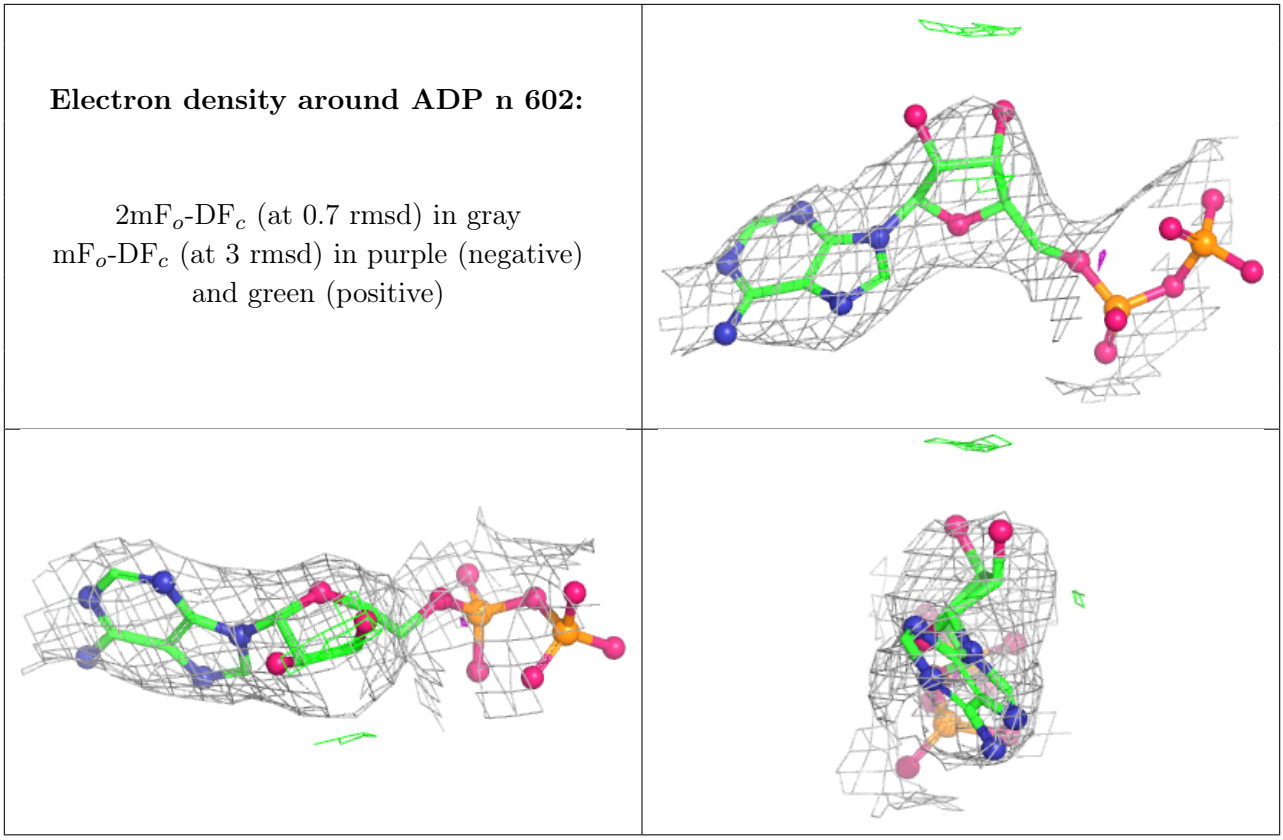






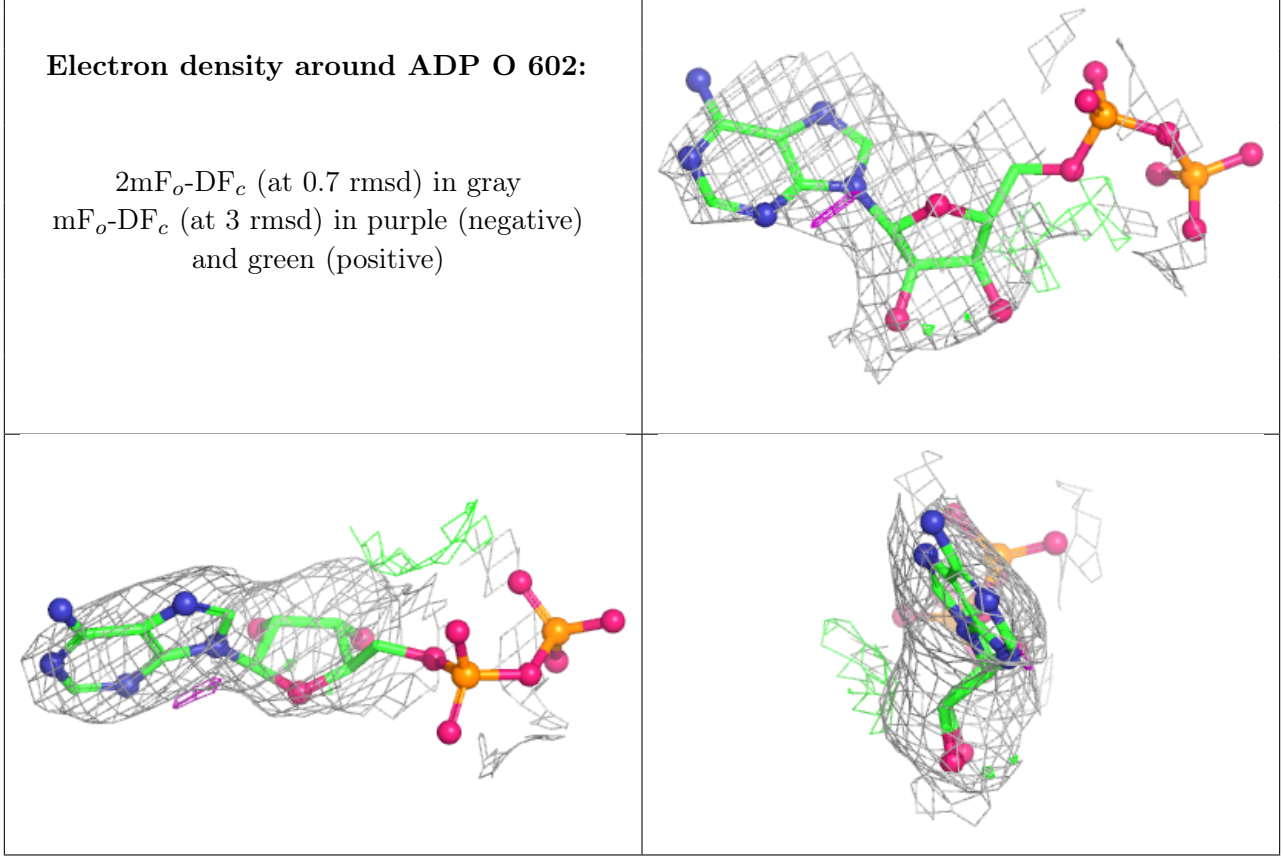
Electron density around ADP n 602:

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



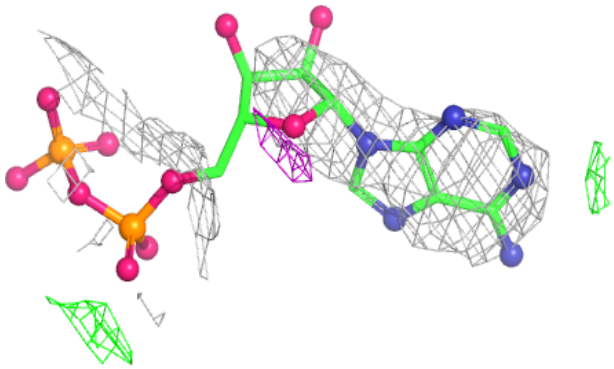
Electron density around ADP O 602:

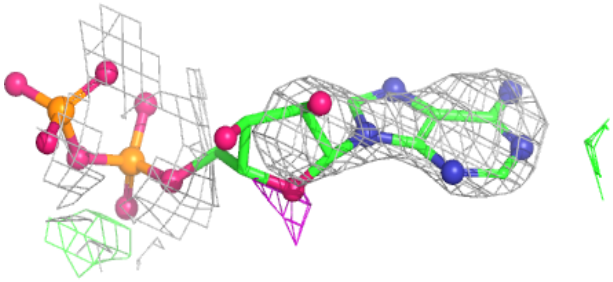
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

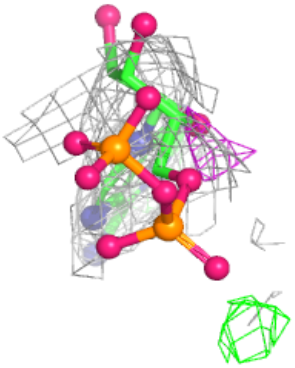


Electron density around ADP m 602:

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

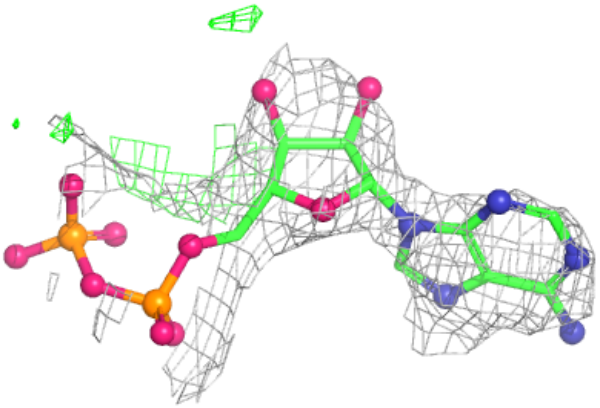


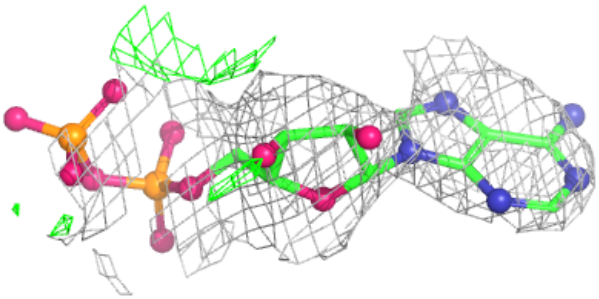


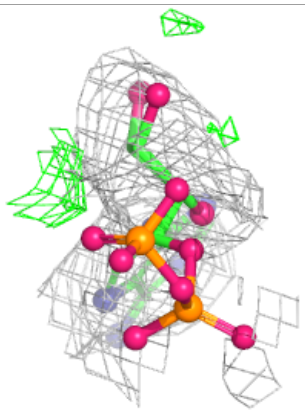


Electron density around ADP i 602:

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

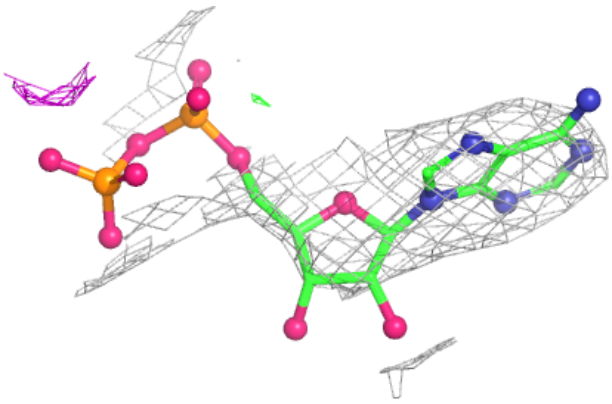


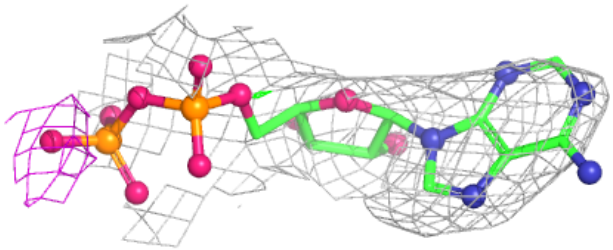


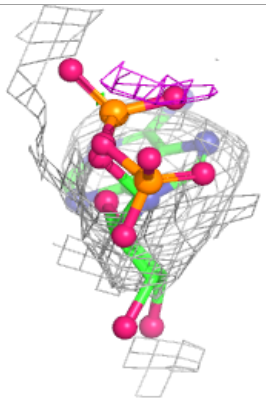


Electron density around ADP h 602:

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

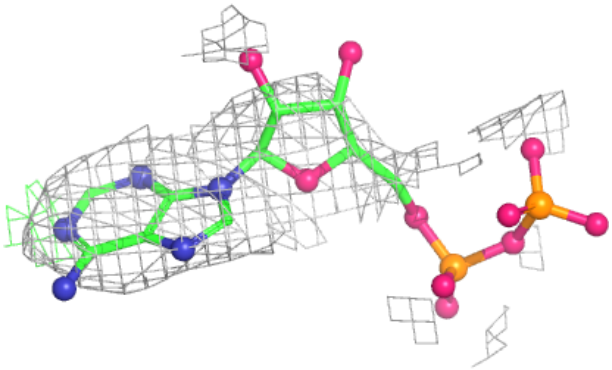


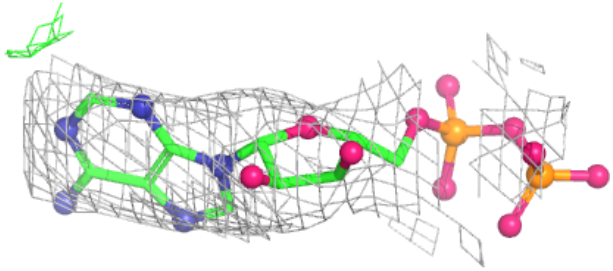


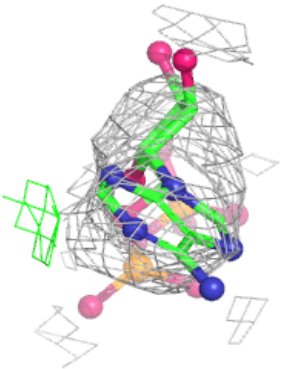


Electron density around ADP P 602:

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



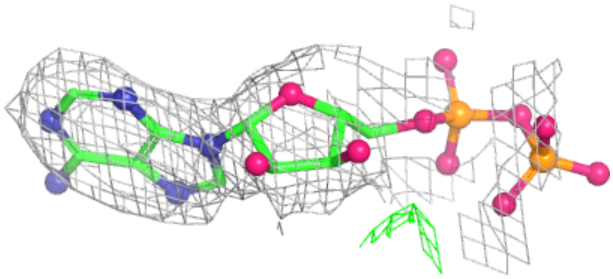


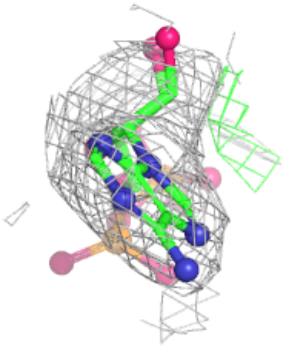


Electron density around ADP o 602:

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

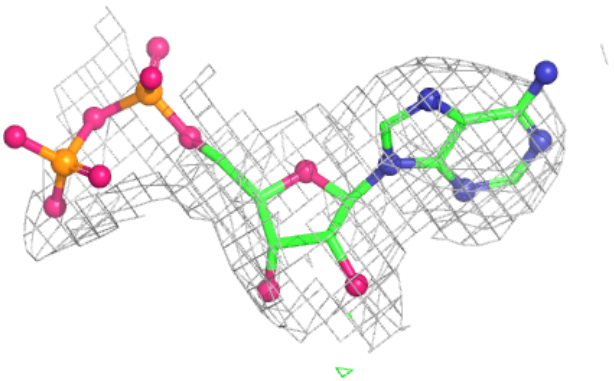


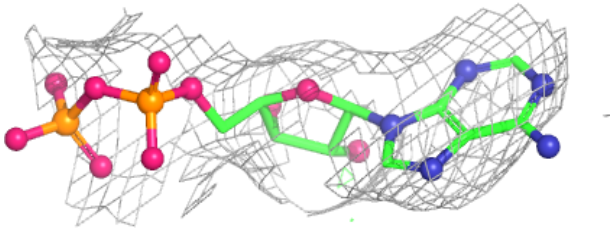


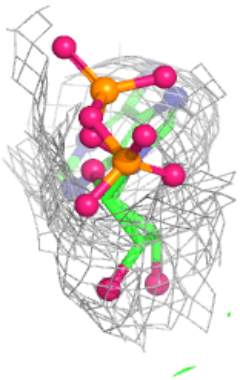


Electron density around ADP F 602:

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

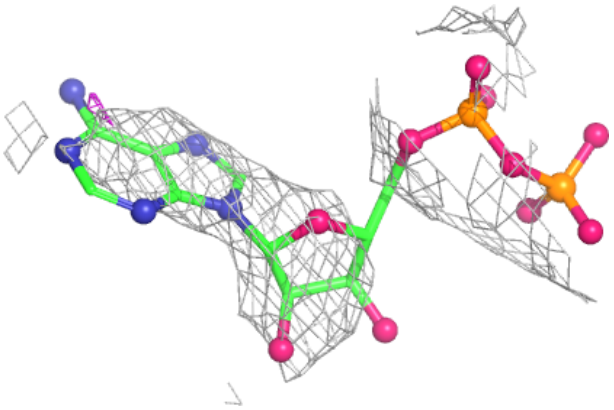


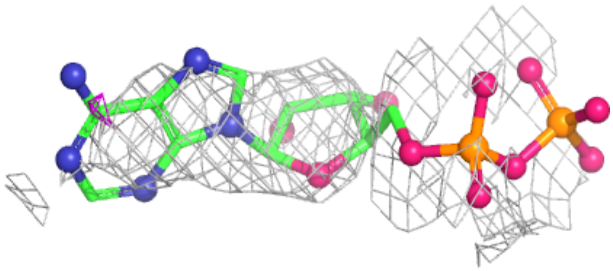


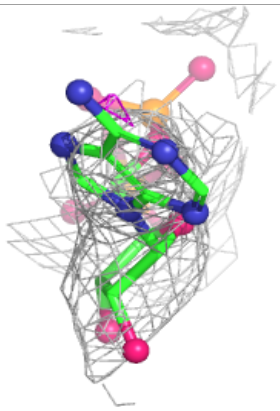


Electron density around ADP k 1102:

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

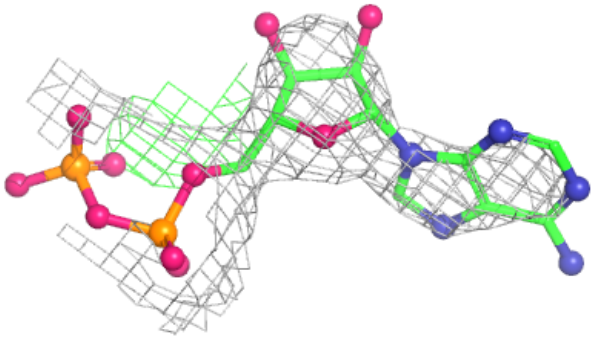


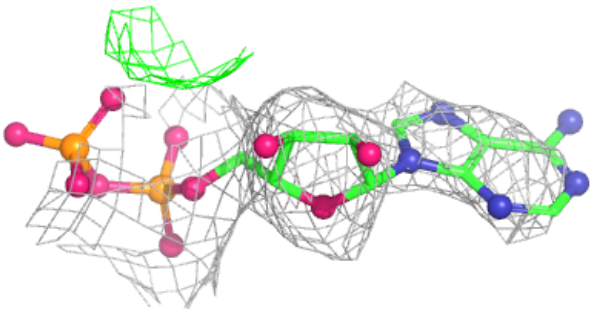


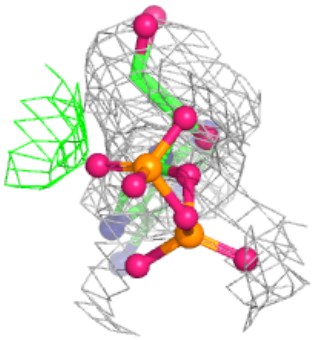


Electron density around ADP A 602:

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

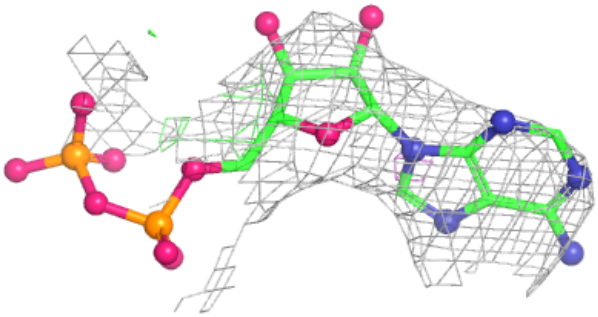


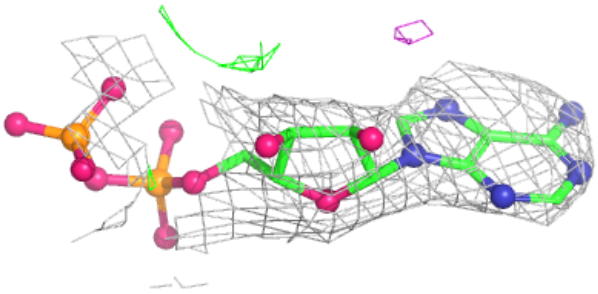


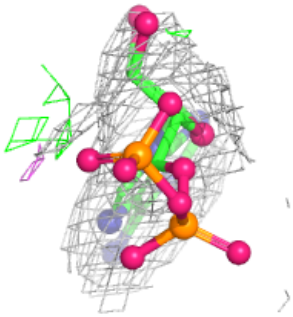


Electron density around ADP g 602:

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

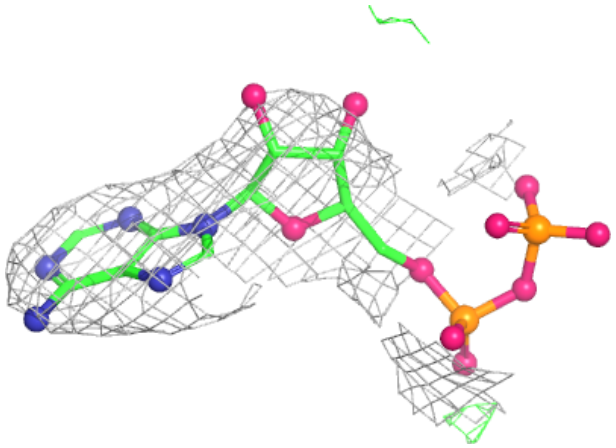


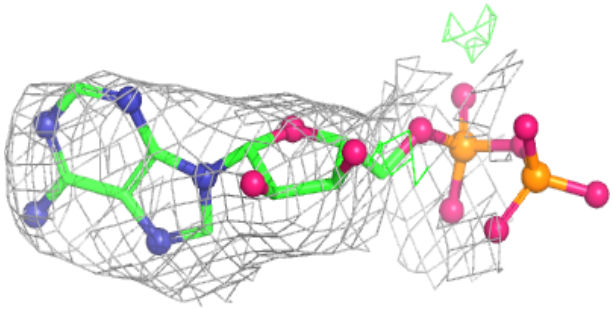


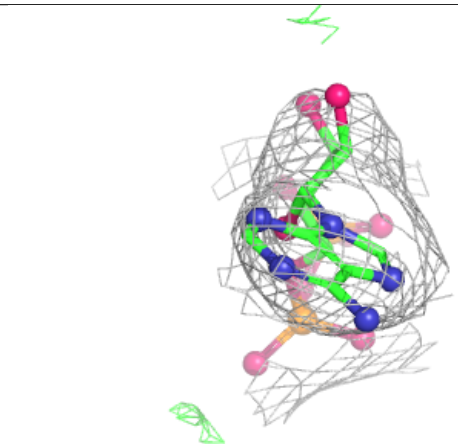


Electron density around ADP d 602:

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

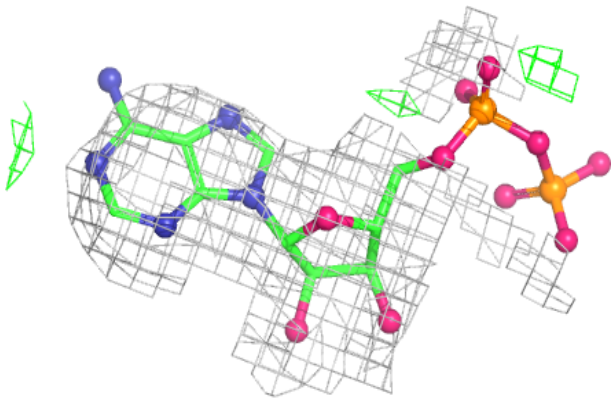


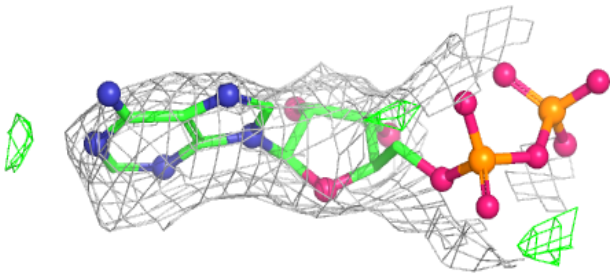


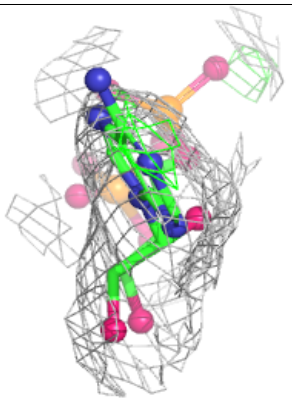


Electron density around ADP M 602:

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

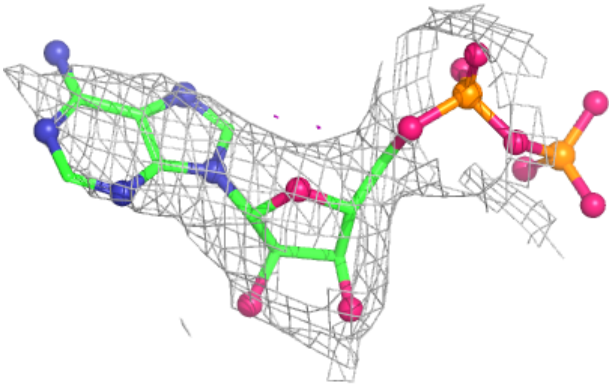


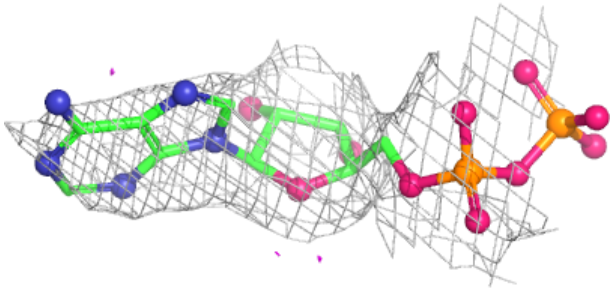


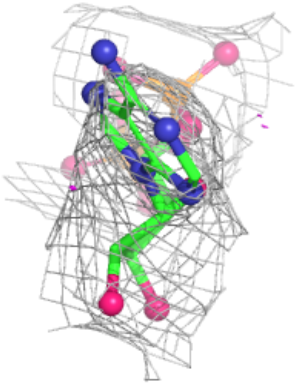


Electron density around ADP b 602:

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

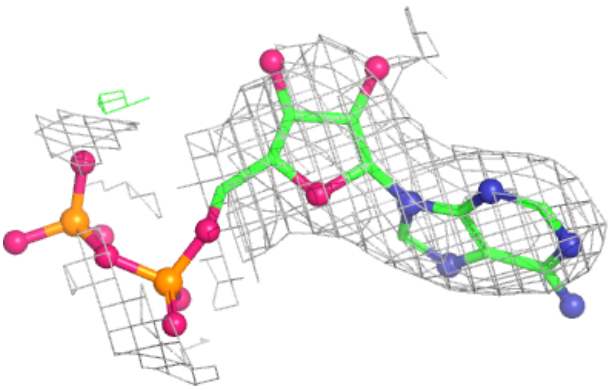


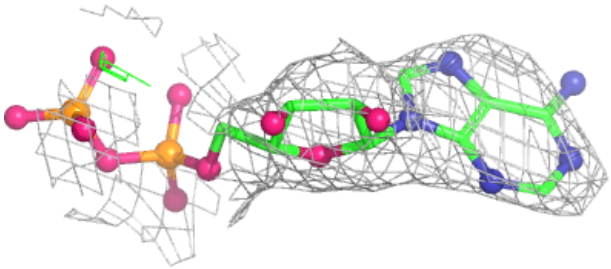


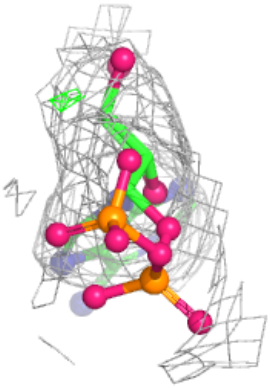


Electron density around ADP H 602:

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

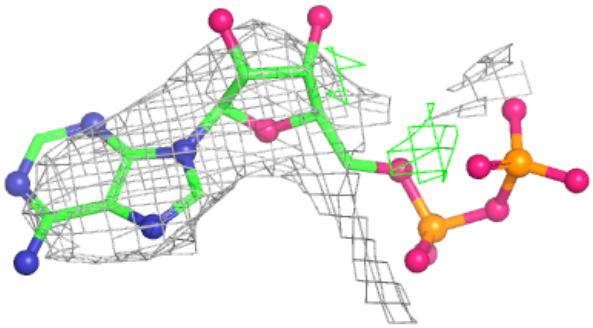


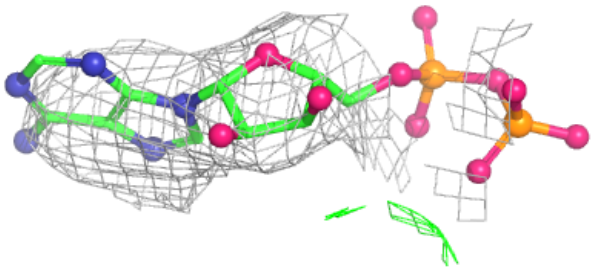


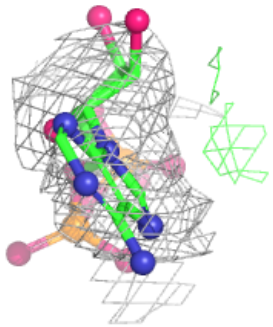


Electron density around ADP a 602:

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

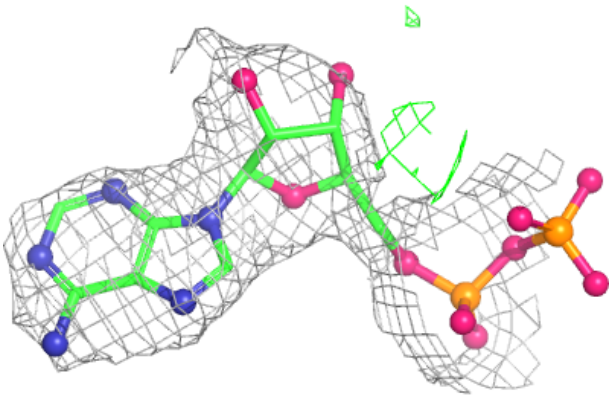


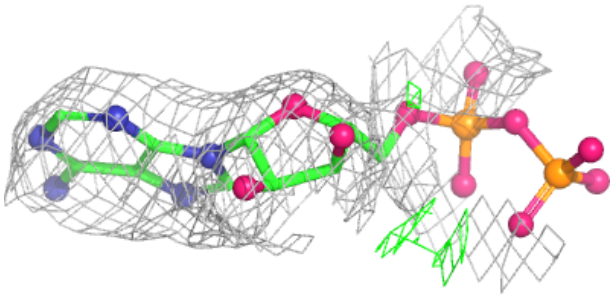


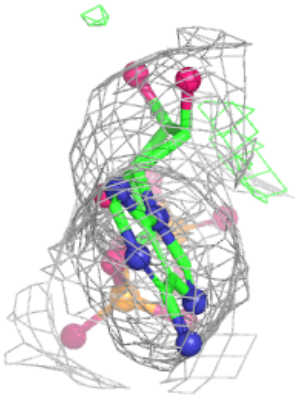


Electron density around ADP B 602:

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

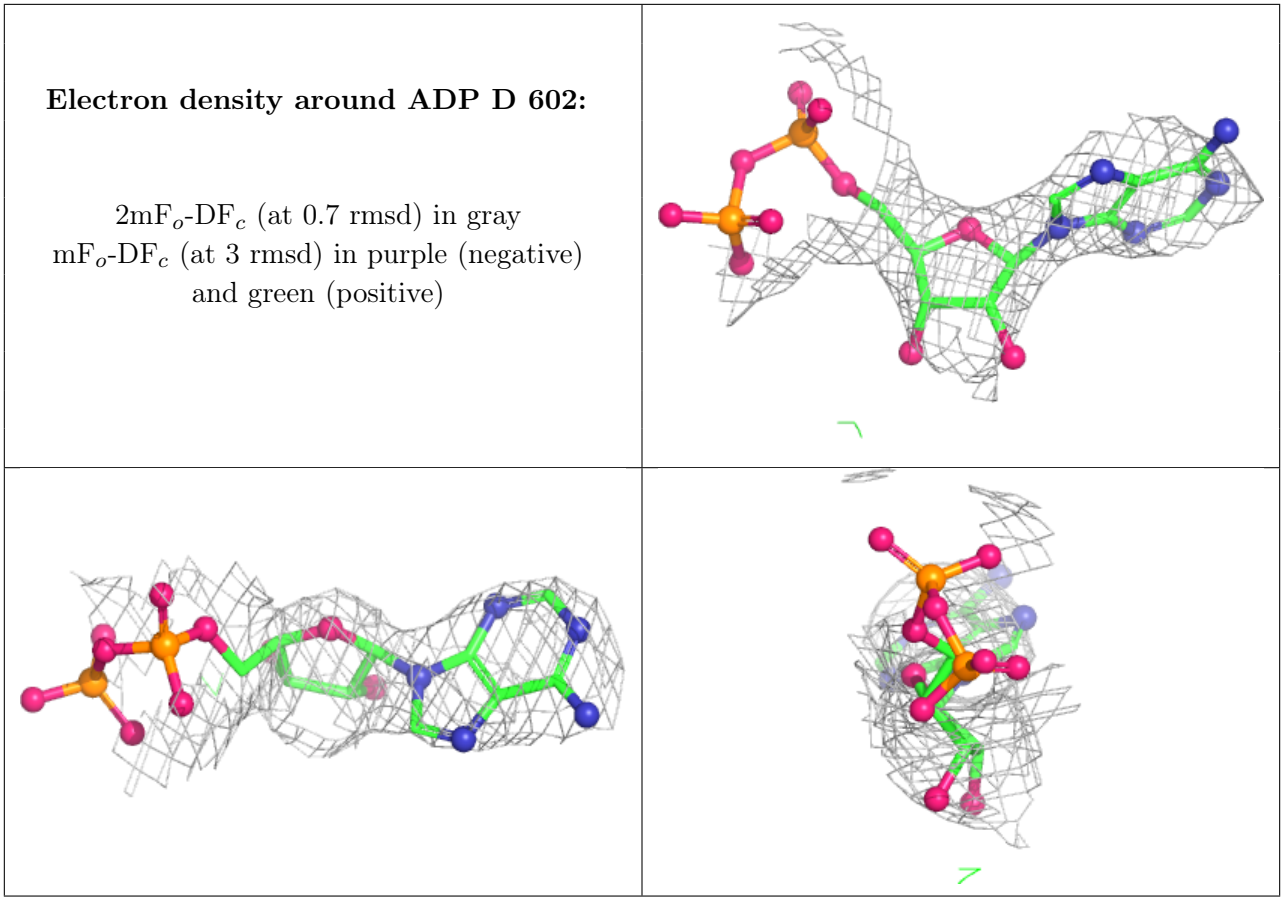






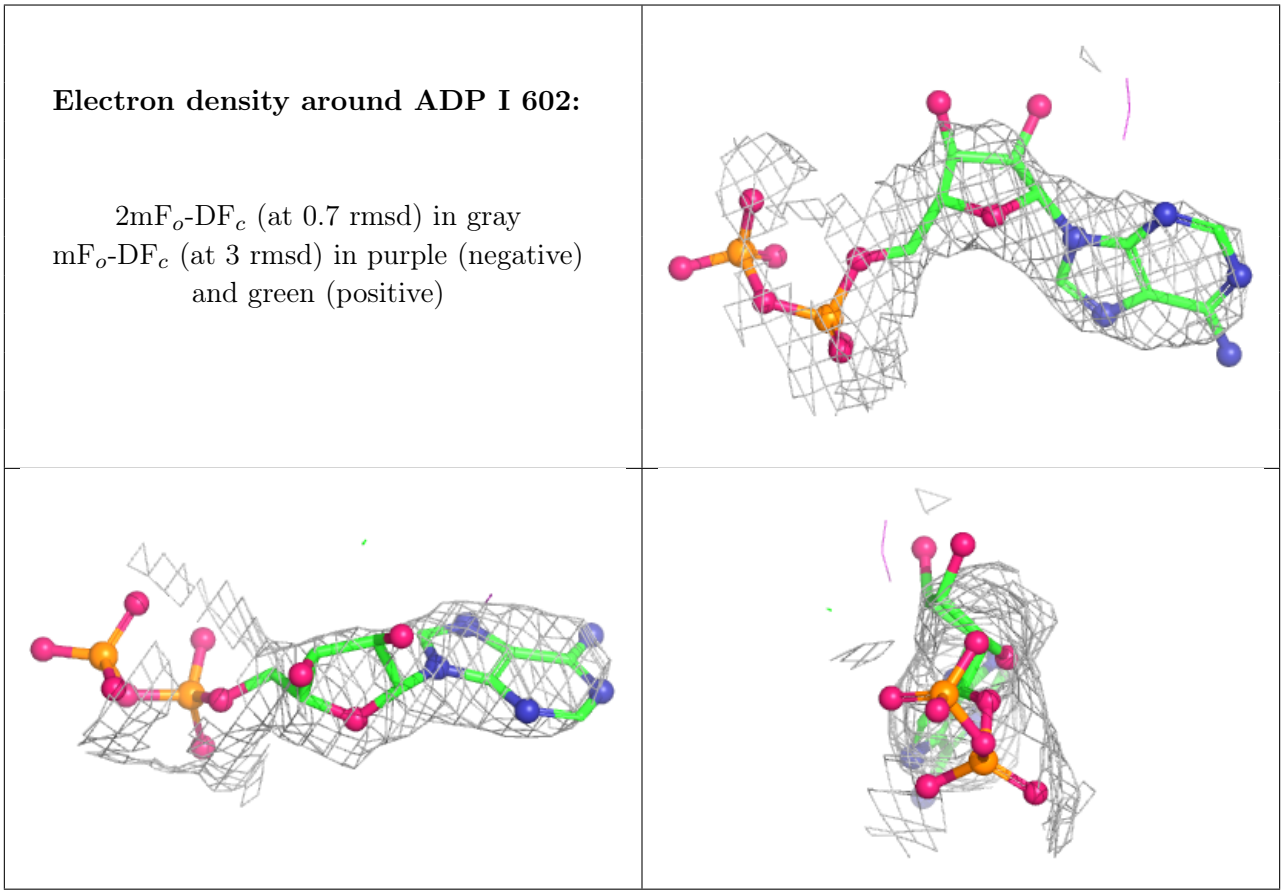
Electron density around ADP D 602:

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



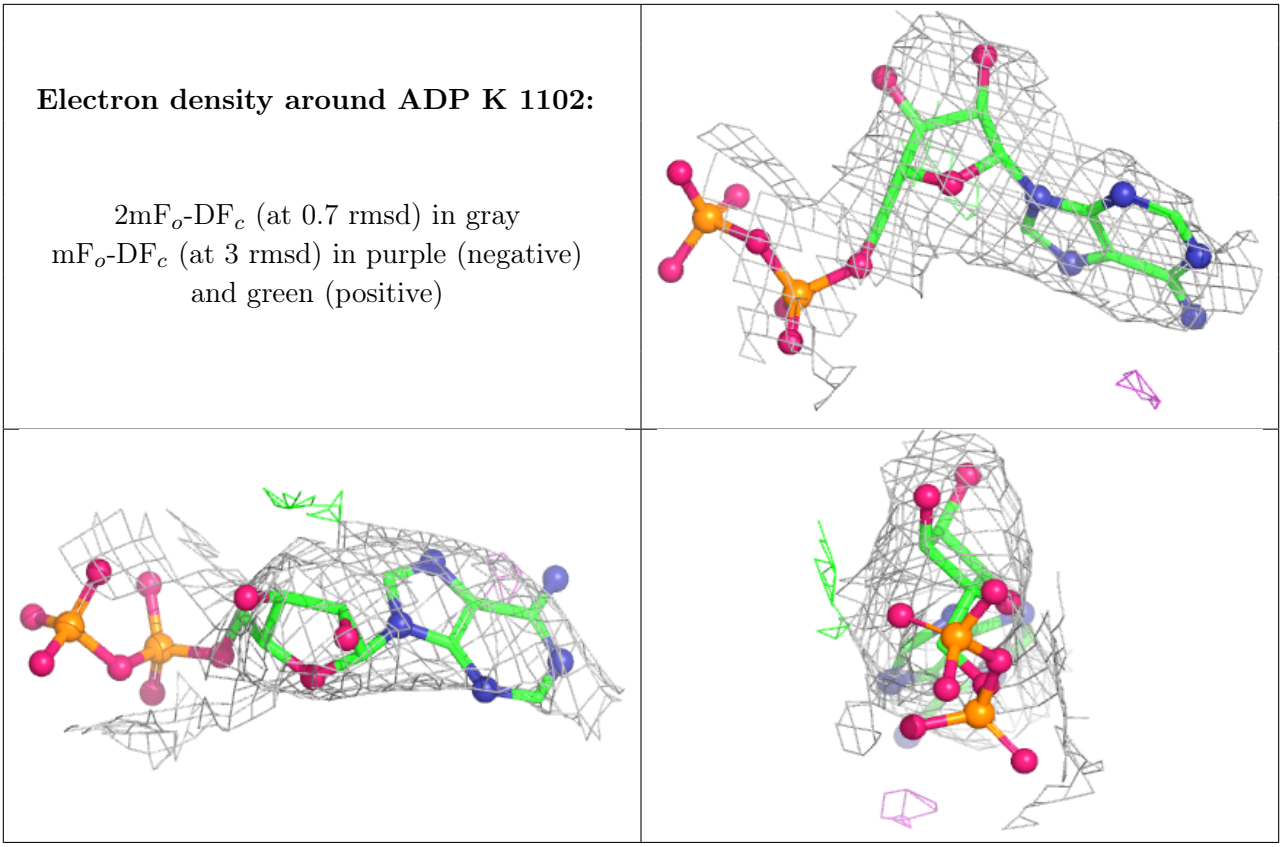
Electron density around ADP I 602:

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



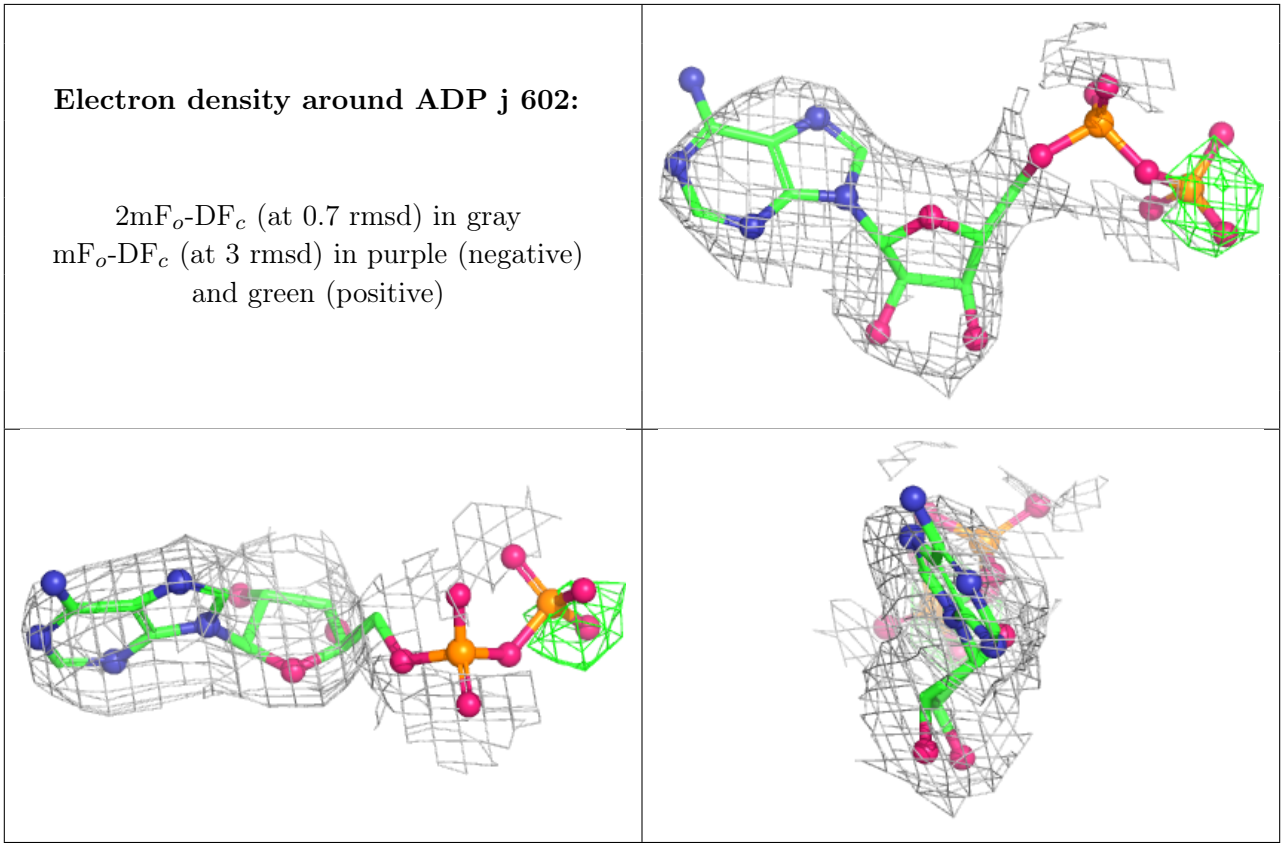
Electron density around ADP K 1102:

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



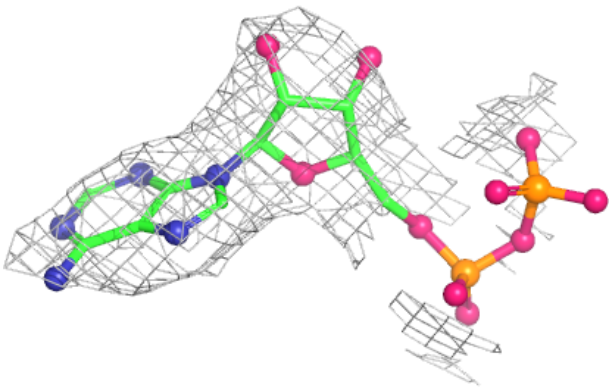
Electron density around ADP j 602:

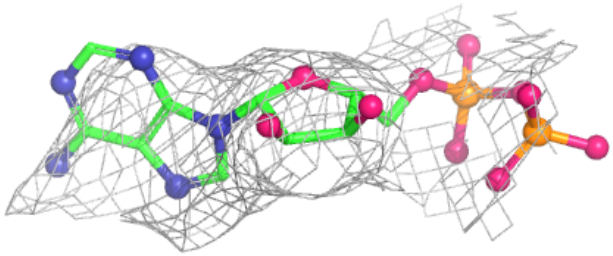
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

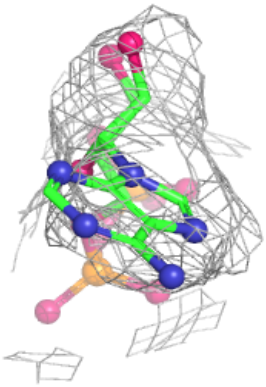


Electron density around ADP l 602:

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

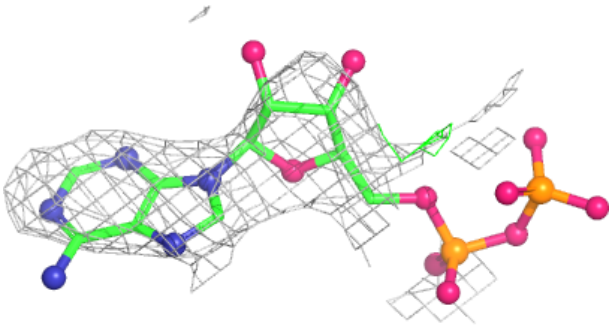


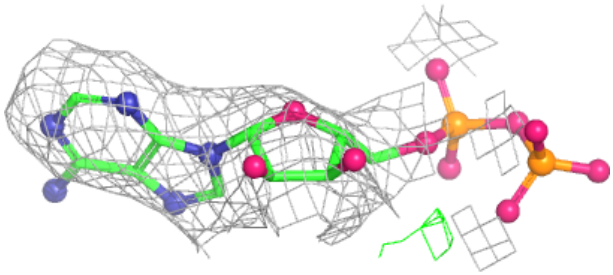


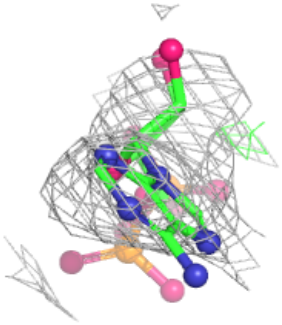


Electron density around ADP G 602:

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

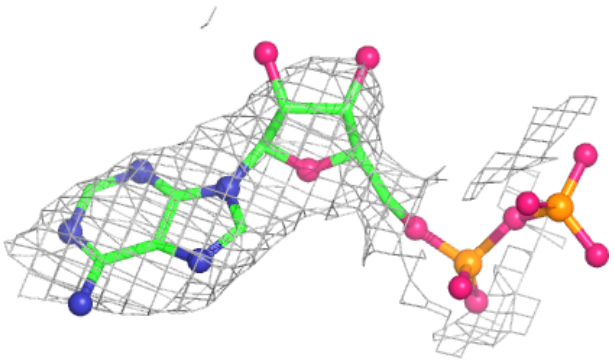


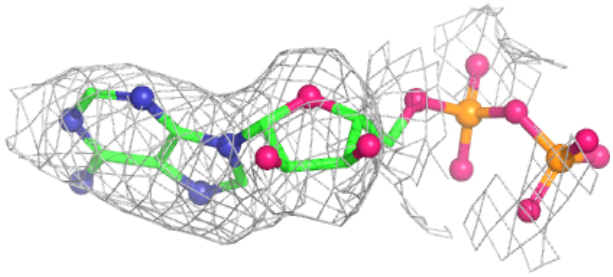


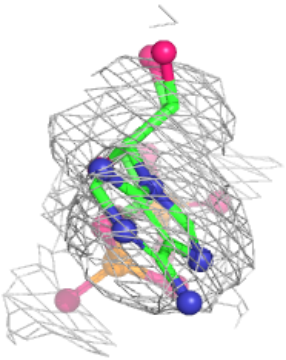


Electron density around ADP J 602:

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

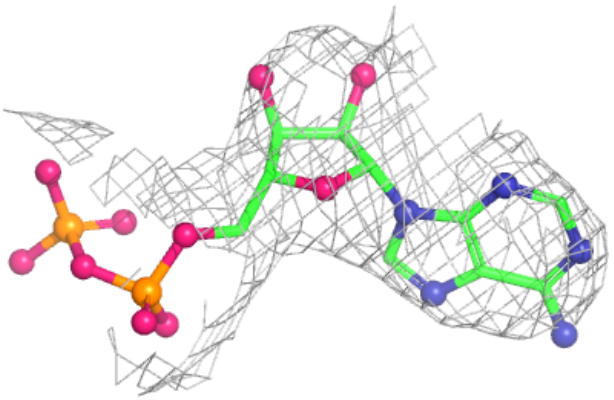


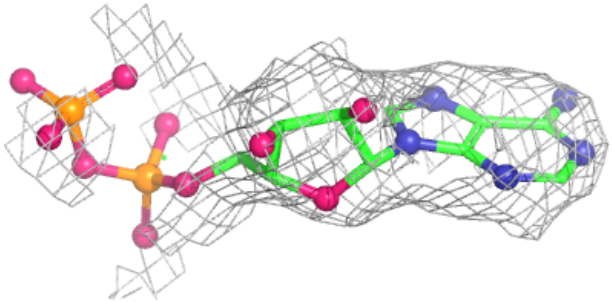


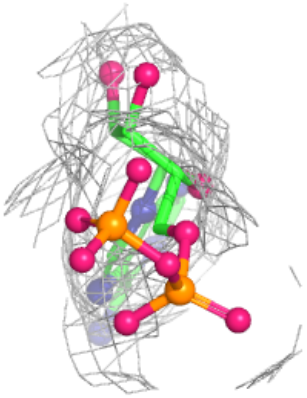


Electron density around ADP e 602:

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

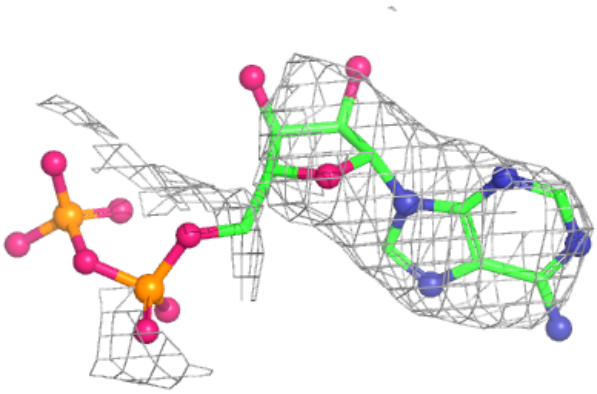


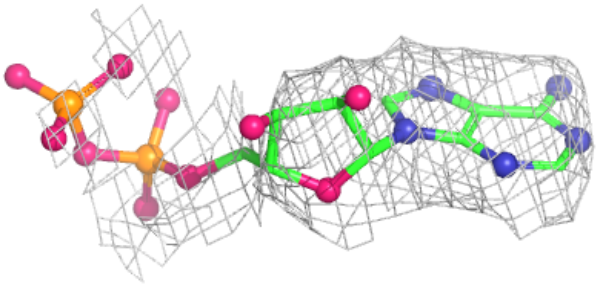


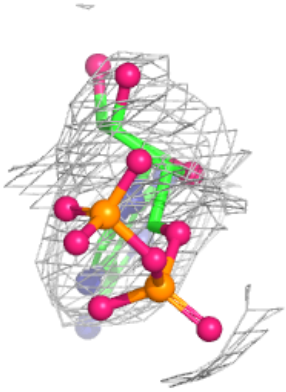


Electron density around ADP E 602:

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

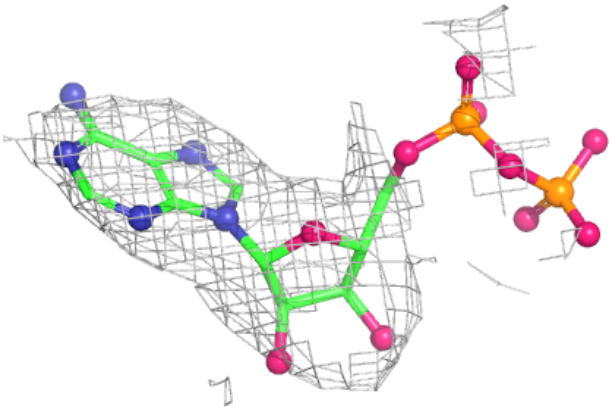


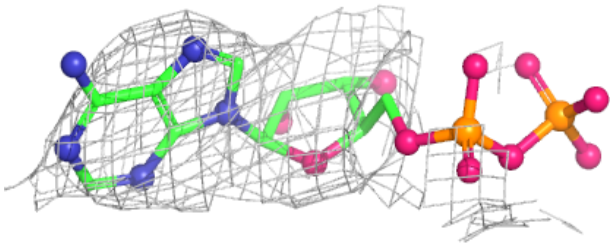


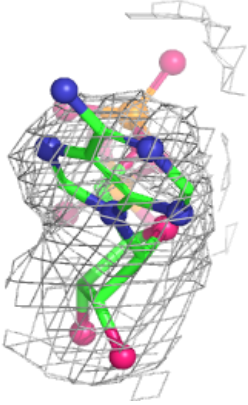


Electron density around ADP C 1102:

$2mF_o$-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 (i)

There are no such residues in this entry.