wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 02:07 am BST

PDB ID	:	4R7Z
Title	:	PfMCM-AAA double-octamer
Authors	:	Miller, J.M.; Arachea, B.T.; Epling, L.B.; Enemark, E.J.
Deposited on	:	2014-08-28
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 following versions of software and data (see references (1)) were used in the production of this report:

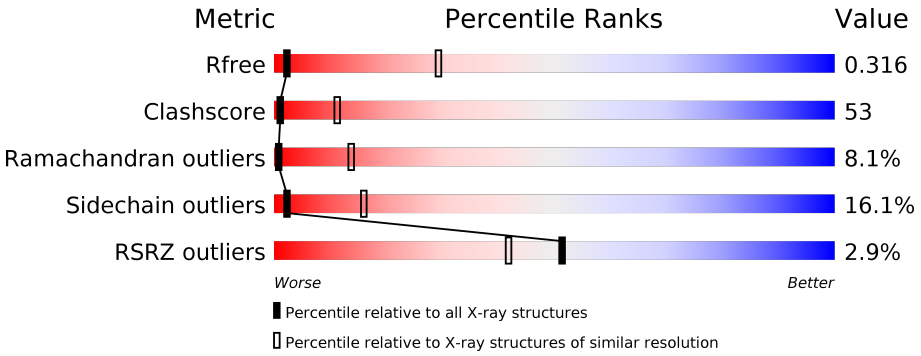
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	A	338	3% 32% 47% 14% • 7%
1	B	338	2% 33% 46% 14% • 7%
1	C	338	3% 32% 47% 14% • 7%
1	D	338	% 32% 47% 14% • 7%
1	E	338	2% 31% 47% 14% • 7%
1	F	338	2% 32% 47% 14% • 7%

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Mol	Chain	Length	Quality of chain
1	G	338	4% 31% 48% 14% 7%
1	H	338	% 32% 47% 14% 7%
1	I	338	% 32% 47% 14% 7%
1	J	338	2% 31% 48% 14% 7%
1	K	338	2% 31% 48% 14% 7%
1	L	338	4% 31% 48% 14% 7%
1	M	338	% 32% 47% 14% 7%
1	N	338	4% 33% 46% 14% 7%
1	O	338	5% 32% 47% 14% 7%
1	P	338	% 32% 47% 14% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 39296 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 Cell division control protein 21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	B	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	C	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	D	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	E	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	F	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	G	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	H	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	I	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	J	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	K	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	L	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	M	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	N	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	O	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			
1	P	316	Total	C	N	O	S	0	0	0
			2428	1533	440	448	7			

There are 528 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
A	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	361	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
B	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	737	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
C	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	746	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
D	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
E	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	355	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
F	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	731	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
G	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	740	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
H	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	749	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
I	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
I	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
J	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	358	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
K	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	734	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
L	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
L	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	743	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
M	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
M	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
N	752	UNK	-	SEE REMARK 999	UNP Q8U3I4

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Chain	Residue	Modelled	Actual	Comment	Reference
O	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	361	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
O	752	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	353	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	354	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	355	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	356	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	357	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	358	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	359	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	360	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	361	UNK	-	SEE REMARK 999	UNP Q8U3I4

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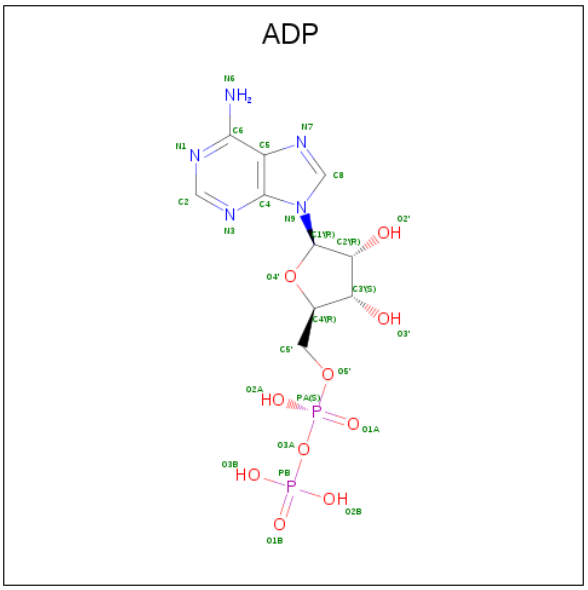
Chain	Residue	Modelled	Actual	Comment	Reference
P	729	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	730	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	731	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	732	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	733	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	734	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	735	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	736	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	737	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	738	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	739	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	740	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	741	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	742	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	743	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	744	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	745	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	746	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	747	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	748	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	749	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	750	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	751	UNK	-	SEE REMARK 999	UNP Q8U3I4
P	752	UNK	-	SEE REMARK 999	UNP Q8U3I4

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

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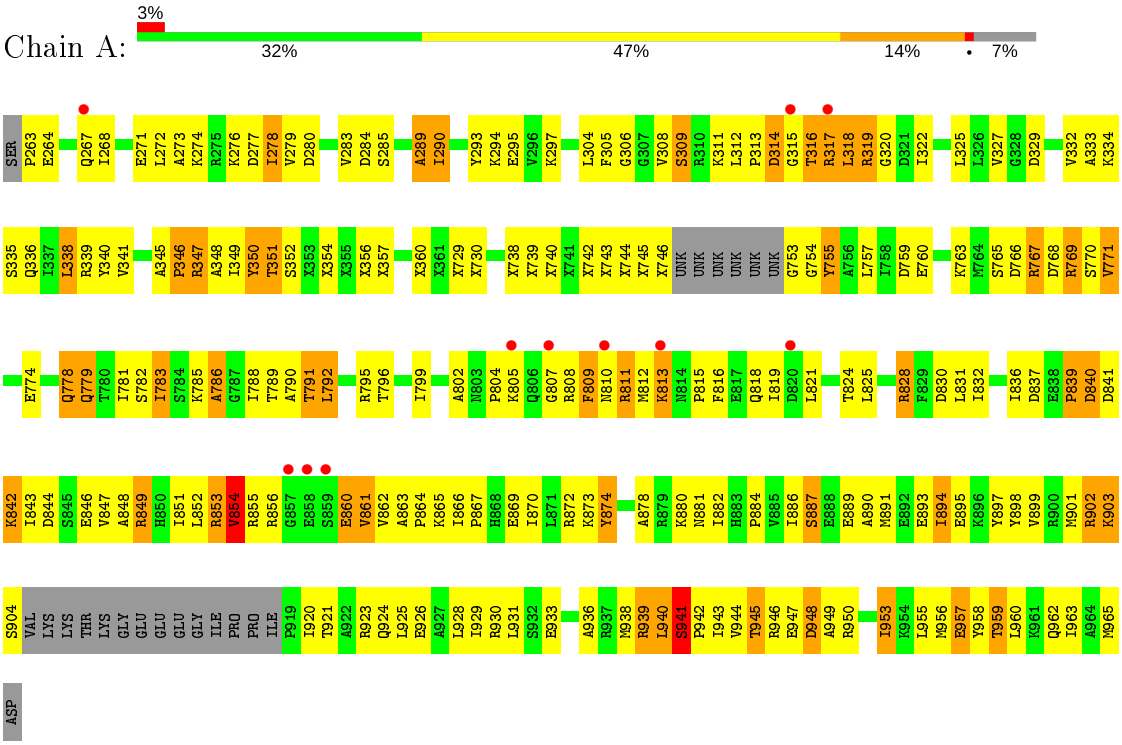
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	N	1	Total Mg 1 1	0	0
3	O	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	M	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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

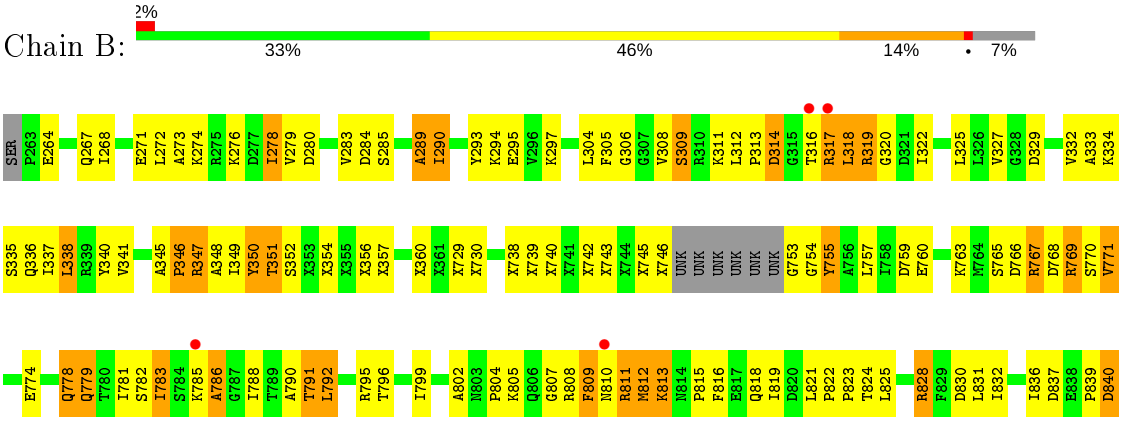
- Molecule 1: Cell division control protein 21

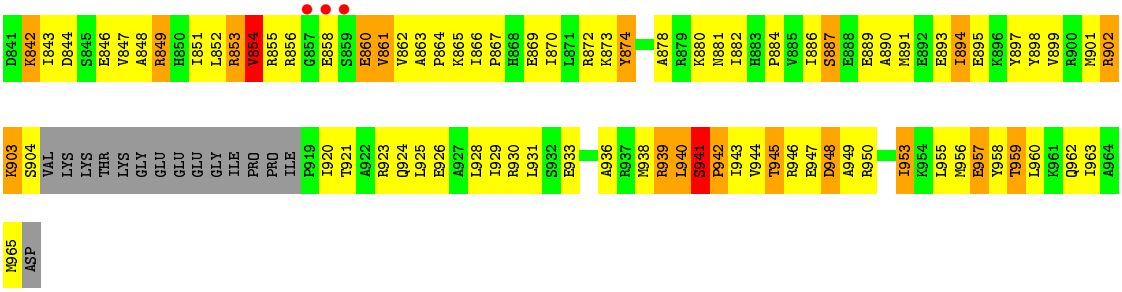
Chain A:



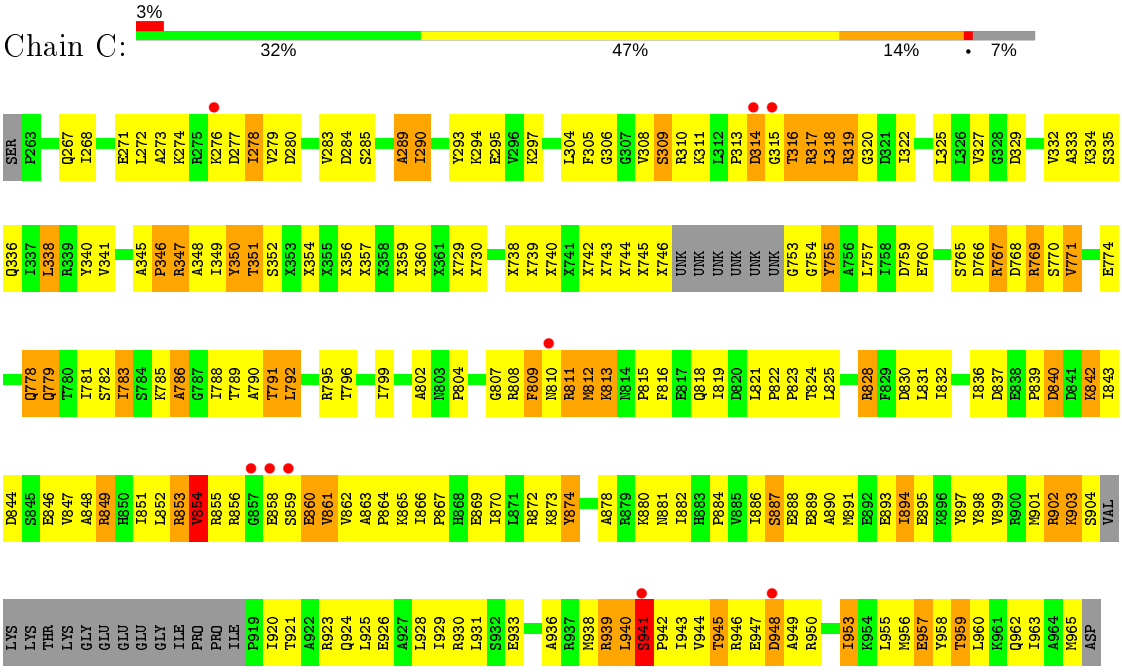
- Molecule 1: Cell division control protein 21

Chain B:

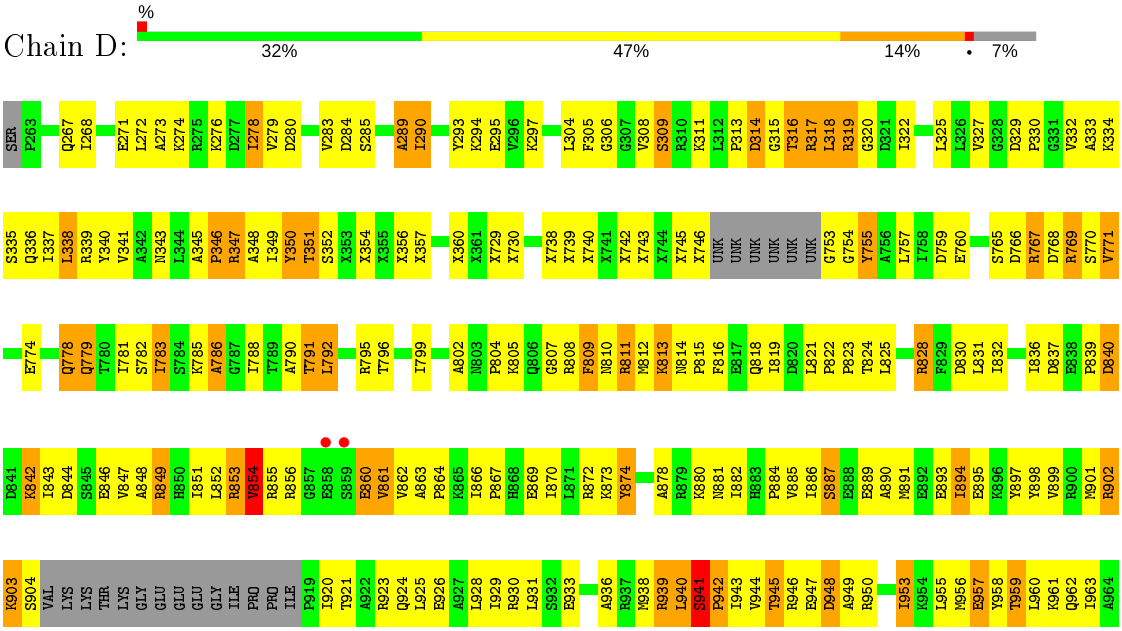




• Molecule 1: Cell division control protein 21

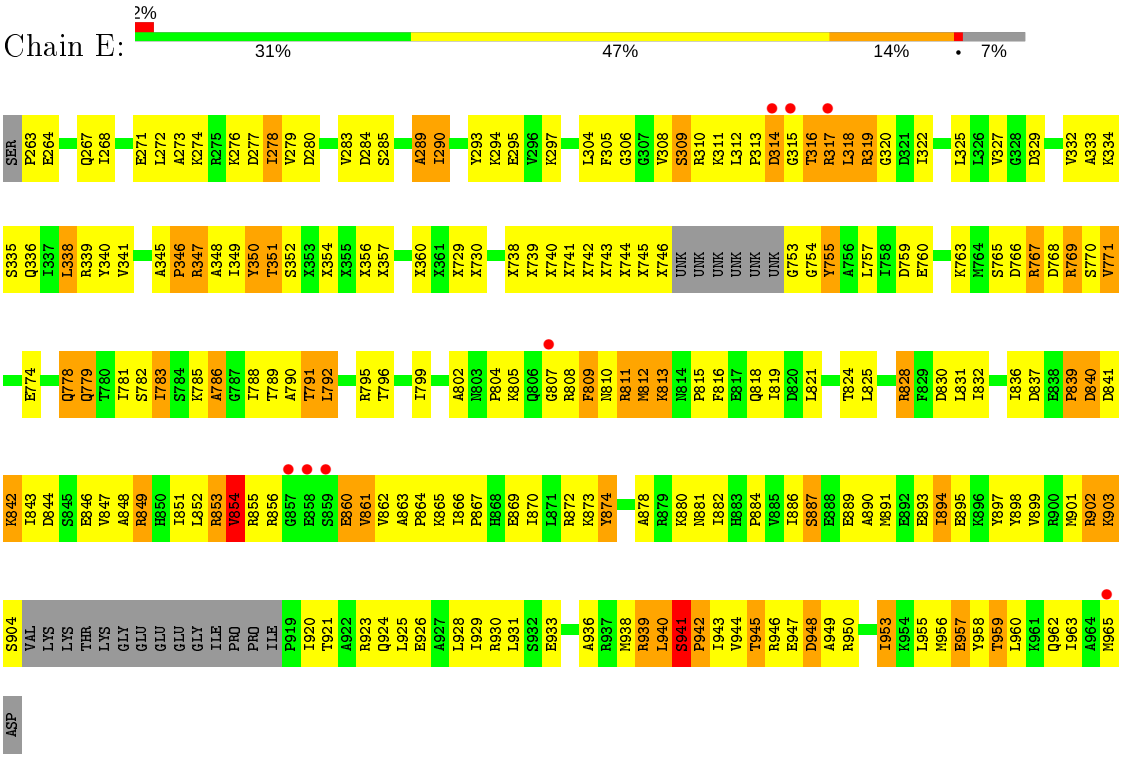


• Molecule 1: Cell division control protein 21



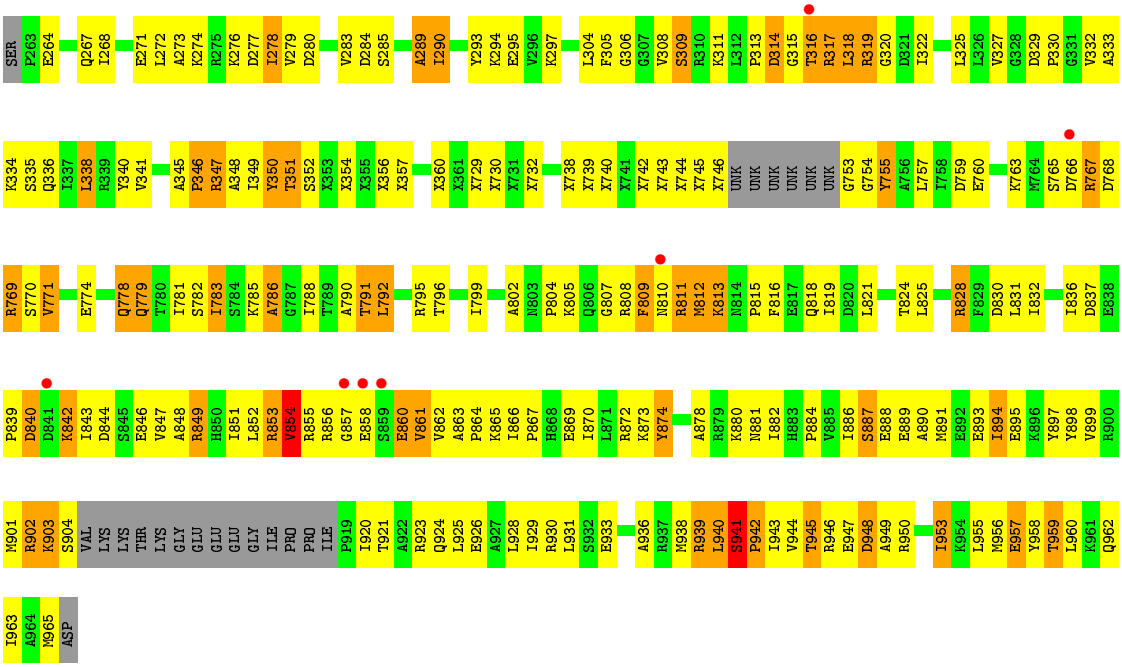
- Molecule 1: Cell division control protein 21

Chain E:



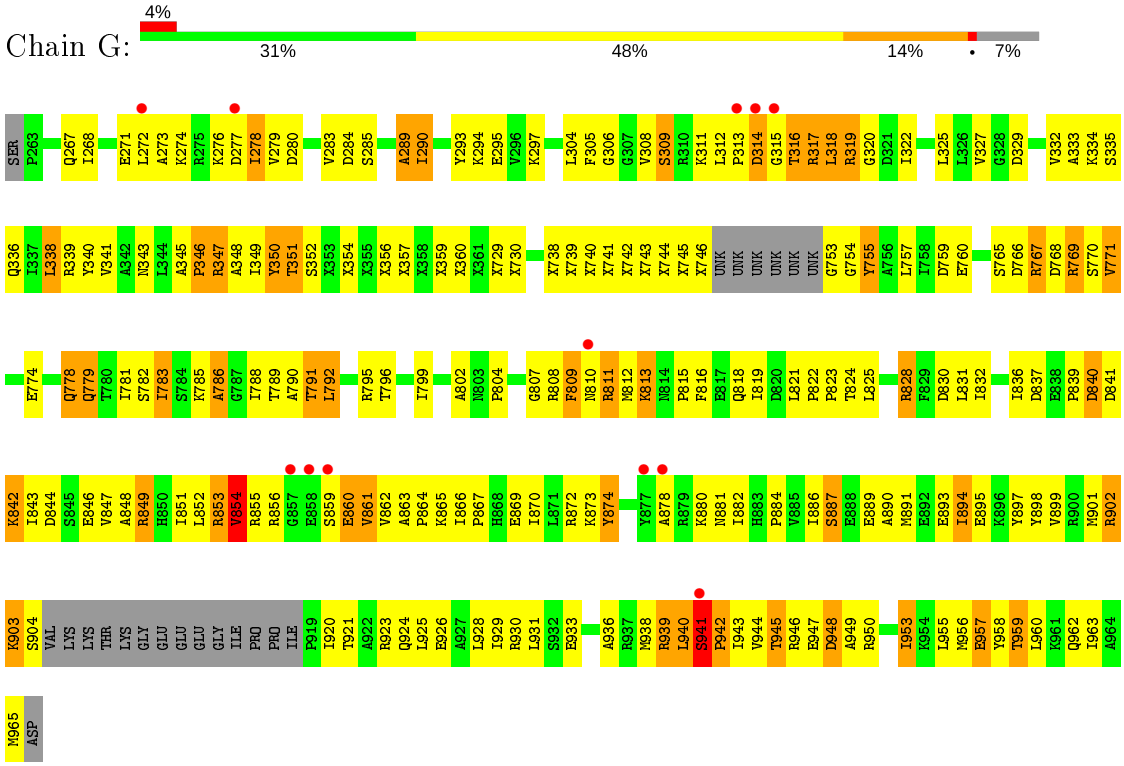
- Molecule 1: Cell division control protein 21

Chain F:



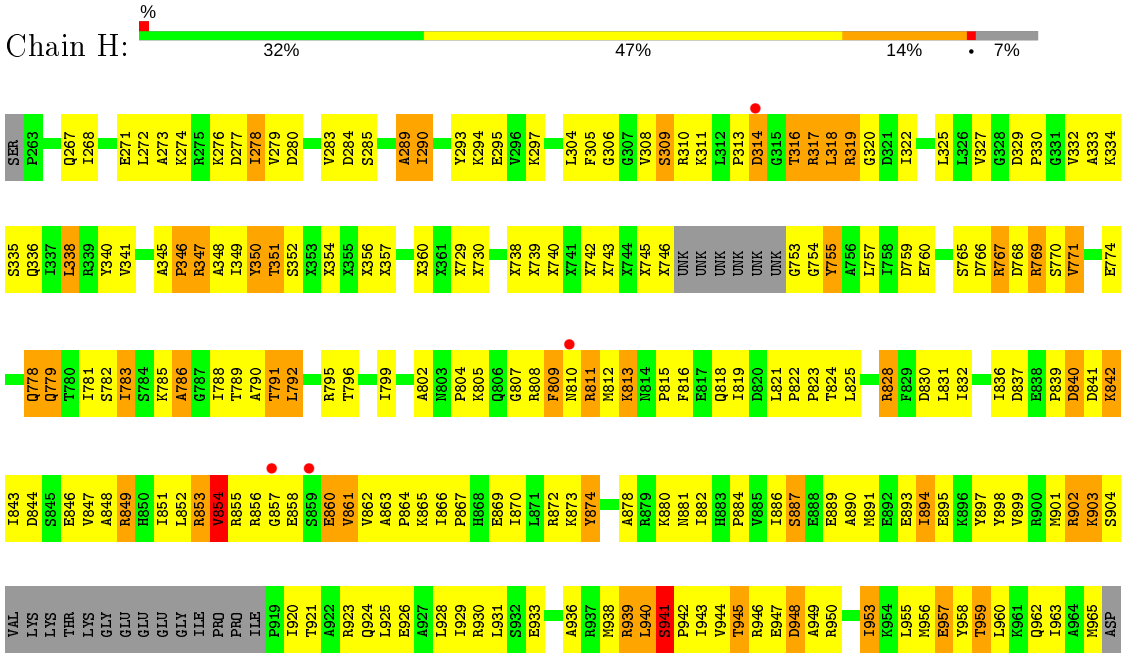
• Molecule 1: Cell division control protein 21

Chain G:



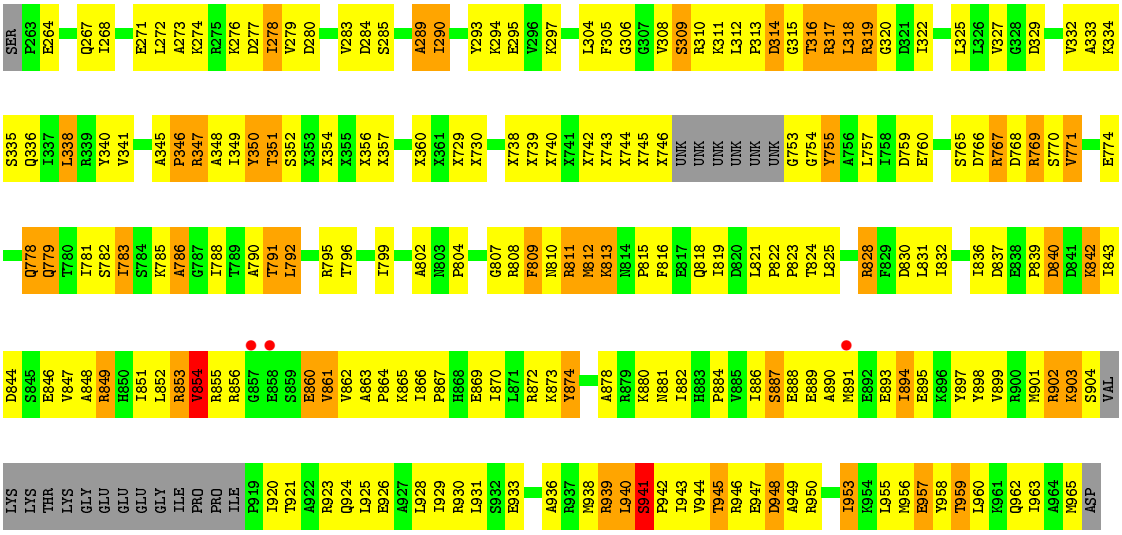
• Molecule 1: Cell division control protein 21

Chain H:



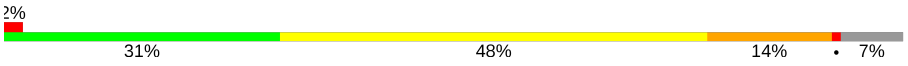
• Molecule 1: Cell division control protein 21

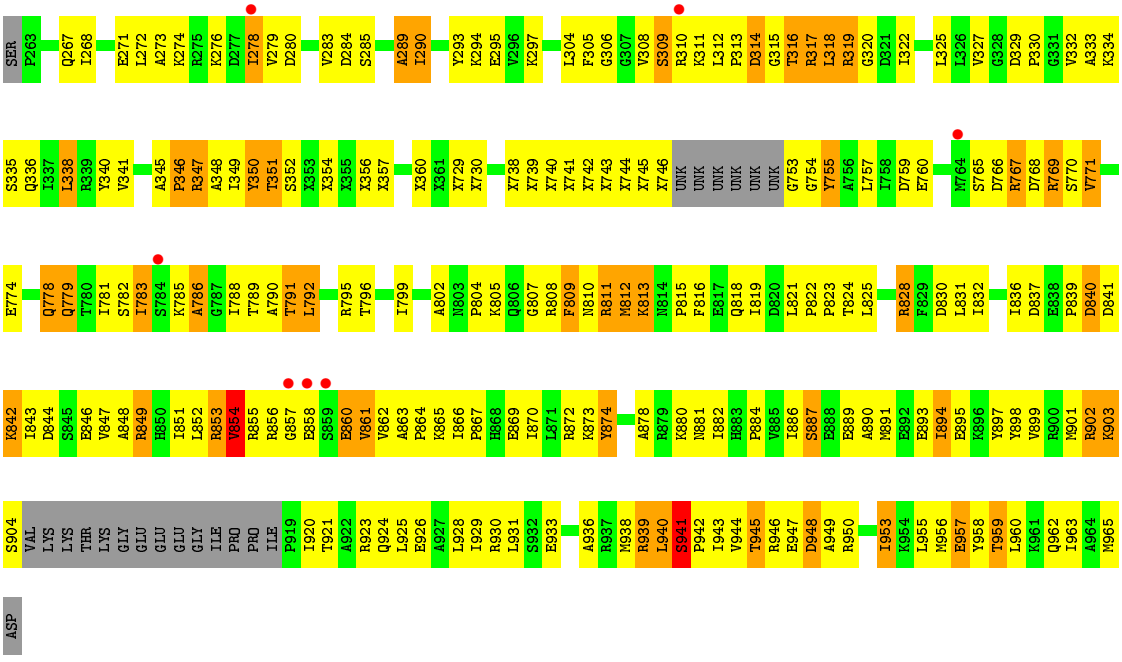
Chain I:



• Molecule 1: Cell division control protein 21

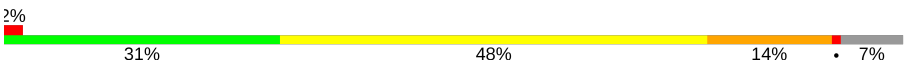
Chain J:

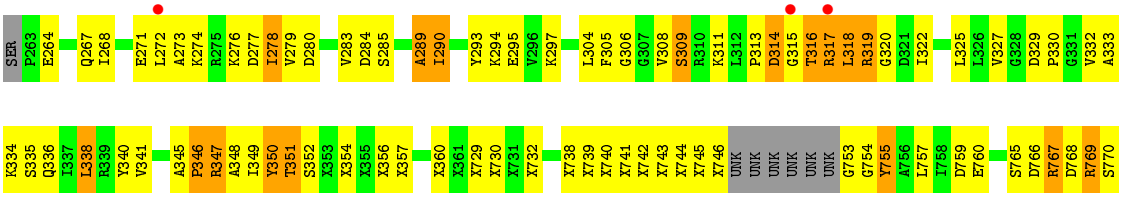


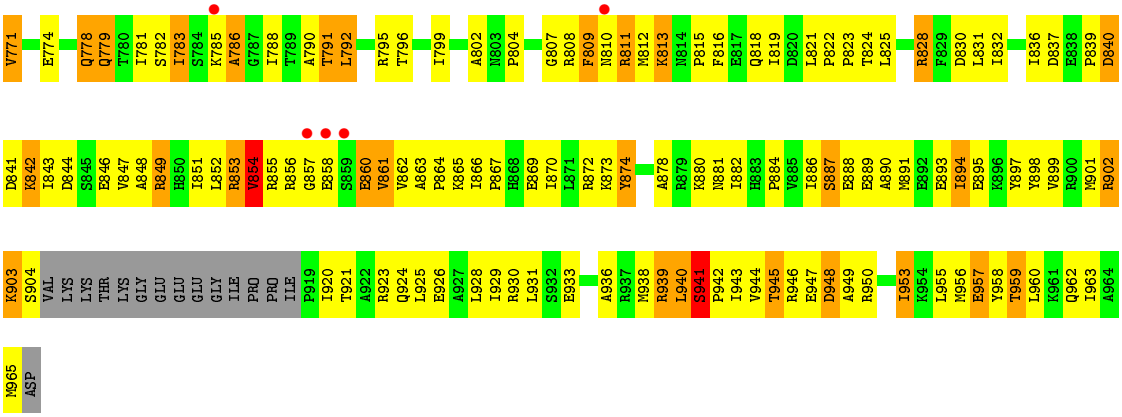


• Molecule 1: Cell division control protein 21

Chain K:

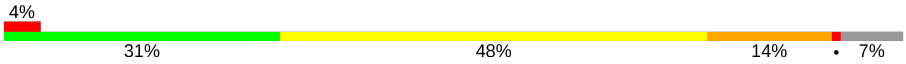


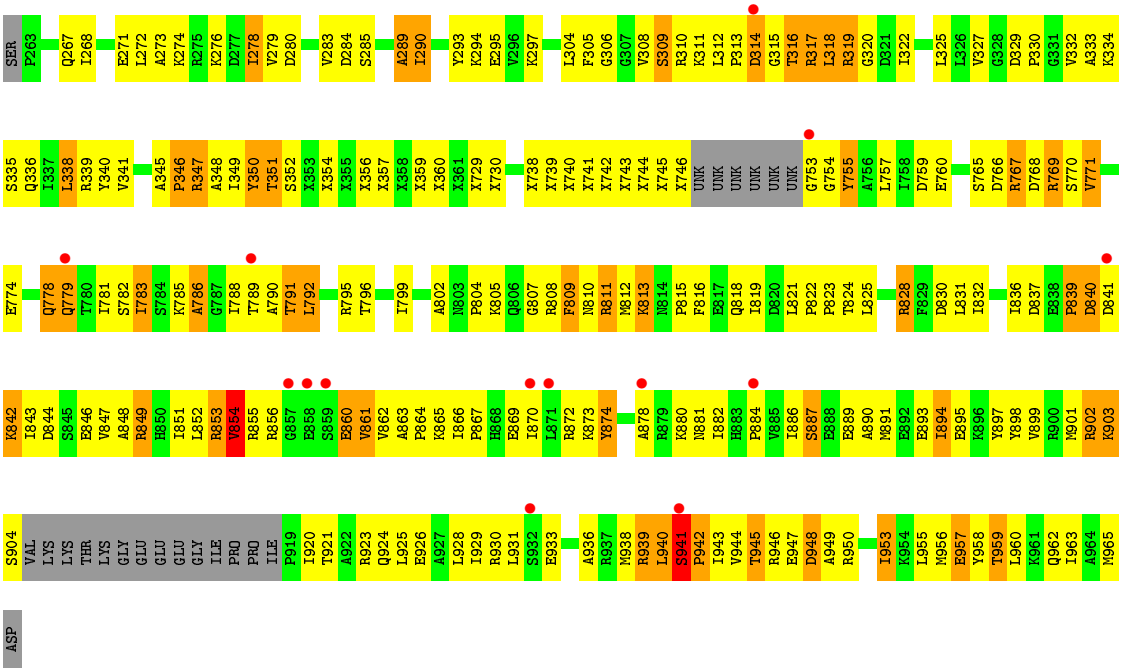




• Molecule 1: Cell division control protein 21

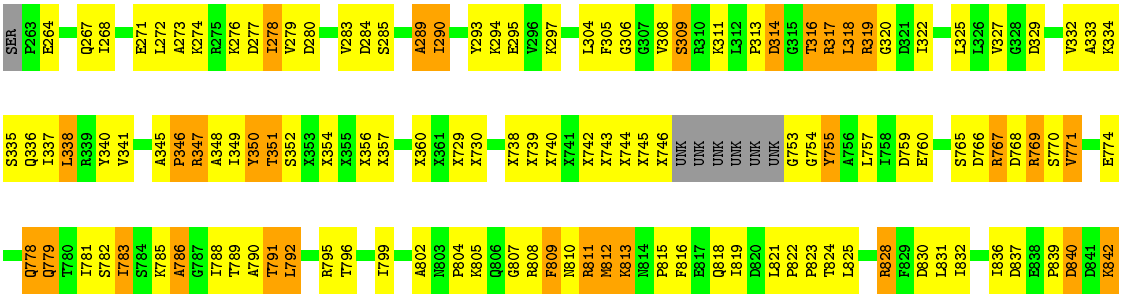
Chain L:

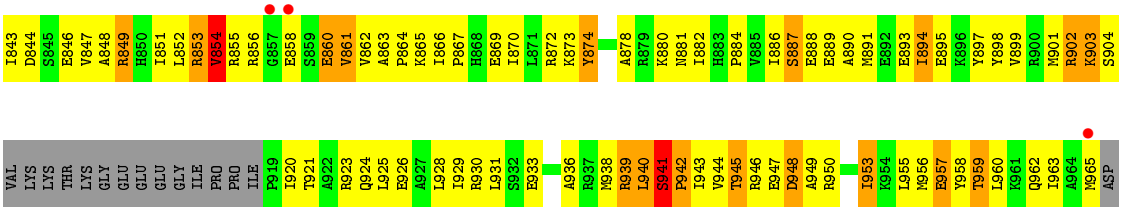




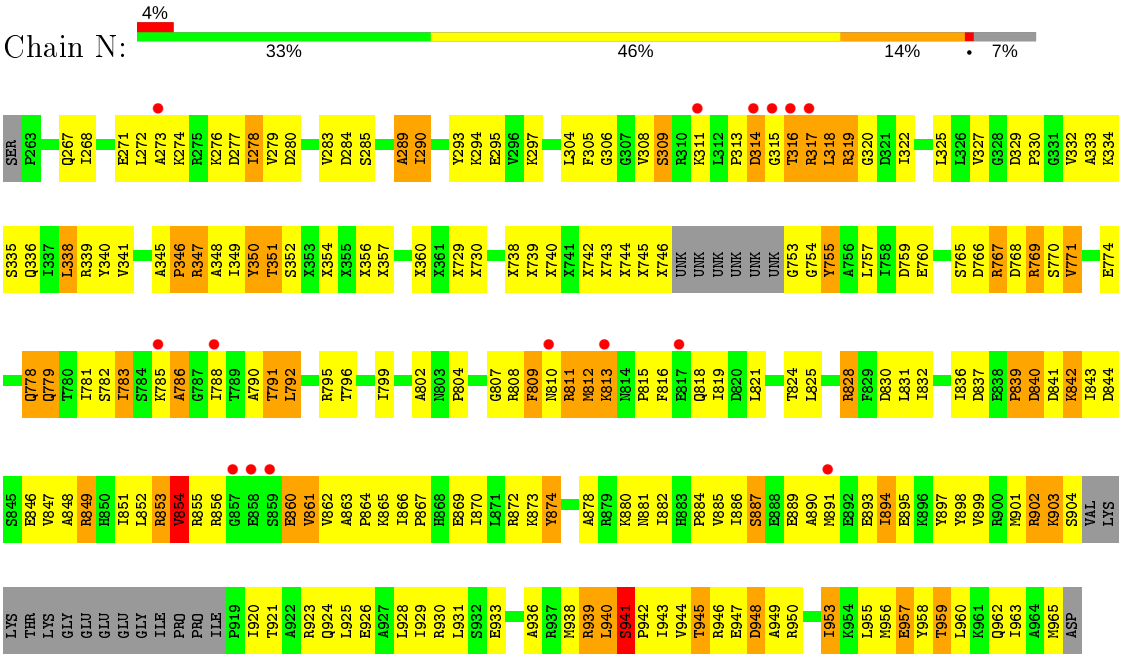
• Molecule 1: Cell division control protein 21

Chain M:

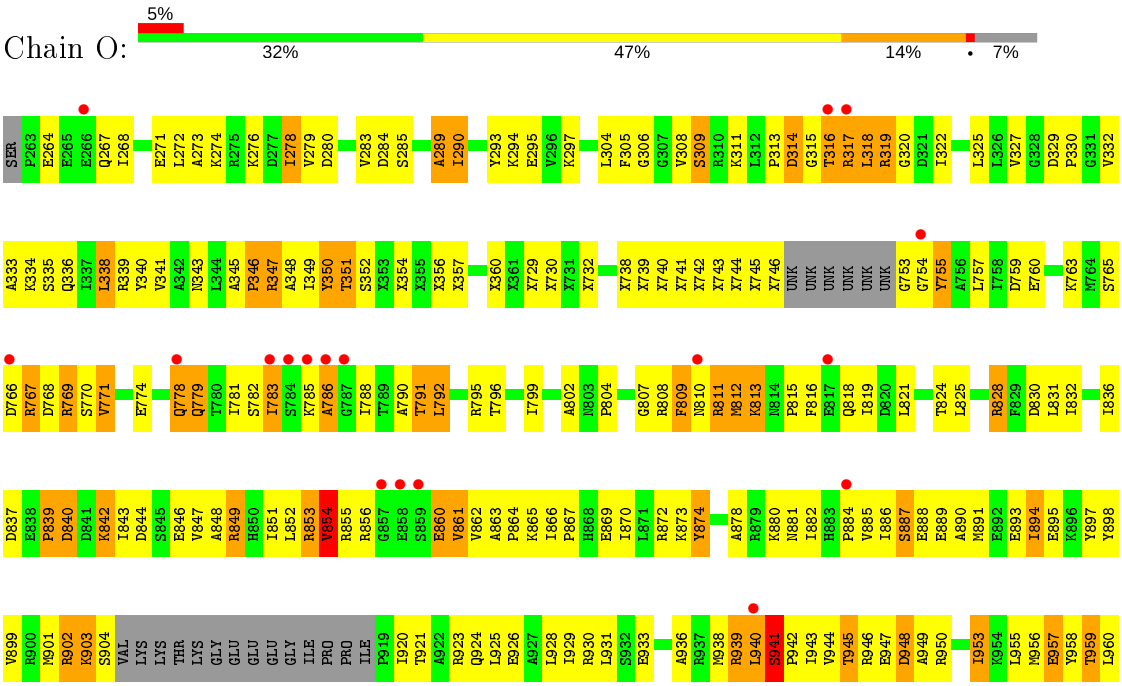


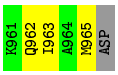


• Molecule 1: Cell division control protein 21



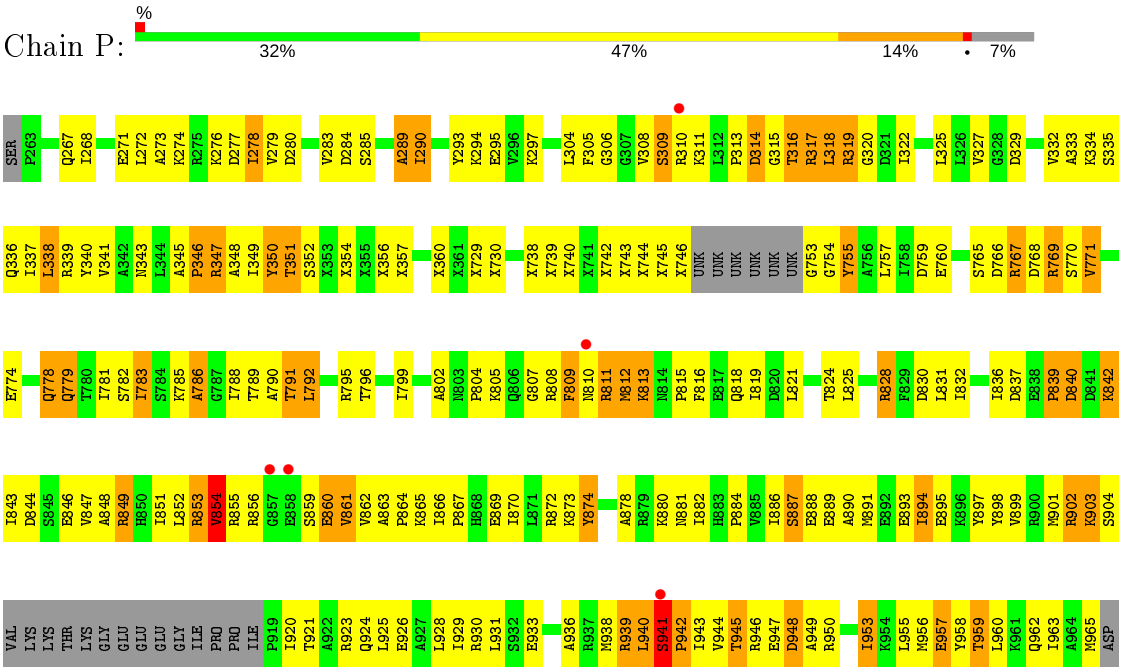
• Molecule 1: Cell division control protein 21





- Molecule 1: Cell division control protein 21

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	124.96Å 127.08Å 128.03Å 71.85° 72.82° 80.39°	Depositor
Resolution (Å)	48.37 – 3.80 48.37 – 3.75	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.37-3.80) 95.4 (48.37-3.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 3.77Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.301 , 0.314 0.301 , 0.316	Depositor DCC
R_{free} test set	3522 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	82.7	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 82.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.004 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	39296	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.46	0/2326	0.72	0/3133
1	B	0.46	0/2326	0.72	0/3133
1	C	0.46	0/2326	0.72	0/3133
1	D	0.46	0/2326	0.72	0/3133
1	E	0.46	0/2326	0.72	0/3133
1	F	0.46	0/2326	0.72	0/3133
1	G	0.46	0/2326	0.72	0/3133
1	H	0.46	0/2326	0.72	0/3133
1	I	0.46	0/2326	0.72	0/3133
1	J	0.46	0/2326	0.72	0/3133
1	K	0.46	0/2326	0.72	0/3133
1	L	0.46	0/2326	0.72	0/3133
1	M	0.46	0/2326	0.72	0/3133
1	N	0.46	0/2326	0.72	0/3133
1	O	0.46	0/2326	0.72	0/3133
1	P	0.46	0/2326	0.72	0/3133
All	All	0.46	0/37216	0.72	0/50128

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2428	0	2425	267	6
1	B	2428	0	2425	259	20
1	C	2428	0	2425	285	1
1	D	2428	0	2425	299	0
1	E	2428	0	2425	270	6
1	F	2428	0	2425	273	4
1	G	2428	0	2425	306	1
1	H	2428	0	2425	267	0
1	I	2428	0	2425	319	6
1	J	2428	0	2425	343	0
1	K	2428	0	2425	298	21
1	L	2428	0	2425	289	0
1	M	2428	0	2425	286	6
1	N	2428	0	2425	283	0
1	O	2428	0	2425	290	3
1	P	2428	0	2425	302	2
2	A	27	0	12	3	0
2	B	27	0	12	3	0
2	C	27	0	12	4	0
2	D	27	0	12	3	0
2	E	27	0	12	3	0
2	F	27	0	12	3	0
2	G	27	0	12	3	0
2	H	27	0	12	3	0
2	I	27	0	12	3	0
2	J	27	0	12	3	0
2	K	27	0	12	4	0
2	L	27	0	12	3	0
2	M	27	0	12	3	0
2	N	27	0	12	3	0
2	O	27	0	12	3	0
2	P	27	0	12	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
All	All	39296	0	38992	4162	38

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 53.

The worst 5 of 4162 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)
1:D:785:LYS:HG3	1:M:785:LYS:CG	1.32	1.56
1:G:730:UNK:CB	1:K:729:UNK:C	1.92	1.44
1:D:785:LYS:CG	1:M:785:LYS:HG3	0.98	1.44
1:E:788:ILE:HG22	1:L:741:UNK:CB	1.47	1.42
1:E:740:UNK:CA	1:L:789:THR:O	1.68	1.41

The worst 5 of 38 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PRO:CB	1:M:264:GLU:OE2[1_654]	0.81	1.39
1:B:264:GLU:OE1	1:K:264:GLU:OE1[1_564]	1.20	1.00
1:B:264:GLU:OE2	1:K:264:GLU:CB[1_564]	1.39	0.81
1:B:264:GLU:CD	1:K:264:GLU:OE1[1_564]	1.45	0.75
1:F:264:GLU:OE1	1:O:264:GLU:OE1[1_546]	1.50	0.70

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	B	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	C	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	D	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	E	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	F	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	G	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	H	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	I	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	J	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	K	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	L	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	M	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	N	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	O	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
1	P	284/338 (84%)	209 (74%)	52 (18%)	23 (8%)	1 14
All	All	4544/5408 (84%)	3344 (74%)	832 (18%)	368 (8%)	1 14

5 of 368 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	THR
1	A	766	ASP
1	A	786	ALA
1	A	810	ASN
1	B	316	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/260 (95%)	207 (84%)	39 (16%)	2	16
1	B	246/260 (95%)	206 (84%)	40 (16%)	2	15
1	C	246/260 (95%)	207 (84%)	39 (16%)	2	16
1	D	246/260 (95%)	206 (84%)	40 (16%)	2	15
1	E	246/260 (95%)	206 (84%)	40 (16%)	2	15
1	F	246/260 (95%)	206 (84%)	40 (16%)	2	15
1	G	246/260 (95%)	206 (84%)	40 (16%)	2	15
1	H	246/260 (95%)	207 (84%)	39 (16%)	2	16
1	I	246/260 (95%)	207 (84%)	39 (16%)	2	16
1	J	246/260 (95%)	207 (84%)	39 (16%)	2	16
1	K	246/260 (95%)	207 (84%)	39 (16%)	2	16
1	L	246/260 (95%)	206 (84%)	40 (16%)	2	15
1	M	246/260 (95%)	206 (84%)	40 (16%)	2	15
1	N	246/260 (95%)	207 (84%)	39 (16%)	2	16
1	O	246/260 (95%)	207 (84%)	39 (16%)	2	16
1	P	246/260 (95%)	206 (84%)	40 (16%)	2	15
All	All	3936/4160 (95%)	3304 (84%)	632 (16%)	2	16

5 of 632 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	347	ARG
1	I	957	GLU
1	O	939	ARG
1	H	783	ILE
1	I	314	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	779	GLN
1	I	779	GLN
1	O	779	GLN
1	H	336	GLN
1	H	779	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
2	ADP	D	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	P	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	N	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	M	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	H	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	O	1001	3	24,29,29	1.16	2 (8%)	29,45,45	1.87	6 (20%)
2	ADP	J	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	I	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.85	6 (20%)
2	ADP	K	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	F	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	E	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	G	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	B	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)
2	ADP	A	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ADP	L	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.87	6 (20%)
2	ADP	C	1001	3	24,29,29	1.17	2 (8%)	29,45,45	1.86	6 (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
2	ADP	D	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	P	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	N	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	M	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	H	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	O	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	J	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	I	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	K	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	F	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	E	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	G	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	B	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	A	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	L	1001	3	-	0/12/32/32	0/3/3/3
2	ADP	C	1001	3	-	0/12/32/32	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1001	ADP	O4'-C1'	2.71	1.44	1.41
2	E	1001	ADP	O4'-C1'	2.71	1.44	1.41
2	I	1001	ADP	O4'-C1'	2.70	1.44	1.41
2	J	1001	ADP	O4'-C1'	2.70	1.44	1.41
2	P	1001	ADP	O4'-C1'	2.69	1.44	1.41

The worst 5 of 96 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	1001	ADP	PA-O3A-PB	-6.13	111.81	132.83
2	E	1001	ADP	PA-O3A-PB	-6.12	111.83	132.83
2	M	1001	ADP	PA-O3A-PB	-6.12	111.84	132.83
2	G	1001	ADP	PA-O3A-PB	-6.11	111.85	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1001	ADP	PA-O3A-PB	-6.11	111.86	132.83

There are no chirality outliers.

There are no torsion outliers.

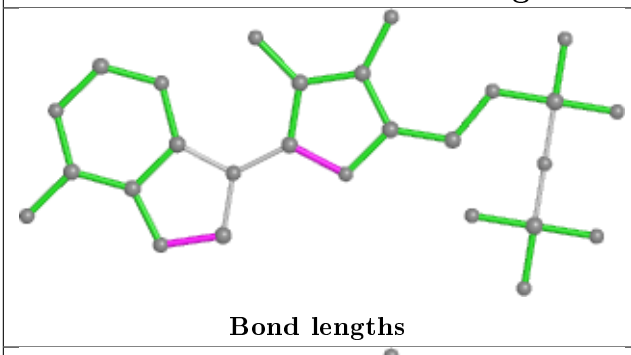
There are no ring outliers.

16 monomers are involved in 51 short contacts:

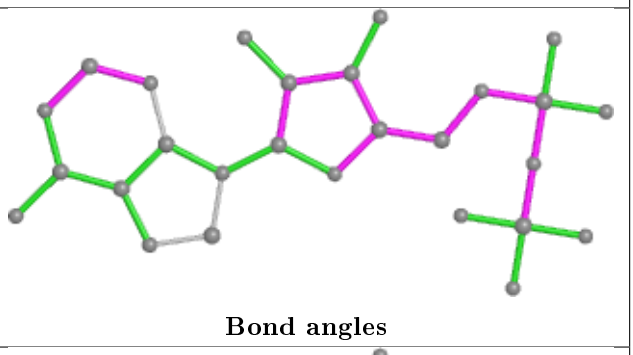
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001	ADP	3	0
2	P	1001	ADP	4	0
2	N	1001	ADP	3	0
2	M	1001	ADP	3	0
2	H	1001	ADP	3	0
2	O	1001	ADP	3	0
2	J	1001	ADP	3	0
2	I	1001	ADP	3	0
2	K	1001	ADP	4	0
2	F	1001	ADP	3	0
2	E	1001	ADP	3	0
2	G	1001	ADP	3	0
2	B	1001	ADP	3	0
2	A	1001	ADP	3	0
2	L	1001	ADP	3	0
2	C	1001	ADP	4	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.

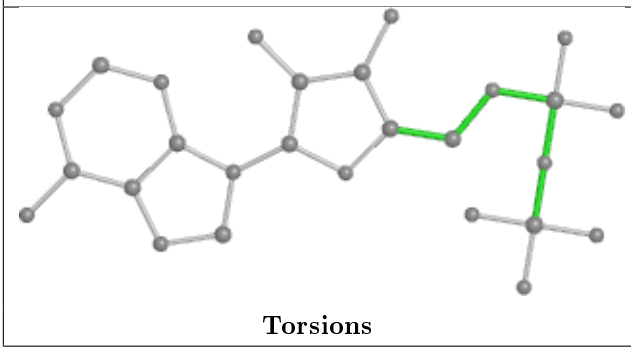
Ligand ADP D 1001



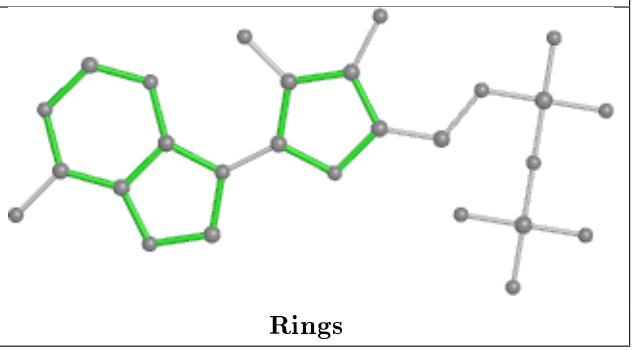
Bond lengths



Bond angles

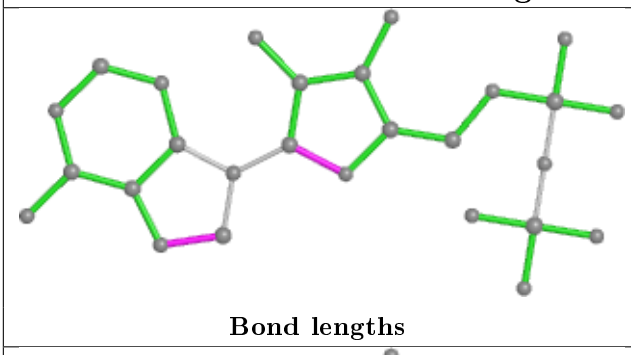


Torsions

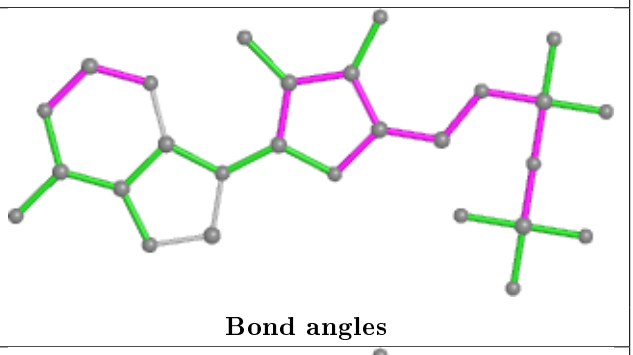


Rings

Ligand ADP P 1001



Bond lengths



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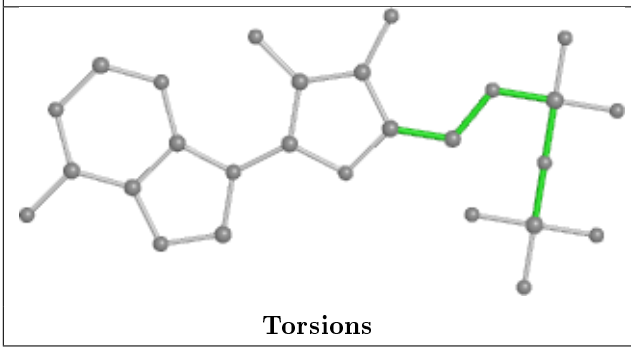

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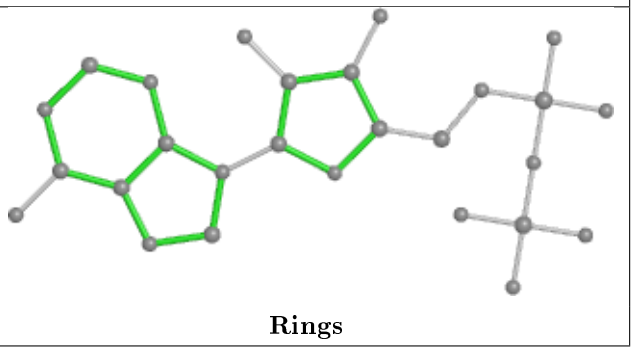

Rings

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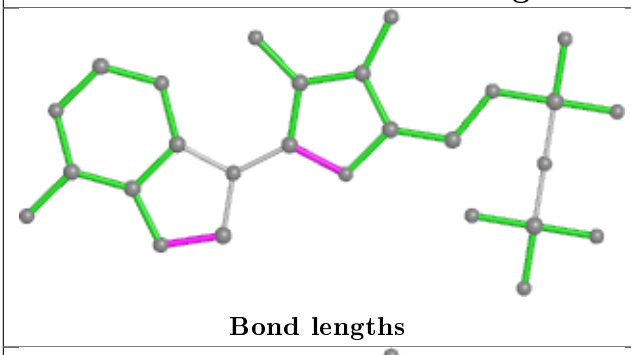

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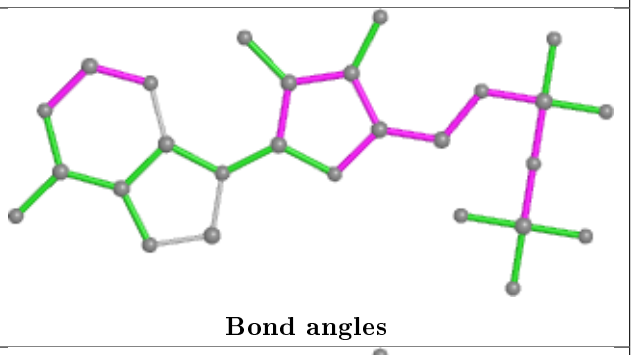
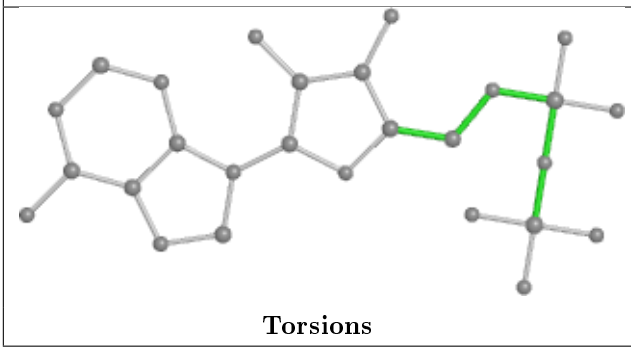


Bond angles



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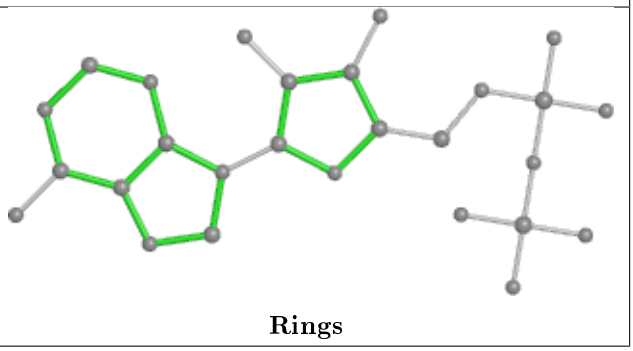

Rings

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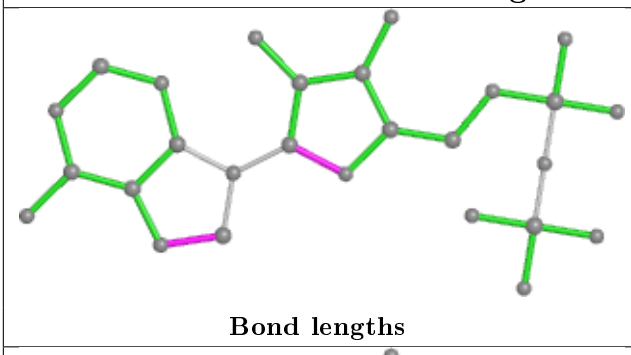

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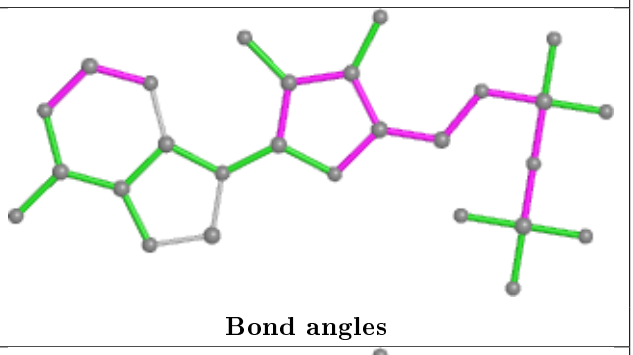
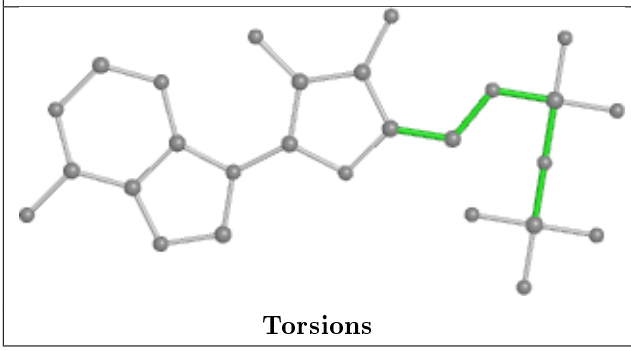


Bond angles



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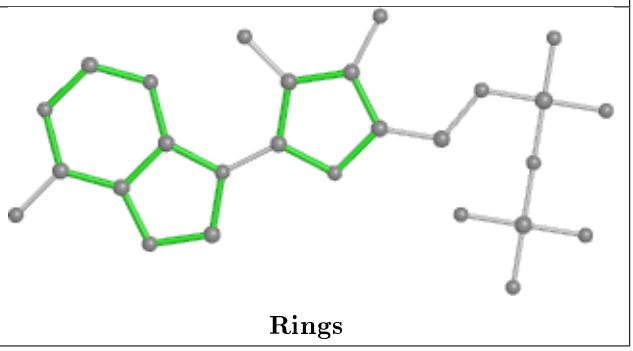
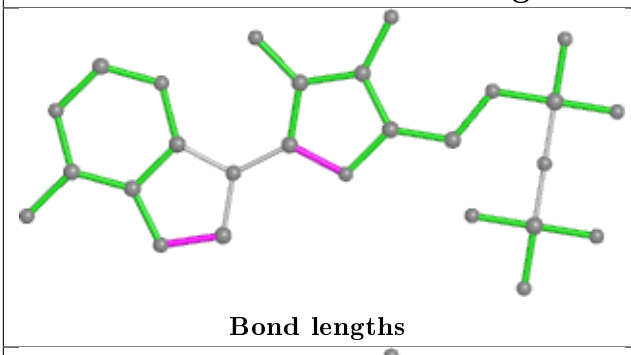


Rings

Ligand ADP H 1001



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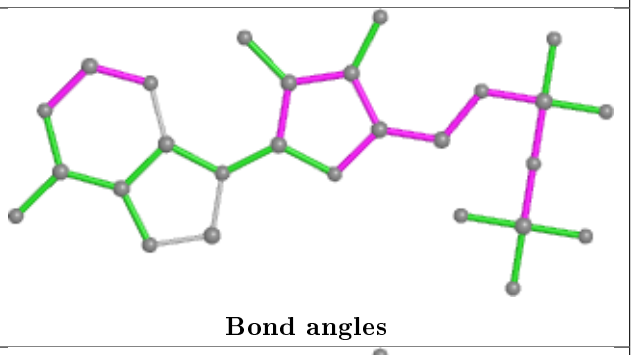

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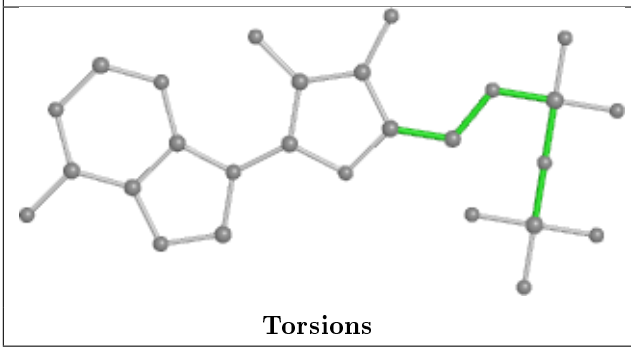

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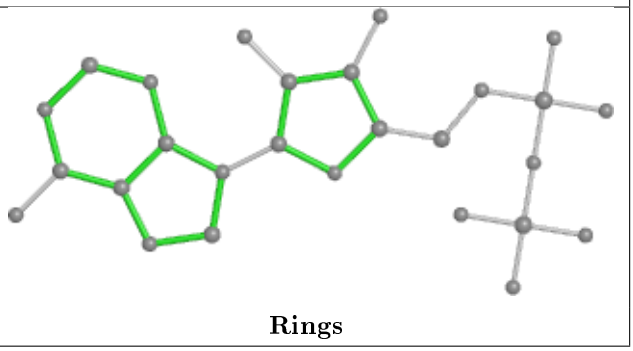

Rings

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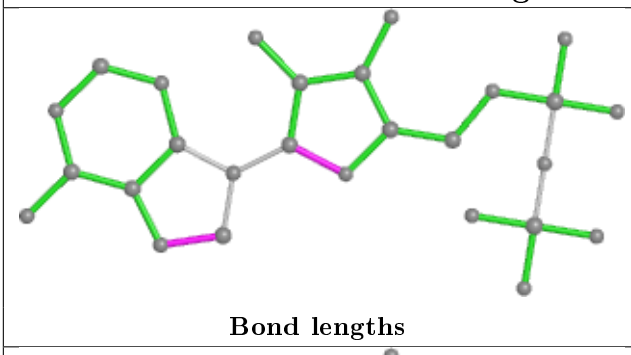

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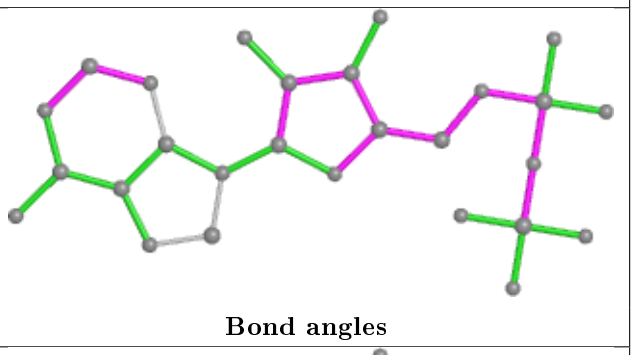

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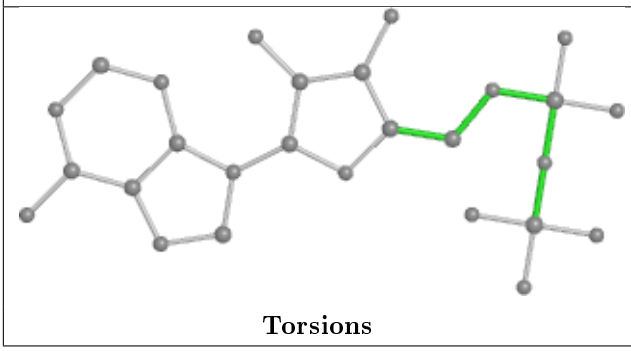

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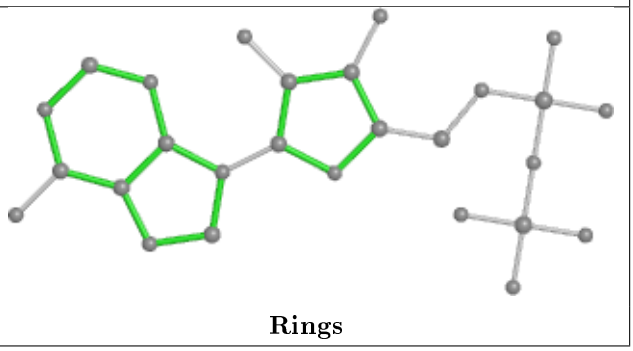
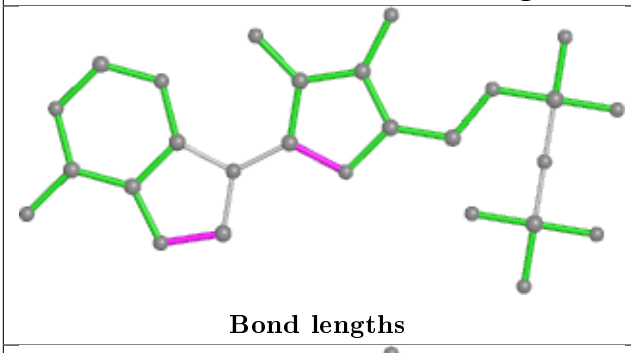


Rings

Ligand ADP J 1001



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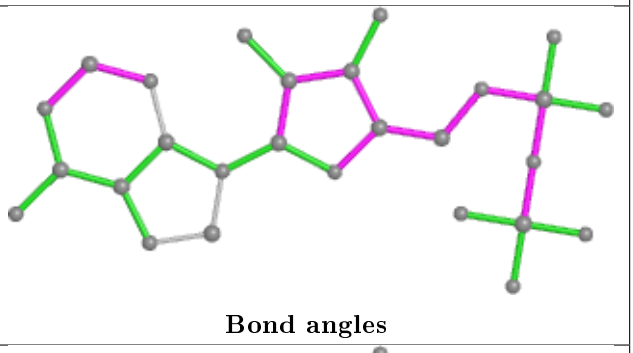

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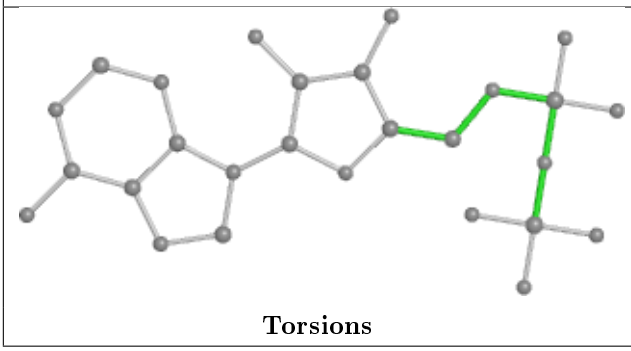

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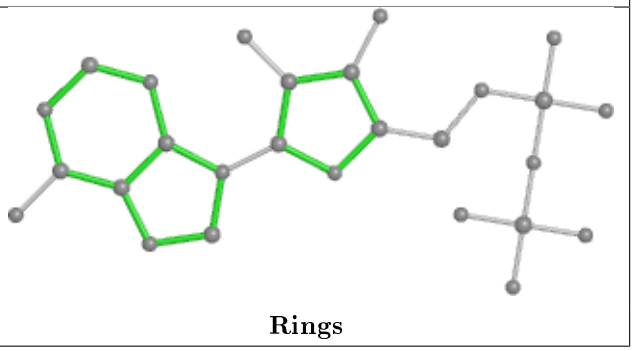

Rings

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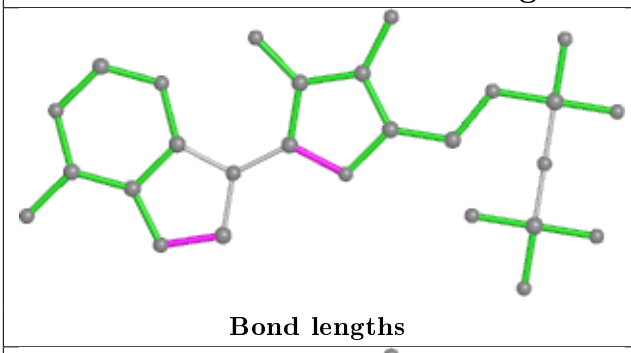

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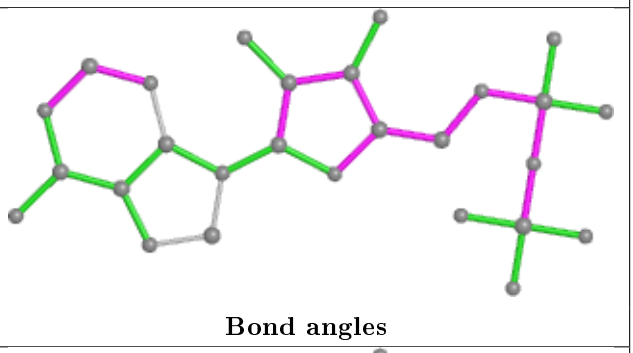

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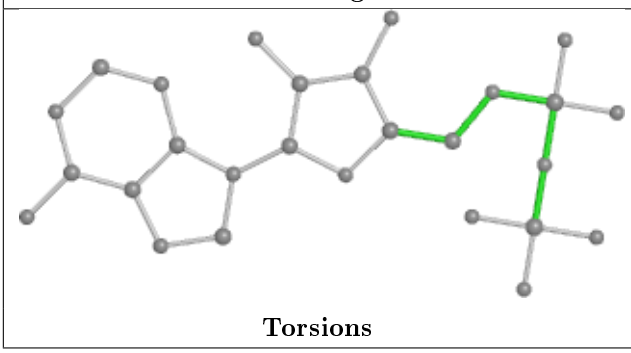
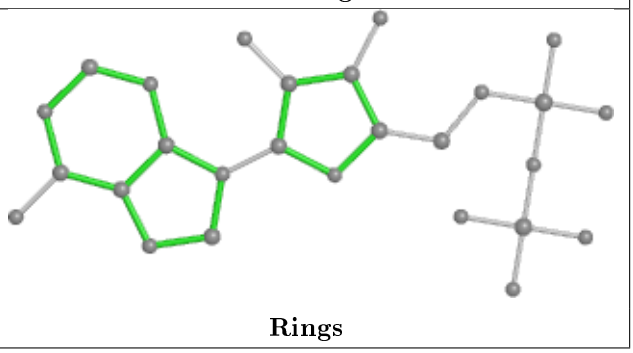
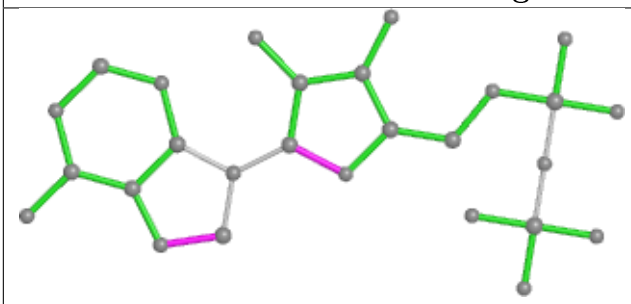


Torsions

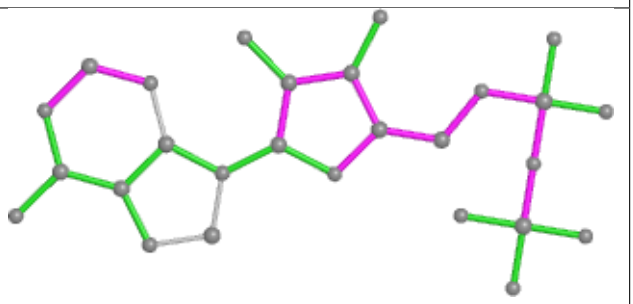


Rings

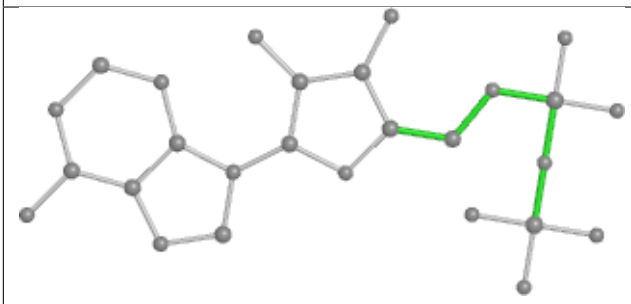
Ligand ADP K 1001



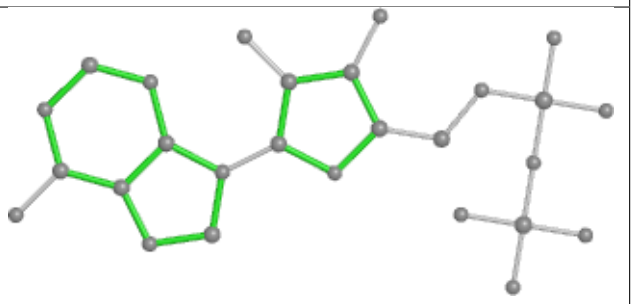
Bond lengths



Bond angles

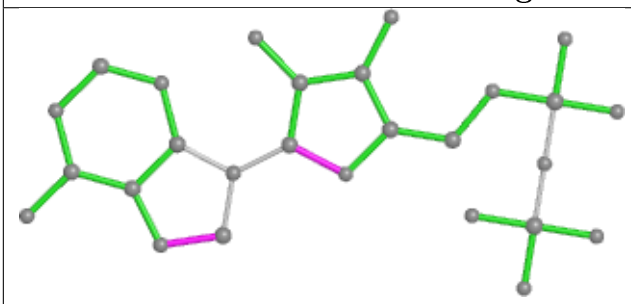


Torsions



Rings

Ligand ADP F 1001



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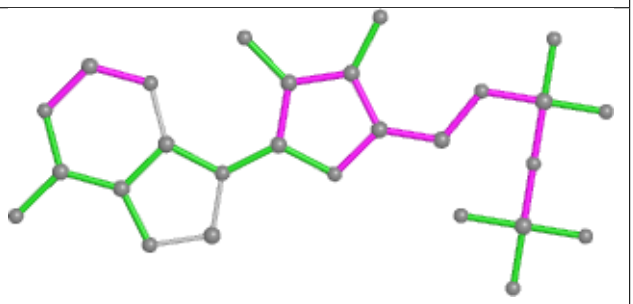

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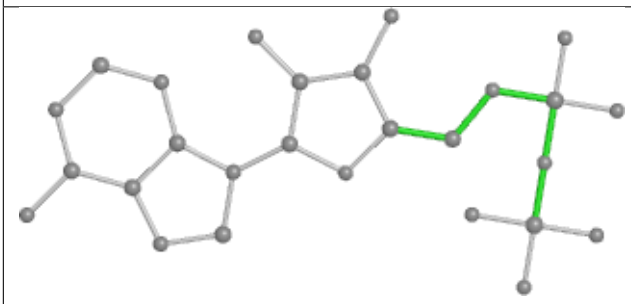
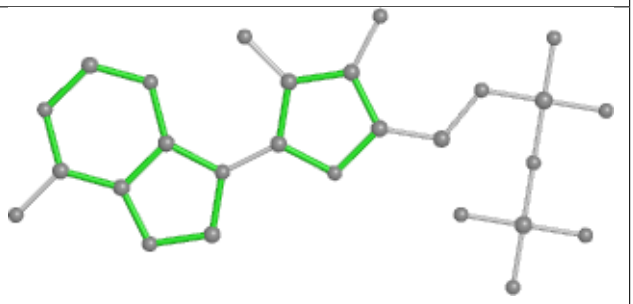
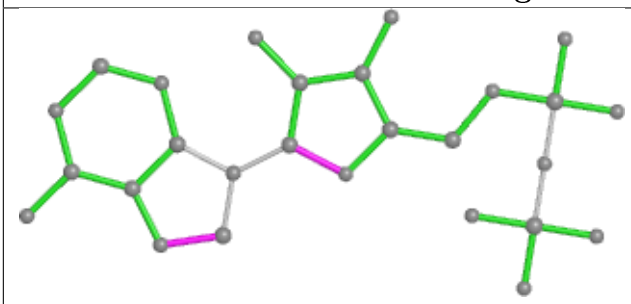


Torsions

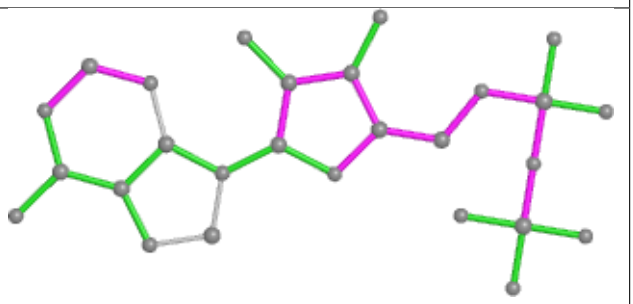


Rings

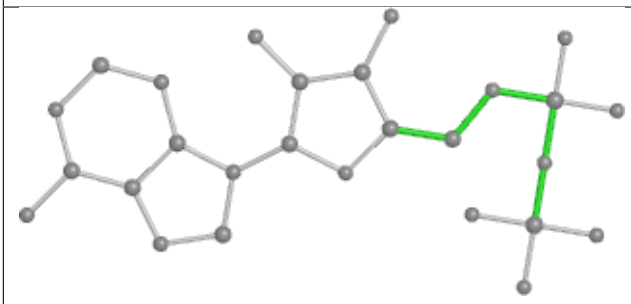
Ligand ADP E 1001



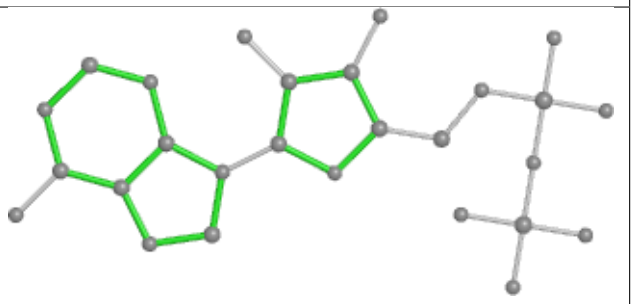
Bond lengths



Bond angles

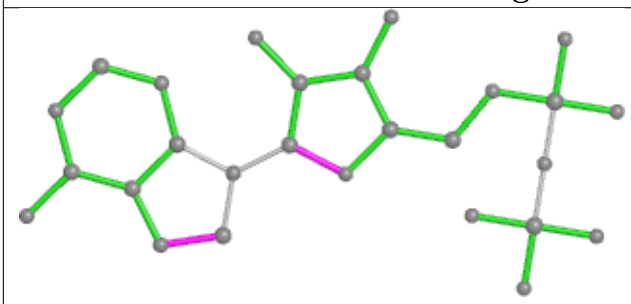


Torsions

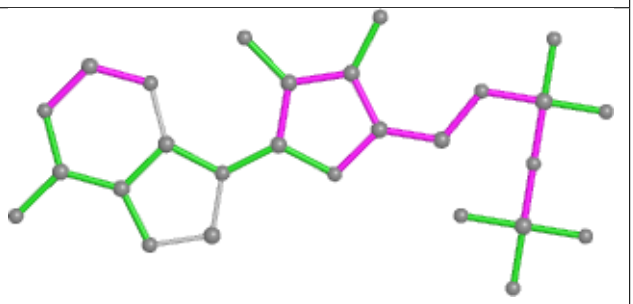


Rings

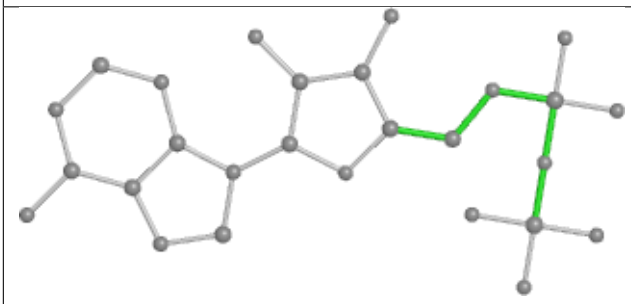
Ligand ADP G 1001



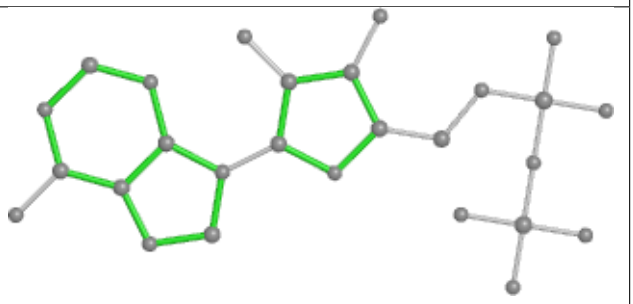
Bond lengths



Bond angles

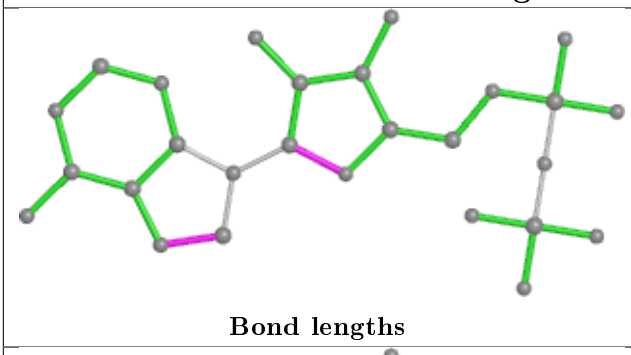


Torsions

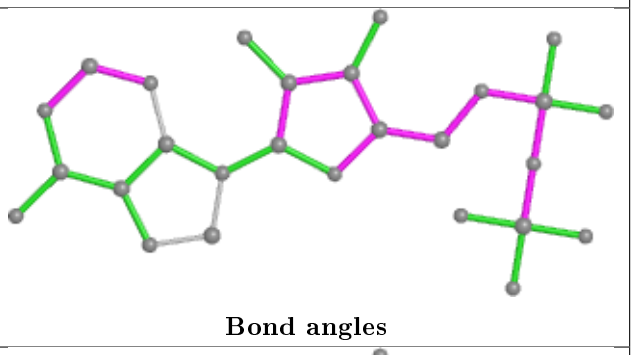


Rings

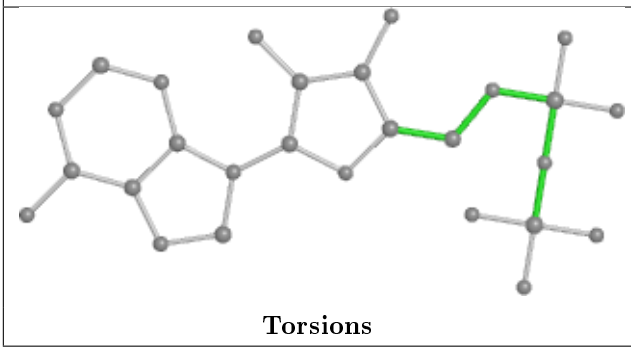
Ligand ADP B 1001



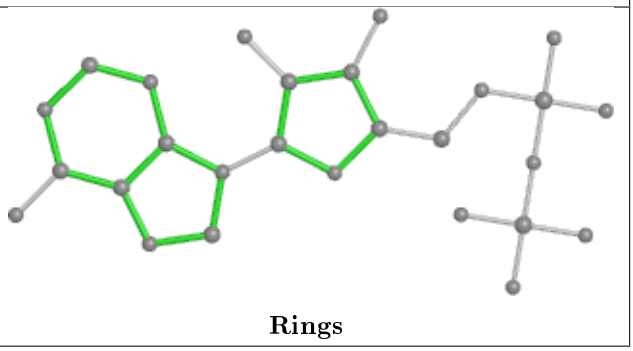
Bond lengths



Bond angles

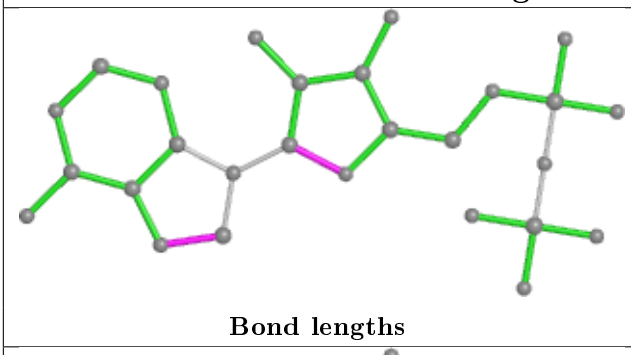


Torsions

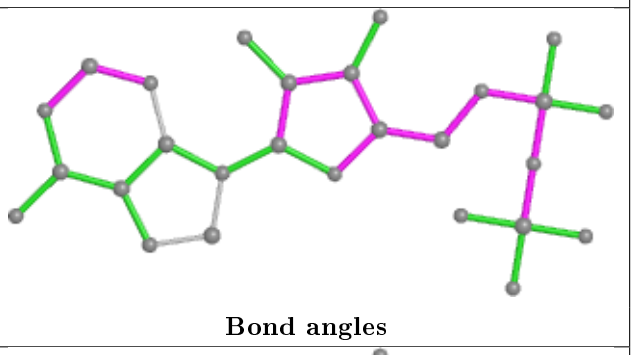


Rings

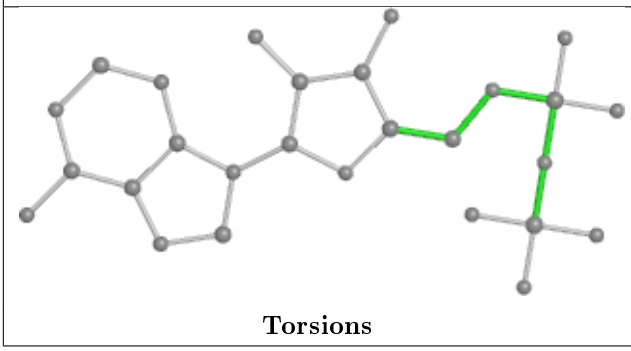
Ligand ADP A 1001



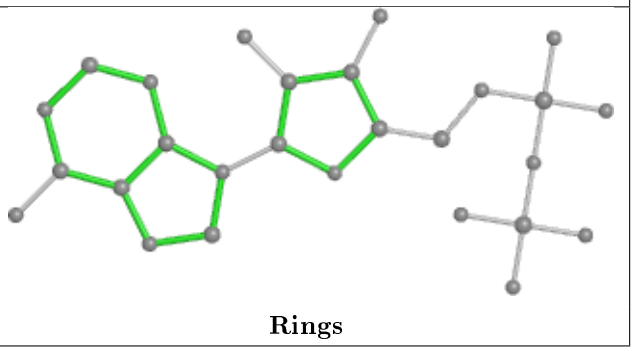
Bond lengths



Bond angles

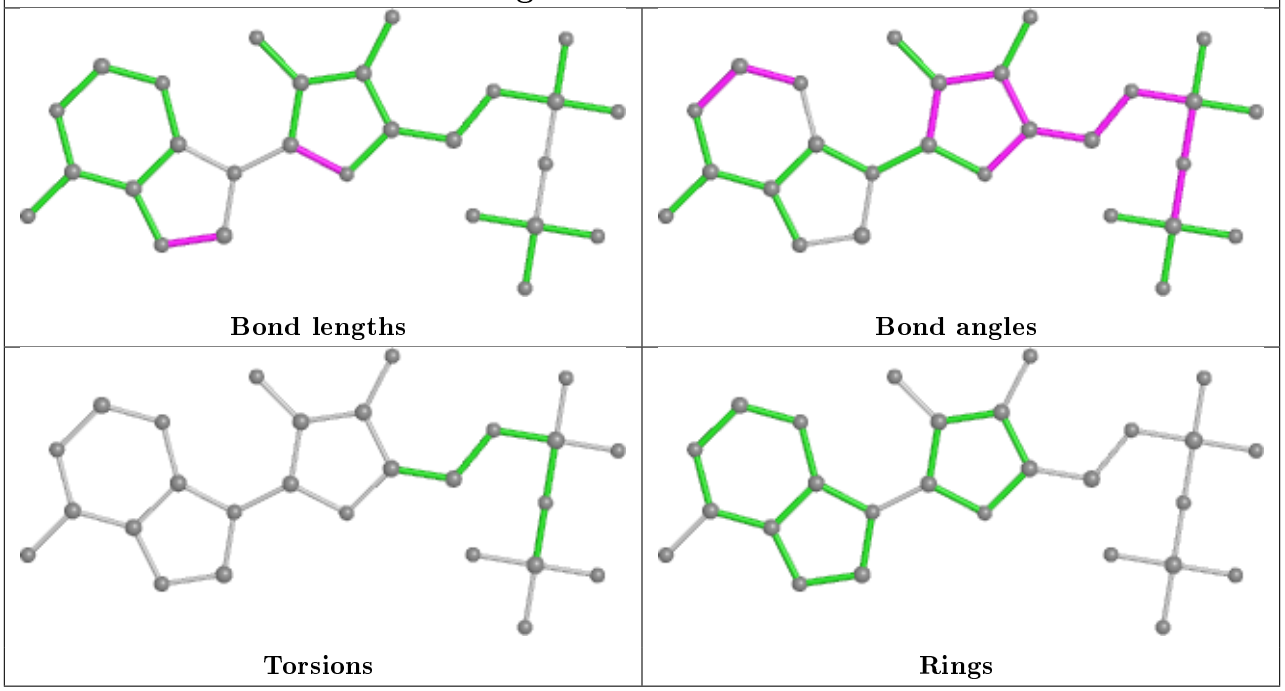


Torsions

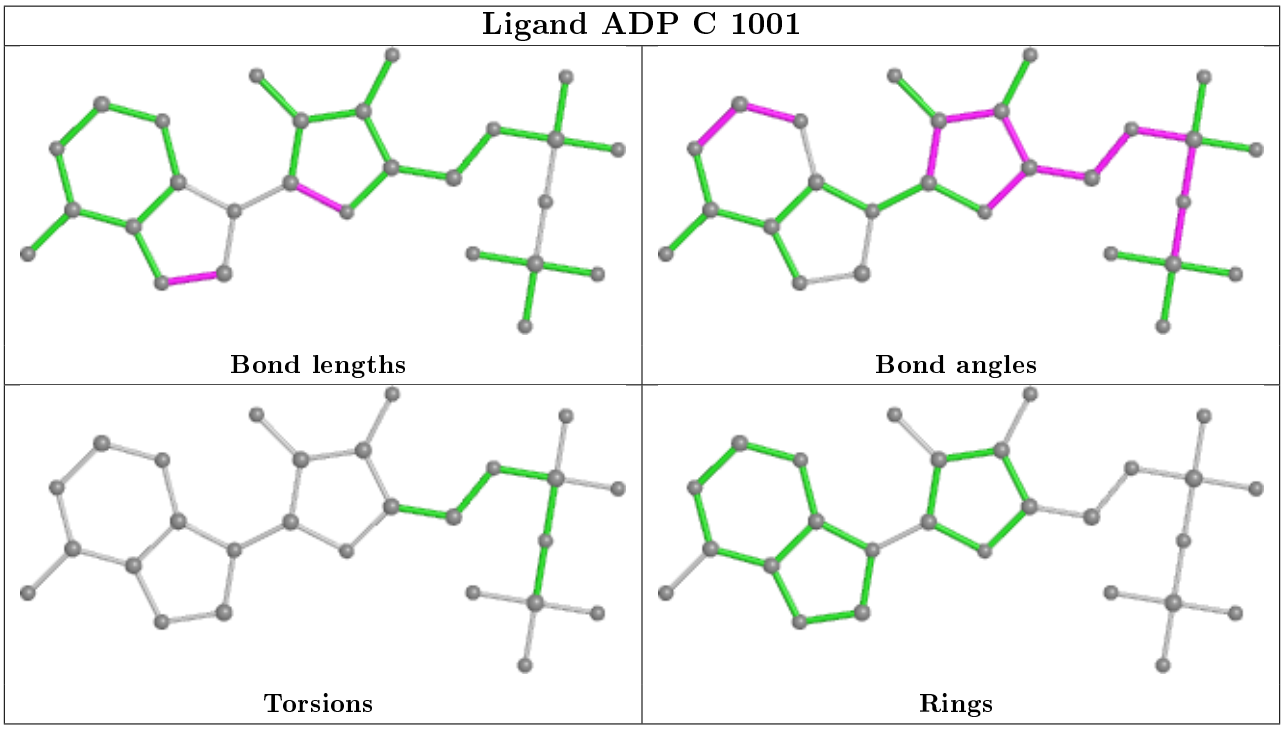


Rings

Ligand ADP L 1001



Ligand ADP C 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	289/338 (85%)	0.10	11 (3%)	40	33	21, 84, 146, 251	0
1	B	289/338 (85%)	-0.06	7 (2%)	59	50	21, 84, 146, 251	0
1	C	289/338 (85%)	-0.02	9 (3%)	49	40	21, 84, 146, 251	0
1	D	289/338 (85%)	-0.01	2 (0%)	87	83	21, 84, 146, 251	0
1	E	289/338 (85%)	0.03	8 (2%)	53	43	21, 84, 146, 251	0
1	F	289/338 (85%)	-0.04	7 (2%)	59	50	21, 84, 146, 251	0
1	G	289/338 (85%)	0.24	12 (4%)	36	30	21, 84, 146, 251	0
1	H	289/338 (85%)	-0.02	4 (1%)	75	68	21, 84, 146, 251	0
1	I	289/338 (85%)	-0.03	3 (1%)	82	76	21, 84, 146, 251	0
1	J	289/338 (85%)	0.05	7 (2%)	59	50	21, 84, 146, 251	0
1	K	289/338 (85%)	0.08	8 (2%)	53	43	21, 84, 146, 251	0
1	L	289/338 (85%)	0.27	14 (4%)	30	26	21, 84, 146, 251	0
1	M	289/338 (85%)	0.08	3 (1%)	82	76	21, 84, 146, 251	0
1	N	289/338 (85%)	0.23	15 (5%)	27	24	21, 84, 146, 251	0
1	O	289/338 (85%)	0.34	18 (6%)	20	16	21, 84, 146, 251	0
1	P	289/338 (85%)	-0.00	5 (1%)	70	62	21, 84, 146, 251	0
All	All	4624/5408 (85%)	0.08	133 (2%)	51	42	21, 84, 146, 251	0

The worst 5 of 133 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	857	GLY	13.0
1	E	858	GLU	10.0
1	N	858	GLU	10.0
1	N	859	SER	9.9
1	M	858	GLU	9.6

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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, 95^{th} 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
3	MG	N	1002	1/1	0.80	0.36	81,81,81,81	0
3	MG	L	1002	1/1	0.84	0.42	81,81,81,81	0
3	MG	A	1002	1/1	0.85	0.28	81,81,81,81	0
2	ADP	A	1001	27/27	0.85	0.27	72,72,72,72	0
3	MG	G	1002	1/1	0.86	0.43	81,81,81,81	0
2	ADP	I	1001	27/27	0.86	0.26	72,72,72,72	0
2	ADP	M	1001	27/27	0.87	0.21	72,72,72,72	0
2	ADP	L	1001	27/27	0.87	0.29	72,72,72,72	0
2	ADP	H	1001	27/27	0.87	0.28	72,72,72,72	0
2	ADP	D	1001	27/27	0.88	0.25	72,72,72,72	0
3	MG	H	1002	1/1	0.88	0.47	81,81,81,81	0
3	MG	P	1002	1/1	0.88	0.30	81,81,81,81	0
2	ADP	G	1001	27/27	0.88	0.29	72,72,72,72	0
3	MG	O	1002	1/1	0.89	0.29	81,81,81,81	0
2	ADP	J	1001	27/27	0.90	0.23	72,72,72,72	0
3	MG	C	1002	1/1	0.90	0.24	81,81,81,81	0
2	ADP	K	1001	27/27	0.90	0.22	72,72,72,72	0
2	ADP	N	1001	27/27	0.91	0.21	72,72,72,72	0
2	ADP	O	1001	27/27	0.91	0.23	72,72,72,72	0
2	ADP	F	1001	27/27	0.92	0.22	72,72,72,72	0
3	MG	J	1002	1/1	0.92	0.12	81,81,81,81	0
2	ADP	P	1001	27/27	0.92	0.20	72,72,72,72	0
3	MG	I	1002	1/1	0.93	0.47	81,81,81,81	0
3	MG	M	1002	1/1	0.93	0.33	81,81,81,81	0
2	ADP	E	1001	27/27	0.93	0.20	72,72,72,72	0
3	MG	F	1002	1/1	0.93	0.26	81,81,81,81	0
2	ADP	C	1001	27/27	0.93	0.20	72,72,72,72	0

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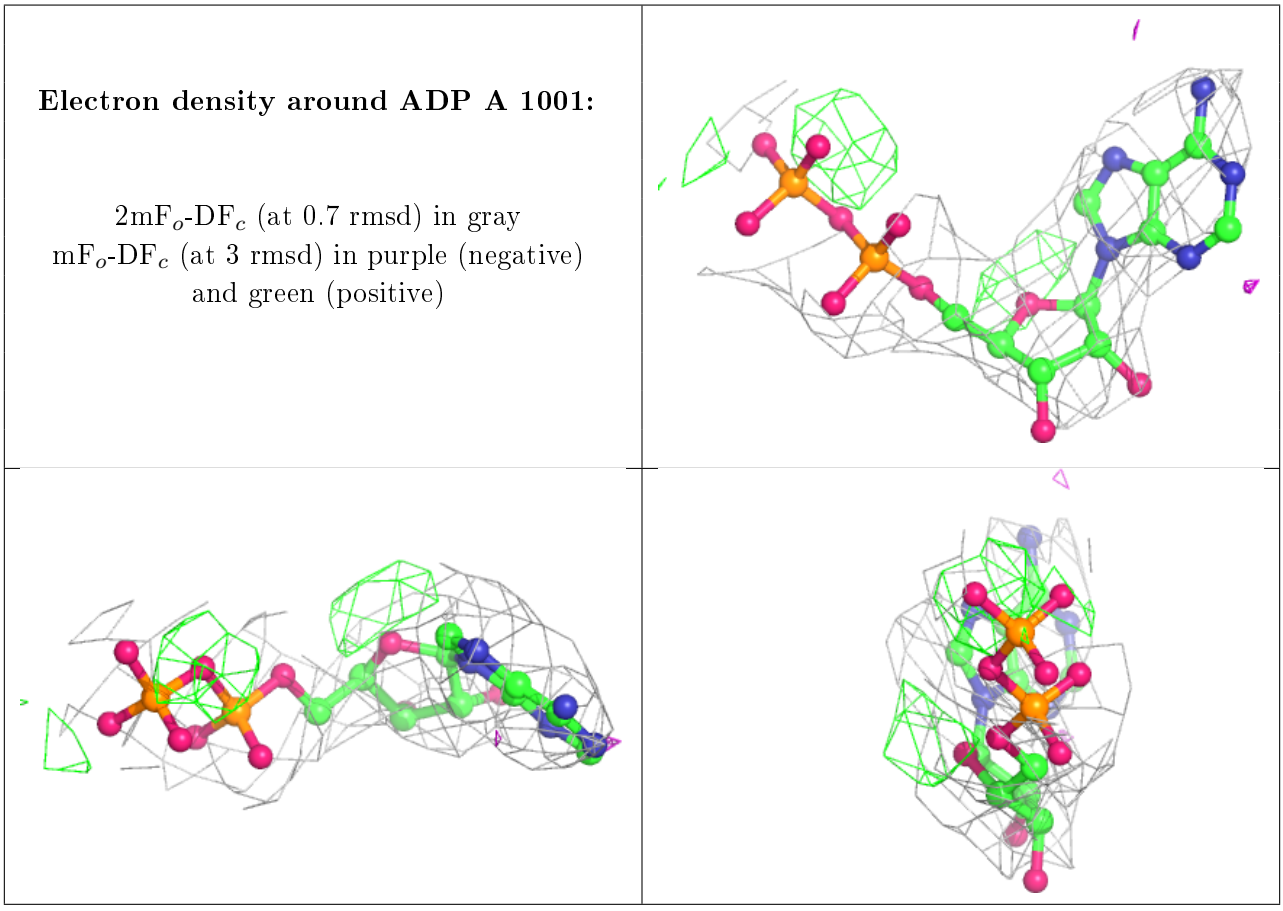
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	B	1001	27/27	0.93	0.23	72,72,72,72	0
3	MG	K	1002	1/1	0.93	0.15	81,81,81,81	0
3	MG	B	1002	1/1	0.94	0.37	81,81,81,81	0
3	MG	D	1002	1/1	0.96	0.51	81,81,81,81	0
3	MG	E	1002	1/1	0.96	0.17	81,81,81,81	0

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.

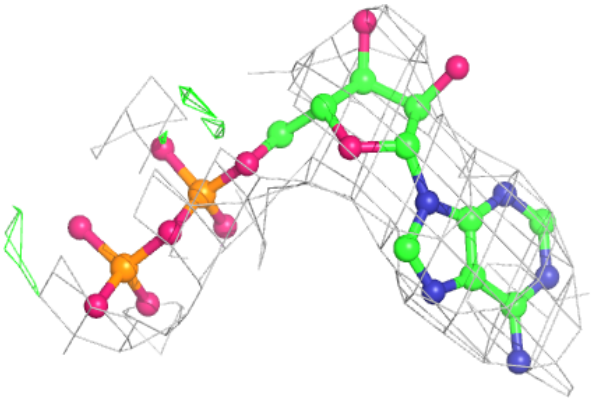
Electron density around ADP A 1001:

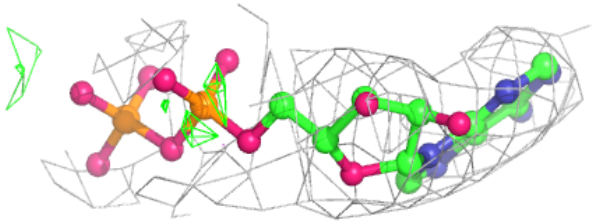
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

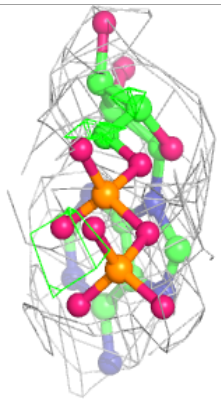


Electron density around ADP I 1001:

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

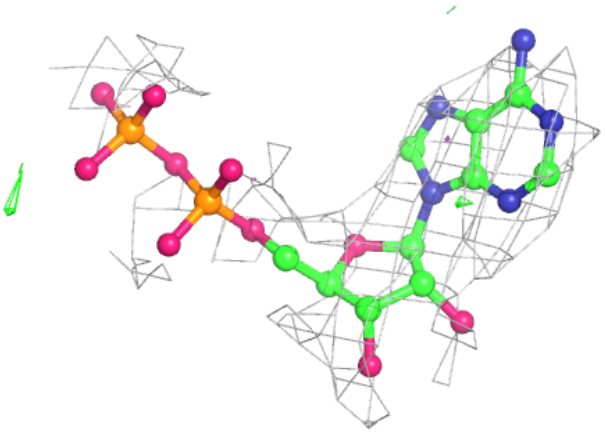


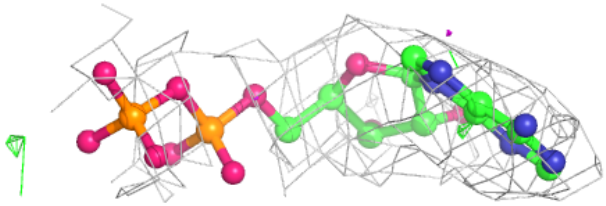


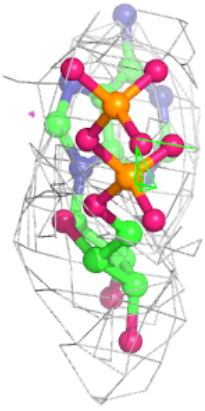


Electron density around ADP M 1001:

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

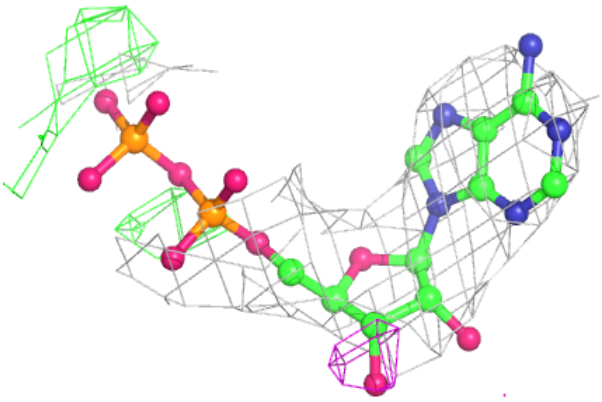


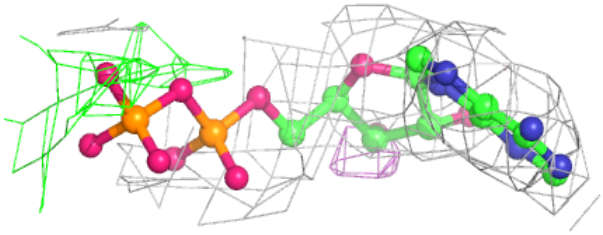


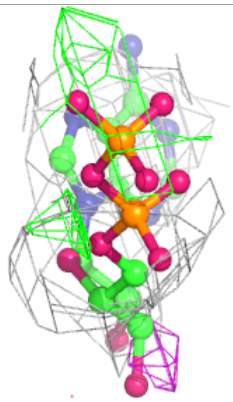


Electron density around ADP L 1001:

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

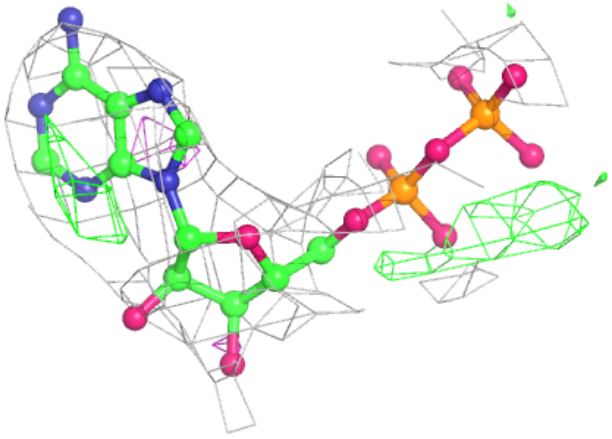


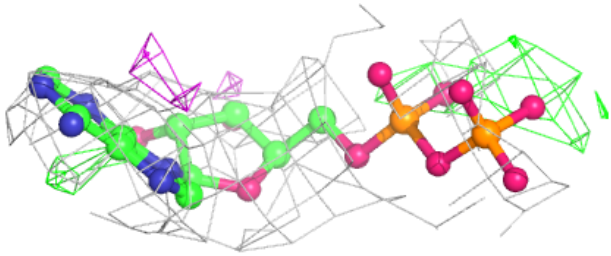


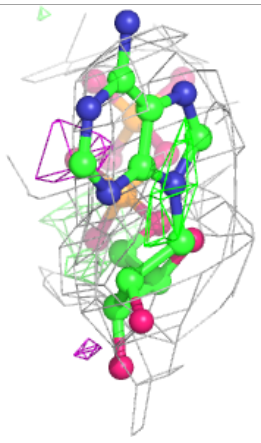


Electron density around ADP H 1001:

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

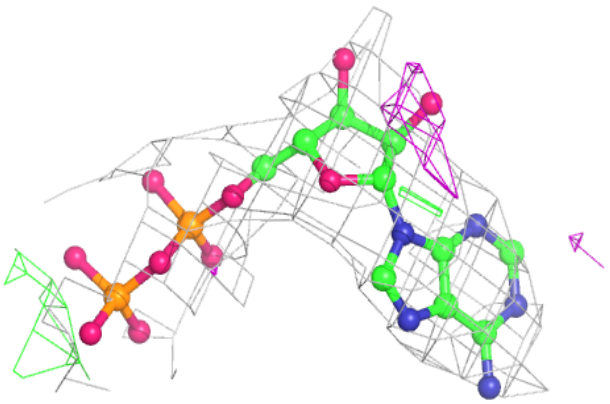


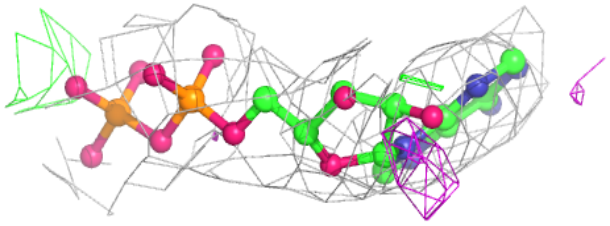


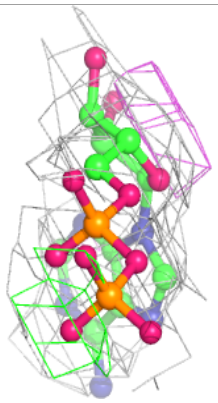


Electron density around ADP D 1001:

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

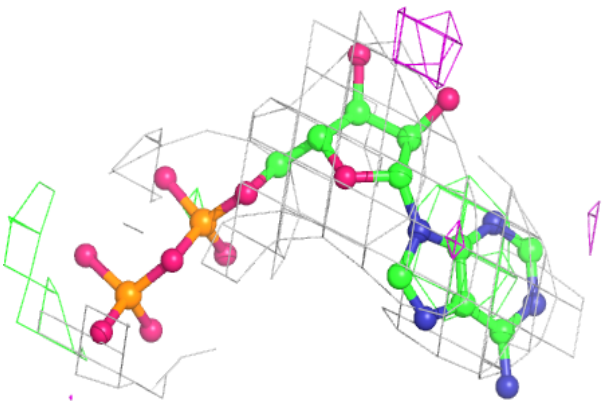


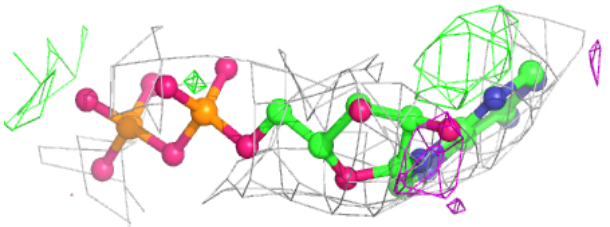


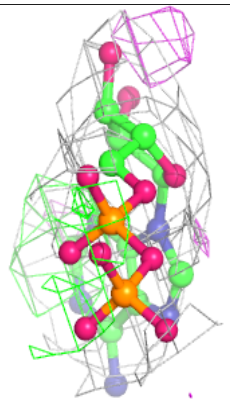


Electron density around ADP G 1001:

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

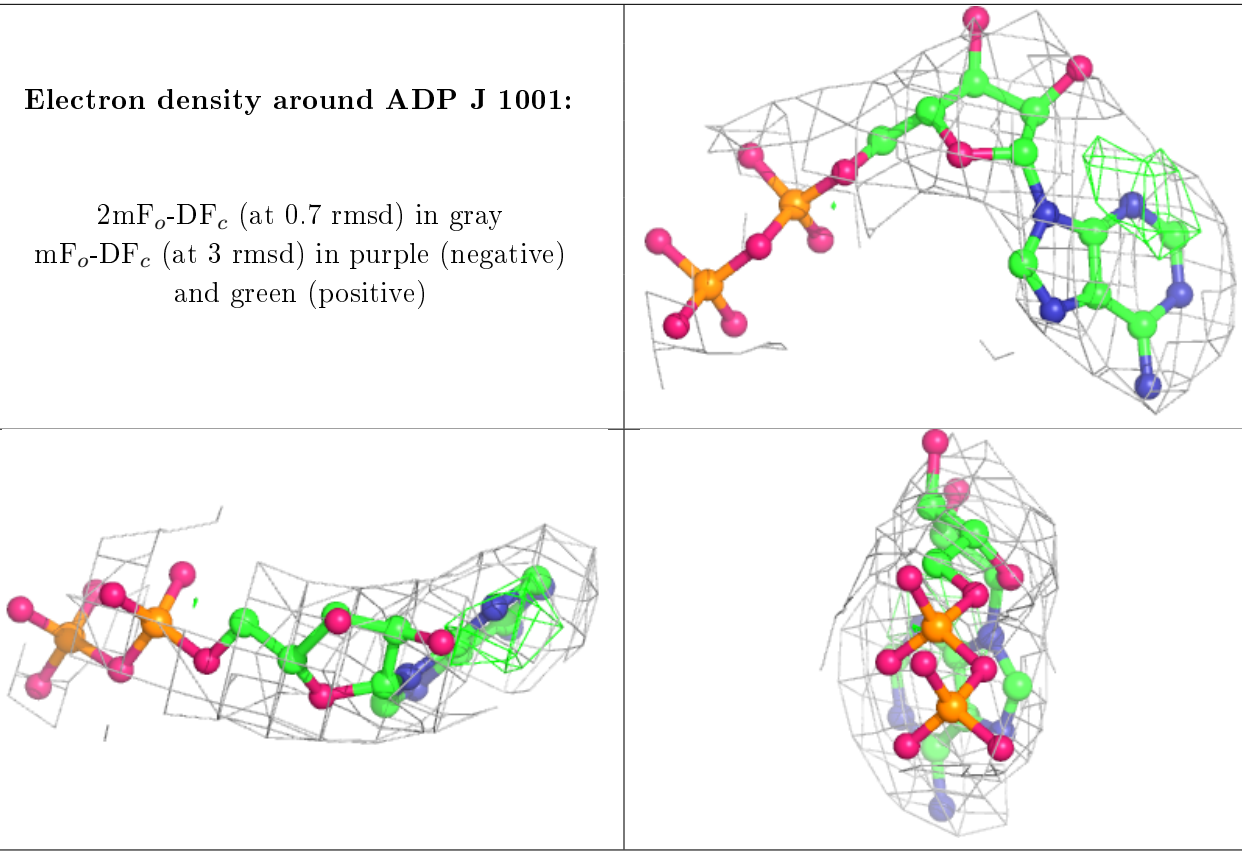






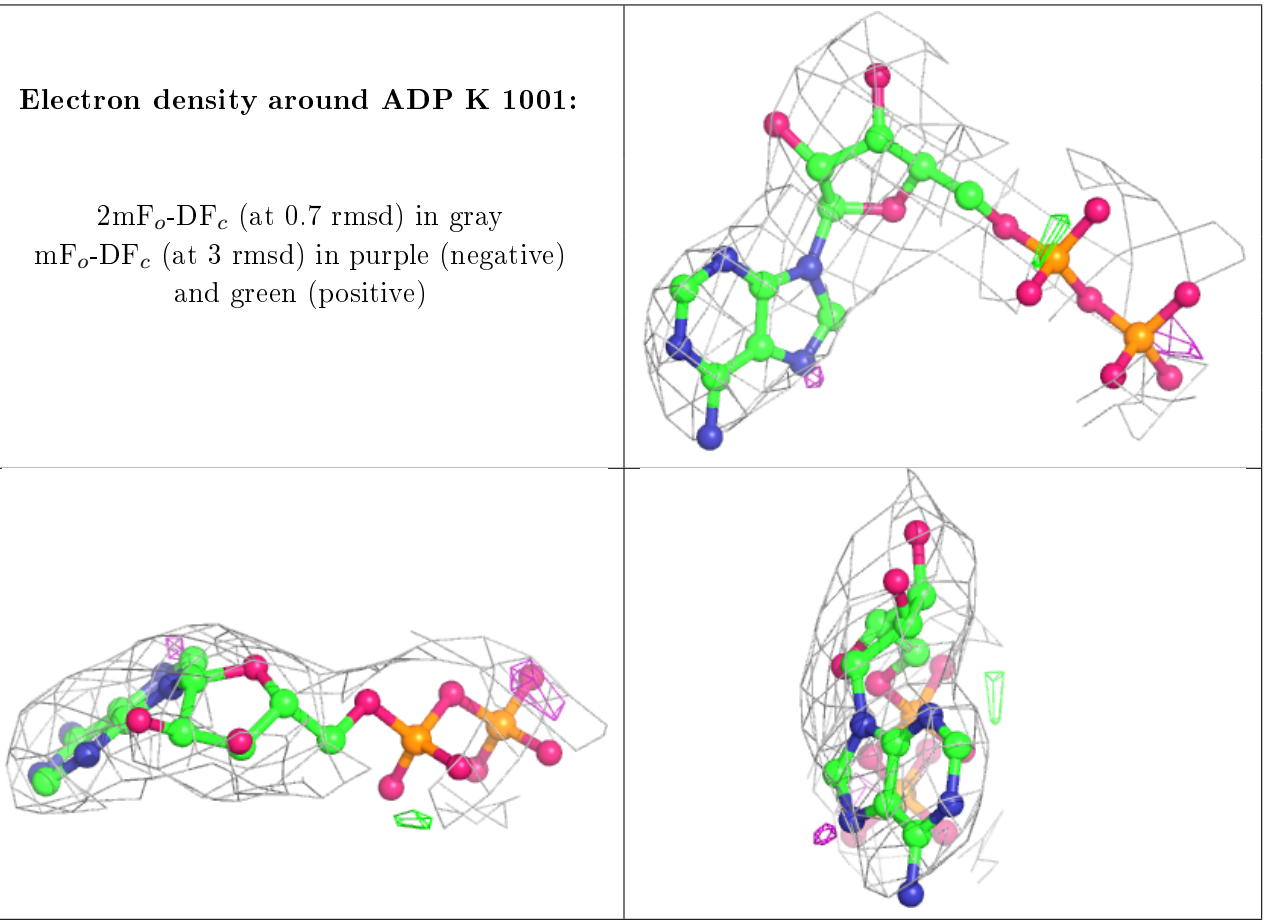
Electron density around ADP J 1001:

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



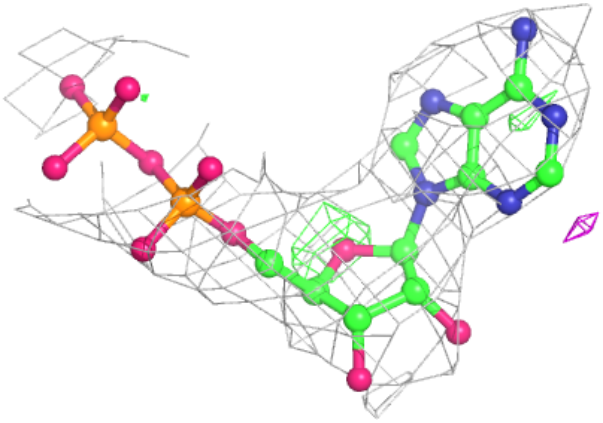
Electron density around ADP K 1001:

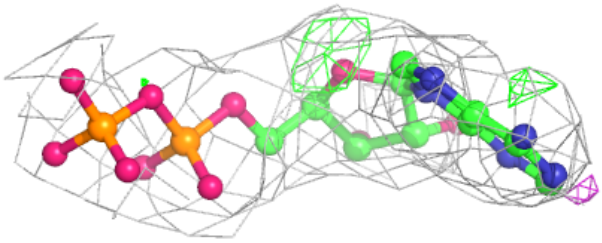
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

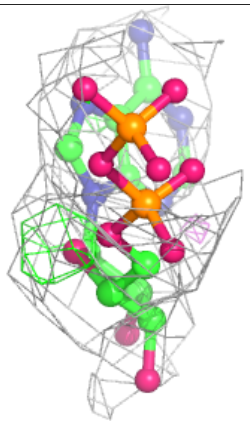


Electron density around ADP N 1001:

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

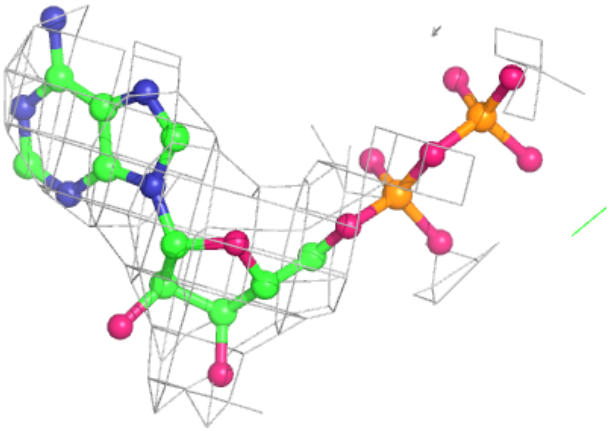


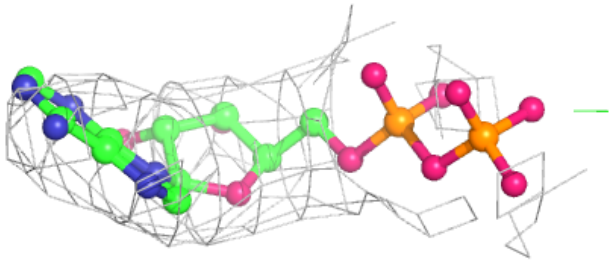


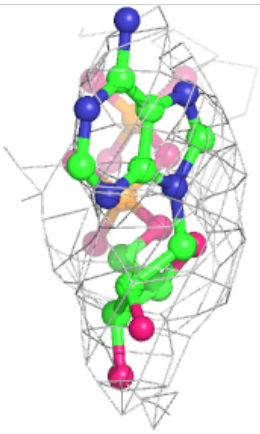


Electron density around ADP O 1001:

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

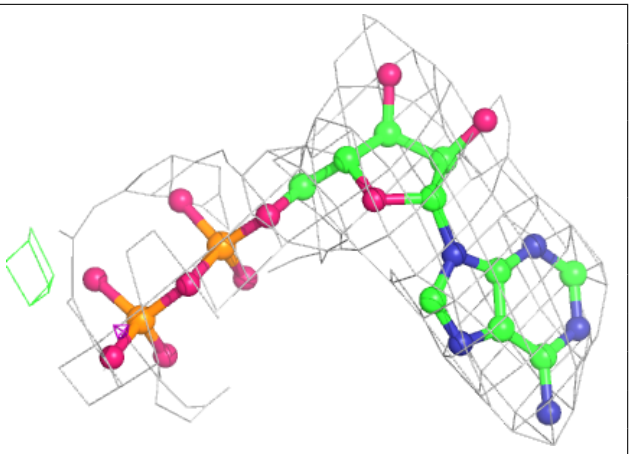


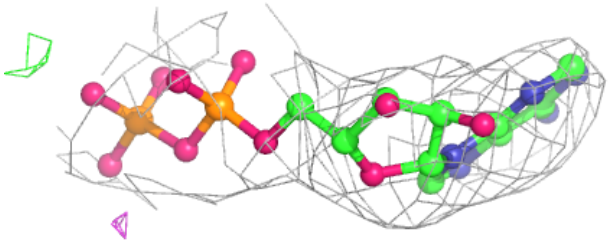


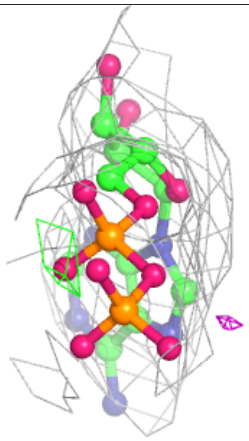


Electron density around ADP F 1001:

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

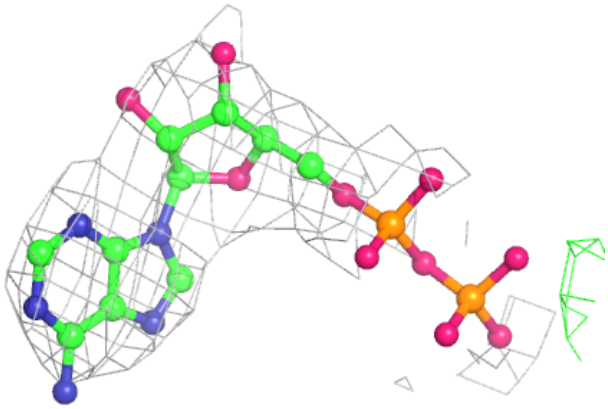


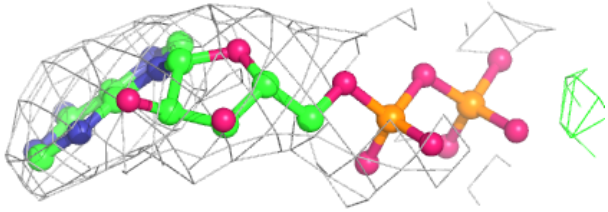


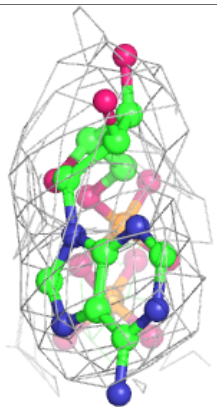


Electron density around ADP P 1001:

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

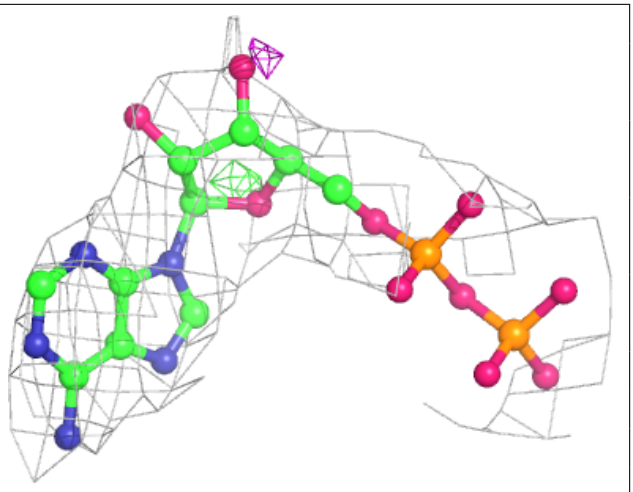


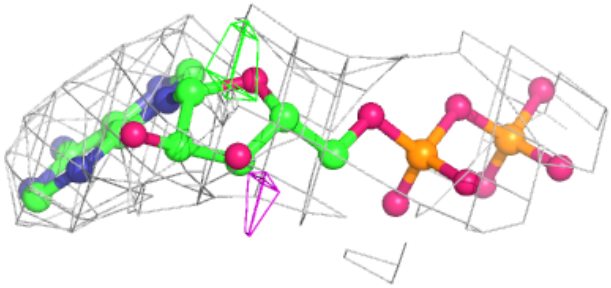


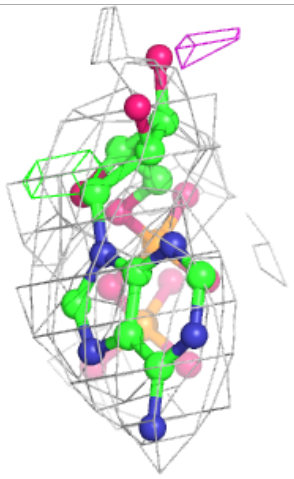


Electron density around ADP E 1001:

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

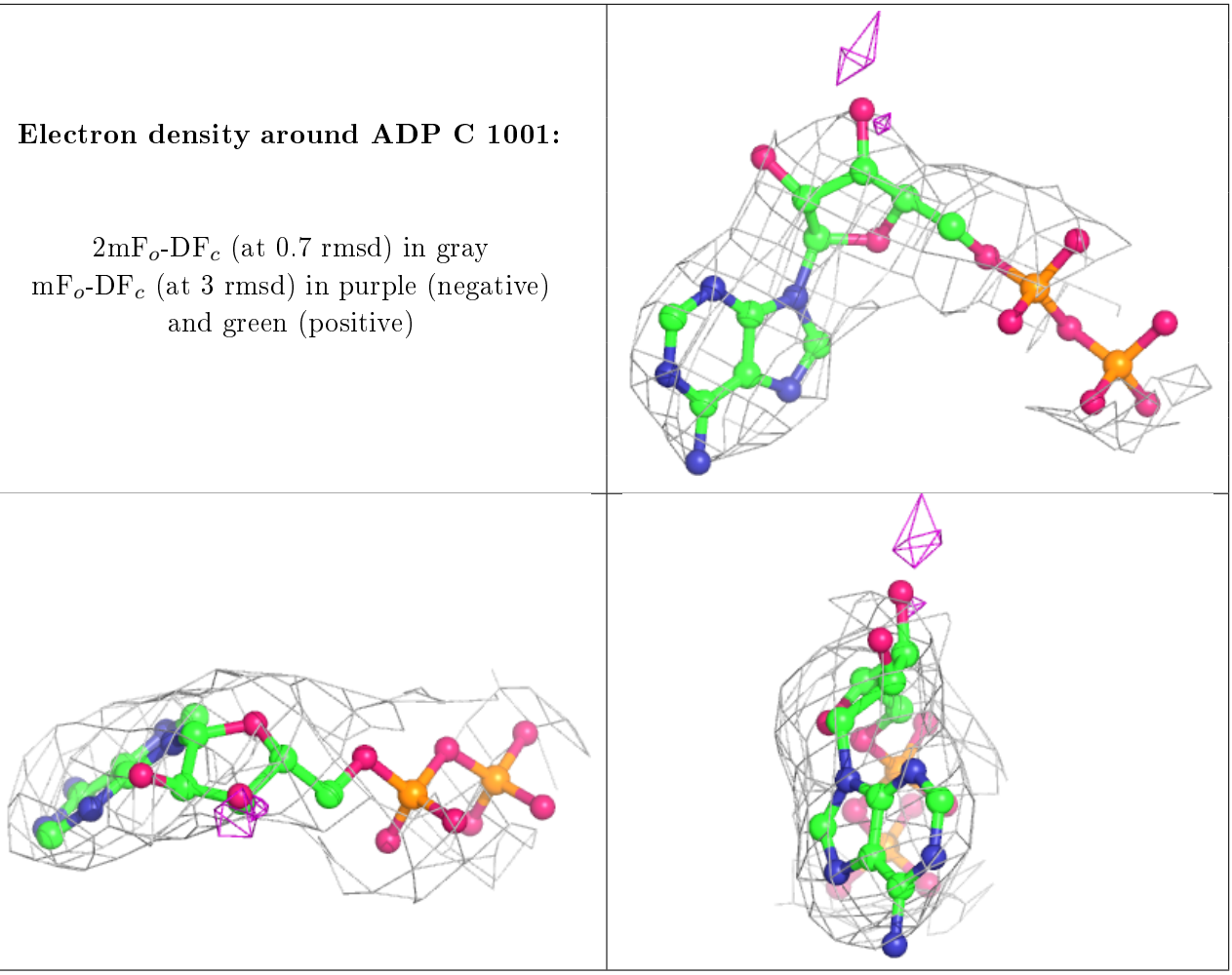






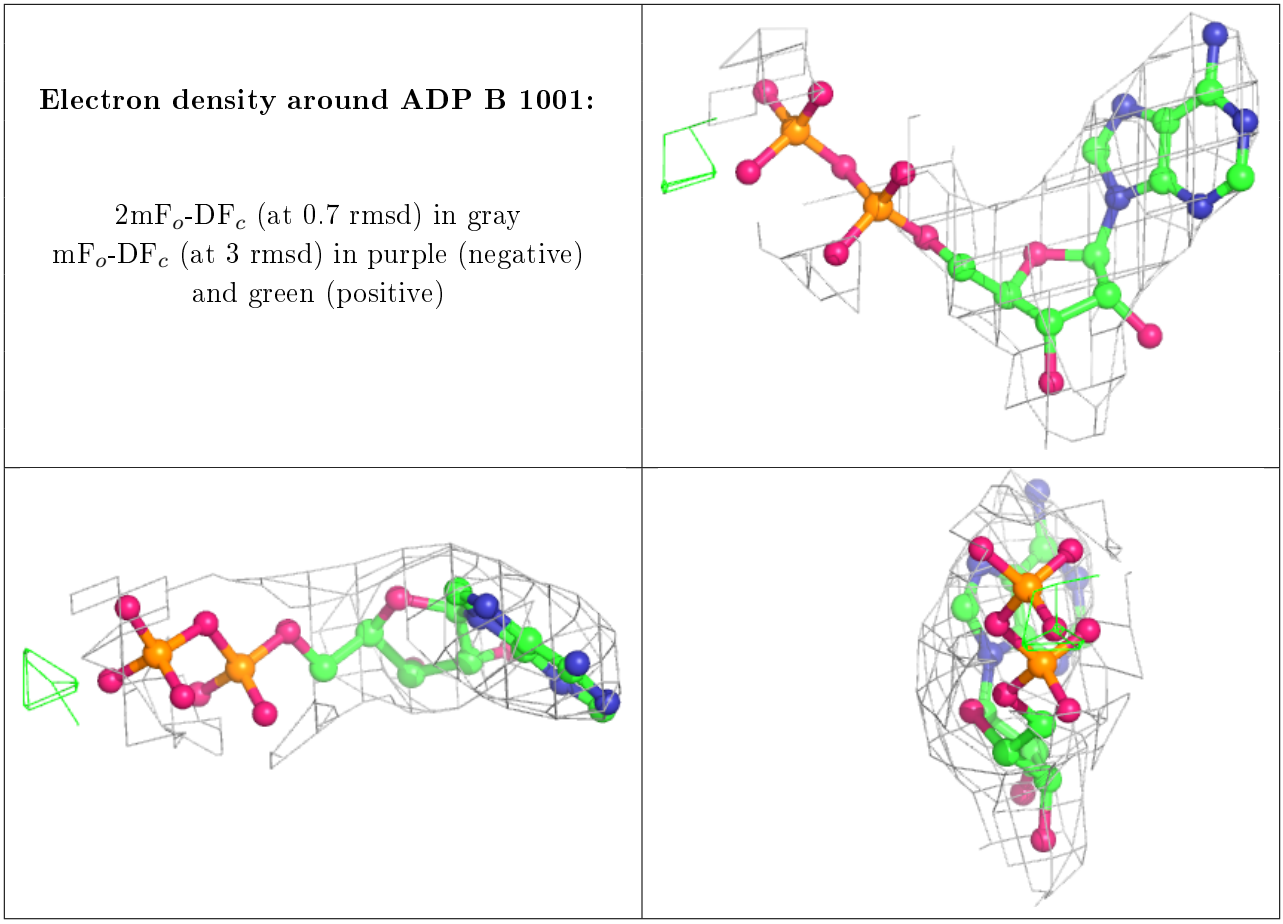
Electron density around ADP C 1001:

$2mF_o$-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 1001:

$2mF_o$-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.