Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 02:14 pm GMT

PDB ID	:	2X86
Title	:	AGME bound to ADP-B-mannose
Authors	:	Kowatz, T.; Morrison, J.P.; Tanner, M.E.; Naismith, J.H.
Deposited on	:	2010-03-06
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i)) were used in the production of this report:

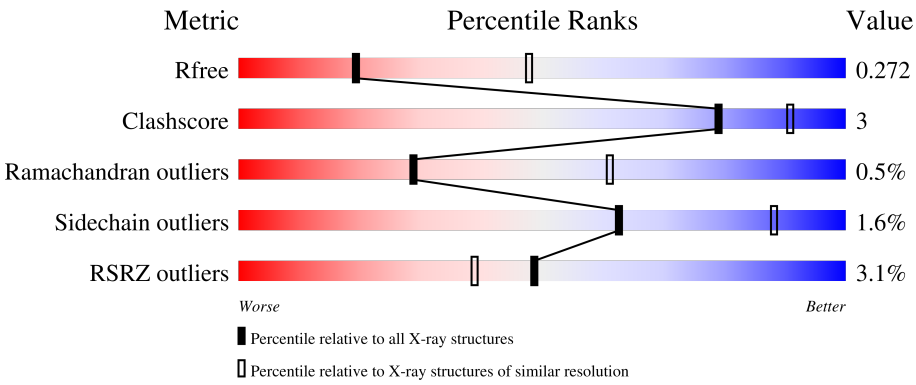
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	A	357	2%, 78%, 7%, 14%
1	B	357	6%, 80%, 6%, 14%
1	C	357	3%, 79%, 6%, 14%
1	D	357	%, 80%, 6%, 14%
1	E	357	%, 79%, 6%, 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	357	3% 78% 7% 14%
1	G	357	8% 80% 5% 14%
1	H	357	2% 80% 6% 14%
1	I	357	% 79% 6% 14%
1	J	357	% 80% 6% 14%
1	K	357	2% 79% 7% 14%
1	L	357	% 79% 6% 14%
1	M	357	% 78% 8% 14%
1	N	357	5% 79% 7% 14%
1	O	357	6% 79% 6% 14%
1	P	357	2% 78% 7% 14%
1	Q	357	% 78% 7% 14%
1	R	357	2% 79% 7% 14%
1	S	357	5% 79% 6% 14%
1	T	357	3% 79% 7% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 51434 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 ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	307	2440	1566	396	469	9	0	0	0
1	B	307	2440	1566	396	469	9	0	0	0
1	C	307	2440	1566	396	469	9	0	0	0
1	D	307	2440	1566	396	469	9	0	0	0
1	E	307	2440	1566	396	469	9	0	0	0
1	F	307	2440	1566	396	469	9	0	0	0
1	G	307	2440	1566	396	469	9	0	0	0
1	H	307	2440	1566	396	469	9	0	0	0
1	I	307	2440	1566	396	469	9	0	0	0
1	J	307	2440	1566	396	469	9	0	0	0
1	K	307	2440	1566	396	469	9	0	0	0
1	L	307	2440	1566	396	469	9	0	0	0
1	M	307	2440	1566	396	469	9	0	0	0
1	N	307	2440	1566	396	469	9	0	0	0
1	O	307	2440	1566	396	469	9	0	0	0
1	P	307	2440	1566	396	469	9	0	0	0

Continued on next page...

Continued from previous page...

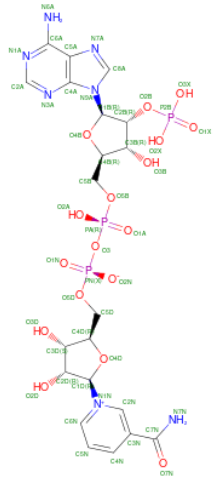
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	307	2440	1566	396	469	9	0	0	0
			Total	C	N	O	S			
1	R	307	2440	1566	396	469	9	0	0	0
			Total	C	N	O	S			
1	S	307	2440	1566	396	469	9	0	0	0
			Total	C	N	O	S			
1	T	307	2440	1566	396	469	9	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	PHE	TYR	engineered mutation	UNP P67911
B	140	PHE	TYR	engineered mutation	UNP P67911
C	140	PHE	TYR	engineered mutation	UNP P67911
D	140	PHE	TYR	engineered mutation	UNP P67911
E	140	PHE	TYR	engineered mutation	UNP P67911
F	140	PHE	TYR	engineered mutation	UNP P67911
G	140	PHE	TYR	engineered mutation	UNP P67911
H	140	PHE	TYR	engineered mutation	UNP P67911
I	140	PHE	TYR	engineered mutation	UNP P67911
J	140	PHE	TYR	engineered mutation	UNP P67911
K	140	PHE	TYR	engineered mutation	UNP P67911
L	140	PHE	TYR	engineered mutation	UNP P67911
M	140	PHE	TYR	engineered mutation	UNP P67911
N	140	PHE	TYR	engineered mutation	UNP P67911
O	140	PHE	TYR	engineered mutation	UNP P67911
P	140	PHE	TYR	engineered mutation	UNP P67911
Q	140	PHE	TYR	engineered mutation	UNP P67911
R	140	PHE	TYR	engineered mutation	UNP P67911
S	140	PHE	TYR	engineered mutation	UNP P67911
T	140	PHE	TYR	engineered mutation	UNP P67911

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

NAP



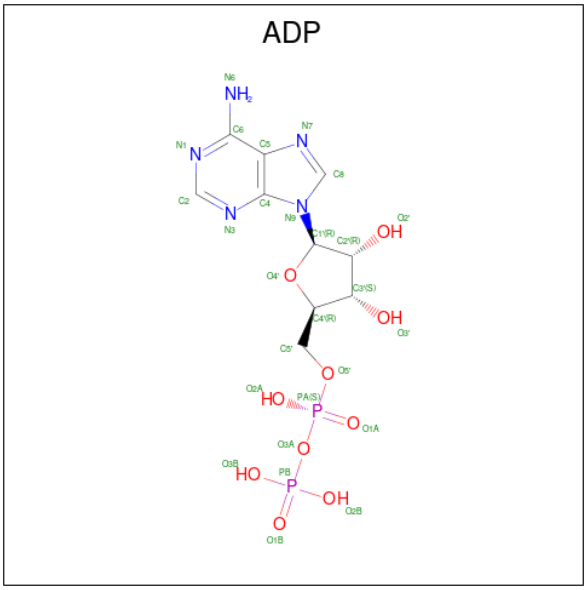
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
2	B	1	48	21	7	17	3	0	0
2	C	1	48	21	7	17	3	0	0
2	D	1	48	21	7	17	3	0	0
2	E	1	48	21	7	17	3	0	0
2	F	1	48	21	7	17	3	0	0
2	G	1	48	21	7	17	3	0	0
2	H	1	48	21	7	17	3	0	0
2	I	1	48	21	7	17	3	0	0
2	J	1	48	21	7	17	3	0	0
2	K	1	48	21	7	17	3	0	0
2	L	1	48	21	7	17	3	0	0
2	M	1	48	21	7	17	3	0	0
2	N	1	48	21	7	17	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	O	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	P	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	Q	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	R	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	S	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	T	1	48	21	7	17	3	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



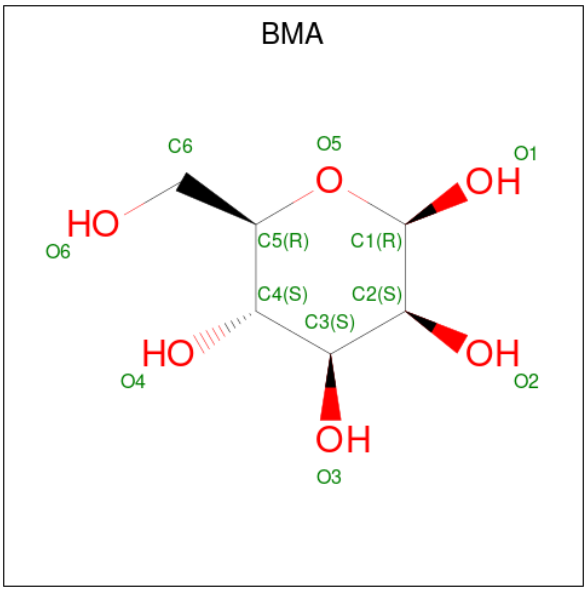
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	B	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	C	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	D	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	E	1	27	10	5	10	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	F	1	27	10	5	10	2	0	0
3	G	1	27	10	5	10	2	0	0
3	H	1	27	10	5	10	2	0	0
3	I	1	27	10	5	10	2	0	0
3	J	1	27	10	5	10	2	0	0
3	K	1	27	10	5	10	2	0	0
3	L	1	27	10	5	10	2	0	0
3	M	1	27	10	5	10	2	0	0
3	N	1	27	10	5	10	2	0	0
3	O	1	27	10	5	10	2	0	0
3	P	1	27	10	5	10	2	0	0
3	Q	1	27	10	5	10	2	0	0
3	R	1	27	10	5	10	2	0	0
3	S	1	27	10	5	10	2	0	0
3	T	1	27	10	5	10	2	0	0

- Molecule 4 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			11	6	5			
4	C	1	Total	C	O		0	0
			11	6	5			
4	D	1	Total	C	O		0	0
			11	6	5			
4	E	1	Total	C	O		0	0
			11	6	5			
4	F	1	Total	C	O		0	0
			11	6	5			
4	G	1	Total	C	O		0	0
			11	6	5			
4	H	1	Total	C	O		0	0
			11	6	5			
4	I	1	Total	C	O		0	0
			11	6	5			
4	J	1	Total	C	O		0	0
			11	6	5			
4	K	1	Total	C	O		0	0
			11	6	5			
4	L	1	Total	C	O		0	0
			11	6	5			
4	M	1	Total	C	O		0	0
			11	6	5			
4	N	1	Total	C	O		0	0
			11	6	5			
4	O	1	Total	C	O		0	0
			11	6	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	P	1	11	6	5	0	0
4	Q	1	11	6	5	0	0
4	R	1	11	6	5	0	0
4	S	1	11	6	5	0	0
4	T	1	11	6	5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	59	59	59	0	0
5	B	36	36	36	0	0
5	C	34	34	34	0	0
5	D	60	60	60	0	0
5	E	61	61	61	0	0
5	F	56	56	56	0	0
5	G	28	28	28	0	0
5	H	49	49	49	0	0
5	I	78	78	78	0	0
5	J	66	66	66	0	0
5	K	59	59	59	0	0
5	L	51	51	51	0	0
5	M	45	45	45	0	0
5	N	39	39	39	0	0

Continued on next page...

Continued from previous page...

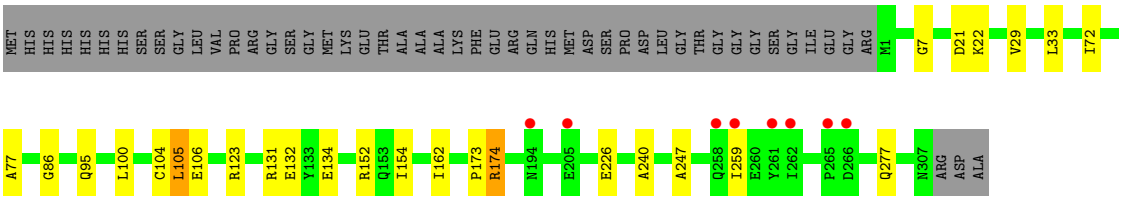
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	33	Total O 33 33	0	0
5	P	49	Total O 49 49	0	0
5	Q	50	Total O 50 50	0	0
5	R	8	Total O 8 8	0	0
5	S	20	Total O 20 20	0	0
5	T	44	Total O 44 44	0	0

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.

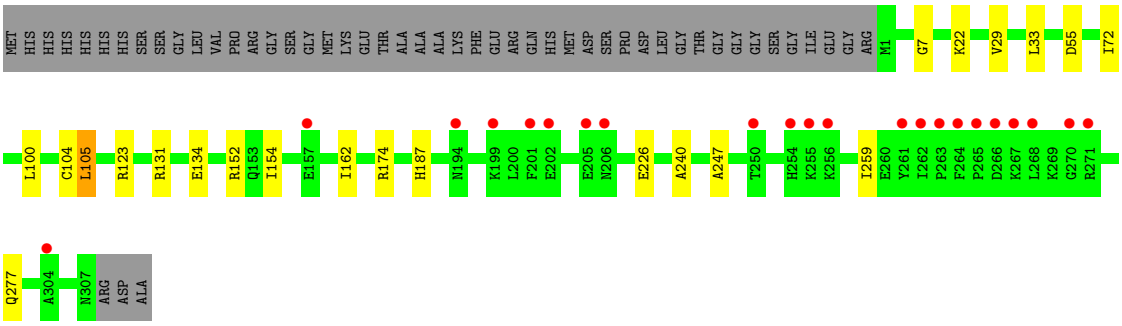
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain A:



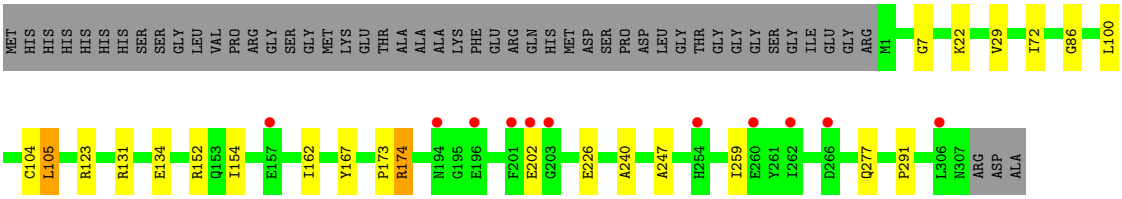
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain B:



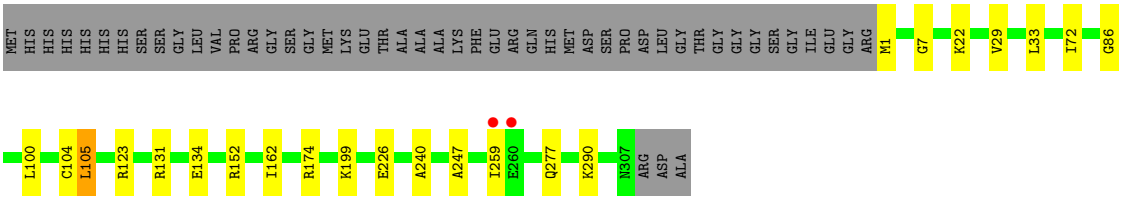
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain C:



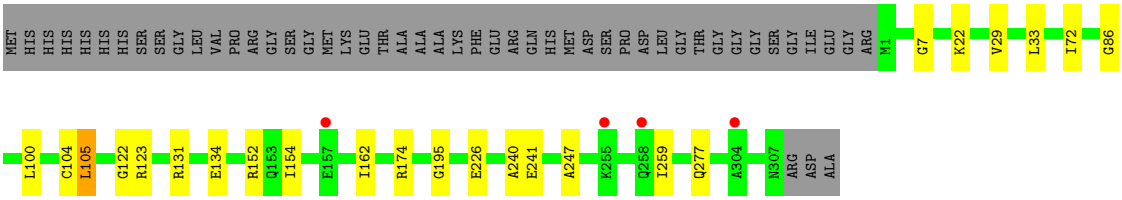
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain D:



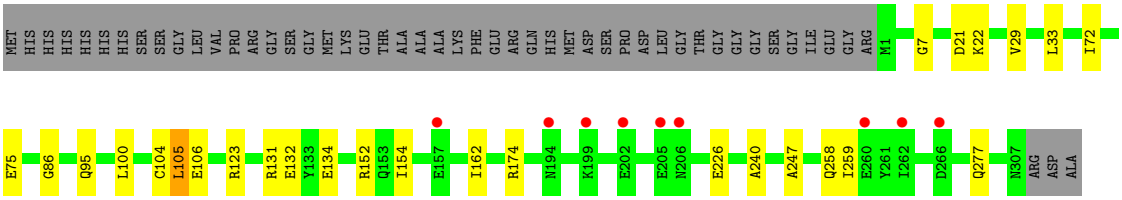
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain E:



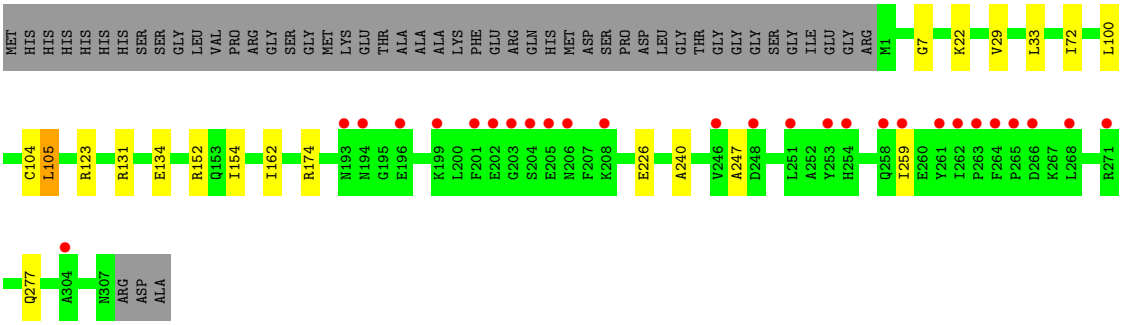
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain F:



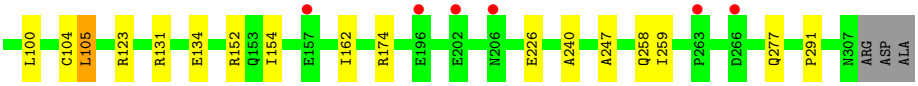
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain G:



• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain H:

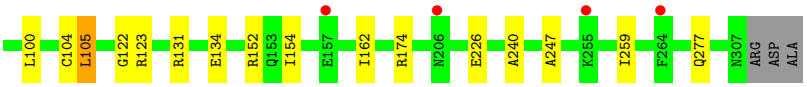


• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain I:

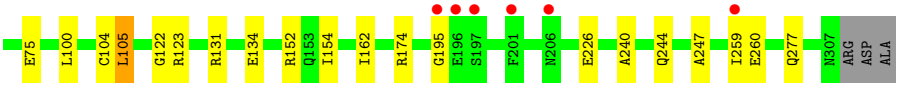
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain J:



• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain K:

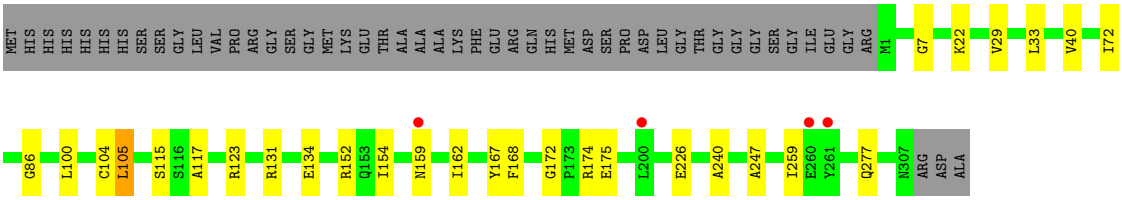


• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain L:

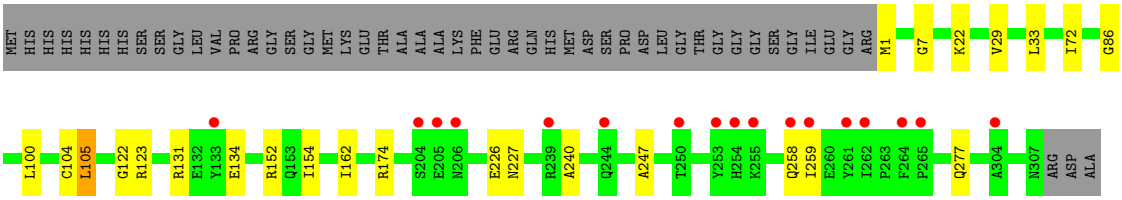
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain M:



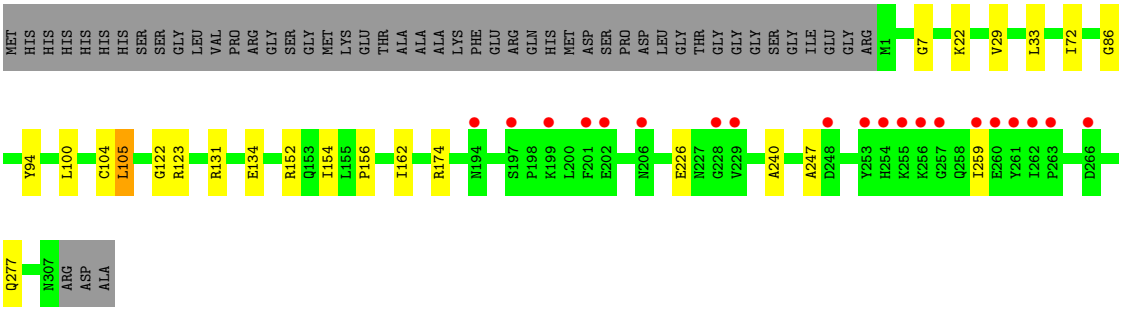
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain N:



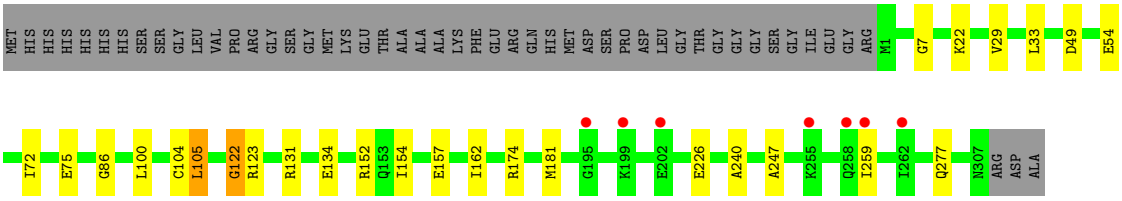
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain O:



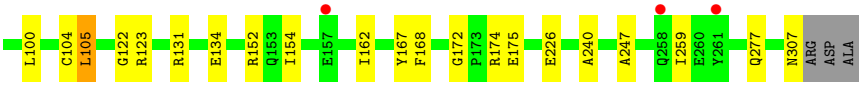
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain P:



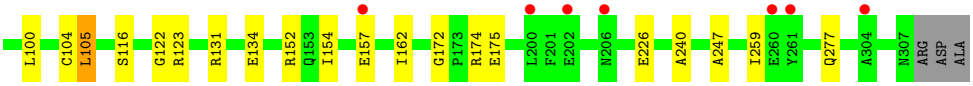
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain Q:



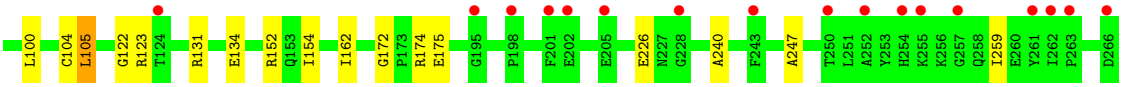
• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

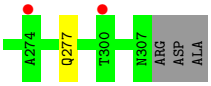
Chain R:



• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain S:





• Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	138.07Å 162.46Å 185.03Å 90.00° 101.45° 90.00°	Depositor
Resolution (Å)	35.05 – 2.80 34.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (35.05-2.80) 96.8 (34.99-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0060	Depositor
R, R_{free}	0.252 , 0.272 0.253 , 0.272	Depositor DCC
R_{free} test set	9658 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	51434	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9719e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: BMA, NAP, 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	0.65	2/2498 (0.1%)	0.66	0/3377
1	B	0.62	0/2498	0.65	0/3377
1	C	0.61	0/2498	0.67	1/3377 (0.0%)
1	D	0.61	0/2498	0.66	0/3377
1	E	0.62	0/2498	0.66	0/3377
1	F	0.65	2/2498 (0.1%)	0.66	0/3377
1	G	0.61	0/2498	0.66	0/3377
1	H	0.61	0/2498	0.65	0/3377
1	I	0.62	0/2498	0.66	0/3377
1	J	0.60	0/2498	0.65	0/3377
1	K	0.62	0/2498	0.66	0/3377
1	L	0.62	0/2498	0.66	0/3377
1	M	0.61	0/2498	0.66	0/3377
1	N	0.61	0/2498	0.65	0/3377
1	O	0.60	0/2498	0.65	0/3377
1	P	0.62	0/2498	0.65	0/3377
1	Q	0.61	0/2498	0.66	0/3377
1	R	0.61	0/2498	0.65	0/3377
1	S	0.60	0/2498	0.65	0/3377
1	T	0.61	0/2498	0.66	0/3377
All	All	0.62	4/49960 (0.0%)	0.66	1/67540 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	132	GLU	CG-CD	8.91	1.65	1.51
1	A	132	GLU	CG-CD	7.90	1.63	1.51
1	F	132	GLU	CB-CG	-7.25	1.38	1.52
1	A	132	GLU	CB-CG	-6.95	1.39	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	202	GLU	OE1-CD-OE2	-5.82	116.31	123.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2440	0	2337	14	1
1	B	2440	0	2337	12	0
1	C	2440	0	2337	13	0
1	D	2440	0	2337	12	1
1	E	2440	0	2337	12	4
1	F	2440	0	2337	13	2
1	G	2440	0	2337	9	0
1	H	2440	0	2337	12	0
1	I	2440	0	2337	14	1
1	J	2440	0	2337	10	0
1	K	2440	0	2337	14	0
1	L	2440	0	2337	11	0
1	M	2440	0	2337	18	4
1	N	2440	0	2337	17	0
1	O	2440	0	2337	15	0
1	P	2440	0	2337	17	0
1	Q	2440	0	2337	14	0
1	R	2440	0	2337	17	0
1	S	2440	0	2337	12	0
1	T	2440	0	2337	14	1
2	A	48	0	25	2	0
2	B	48	0	25	0	0
2	C	48	0	25	3	0
2	D	48	0	25	3	0
2	E	48	0	25	2	0
2	F	48	0	23	3	0
2	G	48	0	23	1	0
2	H	48	0	25	3	0
2	I	48	0	25	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	48	0	25	3	0
2	K	48	0	25	3	0
2	L	48	0	25	3	0
2	M	48	0	25	6	0
2	N	48	0	25	1	0
2	O	48	0	25	1	0
2	P	48	0	25	3	0
2	Q	48	0	25	4	0
2	R	48	0	25	3	0
2	S	48	0	25	1	0
2	T	48	0	25	2	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
3	G	27	0	12	1	0
3	H	27	0	12	0	0
3	I	27	0	12	0	0
3	J	27	0	12	0	0
3	K	27	0	12	0	0
3	L	27	0	12	0	0
3	M	27	0	12	0	0
3	N	27	0	12	0	0
3	O	27	0	12	0	0
3	P	27	0	12	0	0
3	Q	27	0	12	0	0
3	R	27	0	12	0	0
3	S	27	0	12	0	0
3	T	27	0	12	0	0
4	A	11	0	10	1	0
4	C	11	0	10	2	0
4	D	11	0	10	2	0
4	E	11	0	10	2	0
4	F	11	0	10	2	0
4	G	11	0	10	1	0
4	H	11	0	10	2	0
4	I	11	0	10	3	0
4	J	11	0	10	2	0
4	K	11	0	10	2	0
4	L	11	0	10	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	11	0	10	2	0
4	N	11	0	10	1	0
4	O	11	0	10	1	0
4	P	11	0	10	2	0
4	Q	11	0	10	1	0
4	R	11	0	10	2	0
4	S	11	0	10	1	0
4	T	11	0	10	2	0
5	A	59	0	0	1	0
5	B	36	0	0	1	0
5	C	34	0	0	0	0
5	D	60	0	0	3	0
5	E	61	0	0	1	0
5	F	56	0	0	1	0
5	G	28	0	0	0	0
5	H	49	0	0	1	0
5	I	78	0	0	2	0
5	J	66	0	0	0	0
5	K	59	0	0	2	0
5	L	51	0	0	2	0
5	M	45	0	0	1	0
5	N	39	0	0	2	0
5	O	33	0	0	0	0
5	P	49	0	0	3	0
5	Q	50	0	0	1	0
5	R	8	0	0	0	0
5	S	20	0	0	0	0
5	T	44	0	0	0	0
All	All	51434	0	47666	278	7

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 3.

All (278) 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:N:258:GLN:HB3	1:R:157:GLU:OE1	1.58	1.04
1:C:291:PRO:HB3	1:O:156:PRO:O	1.58	1.02
1:N:258:GLN:CB	1:R:157:GLU:OE1	2.10	0.99
2:H:400:NAP:C5N	4:H:402:BMA:H61	2.05	0.86
2:I:400:NAP:C5N	4:I:402:BMA:H61	2.07	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:400:NAP:C4N	4:I:402:BMA:H61	2.14	0.78
2:E:400:NAP:C5N	4:E:402:BMA:H61	2.15	0.77
2:J:400:NAP:C5N	4:J:402:BMA:H61	2.15	0.77
2:T:400:NAP:C5N	4:T:402:BMA:H61	2.15	0.76
2:R:400:NAP:C5N	4:R:402:BMA:H61	2.18	0.74
1:D:1:MET:N	5:D:2001:HOH:O	2.22	0.72
2:F:400:NAP:C5N	4:F:402:BMA:H61	2.20	0.71
2:D:400:NAP:C5N	4:D:402:BMA:H61	2.20	0.71
2:C:400:NAP:C5N	4:C:402:BMA:H61	2.22	0.70
1:N:258:GLN:HB2	1:R:157:GLU:OE1	1.92	0.66
2:C:400:NAP:C4N	4:C:402:BMA:H61	2.26	0.66
1:N:227:ASN:ND2	5:N:2032:HOH:O	2.21	0.65
1:H:291:PRO:HB3	1:T:156:PRO:O	1.96	0.65
2:Q:400:NAP:C5N	4:Q:402:BMA:H61	2.28	0.64
2:J:400:NAP:C4N	4:J:402:BMA:H61	2.28	0.62
2:N:400:NAP:C5N	4:N:402:BMA:H61	2.28	0.62
1:P:122:GLY:HA2	5:P:2048:HOH:O	2.01	0.60
2:M:400:NAP:C4N	4:M:402:BMA:H61	2.31	0.60
1:C:247:ALA:HB1	1:C:259:ILE:HD11	1.85	0.59
3:A:401:ADP:O5'	3:A:401:ADP:H8	1.84	0.59
1:H:247:ALA:HB1	1:H:259:ILE:HD11	1.85	0.59
1:L:247:ALA:HB1	1:L:259:ILE:HD11	1.84	0.59
2:E:400:NAP:C4N	4:E:402:BMA:H61	2.32	0.58
1:T:247:ALA:HB1	1:T:259:ILE:HD11	1.85	0.58
1:Q:247:ALA:HB1	1:Q:259:ILE:HD11	1.84	0.58
2:P:400:NAP:C5N	4:P:402:BMA:H61	2.34	0.58
1:E:247:ALA:HB1	1:E:259:ILE:HD11	1.85	0.58
1:J:247:ALA:HB1	1:J:259:ILE:HD11	1.85	0.58
1:K:75:GLU:O	2:K:400:NAP:H4D	2.04	0.57
1:S:247:ALA:HB1	1:S:259:ILE:HD11	1.85	0.57
1:M:247:ALA:HB1	1:M:259:ILE:HD11	1.86	0.57
1:B:247:ALA:HB1	1:B:259:ILE:HD11	1.85	0.57
1:D:247:ALA:HB1	1:D:259:ILE:HD11	1.85	0.57
1:K:247:ALA:HB1	1:K:259:ILE:HD11	1.85	0.57
1:F:247:ALA:HB1	1:F:259:ILE:HD11	1.86	0.57
1:I:247:ALA:HB1	1:I:259:ILE:HD11	1.85	0.57
1:P:247:ALA:HB1	1:P:259:ILE:HD11	1.85	0.57
2:S:400:NAP:C5N	4:S:402:BMA:H61	2.34	0.57
1:A:106:GLU:O	1:F:258:GLN:OE1	2.23	0.57
1:A:247:ALA:HB1	1:A:259:ILE:HD11	1.86	0.57
1:G:247:ALA:HB1	1:G:259:ILE:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:247:ALA:HB1	1:N:259:ILE:HD11	1.86	0.56
1:L:167:TYR:HB2	2:L:400:NAP:C5N	2.35	0.56
2:M:400:NAP:C5N	4:M:402:BMA:H61	2.36	0.56
1:K:260:GLU:OE1	5:K:2052:HOH:O	2.17	0.56
1:O:247:ALA:HB1	1:O:259:ILE:HD11	1.86	0.56
1:M:167:TYR:HB2	2:M:400:NAP:C5N	2.35	0.56
2:A:400:NAP:C5N	4:A:402:BMA:H61	2.35	0.55
1:R:247:ALA:HB1	1:R:259:ILE:HD11	1.86	0.55
1:F:95:GLN:OE1	5:F:2019:HOH:O	2.18	0.55
1:Q:307:ASN:O	5:Q:2049:HOH:O	2.19	0.54
2:D:400:NAP:C4N	4:D:402:BMA:H61	2.37	0.54
2:H:400:NAP:C4N	4:H:402:BMA:H61	2.38	0.54
1:N:258:GLN:OE1	1:R:157:GLU:OE1	2.26	0.53
2:O:400:NAP:C5N	4:O:402:BMA:H61	2.39	0.53
1:C:86:GLY:HA3	1:D:33:LEU:O	2.09	0.53
1:Q:86:GLY:HA3	1:R:33:LEU:O	2.08	0.53
1:C:167:TYR:HB2	2:C:400:NAP:C5N	2.40	0.51
1:N:258:GLN:OE1	1:R:157:GLU:CD	2.48	0.51
1:P:181:MET:HG3	5:P:2013:HOH:O	2.09	0.51
2:T:400:NAP:C4N	4:T:402:BMA:H61	2.41	0.51
1:I:72:ILE:HD12	1:I:104:CYS:SG	2.51	0.50
1:H:86:GLY:HA3	1:I:33:LEU:O	2.10	0.50
1:L:72:ILE:HD12	1:L:104:CYS:SG	2.52	0.50
1:B:72:ILE:HD12	1:B:104:CYS:SG	2.52	0.50
1:F:72:ILE:HD12	1:F:104:CYS:SG	2.52	0.50
1:Q:72:ILE:HD12	1:Q:104:CYS:SG	2.52	0.50
1:P:72:ILE:HD12	1:P:104:CYS:SG	2.52	0.50
1:A:72:ILE:HD12	1:A:104:CYS:SG	2.52	0.50
1:D:72:ILE:HD12	1:D:104:CYS:SG	2.52	0.50
1:L:86:GLY:HA3	1:M:33:LEU:O	2.12	0.50
2:L:400:NAP:C4N	4:L:402:BMA:H61	2.42	0.50
1:R:72:ILE:HD12	1:R:104:CYS:SG	2.52	0.50
1:O:72:ILE:HD12	1:O:104:CYS:SG	2.52	0.50
1:G:72:ILE:HD12	1:G:104:CYS:SG	2.52	0.50
1:J:72:ILE:HD12	1:J:104:CYS:SG	2.52	0.50
1:N:72:ILE:HD12	1:N:104:CYS:SG	2.52	0.50
1:S:72:ILE:HD12	1:S:104:CYS:SG	2.52	0.50
1:T:72:ILE:HD12	1:T:104:CYS:SG	2.52	0.50
1:C:72:ILE:HD12	1:C:104:CYS:SG	2.52	0.49
1:K:72:ILE:HD12	1:K:104:CYS:SG	2.52	0.49
1:M:72:ILE:HD12	1:M:104:CYS:SG	2.52	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:2039:HOH:O	1:I:40:VAL:HG13	2.11	0.49
1:A:33:LEU:O	1:E:86:GLY:HA3	2.12	0.49
1:H:72:ILE:HD12	1:H:104:CYS:SG	2.52	0.49
1:E:72:ILE:HD12	1:E:104:CYS:SG	2.53	0.49
2:P:400:NAP:C4N	4:P:402:BMA:H61	2.42	0.49
1:T:240:ALA:HB2	1:T:277:GLN:HB2	1.94	0.49
1:N:1:MET:N	5:N:2001:HOH:O	2.45	0.49
1:I:297:GLU:HB3	5:I:2074:HOH:O	2.12	0.48
2:K:400:NAP:C5N	4:K:402:BMA:H61	2.43	0.48
2:I:400:NAP:C5N	4:I:402:BMA:C6	2.87	0.48
1:S:240:ALA:HB2	1:S:277:GLN:HB2	1.95	0.48
1:Q:240:ALA:HB2	1:Q:277:GLN:HB2	1.95	0.48
1:G:240:ALA:HB2	1:G:277:GLN:HB2	1.95	0.48
1:L:240:ALA:HB2	1:L:277:GLN:HB2	1.95	0.48
1:F:240:ALA:HB2	1:F:277:GLN:HB2	1.96	0.48
1:I:240:ALA:HB2	1:I:277:GLN:HB2	1.96	0.48
1:C:240:ALA:HB2	1:C:277:GLN:HB2	1.95	0.48
2:L:400:NAP:C5N	4:L:402:BMA:H61	2.44	0.48
1:R:240:ALA:HB2	1:R:277:GLN:HB2	1.96	0.48
1:S:86:GLY:HA3	1:T:33:LEU:O	2.14	0.48
1:D:240:ALA:HB2	1:D:277:GLN:HB2	1.96	0.47
1:E:240:ALA:HB2	1:E:277:GLN:HB2	1.96	0.47
1:H:240:ALA:HB2	1:H:277:GLN:HB2	1.95	0.47
1:J:240:ALA:HB2	1:J:277:GLN:HB2	1.96	0.47
1:A:86:GLY:HA3	1:B:33:LEU:O	2.14	0.47
1:B:240:ALA:HB2	1:B:277:GLN:HB2	1.96	0.47
1:M:117:ALA:HB3	5:M:2038:HOH:O	2.13	0.47
1:N:240:ALA:HB2	1:N:277:GLN:HB2	1.95	0.47
1:M:240:ALA:HB2	1:M:277:GLN:HB2	1.96	0.47
1:P:240:ALA:HB2	1:P:277:GLN:HB2	1.96	0.47
1:O:240:ALA:HB2	1:O:277:GLN:HB2	1.96	0.47
1:C:291:PRO:CB	1:O:156:PRO:O	2.46	0.47
1:K:195:GLY:HA3	1:P:157:GLU:OE1	2.15	0.47
1:K:240:ALA:HB2	1:K:277:GLN:HB2	1.96	0.47
5:L:2044:HOH:O	1:M:40:VAL:HG13	2.13	0.47
1:A:95:GLN:OE1	5:A:2023:HOH:O	2.21	0.47
1:A:240:ALA:HB2	1:A:277:GLN:HB2	1.97	0.47
1:D:199:LYS:HE2	5:D:2042:HOH:O	2.16	0.46
1:D:290:LYS:HD2	5:D:2057:HOH:O	2.14	0.46
1:F:86:GLY:HA3	1:G:33:LEU:O	2.16	0.46
1:M:167:TYR:HB2	2:M:400:NAP:C4N	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:105:LEU:HD21	1:K:154:ILE:HG21	1.98	0.46
1:P:105:LEU:HD21	1:P:154:ILE:HG21	1.98	0.46
1:P:54:GLU:HB2	5:P:2007:HOH:O	2.16	0.45
1:R:22:LYS:HE3	1:R:226:GLU:OE2	2.17	0.45
1:E:22:LYS:HE3	1:E:226:GLU:OE2	2.17	0.45
1:P:75:GLU:O	2:P:400:NAP:H4D	2.16	0.45
1:T:22:LYS:HE3	1:T:226:GLU:OE2	2.16	0.45
1:B:22:LYS:HE3	1:B:226:GLU:OE2	2.16	0.45
1:Q:168:PHE:O	2:Q:400:NAP:H4N	2.17	0.45
1:M:115:SER:O	2:M:400:NAP:H6N	2.15	0.45
1:S:105:LEU:HD21	1:S:154:ILE:HG21	1.98	0.45
1:J:22:LYS:HE3	1:J:226:GLU:OE2	2.17	0.45
1:O:22:LYS:HE3	1:O:226:GLU:OE2	2.16	0.45
1:B:187:HIS:CE1	3:B:401:ADP:O2'	2.70	0.45
1:C:22:LYS:HE3	1:C:226:GLU:OE2	2.17	0.45
2:D:400:NAP:O3X	2:D:400:NAP:H8A	2.17	0.45
1:H:22:LYS:HE3	1:H:226:GLU:OE2	2.17	0.45
1:I:22:LYS:HE3	1:I:226:GLU:OE2	2.17	0.45
1:M:22:LYS:HE3	1:M:226:GLU:OE2	2.17	0.45
1:H:258:GLN:HG3	1:O:277:GLN:OE1	2.17	0.45
2:J:400:NAP:H8A	2:J:400:NAP:O3X	2.16	0.45
1:G:22:LYS:HE3	1:G:226:GLU:OE2	2.17	0.45
1:D:22:LYS:HE3	1:D:226:GLU:OE2	2.17	0.44
1:K:22:LYS:HE3	1:K:226:GLU:OE2	2.17	0.44
1:M:86:GLY:HA3	1:N:33:LEU:O	2.17	0.44
5:L:2044:HOH:O	1:M:40:VAL:CG1	2.65	0.44
1:A:22:LYS:HE3	1:A:226:GLU:OE2	2.18	0.44
1:S:22:LYS:HE3	1:S:226:GLU:OE2	2.17	0.44
1:A:77:ALA:HB3	2:A:400:NAP:O3D	2.17	0.44
1:D:86:GLY:HA3	1:E:33:LEU:O	2.18	0.44
1:N:22:LYS:HE3	1:N:226:GLU:OE2	2.18	0.44
1:P:22:LYS:HE3	1:P:226:GLU:OE2	2.18	0.44
1:Q:105:LEU:HD21	1:Q:154:ILE:HG21	1.99	0.44
1:L:22:LYS:HE3	1:L:226:GLU:OE2	2.17	0.44
1:K:244:GLN:HB2	5:K:2042:HOH:O	2.17	0.43
1:L:134:GLU:OE1	1:L:152:ARG:NH2	2.51	0.43
1:O:134:GLU:OE1	1:O:152:ARG:NH2	2.51	0.43
1:I:297:GLU:CG	5:I:2074:HOH:O	2.65	0.43
1:M:105:LEU:HD21	1:M:154:ILE:HG21	2.00	0.43
1:F:33:LEU:O	1:J:86:GLY:HA3	2.18	0.43
1:K:33:LEU:O	1:O:86:GLY:HA3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:LEU:HD21	1:L:154:ILE:HG21	1.99	0.43
1:N:134:GLU:OE1	1:N:152:ARG:NH2	2.52	0.43
1:Q:22:LYS:HE3	1:Q:226:GLU:OE2	2.17	0.43
1:T:134:GLU:OE1	1:T:152:ARG:NH2	2.51	0.43
1:F:22:LYS:HE3	1:F:226:GLU:OE2	2.18	0.43
1:G:134:GLU:OE1	1:G:152:ARG:NH2	2.52	0.43
1:O:105:LEU:HD12	1:O:105:LEU:HA	1.90	0.43
1:H:134:GLU:OE1	1:H:152:ARG:NH2	2.52	0.43
1:I:86:GLY:HA3	1:J:33:LEU:O	2.19	0.43
1:M:105:LEU:HD11	1:M:162:ILE:HD11	2.00	0.43
1:T:105:LEU:HD21	1:T:154:ILE:HG21	2.00	0.43
1:B:134:GLU:OE1	1:B:152:ARG:NH2	2.52	0.43
1:A:105:LEU:HD21	1:A:154:ILE:HG21	2.01	0.43
1:E:105:LEU:HD12	1:E:105:LEU:HA	1.90	0.43
3:G:401:ADP:O5'	3:G:401:ADP:H8	2.01	0.43
1:L:105:LEU:HD11	1:L:162:ILE:HD11	2.01	0.43
1:N:105:LEU:HD21	1:N:154:ILE:HG21	2.01	0.43
1:P:105:LEU:HD11	1:P:162:ILE:HD11	2.01	0.43
1:R:105:LEU:HD11	1:R:162:ILE:HD11	2.01	0.43
1:S:134:GLU:OE1	1:S:152:ARG:NH2	2.52	0.43
1:A:105:LEU:HD11	1:A:162:ILE:HD11	2.01	0.43
1:D:134:GLU:OE1	1:D:152:ARG:NH2	2.52	0.43
1:E:134:GLU:OE1	1:E:152:ARG:NH2	2.52	0.43
1:I:134:GLU:OE1	1:I:152:ARG:NH2	2.52	0.43
1:K:105:LEU:HD11	1:K:162:ILE:HD11	2.00	0.43
1:N:7:GLY:HA3	1:N:29:VAL:HG13	2.00	0.43
1:O:105:LEU:HD21	1:O:154:ILE:HG21	2.01	0.43
1:Q:105:LEU:HD11	1:Q:162:ILE:HD11	2.01	0.43
1:Q:134:GLU:OE1	1:Q:152:ARG:NH2	2.52	0.43
1:J:134:GLU:OE1	1:J:152:ARG:NH2	2.52	0.43
1:O:105:LEU:HD11	1:O:162:ILE:HD11	2.01	0.43
2:R:400:NAP:C6N	4:R:402:BMA:H61	2.49	0.43
1:S:7:GLY:HA3	1:S:29:VAL:HG13	2.01	0.43
1:B:105:LEU:HD11	1:B:162:ILE:HD11	2.01	0.42
1:C:134:GLU:OE1	1:C:152:ARG:NH2	2.52	0.42
1:F:105:LEU:HD11	1:F:162:ILE:HD11	2.01	0.42
2:F:400:NAP:C4N	4:F:402:BMA:H61	2.48	0.42
1:K:134:GLU:OE1	1:K:152:ARG:NH2	2.52	0.42
1:R:134:GLU:OE1	1:R:152:ARG:NH2	2.52	0.42
1:F:134:GLU:OE1	1:F:152:ARG:NH2	2.52	0.42
1:R:105:LEU:HD21	1:R:154:ILE:HG21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:GLU:HB3	5:E:2038:HOH:O	2.19	0.42
1:F:105:LEU:HD21	1:F:154:ILE:HG21	2.01	0.42
1:G:105:LEU:HD11	1:G:162:ILE:HD11	2.02	0.42
1:I:105:LEU:HD11	1:I:162:ILE:HD11	2.01	0.42
1:M:134:GLU:OE1	1:M:152:ARG:NH2	2.52	0.42
1:A:134:GLU:OE1	1:A:152:ARG:NH2	2.52	0.42
1:O:7:GLY:HA3	1:O:29:VAL:HG13	2.02	0.42
1:P:105:LEU:HD12	1:P:105:LEU:HA	1.90	0.42
1:T:105:LEU:HD11	1:T:162:ILE:HD11	2.01	0.42
1:C:105:LEU:HD21	1:C:154:ILE:HG21	2.00	0.42
1:H:105:LEU:HD21	1:H:154:ILE:HG21	2.00	0.42
1:J:7:GLY:HA3	1:J:29:VAL:HG13	2.02	0.42
1:P:134:GLU:OE1	1:P:152:ARG:NH2	2.52	0.42
1:D:105:LEU:HD11	1:D:162:ILE:HD11	2.02	0.42
1:P:49:ASP:OD1	1:T:94:TYR:OH	2.32	0.42
1:E:105:LEU:HD21	1:E:154:ILE:HG21	2.01	0.42
1:G:7:GLY:HA3	1:G:29:VAL:HG13	2.01	0.42
1:C:105:LEU:HD11	1:C:162:ILE:HD11	2.01	0.42
1:E:105:LEU:HD11	1:E:162:ILE:HD11	2.01	0.42
1:H:105:LEU:HD11	1:H:162:ILE:HD11	2.01	0.42
1:J:105:LEU:HD21	1:J:154:ILE:HG21	2.01	0.42
1:J:105:LEU:HD11	1:J:162:ILE:HD11	2.01	0.42
1:K:7:GLY:HA3	1:K:29:VAL:HG13	2.01	0.42
1:R:86:GLY:HA3	1:S:33:LEU:O	2.20	0.42
1:H:10:PHE:HB3	2:H:400:NAP:O2N	2.19	0.41
1:S:105:LEU:HD11	1:S:162:ILE:HD11	2.00	0.41
1:D:7:GLY:HA3	1:D:29:VAL:HG13	2.02	0.41
1:E:7:GLY:HA3	1:E:29:VAL:HG13	2.02	0.41
1:F:7:GLY:HA3	1:F:29:VAL:HG13	2.01	0.41
1:N:86:GLY:HA3	1:O:33:LEU:O	2.20	0.41
1:T:7:GLY:HA3	1:T:29:VAL:HG13	2.03	0.41
1:F:75:GLU:O	2:F:400:NAP:H4D	2.20	0.41
1:I:105:LEU:HD21	1:I:154:ILE:HG21	2.02	0.41
1:H:7:GLY:HA3	1:H:29:VAL:HG13	2.01	0.41
1:L:7:GLY:HA3	1:L:29:VAL:HG13	2.02	0.41
1:C:7:GLY:HA3	1:C:29:VAL:HG13	2.02	0.41
1:N:105:LEU:HD11	1:N:162:ILE:HD11	2.01	0.41
1:P:86:GLY:HA3	1:Q:33:LEU:O	2.19	0.41
1:I:7:GLY:HA3	1:I:29:VAL:HG13	2.02	0.41
2:K:400:NAP:C4N	4:K:402:BMA:H61	2.51	0.41
1:M:7:GLY:HA3	1:M:29:VAL:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:33:LEU:O	1:T:86:GLY:HA3	2.20	0.41
1:B:7:GLY:HA3	1:B:29:VAL:HG13	2.02	0.41
1:G:105:LEU:HD21	1:G:154:ILE:HG21	2.02	0.41
1:Q:7:GLY:HA3	1:Q:29:VAL:HG13	2.02	0.41
1:T:251:LEU:HD13	1:T:257:GLY:O	2.21	0.41
1:A:7:GLY:HA3	1:A:29:VAL:HG13	2.01	0.41
1:I:105:LEU:HD12	1:I:105:LEU:HA	1.89	0.41
1:P:7:GLY:HA3	1:P:29:VAL:HG13	2.01	0.41
1:B:55:ASP:HB3	5:B:2010:HOH:O	2.20	0.41
1:B:105:LEU:HD21	1:B:154:ILE:HG21	2.03	0.41
1:M:168:PHE:O	2:M:400:NAP:H4N	2.20	0.41
1:R:172:GLY:O	1:R:175:GLU:HG2	2.22	0.40
1:S:172:GLY:O	1:S:175:GLU:HG2	2.22	0.40
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.90	0.40
1:Q:167:TYR:HB2	2:Q:400:NAP:C5N	2.52	0.40
1:T:134:GLU:CD	1:T:152:ARG:HH22	2.25	0.40
1:A:173:PRO:O	1:A:174:ARG:HB2	2.22	0.40
1:C:173:PRO:O	1:C:174:ARG:HB2	2.22	0.40
1:K:49:ASP:OD1	1:O:94:TYR:OH	2.21	0.40
1:L:172:GLY:O	1:L:175:GLU:HG2	2.22	0.40
1:Q:172:GLY:O	1:Q:175:GLU:HG2	2.22	0.40
1:R:7:GLY:HA3	1:R:29:VAL:HG13	2.02	0.40
1:S:105:LEU:HD12	1:S:105:LEU:HA	1.90	0.40
2:G:400:NAP:C4N	4:G:402:BMA:H61	2.51	0.40
1:M:172:GLY:O	1:M:175:GLU:HG2	2.22	0.40
2:Q:400:NAP:P2B	2:Q:400:NAP:H8A	2.62	0.40
1:R:116:SER:HB2	2:R:400:NAP:H6N	2.04	0.40

All (7) 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:E:195:GLY:O	1:M:159:ASN:OD1[2_646]	1.33	0.87
1:A:21:ASP:O	1:I:277:GLN:OE1[2_546]	1.58	0.62
1:D:277:GLN:OE1	1:F:21:ASP:O[2_556]	1.79	0.41
1:E:195:GLY:O	1:M:159:ASN:CG[2_646]	1.88	0.32
1:E:195:GLY:C	1:M:159:ASN:OD1[2_646]	1.99	0.21
1:E:195:GLY:O	1:M:159:ASN:ND2[2_646]	2.07	0.13
1:F:106:GLU:OE1	1:T:257:GLY:C[2_547]	2.15	0.05

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	305/357 (85%)	298 (98%)	6 (2%)	1 (0%)	41	72
1	B	305/357 (85%)	297 (97%)	7 (2%)	1 (0%)	41	72
1	C	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	41	72
1	D	305/357 (85%)	297 (97%)	7 (2%)	1 (0%)	41	72
1	E	305/357 (85%)	297 (97%)	6 (2%)	2 (1%)	22	53
1	F	305/357 (85%)	298 (98%)	6 (2%)	1 (0%)	41	72
1	G	305/357 (85%)	297 (97%)	7 (2%)	1 (0%)	41	72
1	H	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	41	72
1	I	305/357 (85%)	297 (97%)	6 (2%)	2 (1%)	22	53
1	J	305/357 (85%)	297 (97%)	6 (2%)	2 (1%)	22	53
1	K	305/357 (85%)	298 (98%)	5 (2%)	2 (1%)	22	53
1	L	305/357 (85%)	296 (97%)	7 (2%)	2 (1%)	22	53
1	M	305/357 (85%)	297 (97%)	7 (2%)	1 (0%)	41	72
1	N	305/357 (85%)	297 (97%)	6 (2%)	2 (1%)	22	53
1	O	305/357 (85%)	297 (97%)	6 (2%)	2 (1%)	22	53
1	P	305/357 (85%)	296 (97%)	7 (2%)	2 (1%)	22	53
1	Q	305/357 (85%)	297 (97%)	6 (2%)	2 (1%)	22	53
1	R	305/357 (85%)	297 (97%)	6 (2%)	2 (1%)	22	53
1	S	305/357 (85%)	296 (97%)	7 (2%)	2 (1%)	22	53
1	T	305/357 (85%)	296 (97%)	7 (2%)	2 (1%)	22	53
All	All	6100/7140 (85%)	5937 (97%)	131 (2%)	32 (0%)	29	61

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	174	ARG
1	C	174	ARG
1	D	174	ARG
1	E	174	ARG
1	F	174	ARG
1	G	174	ARG
1	H	174	ARG
1	I	174	ARG
1	J	174	ARG
1	K	174	ARG
1	L	174	ARG
1	M	174	ARG
1	N	174	ARG
1	O	174	ARG
1	P	174	ARG
1	Q	174	ARG
1	R	174	ARG
1	S	174	ARG
1	T	174	ARG
1	L	122	GLY
1	Q	122	GLY
1	E	122	GLY
1	I	122	GLY
1	K	122	GLY
1	O	122	GLY
1	P	122	GLY
1	T	122	GLY
1	J	122	GLY
1	N	122	GLY
1	R	122	GLY
1	S	122	GLY

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	B	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	C	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	D	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	E	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	F	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	G	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	H	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	I	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	J	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	K	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	L	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	M	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	N	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	O	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	P	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	Q	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	R	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	S	255/292 (87%)	251 (98%)	4 (2%)	62	88
1	T	255/292 (87%)	251 (98%)	4 (2%)	62	88
All	All	5100/5840 (87%)	5020 (98%)	80 (2%)	62	88

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LEU
1	A	105	LEU
1	A	123	ARG
1	A	131	ARG
1	B	100	LEU
1	B	105	LEU
1	B	123	ARG
1	B	131	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	100	LEU
1	C	105	LEU
1	C	123	ARG
1	C	131	ARG
1	D	100	LEU
1	D	105	LEU
1	D	123	ARG
1	D	131	ARG
1	E	100	LEU
1	E	105	LEU
1	E	123	ARG
1	E	131	ARG
1	F	100	LEU
1	F	105	LEU
1	F	123	ARG
1	F	131	ARG
1	G	100	LEU
1	G	105	LEU
1	G	123	ARG
1	G	131	ARG
1	H	100	LEU
1	H	105	LEU
1	H	123	ARG
1	H	131	ARG
1	I	100	LEU
1	I	105	LEU
1	I	123	ARG
1	I	131	ARG
1	J	100	LEU
1	J	105	LEU
1	J	123	ARG
1	J	131	ARG
1	K	100	LEU
1	K	105	LEU
1	K	123	ARG
1	K	131	ARG
1	L	100	LEU
1	L	105	LEU
1	L	123	ARG
1	L	131	ARG
1	M	100	LEU
1	M	105	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	123	ARG
1	M	131	ARG
1	N	100	LEU
1	N	105	LEU
1	N	123	ARG
1	N	131	ARG
1	O	100	LEU
1	O	105	LEU
1	O	123	ARG
1	O	131	ARG
1	P	100	LEU
1	P	105	LEU
1	P	123	ARG
1	P	131	ARG
1	Q	100	LEU
1	Q	105	LEU
1	Q	123	ARG
1	Q	131	ARG
1	R	100	LEU
1	R	105	LEU
1	R	123	ARG
1	R	131	ARG
1	S	100	LEU
1	S	105	LEU
1	S	123	ARG
1	S	131	ARG
1	T	100	LEU
1	T	105	LEU
1	T	123	ARG
1	T	131	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	277	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

59 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	R	400	-	45,52,52	1.79	6 (13%)	56,80,80	1.46	6 (10%)
2	NAP	O	400	-	45,52,52	1.76	7 (15%)	56,80,80	1.52	9 (16%)
3	ADP	R	401	4	24,29,29	1.31	3 (12%)	29,45,45	1.52	5 (17%)
4	BMA	R	402	3	11,11,12	0.69	0	15,15,17	2.33	5 (33%)
2	NAP	E	400	-	45,52,52	1.98	6 (13%)	56,80,80	1.41	6 (10%)
3	ADP	N	401	4	24,29,29	1.32	3 (12%)	29,45,45	1.92	7 (24%)
3	ADP	P	401	4	24,29,29	1.23	3 (12%)	29,45,45	1.59	5 (17%)
2	NAP	N	400	-	45,52,52	1.82	5 (11%)	56,80,80	1.17	2 (3%)
3	ADP	G	401	4	24,29,29	1.34	3 (12%)	29,45,45	1.80	6 (20%)
4	BMA	S	402	3	11,11,12	0.47	0	15,15,17	0.97	0
2	NAP	Q	400	-	45,52,52	1.92	5 (11%)	56,80,80	1.27	3 (5%)
4	BMA	G	402	3	11,11,12	0.60	0	15,15,17	0.62	0
3	ADP	H	401	4	24,29,29	1.23	2 (8%)	29,45,45	1.85	8 (27%)
4	BMA	K	402	3	11,11,12	0.70	0	15,15,17	0.86	0
3	ADP	K	401	4	24,29,29	1.24	3 (12%)	29,45,45	1.91	7 (24%)
2	NAP	M	400	-	45,52,52	1.80	4 (8%)	56,80,80	1.32	4 (7%)
2	NAP	F	400	-	45,52,52	3.82	10 (22%)	56,80,80	3.09	12 (21%)
3	ADP	I	401	4	24,29,29	1.27	3 (12%)	29,45,45	1.72	8 (27%)
4	BMA	H	402	3	11,11,12	0.78	0	15,15,17	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	NAP	C	400	-	45,52,52	2.39	5 (11%)	56,80,80	1.72	8 (14%)
2	NAP	G	400	-	45,52,52	3.23	11 (24%)	56,80,80	2.55	12 (21%)
3	ADP	L	401	4	24,29,29	1.24	3 (12%)	29,45,45	1.69	4 (13%)
3	ADP	T	401	4	24,29,29	1.28	3 (12%)	29,45,45	1.57	6 (20%)
4	BMA	O	402	3	11,11,12	0.55	0	15,15,17	0.96	1 (6%)
3	ADP	O	401	4	24,29,29	1.26	3 (12%)	29,45,45	1.63	4 (13%)
2	NAP	B	400	-	45,52,52	1.83	5 (11%)	56,80,80	1.36	7 (12%)
2	NAP	J	400	-	45,52,52	1.86	6 (13%)	56,80,80	1.44	6 (10%)
3	ADP	J	401	4	24,29,29	1.25	3 (12%)	29,45,45	2.09	9 (31%)
4	BMA	N	402	3	11,11,12	0.53	0	15,15,17	0.81	0
4	BMA	P	402	3	11,11,12	0.70	0	15,15,17	1.25	2 (13%)
4	BMA	D	402	3	11,11,12	0.57	0	15,15,17	1.16	3 (20%)
4	BMA	T	402	3	11,11,12	0.65	0	15,15,17	0.83	0
2	NAP	P	400	-	45,52,52	2.38	10 (22%)	56,80,80	1.46	8 (14%)
3	ADP	Q	401	4	24,29,29	1.18	3 (12%)	29,45,45	1.76	7 (24%)
2	NAP	D	400	-	45,52,52	1.85	4 (8%)	56,80,80	1.11	2 (3%)
3	ADP	E	401	4	24,29,29	1.23	4 (16%)	29,45,45	2.00	8 (27%)
4	BMA	A	402	3	11,11,12	0.69	0	15,15,17	0.92	1 (6%)
3	ADP	F	401	4	24,29,29	1.28	3 (12%)	29,45,45	1.71	6 (20%)
4	BMA	F	402	3	11,11,12	0.52	0	15,15,17	0.92	0
4	BMA	C	402	3	11,11,12	0.75	0	15,15,17	0.98	1 (6%)
2	NAP	L	400	-	45,52,52	1.92	5 (11%)	56,80,80	1.25	5 (8%)
3	ADP	C	401	4	24,29,29	1.26	3 (12%)	29,45,45	1.65	5 (17%)
4	BMA	L	402	3	11,11,12	0.66	0	15,15,17	0.70	0
2	NAP	S	400	-	45,52,52	1.82	4 (8%)	56,80,80	1.11	2 (3%)
4	BMA	E	402	3	11,11,12	0.63	0	15,15,17	1.13	1 (6%)
3	ADP	A	401	4	24,29,29	1.28	3 (12%)	29,45,45	1.78	8 (27%)
4	BMA	M	402	3	11,11,12	0.48	0	15,15,17	1.17	2 (13%)
3	ADP	B	401	-	24,29,29	0.95	1 (4%)	29,45,45	1.42	5 (17%)
3	ADP	M	401	4	24,29,29	1.37	3 (12%)	29,45,45	1.90	5 (17%)
4	BMA	Q	402	3	11,11,12	0.59	0	15,15,17	0.84	0
2	NAP	K	400	-	45,52,52	2.25	9 (20%)	56,80,80	1.84	11 (19%)
3	ADP	D	401	4	24,29,29	1.28	2 (8%)	29,45,45	1.90	8 (27%)
4	BMA	I	402	3	11,11,12	0.33	0	15,15,17	1.01	2 (13%)
4	BMA	J	402	3	11,11,12	0.60	0	15,15,17	0.93	1 (6%)
2	NAP	H	400	-	45,52,52	2.04	6 (13%)	56,80,80	1.24	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	I	400	-	45,52,52	1.88	5 (11%)	56,80,80	1.26	4 (7%)
2	NAP	A	400	-	45,52,52	1.75	6 (13%)	56,80,80	1.61	9 (16%)
2	NAP	T	400	-	45,52,52	2.10	6 (13%)	56,80,80	1.60	8 (14%)
3	ADP	S	401	4	24,29,29	1.31	2 (8%)	29,45,45	1.66	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	R	400	-	-	11/31/67/67	0/5/5/5
2	NAP	O	400	-	-	5/31/67/67	0/5/5/5
3	ADP	R	401	4	-	1/12/32/32	0/3/3/3
4	BMA	R	402	3	-	2/2/19/22	0/1/1/1
2	NAP	E	400	-	-	11/31/67/67	0/5/5/5
3	ADP	N	401	4	-	1/12/32/32	0/3/3/3
3	ADP	P	401	4	-	0/12/32/32	0/3/3/3
2	NAP	N	400	-	-	8/31/67/67	0/5/5/5
3	ADP	G	401	4	-	0/12/32/32	0/3/3/3
4	BMA	S	402	3	-	2/2/19/22	0/1/1/1
2	NAP	Q	400	-	-	12/31/67/67	0/5/5/5
4	BMA	G	402	3	-	0/2/19/22	0/1/1/1
3	ADP	H	401	4	-	1/12/32/32	0/3/3/3
4	BMA	K	402	3	-	2/2/19/22	0/1/1/1
3	ADP	K	401	4	-	3/12/32/32	0/3/3/3
2	NAP	M	400	-	-	7/31/67/67	0/5/5/5
2	NAP	F	400	-	-	7/31/67/67	0/5/5/5
3	ADP	I	401	4	-	0/12/32/32	0/3/3/3
4	BMA	H	402	3	-	2/2/19/22	0/1/1/1
2	NAP	C	400	-	-	9/31/67/67	0/5/5/5
2	NAP	G	400	-	-	6/31/67/67	0/5/5/5
3	ADP	L	401	4	-	1/12/32/32	0/3/3/3
3	ADP	T	401	4	-	1/12/32/32	0/3/3/3
4	BMA	O	402	3	-	2/2/19/22	0/1/1/1
3	ADP	O	401	4	-	2/12/32/32	0/3/3/3
2	NAP	B	400	-	-	13/31/67/67	0/5/5/5
2	NAP	J	400	-	-	12/31/67/67	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	J	401	4	-	1/12/32/32	0/3/3/3
4	BMA	N	402	3	-	2/2/19/22	0/1/1/1
4	BMA	P	402	3	-	2/2/19/22	0/1/1/1
4	BMA	D	402	3	-	2/2/19/22	0/1/1/1
4	BMA	T	402	3	-	2/2/19/22	0/1/1/1
2	NAP	P	400	-	-	8/31/67/67	0/5/5/5
3	ADP	Q	401	4	-	0/12/32/32	0/3/3/3
2	NAP	D	400	-	-	1/31/67/67	0/5/5/5
3	ADP	E	401	4	-	3/12/32/32	0/3/3/3
4	BMA	A	402	3	-	2/2/19/22	0/1/1/1
3	ADP	F	401	4	-	0/12/32/32	0/3/3/3
4	BMA	F	402	3	-	0/2/19/22	0/1/1/1
4	BMA	C	402	3	-	1/2/19/22	0/1/1/1
2	NAP	L	400	-	-	4/31/67/67	0/5/5/5
3	ADP	C	401	4	-	1/12/32/32	0/3/3/3
4	BMA	L	402	3	-	2/2/19/22	0/1/1/1
2	NAP	S	400	-	-	6/31/67/67	0/5/5/5
4	BMA	E	402	3	-	2/2/19/22	0/1/1/1
3	ADP	A	401	4	-	1/12/32/32	0/3/3/3
4	BMA	M	402	3	-	2/2/19/22	0/1/1/1
3	ADP	B	401	-	-	0/12/32/32	0/3/3/3
3	ADP	M	401	4	-	0/12/32/32	0/3/3/3
4	BMA	Q	402	3	-	2/2/19/22	0/1/1/1
2	NAP	K	400	-	-	9/31/67/67	0/5/5/5
3	ADP	D	401	4	-	0/12/32/32	0/3/3/3
4	BMA	I	402	3	-	1/2/19/22	0/1/1/1
4	BMA	J	402	3	-	2/2/19/22	0/1/1/1
2	NAP	H	400	-	-	12/31/67/67	0/5/5/5
2	NAP	I	400	-	-	11/31/67/67	0/5/5/5
2	NAP	A	400	-	-	9/31/67/67	0/5/5/5
2	NAP	T	400	-	-	8/31/67/67	0/5/5/5
3	ADP	S	401	4	-	3/12/32/32	0/3/3/3

All (181) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	NAP	O7N-C7N	15.54	1.53	1.24
2	F	400	NAP	C7N-N7N	-11.43	1.11	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	400	NAP	O7N-C7N	11.25	1.45	1.24
2	G	400	NAP	C2N-N1N	11.00	1.48	1.35
2	H	400	NAP	O7N-C7N	10.79	1.44	1.24
2	P	400	NAP	O7N-C7N	10.66	1.44	1.24
2	F	400	NAP	C2N-C3N	10.63	1.55	1.39
2	K	400	NAP	O7N-C7N	10.61	1.44	1.24
2	C	400	NAP	C7N-N7N	10.47	1.52	1.33
2	T	400	NAP	O7N-C7N	10.07	1.43	1.24
2	E	400	NAP	O7N-C7N	9.70	1.42	1.24
2	D	400	NAP	O7N-C7N	9.66	1.42	1.24
2	I	400	NAP	O7N-C7N	9.61	1.42	1.24
2	Q	400	NAP	O7N-C7N	9.50	1.42	1.24
2	S	400	NAP	O7N-C7N	9.46	1.42	1.24
2	N	400	NAP	O7N-C7N	9.36	1.42	1.24
2	C	400	NAP	O7N-C7N	-9.36	1.06	1.24
2	B	400	NAP	O7N-C7N	9.24	1.41	1.24
2	L	400	NAP	O7N-C7N	9.11	1.41	1.24
2	M	400	NAP	O7N-C7N	8.95	1.41	1.24
2	J	400	NAP	O7N-C7N	8.76	1.40	1.24
2	R	400	NAP	O7N-C7N	8.69	1.40	1.24
2	F	400	NAP	C4N-C3N	-7.91	1.25	1.39
2	O	400	NAP	O7N-C7N	7.75	1.39	1.24
2	G	400	NAP	C7N-N7N	-7.15	1.19	1.33
2	A	400	NAP	C7N-N7N	6.78	1.45	1.33
2	F	400	NAP	C6N-C5N	5.77	1.51	1.38
2	P	400	NAP	C2N-N1N	5.63	1.41	1.35
2	G	400	NAP	C4N-C3N	-5.50	1.29	1.39
2	G	400	NAP	C5N-C4N	5.43	1.50	1.38
2	P	400	NAP	C2A-N3A	4.72	1.39	1.32
2	E	400	NAP	P2B-O2B	4.68	1.68	1.59
2	G	400	NAP	P2B-O2B	4.62	1.68	1.59
2	G	400	NAP	C3N-C7N	4.58	1.57	1.50
2	T	400	NAP	C2A-N3A	4.51	1.39	1.32
2	A	400	NAP	C2A-N3A	4.33	1.39	1.32
2	I	400	NAP	P2B-O2B	4.31	1.67	1.59
2	C	400	NAP	C2A-N3A	4.31	1.39	1.32
2	A	400	NAP	C6N-C5N	4.31	1.48	1.38
2	L	400	NAP	P2B-O2B	4.25	1.67	1.59
2	A	400	NAP	P2B-O2B	4.17	1.67	1.59
2	Q	400	NAP	C2A-N3A	4.12	1.38	1.32
2	K	400	NAP	C2N-N1N	4.12	1.40	1.35
2	L	400	NAP	C2A-N3A	4.06	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	400	NAP	C2N-N1N	4.06	1.39	1.35
2	K	400	NAP	C2A-N3A	4.05	1.38	1.32
2	H	400	NAP	C2A-N3A	4.03	1.38	1.32
2	J	400	NAP	C2A-N3A	4.03	1.38	1.32
2	G	400	NAP	C2A-N3A	4.03	1.38	1.32
2	J	400	NAP	P2B-O2B	3.95	1.66	1.59
2	B	400	NAP	P2B-O2B	3.95	1.66	1.59
2	M	400	NAP	C2A-N3A	3.92	1.38	1.32
2	T	400	NAP	C2N-C3N	3.91	1.45	1.39
2	M	400	NAP	P2B-O2B	3.90	1.66	1.59
2	E	400	NAP	C2A-N3A	3.88	1.38	1.32
2	S	400	NAP	C2A-N3A	3.87	1.38	1.32
2	O	400	NAP	C2A-N3A	3.81	1.38	1.32
2	F	400	NAP	P2B-O2B	3.80	1.66	1.59
2	N	400	NAP	C2A-N3A	3.79	1.38	1.32
2	O	400	NAP	P2B-O2B	3.75	1.66	1.59
3	S	401	ADP	O4'-C1'	3.75	1.46	1.41
2	B	400	NAP	C2A-N3A	3.74	1.38	1.32
2	Q	400	NAP	P2B-O2B	3.66	1.66	1.59
3	R	401	ADP	PB-O1B	3.66	1.62	1.50
3	O	401	ADP	PB-O1B	3.65	1.62	1.50
2	F	400	NAP	C2N-N1N	3.65	1.39	1.35
3	N	401	ADP	PB-O1B	3.63	1.62	1.50
3	Q	401	ADP	PB-O1B	3.63	1.62	1.50
3	K	401	ADP	PB-O1B	3.60	1.62	1.50
3	M	401	ADP	PB-O1B	3.60	1.62	1.50
3	N	401	ADP	O4'-C1'	3.59	1.46	1.41
3	T	401	ADP	PB-O1B	3.55	1.62	1.50
3	G	401	ADP	PB-O1B	3.54	1.62	1.50
2	G	400	NAP	C2N-C3N	3.53	1.44	1.39
2	D	400	NAP	C2A-N3A	3.53	1.37	1.32
3	C	401	ADP	PB-O1B	3.50	1.61	1.50
3	J	401	ADP	PB-O1B	3.50	1.61	1.50
3	L	401	ADP	PB-O1B	3.50	1.61	1.50
2	D	400	NAP	P2B-O2B	3.49	1.65	1.59
2	R	400	NAP	C2A-N3A	3.46	1.37	1.32
3	H	401	ADP	PB-O1B	3.43	1.61	1.50
2	R	400	NAP	P2B-O2B	3.43	1.65	1.59
3	S	401	ADP	PB-O1B	3.41	1.61	1.50
2	R	400	NAP	C2N-N1N	3.39	1.39	1.35
3	D	401	ADP	PB-O1B	3.39	1.61	1.50
3	D	401	ADP	O4'-C1'	3.36	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	ADP	O4'-C1'	3.36	1.45	1.41
2	N	400	NAP	P2B-O2B	3.33	1.65	1.59
2	P	400	NAP	C4N-C3N	-3.30	1.33	1.39
2	F	400	NAP	C2A-N3A	3.27	1.37	1.32
2	P	400	NAP	C5N-C4N	3.26	1.45	1.38
3	I	401	ADP	PB-O1B	3.25	1.61	1.50
2	G	400	NAP	C6N-N1N	-3.22	1.27	1.35
2	T	400	NAP	P2B-O2B	3.19	1.65	1.59
3	A	401	ADP	PB-O1B	3.18	1.60	1.50
3	P	401	ADP	PB-O1B	3.18	1.60	1.50
2	I	400	NAP	C2A-N3A	3.17	1.37	1.32
3	K	401	ADP	O4'-C1'	3.15	1.45	1.41
3	F	401	ADP	PB-O1B	3.11	1.60	1.50
3	E	401	ADP	PB-O1B	3.08	1.60	1.50
2	K	400	NAP	C5N-C4N	3.07	1.45	1.38
2	L	400	NAP	C2N-N1N	3.05	1.38	1.35
3	A	401	ADP	C8-N7	-3.05	1.29	1.34
2	P	400	NAP	C2A-N1A	3.02	1.39	1.33
3	I	401	ADP	O4'-C1'	3.01	1.45	1.41
2	Q	400	NAP	C2N-N1N	2.98	1.38	1.35
3	L	401	ADP	O4'-C1'	2.98	1.45	1.41
2	K	400	NAP	C4N-C3N	-2.97	1.34	1.39
3	R	401	ADP	O4'-C1'	2.97	1.45	1.41
3	H	401	ADP	O4'-C1'	2.93	1.45	1.41
2	K	400	NAP	C2A-N1A	2.93	1.39	1.33
2	C	400	NAP	P2B-O2B	2.93	1.64	1.59
3	M	401	ADP	O4'-C1'	2.92	1.45	1.41
2	H	400	NAP	C2N-N1N	2.90	1.38	1.35
2	K	400	NAP	P2B-O2B	2.89	1.64	1.59
3	C	401	ADP	O4'-C1'	2.88	1.45	1.41
2	P	400	NAP	P2B-O2B	2.88	1.64	1.59
3	G	401	ADP	O4'-C1'	2.88	1.45	1.41
3	O	401	ADP	O4'-C1'	2.84	1.45	1.41
3	A	401	ADP	O4'-C1'	2.83	1.45	1.41
3	G	401	ADP	C8-N7	-2.83	1.29	1.34
3	P	401	ADP	O4'-C1'	2.78	1.45	1.41
3	T	401	ADP	O4'-C1'	2.77	1.44	1.41
2	A	400	NAP	C2A-N1A	2.76	1.39	1.33
3	M	401	ADP	C8-N7	-2.73	1.29	1.34
2	L	400	NAP	C2A-N1A	2.73	1.39	1.33
2	O	400	NAP	C2A-N1A	2.72	1.39	1.33
2	H	400	NAP	P2B-O2B	2.71	1.64	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	400	NAP	C2N-C3N	2.71	1.43	1.39
2	T	400	NAP	C2A-N1A	2.70	1.38	1.33
2	S	400	NAP	P2B-O2B	2.69	1.64	1.59
2	J	400	NAP	C2N-N1N	2.68	1.38	1.35
2	G	400	NAP	C2A-N1A	2.67	1.38	1.33
2	P	400	NAP	C3N-C7N	2.65	1.54	1.50
2	S	400	NAP	C2A-N1A	2.64	1.38	1.33
2	B	400	NAP	C2N-N1N	2.64	1.38	1.35
2	Q	400	NAP	C2A-N1A	2.64	1.38	1.33
2	C	400	NAP	C2A-N1A	2.59	1.38	1.33
2	A	400	NAP	C4N-C3N	-2.59	1.34	1.39
2	E	400	NAP	C2N-N1N	2.56	1.38	1.35
2	N	400	NAP	C2A-N1A	2.56	1.38	1.33
3	J	401	ADP	O4'-C1'	2.55	1.44	1.41
2	H	400	NAP	C2A-N1A	2.52	1.38	1.33
3	O	401	ADP	C8-N7	-2.47	1.30	1.34
3	B	401	ADP	C5-C4	2.46	1.47	1.40
3	E	401	ADP	O4'-C1'	2.45	1.44	1.41
2	B	400	NAP	C2A-N1A	2.44	1.38	1.33
2	J	400	NAP	C2D-C1D	-2.44	1.50	1.53
3	C	401	ADP	C8-N7	-2.43	1.30	1.34
2	E	400	NAP	C2A-N1A	2.41	1.38	1.33
2	D	400	NAP	C2A-N1A	2.41	1.38	1.33
3	R	401	ADP	C8-N7	-2.41	1.30	1.34
3	E	401	ADP	C4-N3	-2.40	1.32	1.35
2	K	400	NAP	C6N-N1N	-2.37	1.29	1.35
3	I	401	ADP	C8-N7	-2.36	1.30	1.34
2	J	400	NAP	C2A-N1A	2.35	1.38	1.33
2	I	400	NAP	C2N-N1N	2.34	1.37	1.35
3	T	401	ADP	C8-N7	-2.32	1.30	1.34
3	F	401	ADP	C8-N7	-2.31	1.30	1.34
3	Q	401	ADP	O4'-C1'	2.30	1.44	1.41
2	M	400	NAP	C2A-N1A	2.29	1.38	1.33
3	Q	401	ADP	C8-N7	-2.27	1.30	1.34
2	R	400	NAP	C2A-N1A	2.25	1.38	1.33
3	E	401	ADP	C8-N7	-2.21	1.30	1.34
2	F	400	NAP	C6N-N1N	-2.21	1.30	1.35
2	E	400	NAP	C2D-C1D	-2.21	1.50	1.53
2	K	400	NAP	C2D-C1D	-2.21	1.50	1.53
3	N	401	ADP	C8-N7	-2.21	1.30	1.34
2	I	400	NAP	C2A-N1A	2.20	1.38	1.33
2	O	400	NAP	C2N-N1N	2.19	1.37	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	400	NAP	C2N-N1N	2.19	1.37	1.35
3	J	401	ADP	C4-N3	-2.18	1.32	1.35
2	P	400	NAP	C7N-N7N	-2.14	1.28	1.33
3	K	401	ADP	C8-N7	-2.13	1.30	1.34
2	O	400	NAP	C7N-N7N	2.11	1.37	1.33
2	H	400	NAP	C2N-C3N	2.08	1.42	1.39
3	P	401	ADP	C4-N3	-2.06	1.32	1.35
2	F	400	NAP	C2D-C1D	-2.05	1.50	1.53
2	R	400	NAP	C5N-C4N	2.04	1.43	1.38
3	L	401	ADP	C8-N7	-2.04	1.31	1.34
2	O	400	NAP	C6N-C5N	-2.04	1.34	1.38

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	400	NAP	C5N-C4N-C3N	11.72	134.21	120.34
2	G	400	NAP	C3N-C2N-N1N	-9.68	110.96	120.43
2	F	400	NAP	C3N-C2N-N1N	-8.92	111.71	120.43
2	F	400	NAP	C3N-C7N-N7N	7.69	126.98	117.75
2	F	400	NAP	O7N-C7N-C3N	-7.56	110.58	119.63
2	G	400	NAP	C2N-C3N-C4N	7.39	126.63	118.26
2	F	400	NAP	C6N-N1N-C2N	7.28	128.61	121.97
2	G	400	NAP	O7N-C7N-C3N	-6.56	111.79	119.63
2	G	400	NAP	C3N-C7N-N7N	6.55	125.61	117.75
2	F	400	NAP	C6N-C5N-C4N	-6.37	110.18	119.44
2	R	400	NAP	N3A-C2A-N1A	-6.24	118.92	128.68
3	E	401	ADP	PA-O3A-PB	-6.17	111.64	132.83
2	F	400	NAP	N3A-C2A-N1A	-5.99	119.32	128.68
3	A	401	ADP	PA-O3A-PB	-5.93	112.48	132.83
3	M	401	ADP	PA-O3A-PB	-5.91	112.56	132.83
3	G	401	ADP	PA-O3A-PB	-5.82	112.86	132.83
2	K	400	NAP	C3N-C2N-N1N	-5.80	114.76	120.43
2	T	400	NAP	N3A-C2A-N1A	-5.58	119.95	128.68
2	I	400	NAP	N3A-C2A-N1A	-5.50	120.08	128.68
2	O	400	NAP	N3A-C2A-N1A	-5.49	120.09	128.68
2	M	400	NAP	N3A-C2A-N1A	-5.49	120.09	128.68
3	J	401	ADP	O3A-PB-O1B	-5.44	80.99	111.19
3	F	401	ADP	PA-O3A-PB	-5.44	114.15	132.83
2	G	400	NAP	C6N-C5N-C4N	-5.37	111.64	119.44
2	C	400	NAP	C3N-C7N-N7N	-5.32	111.37	117.75
3	K	401	ADP	PA-O3A-PB	-5.28	114.72	132.83
2	J	400	NAP	N3A-C2A-N1A	-5.26	120.46	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	402	BMA	O5-C5-C6	5.26	115.44	107.20
2	T	400	NAP	C3N-C2N-N1N	-5.23	115.31	120.43
2	B	400	NAP	N3A-C2A-N1A	-5.23	120.50	128.68
2	K	400	NAP	C6N-C5N-C4N	-5.20	111.89	119.44
3	S	401	ADP	PA-O3A-PB	-5.16	115.13	132.83
2	Q	400	NAP	N3A-C2A-N1A	-5.14	120.64	128.68
2	A	400	NAP	N3A-C2A-N1A	-5.11	120.69	128.68
2	H	400	NAP	N3A-C2A-N1A	-5.10	120.70	128.68
3	N	401	ADP	PA-O3A-PB	-5.10	115.32	132.83
2	E	400	NAP	N3A-C2A-N1A	-5.09	120.72	128.68
2	D	400	NAP	N3A-C2A-N1A	-5.07	120.76	128.68
3	J	401	ADP	PA-O3A-PB	-5.05	115.48	132.83
2	C	400	NAP	N3A-C2A-N1A	-5.01	120.84	128.68
3	C	401	ADP	PA-O3A-PB	-4.99	115.72	132.83
2	S	400	NAP	N3A-C2A-N1A	-4.97	120.90	128.68
3	O	401	ADP	PA-O3A-PB	-4.92	115.94	132.83
2	N	400	NAP	N3A-C2A-N1A	-4.88	121.06	128.68
2	G	400	NAP	N3A-C2A-N1A	-4.83	121.13	128.68
3	P	401	ADP	PA-O3A-PB	-4.82	116.30	132.83
3	D	401	ADP	PA-O3A-PB	-4.80	116.35	132.83
2	L	400	NAP	N3A-C2A-N1A	-4.78	121.20	128.68
3	Q	401	ADP	N3-C2-N1	-4.69	121.35	128.68
2	G	400	NAP	C5N-C6N-N1N	4.66	127.08	120.40
4	R	402	BMA	C1-O5-C5	-4.63	105.92	112.19
2	K	400	NAP	N3A-C2A-N1A	-4.63	121.45	128.68
3	L	401	ADP	PA-O3A-PB	-4.62	116.98	132.83
2	A	400	NAP	C6N-C5N-C4N	-4.59	112.77	119.44
3	Q	401	ADP	PA-O3A-PB	-4.52	117.30	132.83
3	K	401	ADP	N3-C2-N1	-4.51	121.64	128.68
3	I	401	ADP	PA-O3A-PB	-4.51	117.36	132.83
3	H	401	ADP	N3-C2-N1	-4.50	121.64	128.68
3	H	401	ADP	PA-O3A-PB	-4.49	117.41	132.83
2	A	400	NAP	C5N-C4N-C3N	4.45	125.61	120.34
3	R	401	ADP	PA-O3A-PB	-4.42	117.67	132.83
2	P	400	NAP	N3A-C2A-N1A	-4.36	121.86	128.68
2	P	400	NAP	C3N-C2N-N1N	-4.34	116.18	120.43
3	O	401	ADP	N3-C2-N1	-4.32	121.92	128.68
3	L	401	ADP	N3-C2-N1	-4.32	121.93	128.68
3	A	401	ADP	N3-C2-N1	-4.31	121.94	128.68
3	D	401	ADP	N3-C2-N1	-4.22	122.08	128.68
3	S	401	ADP	N3-C2-N1	-4.21	122.10	128.68
3	J	401	ADP	N3-C2-N1	-4.20	122.12	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	401	ADP	N3-C2-N1	-4.19	122.13	128.68
2	C	400	NAP	O7N-C7N-C3N	4.18	124.63	119.63
3	C	401	ADP	N3-C2-N1	-4.16	122.17	128.68
3	T	401	ADP	N3-C2-N1	-4.15	122.19	128.68
3	R	401	ADP	N3-C2-N1	-4.14	122.21	128.68
2	C	400	NAP	C5N-C4N-C3N	-4.12	115.46	120.34
3	I	401	ADP	N3-C2-N1	-4.06	122.33	128.68
3	N	401	ADP	O3A-PB-O1B	-3.97	89.20	111.19
3	F	401	ADP	N3-C2-N1	-3.93	122.53	128.68
3	M	401	ADP	N3-C2-N1	-3.91	122.57	128.68
3	T	401	ADP	PA-O3A-PB	-3.90	119.44	132.83
3	P	401	ADP	N3-C2-N1	-3.89	122.59	128.68
3	E	401	ADP	N3-C2-N1	-3.85	122.66	128.68
2	F	400	NAP	C3B-C2B-C1B	-3.83	95.68	102.89
3	M	401	ADP	O2B-PB-O3A	3.81	117.41	104.64
3	G	401	ADP	N3-C2-N1	-3.79	122.75	128.68
3	D	401	ADP	O3A-PB-O1B	-3.76	90.33	111.19
3	B	401	ADP	N3-C2-N1	-3.75	122.82	128.68
2	O	400	NAP	C6N-C5N-C4N	3.73	124.86	119.44
3	K	401	ADP	O3A-PB-O1B	-3.71	90.59	111.19
2	C	400	NAP	C2N-C3N-C4N	3.71	122.46	118.26
2	E	400	NAP	C3B-C2B-C1B	-3.70	95.93	102.89
2	K	400	NAP	C2N-C3N-C4N	3.66	122.41	118.26
4	R	402	BMA	C2-C3-C4	-3.48	104.88	110.89
2	K	400	NAP	C5N-C6N-N1N	3.45	125.34	120.40
2	J	400	NAP	C3N-C7N-N7N	3.42	121.86	117.75
3	M	401	ADP	O3A-PB-O1B	-3.42	92.22	111.19
2	P	400	NAP	C6N-C5N-C4N	-3.42	114.47	119.44
2	L	400	NAP	C3N-C2N-N1N	-3.36	117.15	120.43
2	R	400	NAP	C3B-C2B-C1B	-3.35	96.59	102.89
4	P	402	BMA	C1-O5-C5	3.35	116.73	112.19
2	J	400	NAP	C3B-C2B-C1B	-3.31	96.66	102.89
2	M	400	NAP	C3B-C2B-C1B	-3.30	96.68	102.89
4	R	402	BMA	C3-C4-C5	-3.29	104.38	110.24
2	T	400	NAP	C3N-C7N-N7N	3.28	121.69	117.75
3	E	401	ADP	C4-C5-N7	-3.27	105.99	109.40
2	A	400	NAP	C3B-C2B-C1B	-3.24	96.80	102.89
2	O	400	NAP	O3X-P2B-O2B	3.20	120.34	105.99
3	J	401	ADP	O3B-PB-O3A	3.20	115.36	104.64
2	K	400	NAP	C3N-C7N-N7N	3.17	121.56	117.75
2	P	400	NAP	C3N-C7N-N7N	3.17	121.56	117.75
3	H	401	ADP	O3B-PB-O3A	3.17	115.26	104.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	400	NAP	C3B-C2B-C1B	-3.12	97.03	102.89
2	M	400	NAP	O3X-P2B-O2B	3.12	119.95	105.99
3	N	401	ADP	O2B-PB-O3A	3.10	115.04	104.64
2	O	400	NAP	C3B-C2B-C1B	-3.10	97.07	102.89
2	K	400	NAP	O3X-P2B-O2B	3.07	119.75	105.99
2	T	400	NAP	C1B-N9A-C4A	-3.06	121.26	126.64
2	K	400	NAP	O7N-C7N-C3N	-3.06	115.97	119.63
3	F	401	ADP	C4-C5-N7	-3.05	106.22	109.40
3	I	401	ADP	O2B-PB-O3A	3.04	114.83	104.64
2	I	400	NAP	O3X-P2B-O2B	3.03	119.57	105.99
3	N	401	ADP	C4-C5-N7	-2.99	106.28	109.40
2	E	400	NAP	O3X-P2B-O2B	2.98	119.33	105.99
2	B	400	NAP	O4D-C1D-C2D	-2.98	102.58	106.93
2	F	400	NAP	C1B-N9A-C4A	-2.98	121.41	126.64
3	S	401	ADP	C4-C5-N7	-2.96	106.32	109.40
3	D	401	ADP	O3B-PB-O3A	2.94	114.48	104.64
2	R	400	NAP	O3X-P2B-O2B	2.93	119.13	105.99
2	C	400	NAP	C4N-C3N-C7N	-2.89	113.32	121.04
2	O	400	NAP	C6N-N1N-C2N	-2.83	119.39	121.97
2	K	400	NAP	C3B-C2B-C1B	-2.83	97.57	102.89
3	H	401	ADP	O3A-PB-O1B	-2.82	95.56	111.19
2	G	400	NAP	C3B-C2B-C1B	-2.81	97.61	102.89
2	O	400	NAP	C5N-C4N-C3N	-2.80	117.02	120.34
2	O	400	NAP	C2N-N1N-C1D	2.80	125.37	119.14
4	I	402	BMA	C3-C4-C5	-2.79	105.26	110.24
3	E	401	ADP	C5-C6-N6	2.76	124.55	120.35
2	B	400	NAP	C3B-C2B-C1B	-2.76	97.70	102.89
3	I	401	ADP	O3A-PB-O1B	-2.75	95.91	111.19
3	O	401	ADP	C4-C5-N7	-2.74	106.54	109.40
3	B	401	ADP	C4-C5-N7	-2.72	106.56	109.40
2	A	400	NAP	O7N-C7N-C3N	2.72	122.88	119.63
2	D	400	NAP	O3X-P2B-O2B	2.71	118.13	105.99
3	G	401	ADP	O3B-PB-O3A	2.70	113.70	104.64
4	H	402	BMA	C6-C5-C4	2.70	119.32	113.00
3	J	401	ADP	O2B-PB-O3A	2.69	113.67	104.64
4	M	402	BMA	O5-C5-C6	2.69	111.42	107.20
3	D	401	ADP	O2B-PB-O3A	2.68	113.61	104.64
2	B	400	NAP	C6N-N1N-C2N	-2.67	119.54	121.97
3	Q	401	ADP	O3B-PB-O3A	2.67	113.58	104.64
2	C	400	NAP	C3B-C2B-C1B	-2.66	97.89	102.89
4	J	402	BMA	C1-O5-C5	2.65	115.79	112.19
2	S	400	NAP	C3B-C2B-C1B	-2.64	97.92	102.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	402	BMA	O5-C5-C6	2.64	111.34	107.20
4	D	402	BMA	C3-C4-C5	-2.64	105.53	110.24
4	E	402	BMA	C6-C5-C4	2.61	119.13	113.00
3	A	401	ADP	O3B-PB-O3A	2.60	113.36	104.64
2	E	400	NAP	C3N-C2N-N1N	-2.60	117.89	120.43
2	C	400	NAP	O3X-P2B-O2B	2.59	117.58	105.99
3	H	401	ADP	C4-C5-N7	-2.57	106.72	109.40
4	O	402	BMA	C3-C4-C5	-2.56	105.67	110.24
2	Q	400	NAP	C2N-N1N-C1D	2.55	124.81	119.14
3	E	401	ADP	O3B-PB-O3A	2.54	113.17	104.64
3	I	401	ADP	C4-C5-N7	-2.54	106.75	109.40
2	B	400	NAP	O3X-P2B-O2B	2.53	117.32	105.99
3	S	401	ADP	O3B-PB-O3A	2.51	113.06	104.64
3	D	401	ADP	C3'-C2'-C1'	2.50	104.75	100.98
3	D	401	ADP	C4-C5-N7	-2.48	106.82	109.40
3	N	401	ADP	O3B-PB-O3A	2.47	112.92	104.64
3	Q	401	ADP	PA-O5'-C5'	-2.47	107.20	121.68
2	N	400	NAP	O3X-P2B-O2B	2.47	117.06	105.99
2	I	400	NAP	C3B-C2B-C1B	-2.47	98.25	102.89
2	E	400	NAP	O3X-P2B-O1X	-2.46	101.07	110.68
2	A	400	NAP	C4A-C5A-N7A	-2.45	106.84	109.40
3	L	401	ADP	O2B-PB-O3A	2.45	112.86	104.64
2	R	400	NAP	O2B-C2B-C1B	2.45	118.91	110.10
3	C	401	ADP	O3B-PB-O3A	2.44	112.83	104.64
2	A	400	NAP	O3B-C3B-C4B	-2.44	104.00	111.05
3	J	401	ADP	C4-C5-N7	-2.43	106.86	109.40
2	P	400	NAP	C3B-C2B-C1B	-2.43	98.33	102.89
2	H	400	NAP	C3N-C2N-N1N	-2.41	118.07	120.43
3	K	401	ADP	C4-C5-N7	-2.41	106.89	109.40
2	B	400	NAP	C2N-N1N-C1D	2.40	124.47	119.14
3	Q	401	ADP	O2B-PB-O3A	2.39	112.63	104.64
3	D	401	ADP	PA-O5'-C5'	-2.38	107.70	121.68
3	T	401	ADP	C3'-C2'-C1'	2.38	104.56	100.98
2	G	400	NAP	O2B-C2B-C1B	2.37	118.64	110.10
3	F	401	ADP	O3B-PB-O3A	2.37	112.58	104.64
3	J	401	ADP	O3B-PB-O2B	2.36	116.66	107.64
3	E	401	ADP	C3'-C2'-C1'	2.35	104.52	100.98
3	I	401	ADP	C3'-C2'-C1'	2.34	104.51	100.98
3	H	401	ADP	C2'-C3'-C4'	-2.33	98.11	102.64
3	T	401	ADP	C4-C5-N7	-2.33	106.97	109.40
3	K	401	ADP	O2B-PB-O3A	2.32	112.42	104.64
3	G	401	ADP	PA-O5'-C5'	-2.32	108.10	121.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	400	NAP	C4N-C3N-C7N	-2.31	114.86	121.04
2	T	400	NAP	O3X-P2B-O2B	2.31	116.33	105.99
3	P	401	ADP	O3B-PB-O3A	2.30	112.36	104.64
2	L	400	NAP	C1B-N9A-C4A	-2.30	122.60	126.64
3	Q	401	ADP	C1'-N9-C4	-2.30	122.60	126.64
2	P	400	NAP	C4A-C5A-N7A	-2.30	107.01	109.40
2	H	400	NAP	O3X-P2B-O2B	2.29	116.26	105.99
2	G	400	NAP	O3X-P2B-O2B	2.29	116.25	105.99
4	P	402	BMA	C6-C5-C4	2.28	118.35	113.00
3	O	401	ADP	O3B-PB-O3A	2.28	112.28	104.64
3	K	401	ADP	C2'-C3'-C4'	-2.28	98.22	102.64
2	A	400	NAP	C3N-C7N-N7N	-2.28	115.02	117.75
2	P	400	NAP	C2N-C3N-C4N	2.27	120.83	118.26
2	R	400	NAP	O2N-PN-O1N	2.26	123.42	112.24
3	G	401	ADP	O5'-C5'-C4'	2.25	116.74	108.99
3	B	401	ADP	C2-N1-C6	2.25	122.60	118.75
3	T	401	ADP	O3B-PB-O3A	2.24	112.16	104.64
2	F	400	NAP	O3X-P2B-O2B	2.24	116.04	105.99
3	Q	401	ADP	O3A-PB-O1B	-2.24	98.76	111.19
3	P	401	ADP	PA-O5'-C5'	-2.22	108.64	121.68
3	B	401	ADP	C1'-N9-C4	-2.21	122.75	126.64
3	G	401	ADP	O3A-PB-O1B	-2.21	98.92	111.19
3	B	401	ADP	C3'-C2'-C1'	2.21	104.30	100.98
3	H	401	ADP	O2B-PB-O3A	2.20	112.02	104.64
4	R	402	BMA	O5-C1-C2	-2.20	107.37	110.77
2	E	400	NAP	C2N-N1N-C1D	2.20	124.03	119.14
4	D	402	BMA	C6-C5-C4	2.19	118.13	113.00
3	C	401	ADP	O2B-PB-O3A	2.19	111.97	104.64
3	F	401	ADP	PA-O5'-C5'	-2.18	108.91	121.68
3	A	401	ADP	PA-O5'-C5'	-2.17	108.95	121.68
2	L	400	NAP	C3B-C2B-C1B	-2.17	98.81	102.89
2	F	400	NAP	C2N-C3N-C4N	-2.17	115.80	118.26
3	E	401	ADP	O4'-C4'-C3'	2.17	109.40	105.11
3	F	401	ADP	C3'-C2'-C1'	2.15	104.22	100.98
3	A	401	ADP	O2B-PB-O3A	2.15	111.83	104.64
2	T	400	NAP	O2N-PN-O1N	2.15	122.85	112.24
2	L	400	NAP	O3X-P2B-O2B	2.15	115.60	105.99
4	C	402	BMA	O5-C5-C6	2.14	110.57	107.20
2	I	400	NAP	O2B-C2B-C1B	2.14	117.81	110.10
4	I	402	BMA	O5-C1-C2	-2.14	107.47	110.77
2	A	400	NAP	O3X-P2B-O2B	2.13	115.55	105.99
3	T	401	ADP	PA-O5'-C5'	-2.13	109.22	121.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	400	NAP	O3X-P2B-O2B	2.12	115.47	105.99
3	R	401	ADP	C4-C5-N7	-2.11	107.20	109.40
3	H	401	ADP	PA-O5'-C5'	-2.11	109.33	121.68
2	H	400	NAP	O7N-C7N-N7N	-2.10	119.59	122.58
3	R	401	ADP	PA-O5'-C5'	-2.10	109.38	121.68
3	A	401	ADP	C4-C5-N7	-2.10	107.21	109.40
3	C	401	ADP	N6-C6-N1	2.10	122.92	118.57
2	J	400	NAP	O7N-C7N-N7N	-2.09	119.61	122.58
2	K	400	NAP	O2N-PN-O1N	2.08	122.54	112.24
3	A	401	ADP	C3'-C2'-C1'	2.08	104.11	100.98
2	R	400	NAP	C6N-N1N-C2N	-2.08	120.08	121.97
2	G	400	NAP	C2N-C3N-C7N	-2.08	113.43	119.46
2	J	400	NAP	C3N-C2N-N1N	-2.08	118.40	120.43
2	P	400	NAP	C5N-C4N-C3N	2.08	122.80	120.34
2	B	400	NAP	C4N-C3N-C7N	-2.07	115.49	121.04
4	M	402	BMA	C3-C4-C5	-2.07	106.54	110.24
2	K	400	NAP	C4A-C5A-N7A	-2.07	107.24	109.40
2	M	400	NAP	O2N-PN-O1N	2.07	122.47	112.24
3	R	401	ADP	O3B-PB-O3A	2.07	111.57	104.64
3	K	401	ADP	PA-O5'-C5'	-2.07	109.56	121.68
3	J	401	ADP	PA-O5'-C5'	-2.06	109.61	121.68
3	M	401	ADP	O3B-PB-O3A	2.04	111.49	104.64
3	J	401	ADP	C3'-C2'-C1'	2.04	104.05	100.98
3	E	401	ADP	C2-N1-C6	2.04	122.25	118.75
3	P	401	ADP	C4-C5-N7	-2.04	107.27	109.40
4	D	402	BMA	O5-C1-C2	-2.04	107.62	110.77
3	L	401	ADP	C4-C5-N7	-2.04	107.28	109.40
3	I	401	ADP	O3B-PB-O2B	2.04	115.42	107.64
2	F	400	NAP	O2N-PN-O1N	2.03	122.29	112.24
2	H	400	NAP	C3B-C2B-C1B	-2.03	99.07	102.89
3	I	401	ADP	PA-O5'-C5'	-2.03	109.78	121.68
3	A	401	ADP	O4'-C4'-C3'	2.02	109.12	105.11
2	Q	400	NAP	C3B-C2B-C1B	-2.02	99.09	102.89
2	T	400	NAP	O7N-C7N-C3N	-2.01	117.22	119.63
3	N	401	ADP	PA-O5'-C5'	-2.01	109.89	121.68
2	O	400	NAP	C2N-C3N-C7N	2.01	125.29	119.46
2	G	400	NAP	O2N-PN-O1N	2.01	122.16	112.24

There are no chirality outliers.

All (220) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	NAP	C2B-O2B-P2B-O1X
2	A	400	NAP	C5D-O5D-PN-O2N
2	A	400	NAP	O4D-C1D-N1N-C2N
2	B	400	NAP	C5B-O5B-PA-O2A
2	B	400	NAP	C2B-O2B-P2B-O1X
2	C	400	NAP	O4B-C4B-C5B-O5B
2	C	400	NAP	C2B-O2B-P2B-O1X
2	E	400	NAP	C2B-O2B-P2B-O1X
2	E	400	NAP	C5D-O5D-PN-O1N
2	E	400	NAP	C5D-O5D-PN-O2N
2	F	400	NAP	C2B-O2B-P2B-O1X
2	G	400	NAP	C2B-O2B-P2B-O1X
2	H	400	NAP	C5B-O5B-PA-O2A
2	H	400	NAP	O4B-C4B-C5B-O5B
2	H	400	NAP	C2B-O2B-P2B-O1X
2	H	400	NAP	C5D-O5D-PN-O1N
2	H	400	NAP	C5D-O5D-PN-O2N
2	I	400	NAP	C2B-O2B-P2B-O1X
2	I	400	NAP	C5D-O5D-PN-O2N
2	J	400	NAP	C5B-O5B-PA-O2A
2	J	400	NAP	C2B-O2B-P2B-O1X
2	J	400	NAP	C5D-O5D-PN-O2N
2	K	400	NAP	C5B-O5B-PA-O2A
2	K	400	NAP	O4D-C4D-C5D-O5D
2	L	400	NAP	C2B-O2B-P2B-O1X
2	L	400	NAP	O4D-C1D-N1N-C2N
2	M	400	NAP	C2B-O2B-P2B-O1X
2	N	400	NAP	C2B-O2B-P2B-O1X
2	O	400	NAP	C2B-O2B-P2B-O1X
2	P	400	NAP	C2B-O2B-P2B-O1X
2	Q	400	NAP	C5B-O5B-PA-O2A
2	Q	400	NAP	C2B-O2B-P2B-O1X
2	R	400	NAP	O4B-C4B-C5B-O5B
2	R	400	NAP	C2B-O2B-P2B-O1X
2	R	400	NAP	C5D-O5D-PN-O2N
2	S	400	NAP	O4B-C4B-C5B-O5B
2	S	400	NAP	C2B-O2B-P2B-O1X
2	T	400	NAP	C5B-O5B-PA-O2A
2	T	400	NAP	C2B-O2B-P2B-O1X
3	K	401	ADP	C5'-O5'-PA-O3A
3	S	401	ADP	PA-O3A-PB-O3B
4	O	402	BMA	O5-C5-C6-O6
4	J	402	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	N	402	BMA	O5-C5-C6-O6
4	E	402	BMA	O5-C5-C6-O6
4	S	402	BMA	O5-C5-C6-O6
4	A	402	BMA	O5-C5-C6-O6
4	H	402	BMA	O5-C5-C6-O6
4	P	402	BMA	O5-C5-C6-O6
4	D	402	BMA	O5-C5-C6-O6
4	O	402	BMA	C4-C5-C6-O6
4	A	402	BMA	C4-C5-C6-O6
4	E	402	BMA	C4-C5-C6-O6
4	H	402	BMA	C4-C5-C6-O6
4	J	402	BMA	C4-C5-C6-O6
4	S	402	BMA	C4-C5-C6-O6
2	B	400	NAP	O4B-C4B-C5B-O5B
2	H	400	NAP	C3B-C4B-C5B-O5B
2	I	400	NAP	O4B-C4B-C5B-O5B
2	K	400	NAP	O4B-C4B-C5B-O5B
2	K	400	NAP	C3D-C4D-C5D-O5D
2	P	400	NAP	O4B-C4B-C5B-O5B
2	Q	400	NAP	O4B-C4B-C5B-O5B
2	Q	400	NAP	C3B-C4B-C5B-O5B
2	R	400	NAP	C3B-C4B-C5B-O5B
2	T	400	NAP	O4B-C4B-C5B-O5B
2	T	400	NAP	C3B-C4B-C5B-O5B
4	R	402	BMA	O5-C5-C6-O6
4	N	402	BMA	C4-C5-C6-O6
4	P	402	BMA	C4-C5-C6-O6
4	L	402	BMA	O5-C5-C6-O6
4	Q	402	BMA	O5-C5-C6-O6
4	D	402	BMA	C4-C5-C6-O6
4	K	402	BMA	O5-C5-C6-O6
4	M	402	BMA	O5-C5-C6-O6
4	T	402	BMA	O5-C5-C6-O6
4	Q	402	BMA	C4-C5-C6-O6
4	L	402	BMA	C4-C5-C6-O6
2	B	400	NAP	C3B-C4B-C5B-O5B
2	C	400	NAP	C3B-C4B-C5B-O5B
2	F	400	NAP	O4B-C4B-C5B-O5B
2	K	400	NAP	C3B-C4B-C5B-O5B
2	O	400	NAP	O4B-C4B-C5B-O5B
2	S	400	NAP	C3B-C4B-C5B-O5B
2	B	400	NAP	O4D-C4D-C5D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	P	400	NAP	C3B-C4B-C5B-O5B
2	E	400	NAP	O4B-C4B-C5B-O5B
2	E	400	NAP	C3B-C4B-C5B-O5B
2	F	400	NAP	C3B-C4B-C5B-O5B
2	I	400	NAP	C3B-C4B-C5B-O5B
4	K	402	BMA	C4-C5-C6-O6
4	R	402	BMA	C4-C5-C6-O6
2	O	400	NAP	C3B-C4B-C5B-O5B
3	A	401	ADP	PA-O3A-PB-O1B
3	C	401	ADP	PA-O3A-PB-O1B
3	O	401	ADP	PA-O3A-PB-O1B
2	H	400	NAP	PA-O3-PN-O1N
4	M	402	BMA	C4-C5-C6-O6
2	N	400	NAP	O4B-C4B-C5B-O5B
2	E	400	NAP	C4B-C5B-O5B-PA
2	H	400	NAP	C4B-C5B-O5B-PA
2	K	400	NAP	C4B-C5B-O5B-PA
2	M	400	NAP	C4B-C5B-O5B-PA
2	T	400	NAP	C4B-C5B-O5B-PA
4	T	402	BMA	C4-C5-C6-O6
2	Q	400	NAP	PN-O3-PA-O5B
3	S	401	ADP	PB-O3A-PA-O5'
2	J	400	NAP	O4B-C4B-C5B-O5B
2	M	400	NAP	O4B-C4B-C5B-O5B
2	Q	400	NAP	O4D-C4D-C5D-O5D
2	B	400	NAP	C4N-C3N-C7N-N7N
2	B	400	NAP	C4B-C5B-O5B-PA
2	B	400	NAP	C4N-C3N-C7N-O7N
3	O	401	ADP	PA-O3A-PB-O3B
2	B	400	NAP	C5B-O5B-PA-O3
2	C	400	NAP	C5B-O5B-PA-O3
2	E	400	NAP	C5B-O5B-PA-O3
2	G	400	NAP	C2B-O2B-P2B-O2X
2	H	400	NAP	C5B-O5B-PA-O3
2	H	400	NAP	C5D-O5D-PN-O3
2	I	400	NAP	C5B-O5B-PA-O3
2	I	400	NAP	C5D-O5D-PN-O3
2	J	400	NAP	C5B-O5B-PA-O3
2	J	400	NAP	C5D-O5D-PN-O3
2	K	400	NAP	C5B-O5B-PA-O3
2	Q	400	NAP	C5B-O5B-PA-O3
2	R	400	NAP	C5B-O5B-PA-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	R	400	NAP	C2B-O2B-P2B-O2X
2	R	400	NAP	C5D-O5D-PN-O3
2	T	400	NAP	C5B-O5B-PA-O3
3	H	401	ADP	C5'-O5'-PA-O3A
3	L	401	ADP	C5'-O5'-PA-O3A
3	R	401	ADP	C5'-O5'-PA-O3A
2	A	400	NAP	O4B-C4B-C5B-O5B
2	D	400	NAP	O4B-C4B-C5B-O5B
2	N	400	NAP	C3B-C4B-C5B-O5B
2	T	400	NAP	PA-O3-PN-O2N
3	J	401	ADP	PB-O3A-PA-O1A
2	J	400	NAP	C4B-C5B-O5B-PA
2	L	400	NAP	C4B-C5B-O5B-PA
2	Q	400	NAP	C4B-C5B-O5B-PA
2	B	400	NAP	C5B-O5B-PA-O1A
2	C	400	NAP	C5B-O5B-PA-O1A
2	H	400	NAP	C5B-O5B-PA-O1A
2	I	400	NAP	C5B-O5B-PA-O1A
2	I	400	NAP	C5B-O5B-PA-O2A
2	I	400	NAP	C5D-O5D-PN-O1N
2	J	400	NAP	C5B-O5B-PA-O1A
2	J	400	NAP	C5D-O5D-PN-O1N
2	K	400	NAP	C5B-O5B-PA-O1A
2	Q	400	NAP	C5B-O5B-PA-O1A
2	R	400	NAP	C5D-O5D-PN-O1N
2	T	400	NAP	C5B-O5B-PA-O1A
3	E	401	ADP	C5'-O5'-PA-O1A
3	K	401	ADP	C5'-O5'-PA-O2A
2	C	400	NAP	C4B-C5B-O5B-PA
2	I	400	NAP	C4B-C5B-O5B-PA
4	C	402	BMA	O5-C5-C6-O6
3	E	401	ADP	PA-O3A-PB-O1B
2	A	400	NAP	C4B-C5B-O5B-PA
2	F	400	NAP	C4B-C5B-O5B-PA
2	G	400	NAP	C4B-C5B-O5B-PA
2	E	400	NAP	PA-O3-PN-O2N
2	H	400	NAP	PA-O3-PN-O2N
2	J	400	NAP	PA-O3-PN-O2N
2	Q	400	NAP	PA-O3-PN-O2N
2	N	400	NAP	C4B-C5B-O5B-PA
2	B	400	NAP	C3D-C4D-C5D-O5D
2	J	400	NAP	C3B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	L	400	NAP	O4B-C4B-C5B-O5B
2	S	400	NAP	C4B-C5B-O5B-PA
3	T	401	ADP	PA-O3A-PB-O1B
2	M	400	NAP	C3B-C4B-C5B-O5B
2	G	400	NAP	PA-O3-PN-O1N
2	G	400	NAP	PA-O3-PN-O2N
2	K	400	NAP	PA-O3-PN-O2N
2	N	400	NAP	PA-O3-PN-O1N
2	P	400	NAP	C4B-C5B-O5B-PA
2	R	400	NAP	C4B-C5B-O5B-PA
2	A	400	NAP	C3B-C4B-C5B-O5B
3	E	401	ADP	O4'-C4'-C5'-O5'
3	S	401	ADP	PA-O3A-PB-O2B
2	A	400	NAP	C2B-O2B-P2B-O3X
2	A	400	NAP	C5D-O5D-PN-O3
2	B	400	NAP	C2B-O2B-P2B-O3X
2	C	400	NAP	C2B-O2B-P2B-O3X
2	C	400	NAP	C5D-O5D-PN-O3
2	E	400	NAP	C2B-O2B-P2B-O3X
2	E	400	NAP	C5D-O5D-PN-O3
2	F	400	NAP	C5B-O5B-PA-O3
2	F	400	NAP	C2B-O2B-P2B-O2X
2	M	400	NAP	C5B-O5B-PA-O3
2	N	400	NAP	C5B-O5B-PA-O3
2	P	400	NAP	C2B-O2B-P2B-O2X
2	P	400	NAP	C2B-O2B-P2B-O3X
2	S	400	NAP	C2B-O2B-P2B-O3X
2	B	400	NAP	PA-O3-PN-O2N
2	C	400	NAP	PA-O3-PN-O2N
2	F	400	NAP	PA-O3-PN-O1N
2	I	400	NAP	PA-O3-PN-O2N
2	J	400	NAP	PA-O3-PN-O1N
2	M	400	NAP	PA-O3-PN-O1N
2	N	400	NAP	PA-O3-PN-O2N
2	O	400	NAP	PA-O3-PN-O1N
2	P	400	NAP	PA-O3-PN-O2N
2	Q	400	NAP	PA-O3-PN-O1N
2	R	400	NAP	PA-O3-PN-O1N
3	N	401	ADP	PB-O3A-PA-O2A
2	O	400	NAP	C4B-C5B-O5B-PA
2	A	400	NAP	C5D-O5D-PN-O1N
2	E	400	NAP	C5B-O5B-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	M	400	NAP	C5B-O5B-PA-O1A
2	N	400	NAP	C5B-O5B-PA-O1A
2	P	400	NAP	C5B-O5B-PA-O1A
2	R	400	NAP	C5B-O5B-PA-O1A
2	S	400	NAP	C5B-O5B-PA-O1A
2	G	400	NAP	O4B-C4B-C5B-O5B
2	Q	400	NAP	C3D-C4D-C5D-O5D
4	I	402	BMA	O5-C5-C6-O6
3	K	401	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

41 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	400	NAP	3	0
2	O	400	NAP	1	0
4	R	402	BMA	2	0
2	E	400	NAP	2	0
2	N	400	NAP	1	0
3	G	401	ADP	1	0
4	S	402	BMA	1	0
2	Q	400	NAP	4	0
4	G	402	BMA	1	0
4	K	402	BMA	2	0
2	M	400	NAP	6	0
2	F	400	NAP	3	0
4	H	402	BMA	2	0
2	C	400	NAP	3	0
2	G	400	NAP	1	0
4	O	402	BMA	1	0
2	J	400	NAP	3	0
4	N	402	BMA	1	0
4	P	402	BMA	2	0
4	D	402	BMA	2	0
4	T	402	BMA	2	0
2	P	400	NAP	3	0
2	D	400	NAP	3	0
4	A	402	BMA	1	0
4	F	402	BMA	2	0
4	C	402	BMA	2	0
2	L	400	NAP	3	0
4	L	402	BMA	2	0

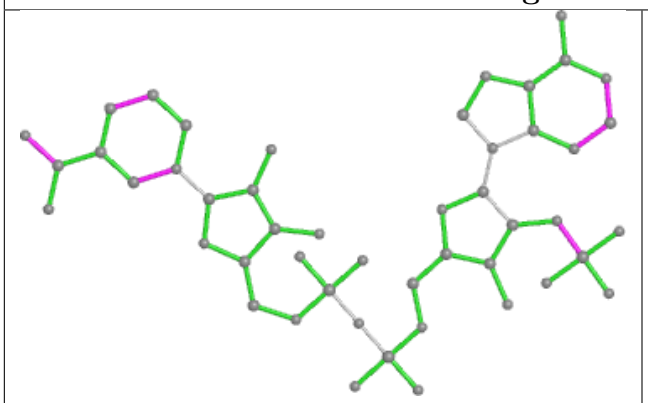
Continued on next page...

Continued from previous page...

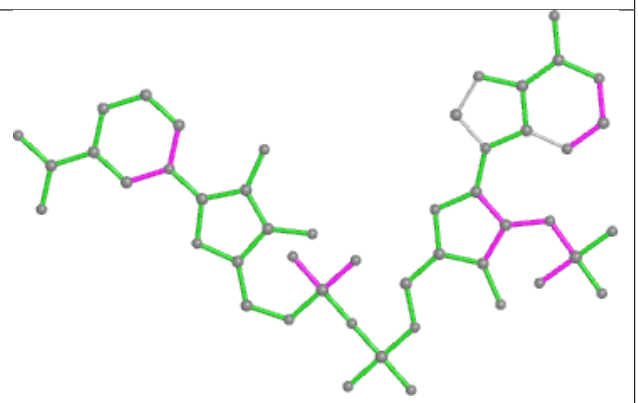
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	400	NAP	1	0
4	E	402	BMA	2	0
3	A	401	ADP	1	0
4	M	402	BMA	2	0
3	B	401	ADP	1	0
4	Q	402	BMA	1	0
2	K	400	NAP	3	0
4	I	402	BMA	3	0
4	J	402	BMA	2	0
2	H	400	NAP	3	0
2	I	400	NAP	3	0
2	A	400	NAP	2	0
2	T	400	NAP	2	0

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.

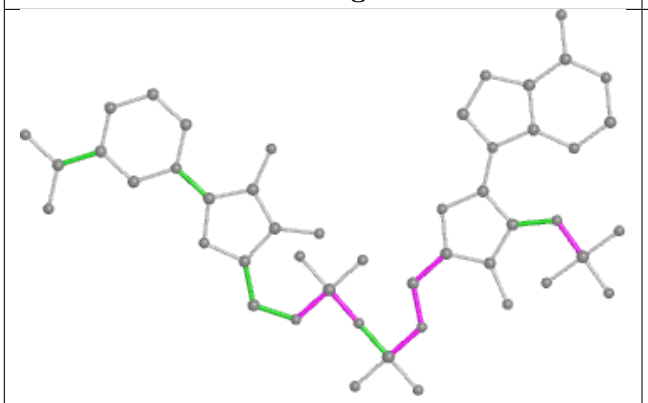
Ligand NAP R 400



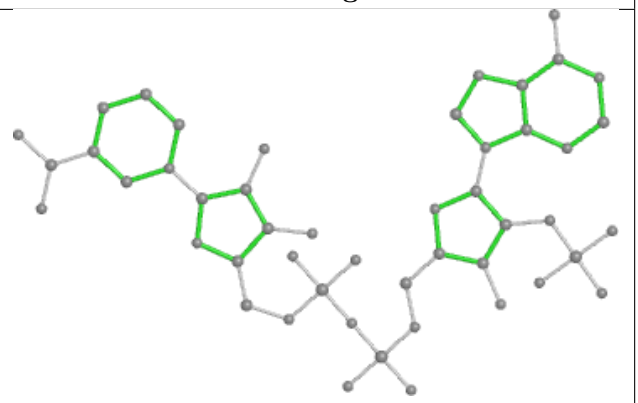
Bond lengths



Bond angles

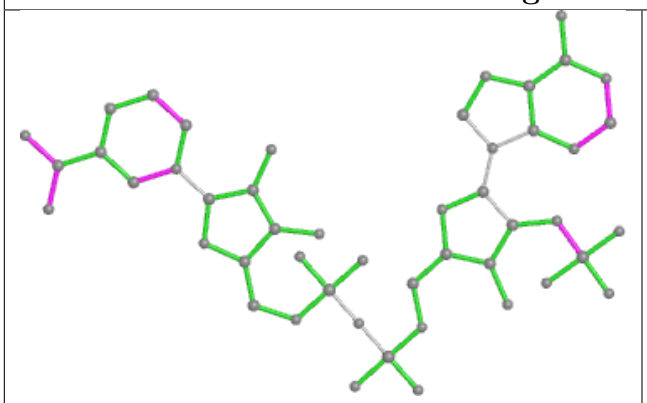


Torsions

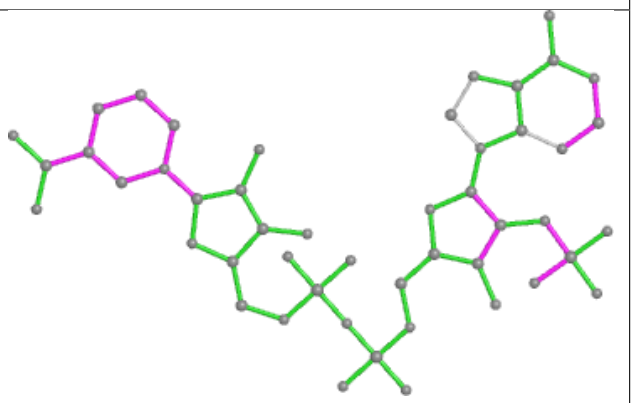


Rings

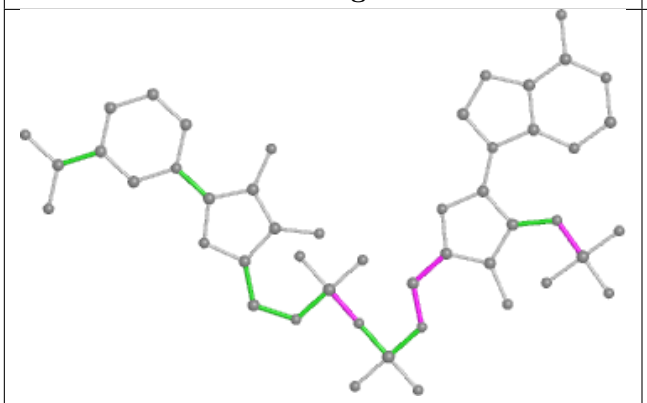
Ligand NAP O 400



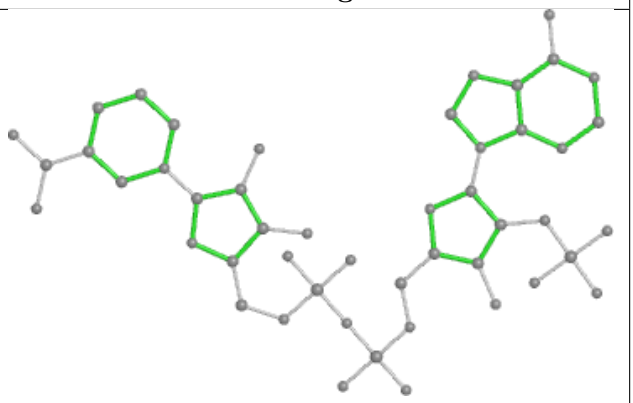
Bond lengths



Bond angles

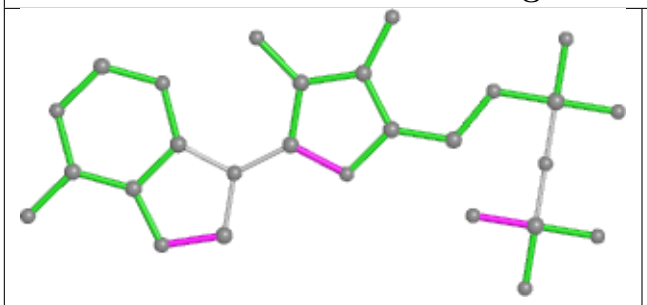


Torsions

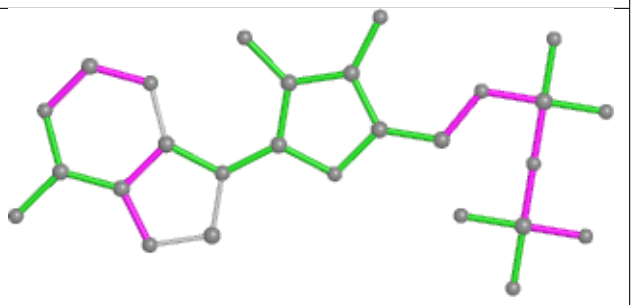


Rings

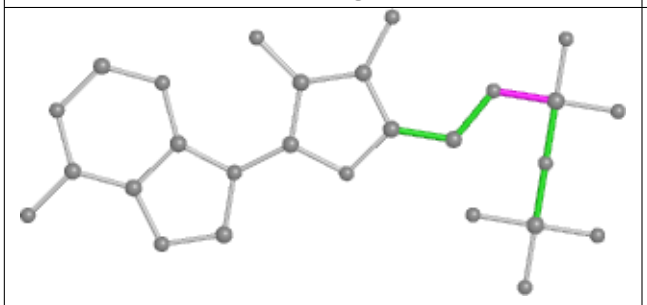
Ligand ADP R 401



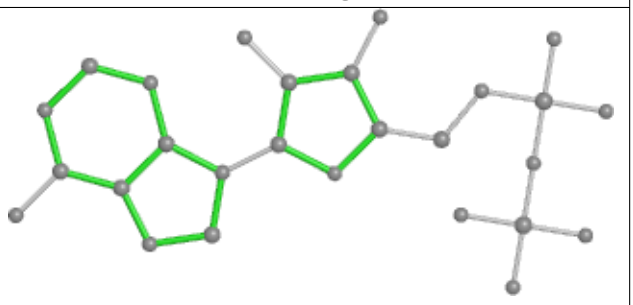
Bond lengths



Bond angles

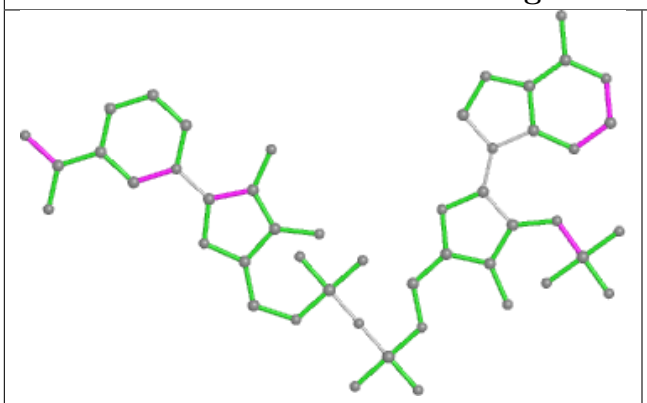


Torsions

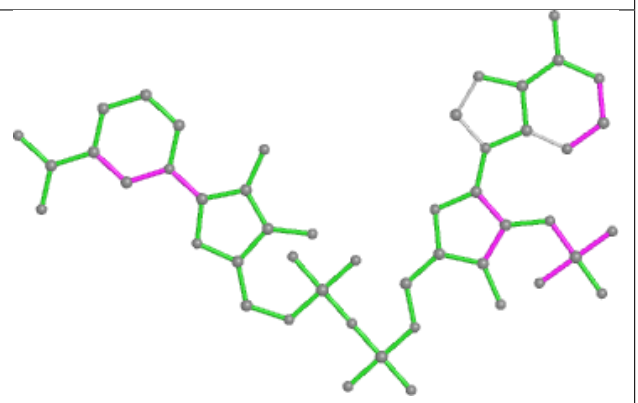


Rings

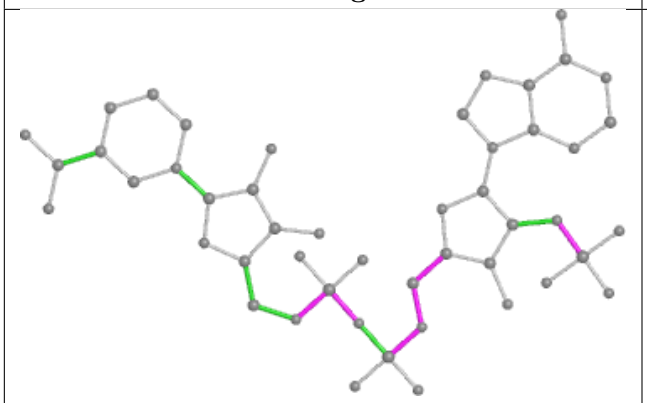
Ligand NAP E 400



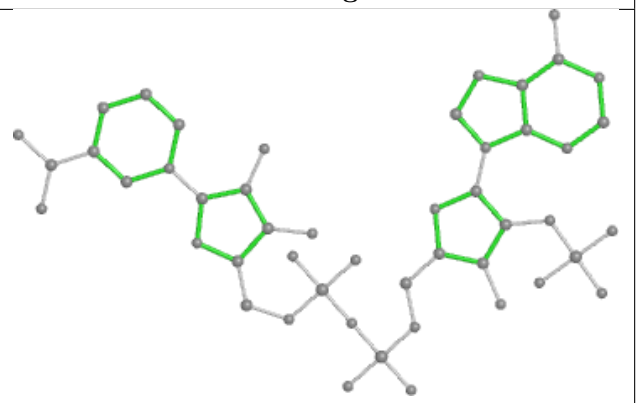
Bond lengths



Bond angles

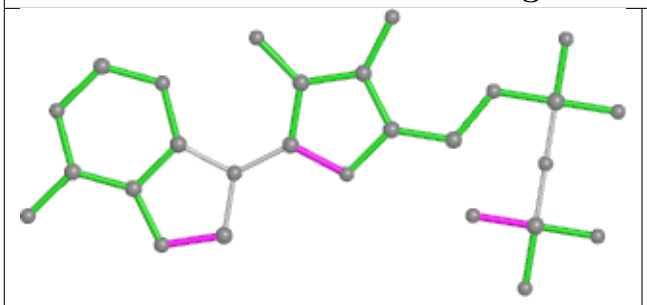


Torsions

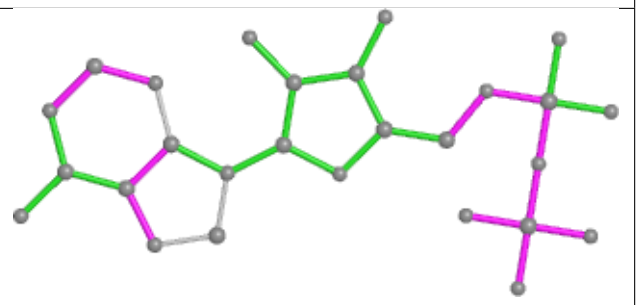


Rings

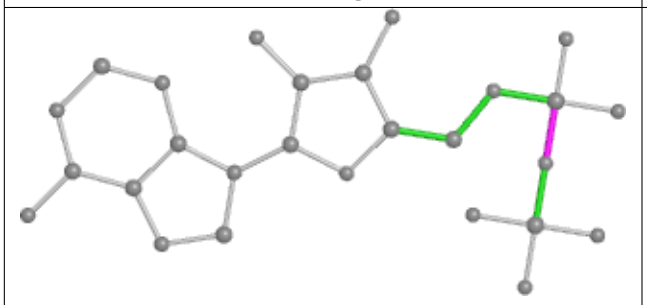
Ligand ADP N 401



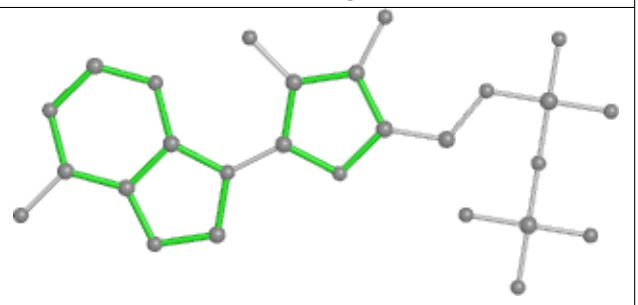
Bond lengths



Bond angles

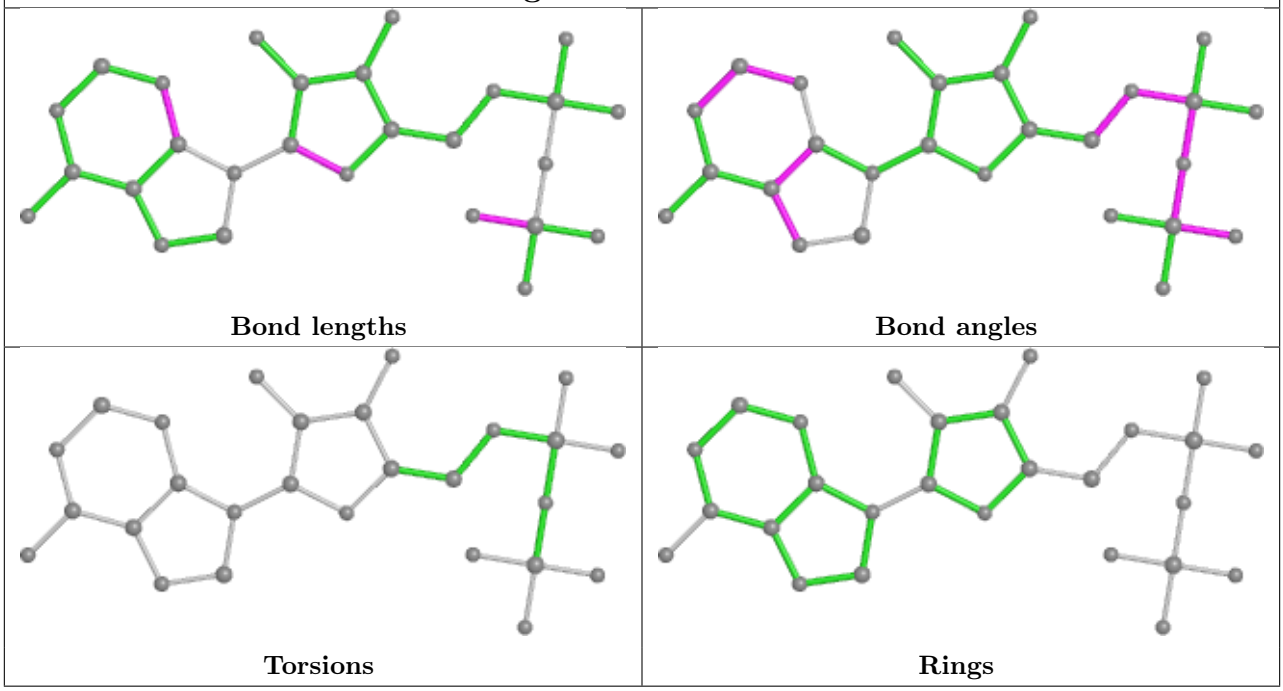


Torsions

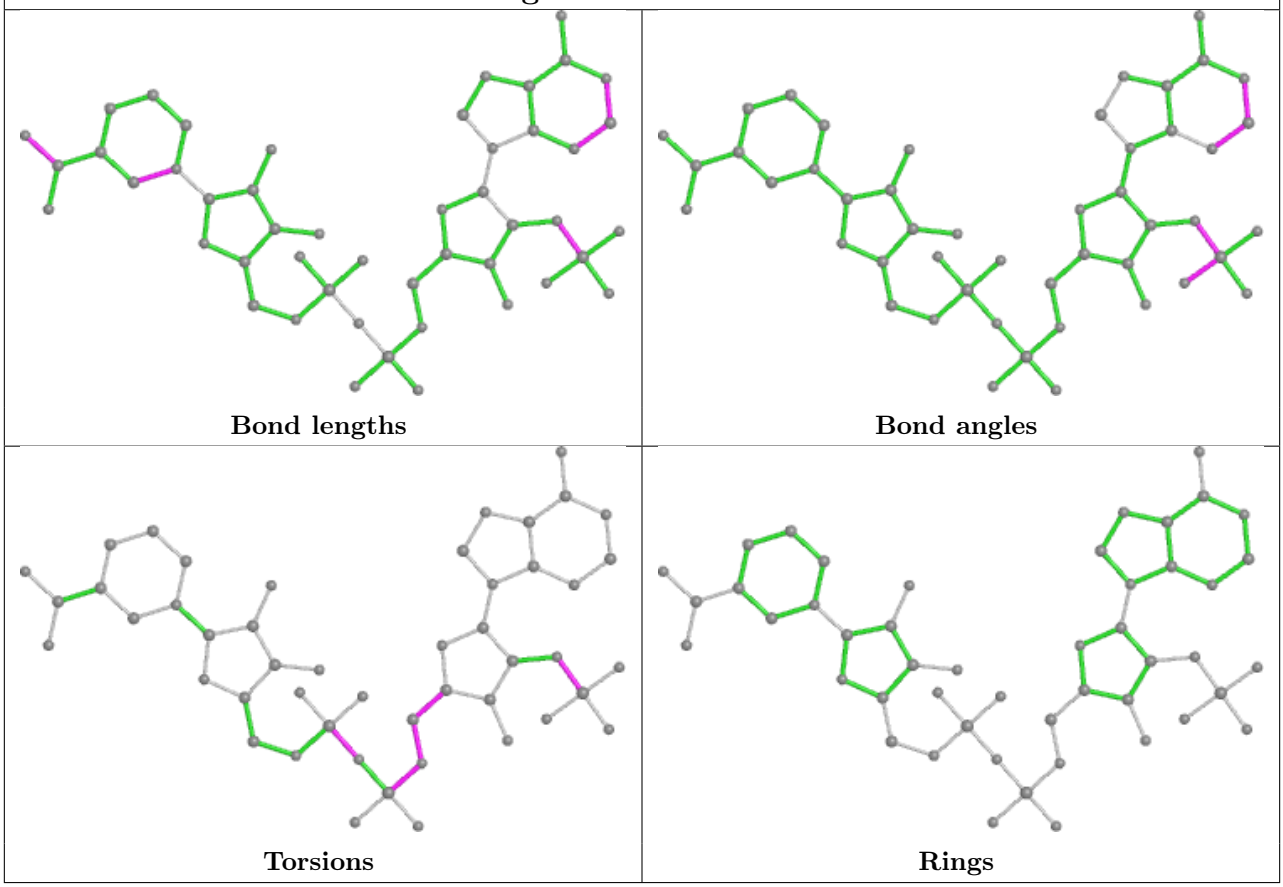


Rings

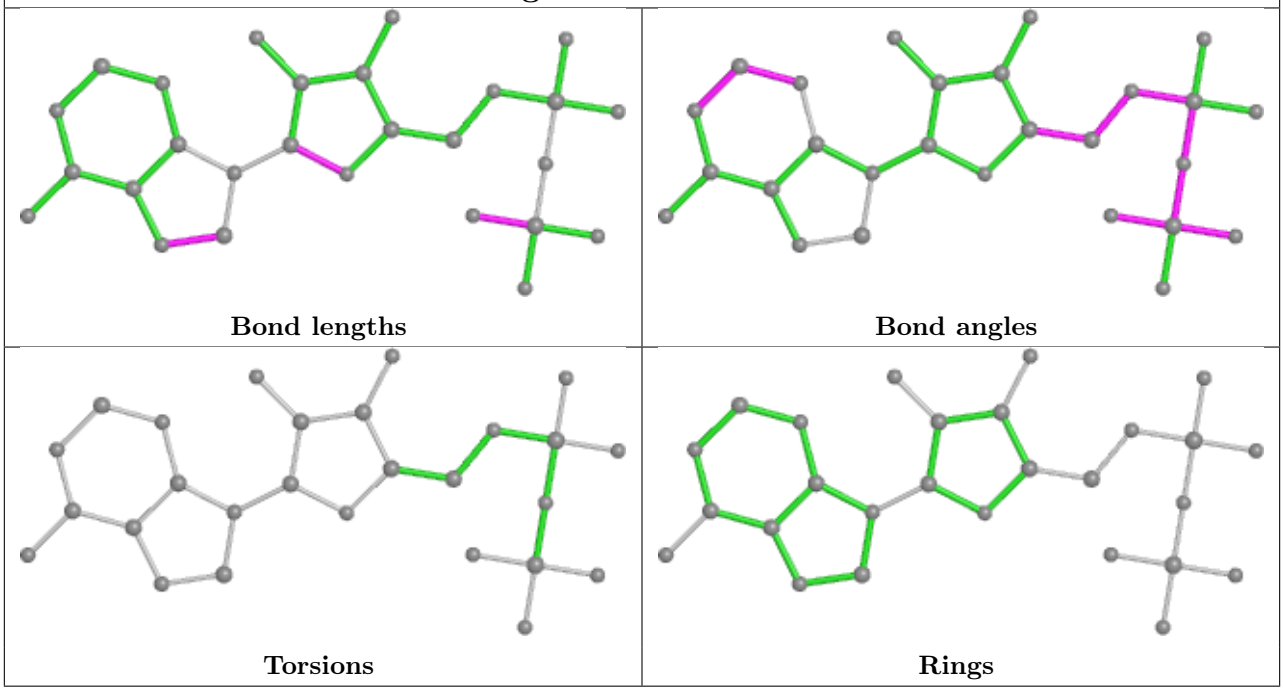
Ligand ADP P 401



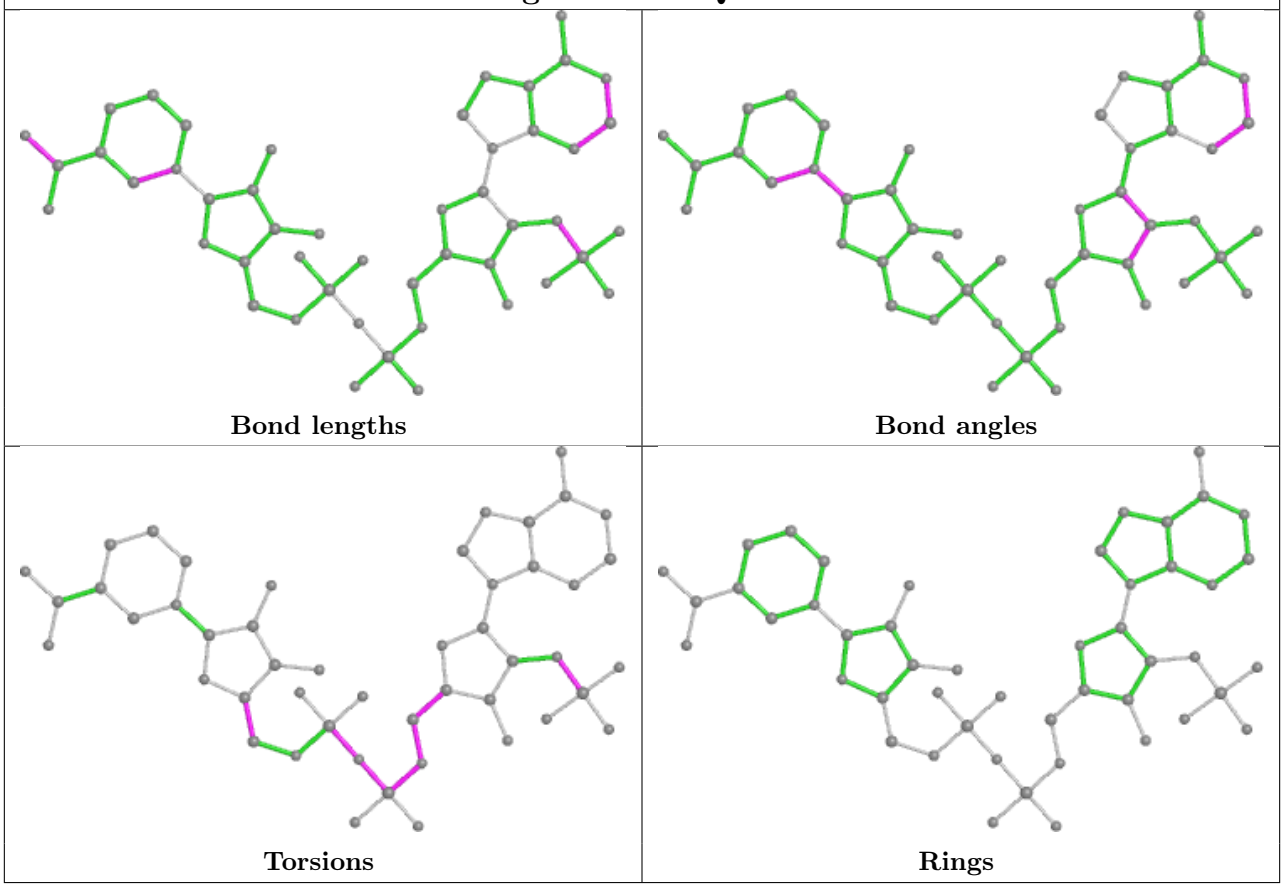
Ligand NAP N 400



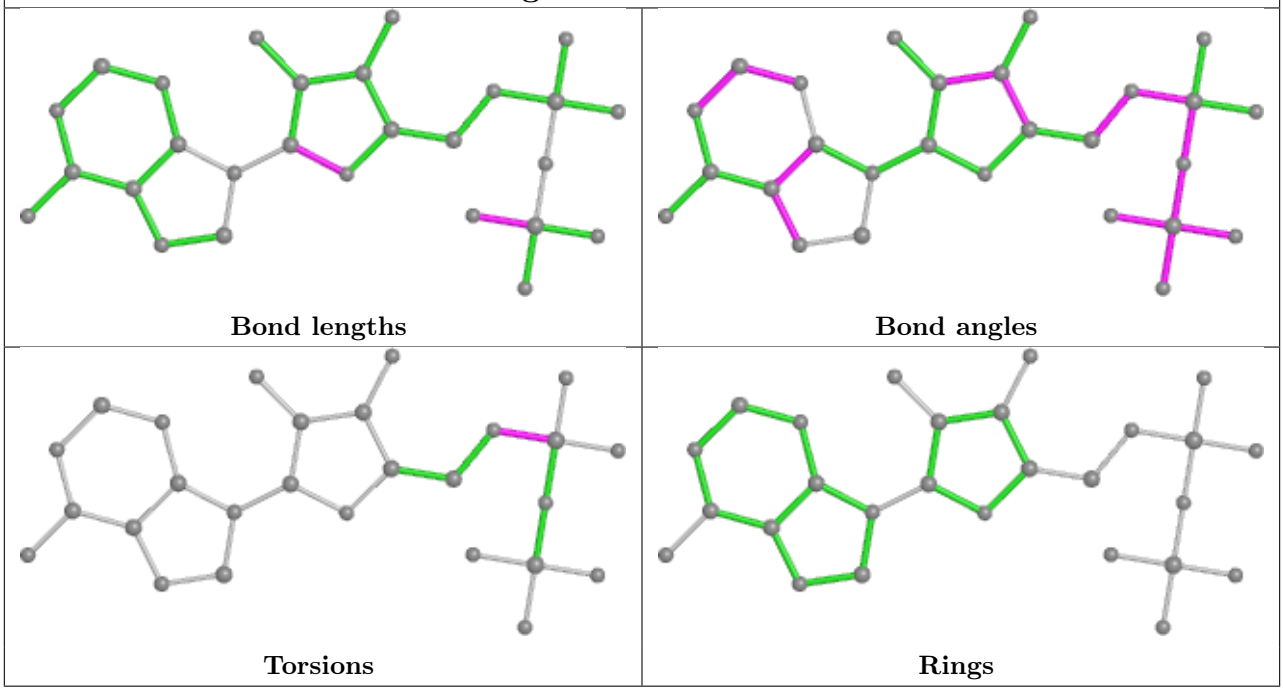
Ligand ADP G 401



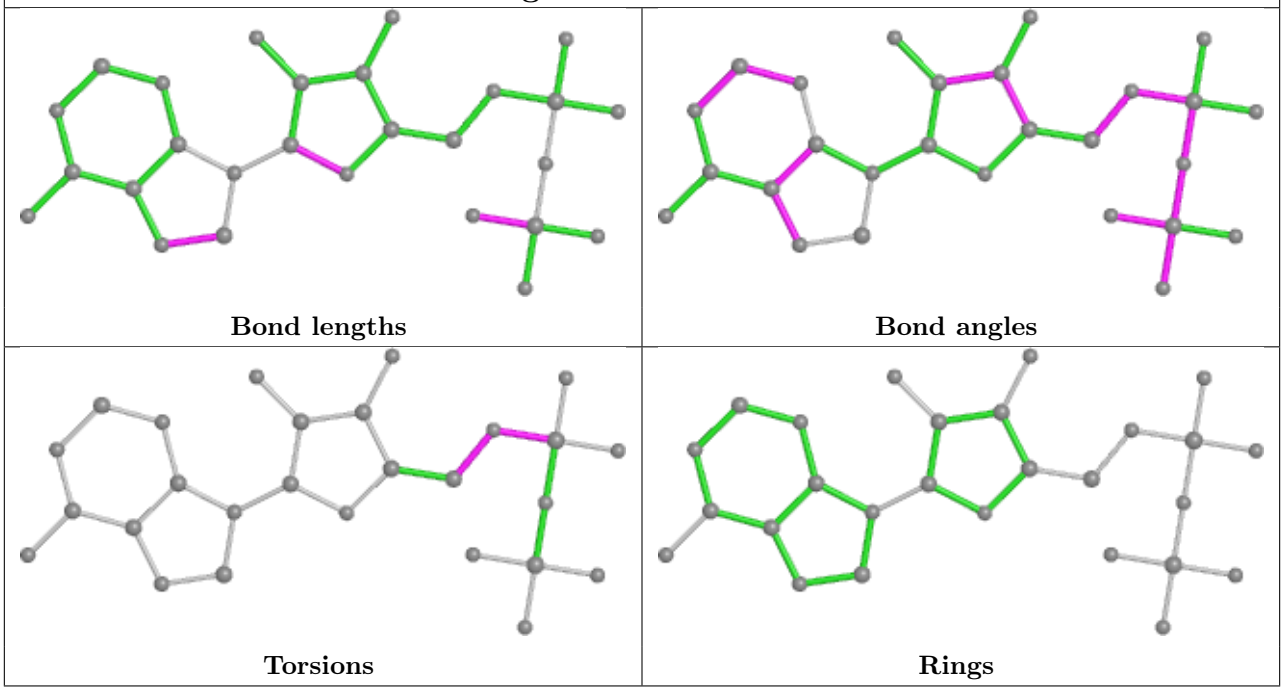
Ligand NAP Q 400



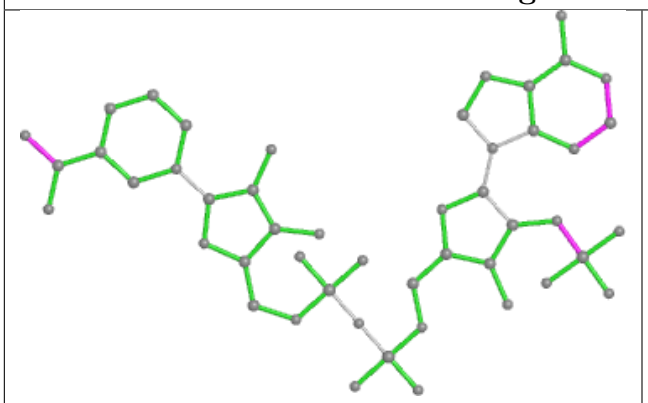
Ligand ADP H 401



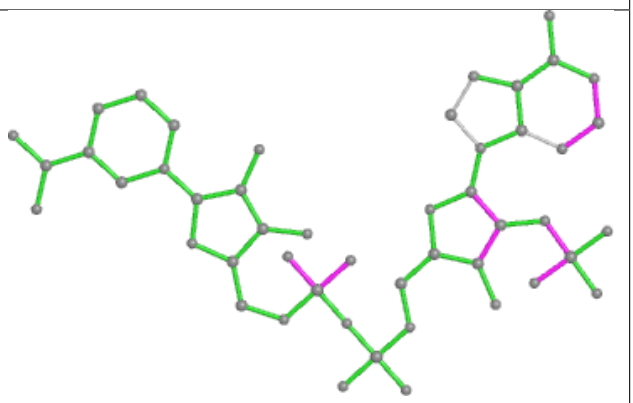
Ligand ADP K 401



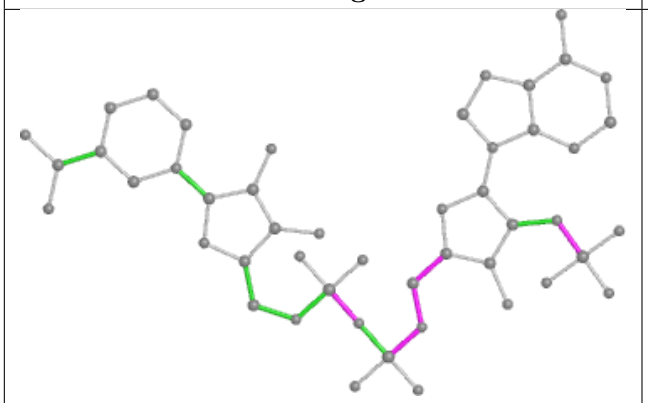
Ligand NAP M 400



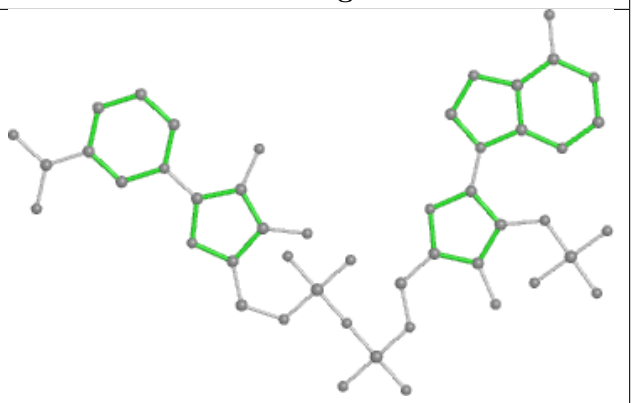
Bond lengths



Bond angles

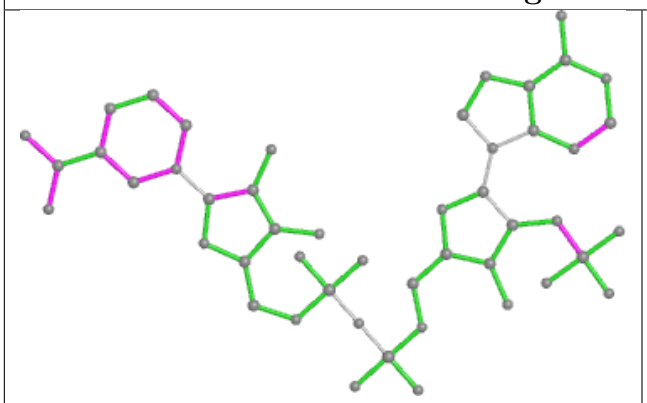


Torsions

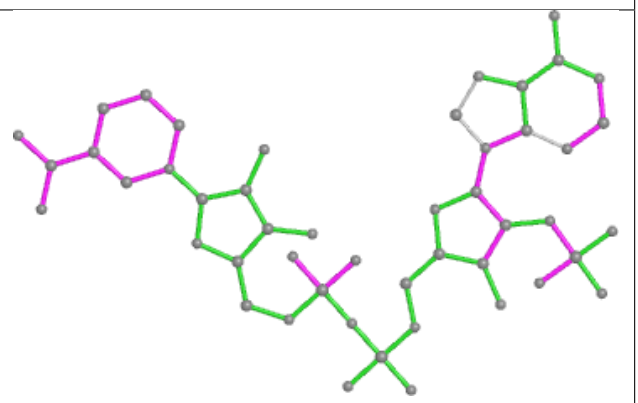


Rings

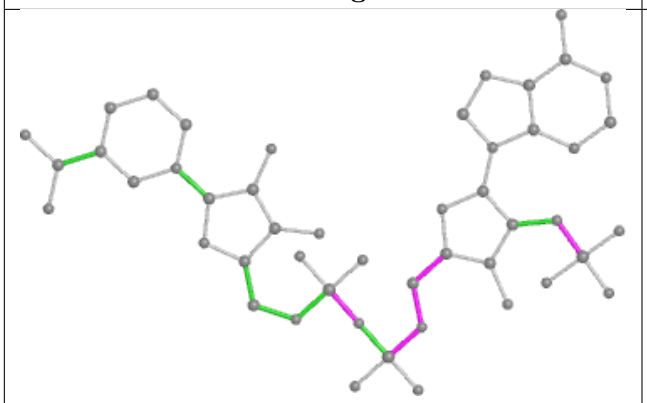
Ligand NAP F 400



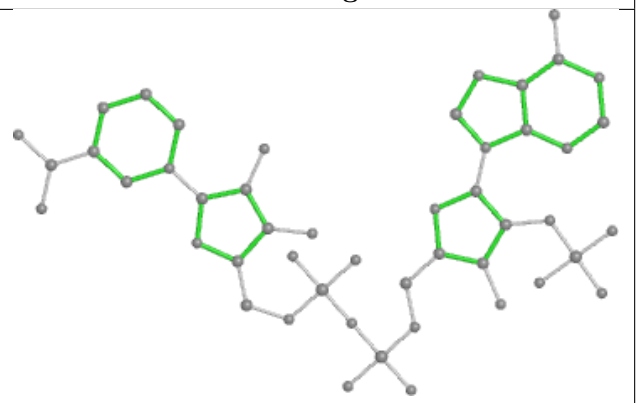
Bond lengths



Bond angles

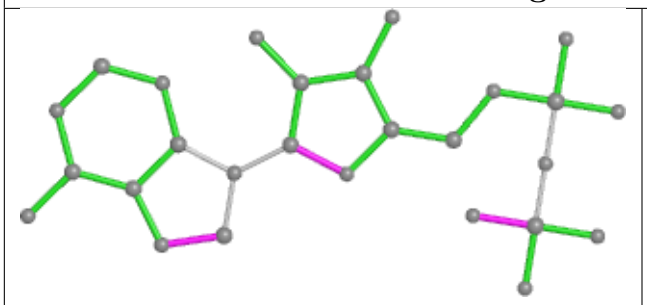


Torsions

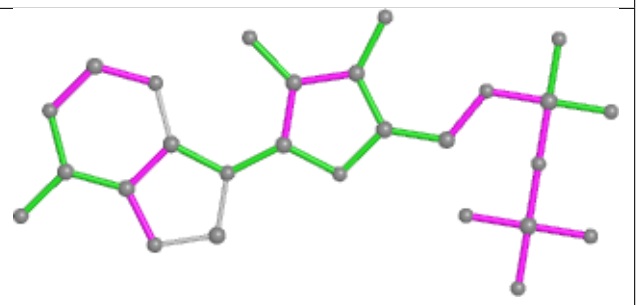


Rings

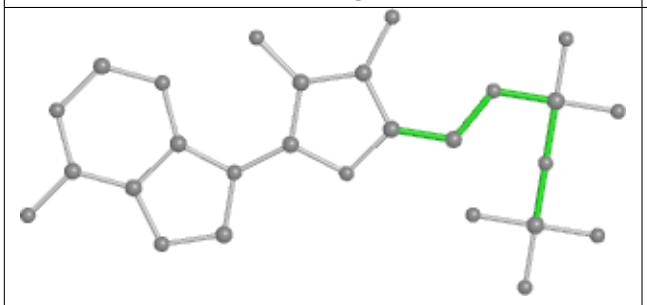
Ligand ADP I 401



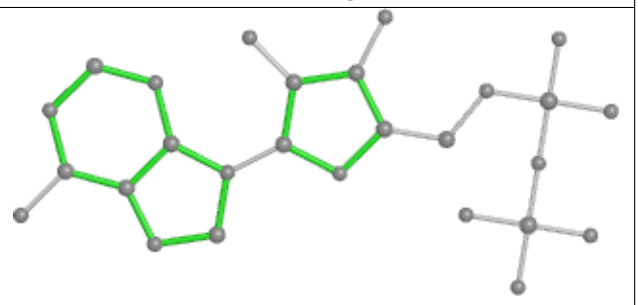
Bond lengths



Bond angles

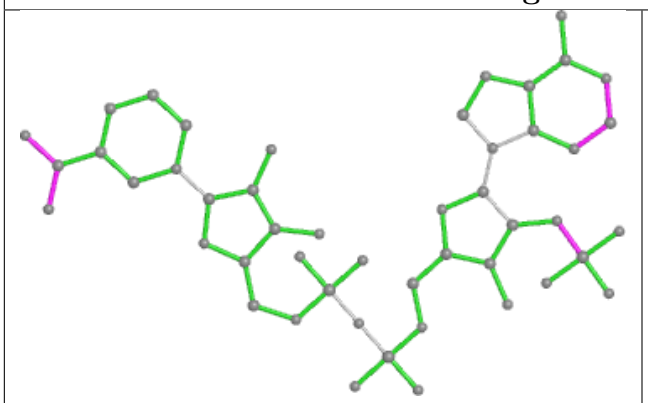


Torsions

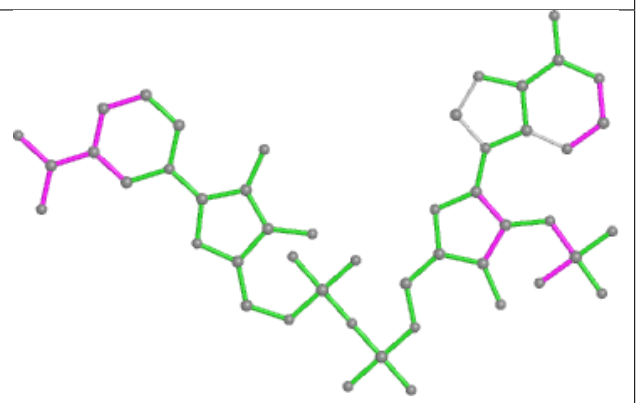


Rings

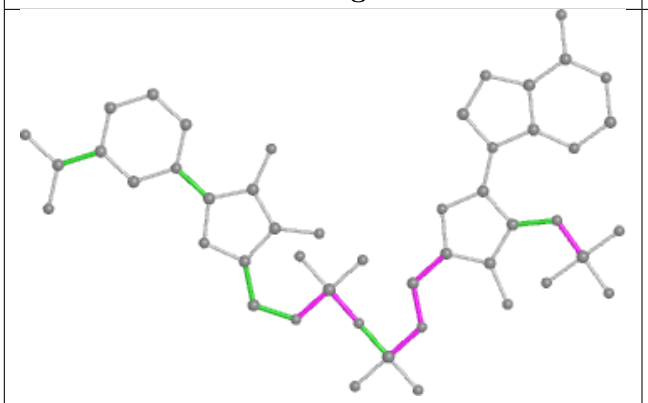
Ligand NAP C 400



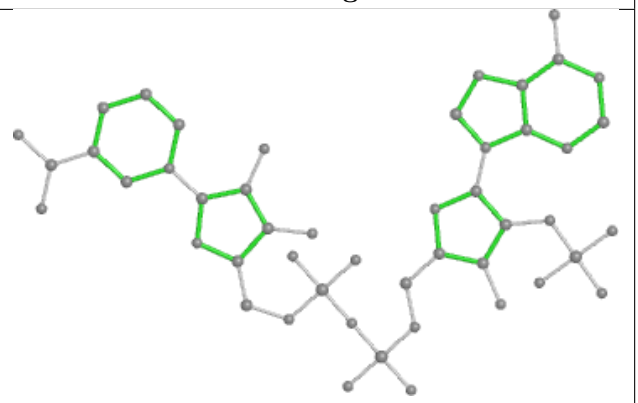
Bond lengths



Bond angles

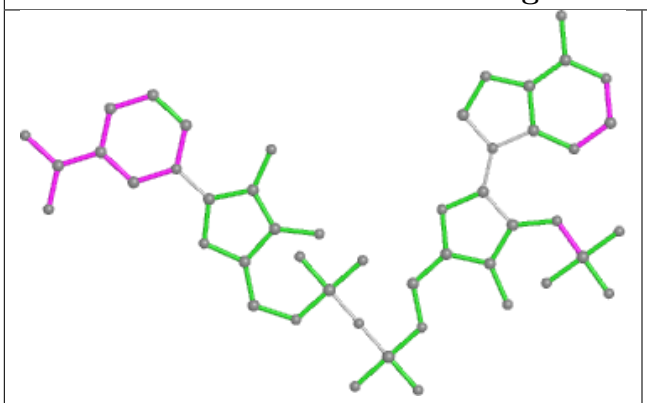


Torsions

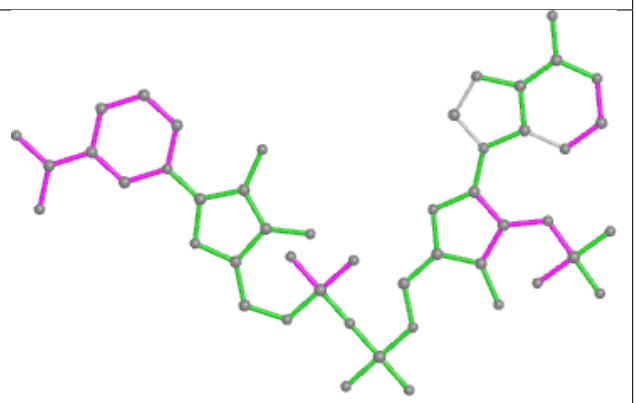


Rings

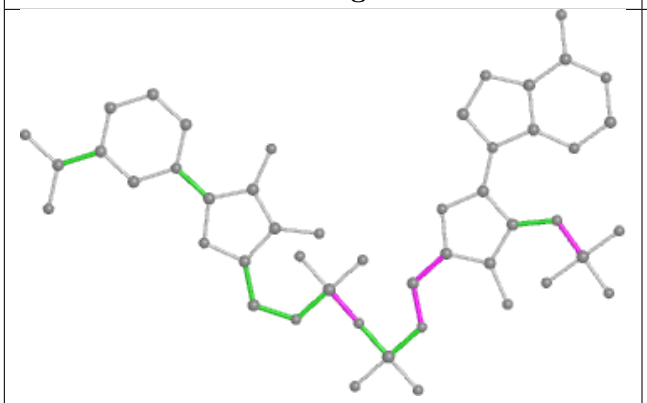
Ligand NAP G 400



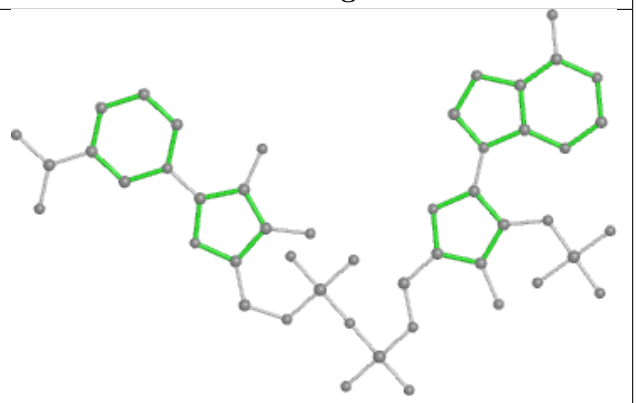
Bond lengths



Bond angles

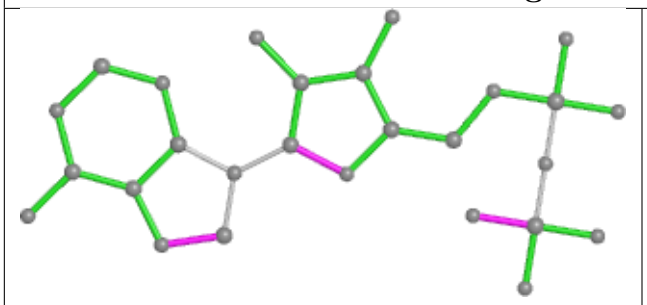


Torsions

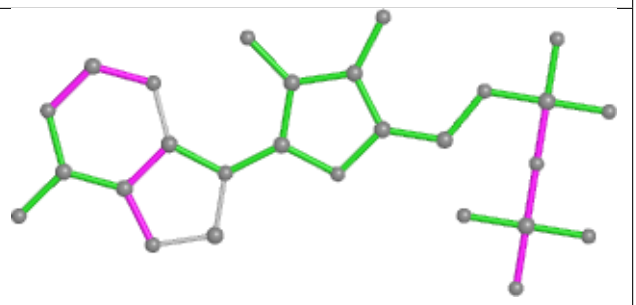


Rings

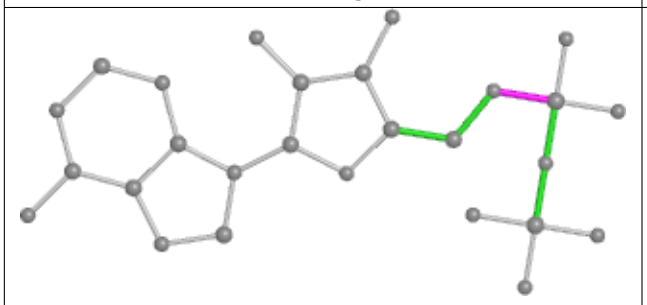
Ligand ADP L 401



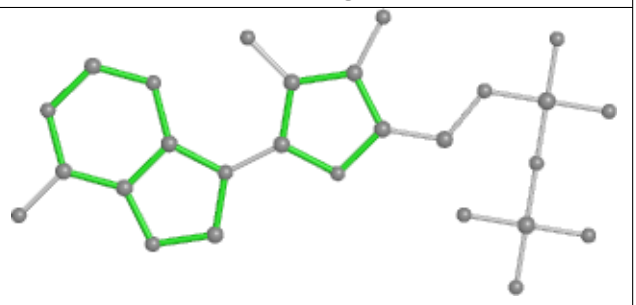
Bond lengths



Bond angles

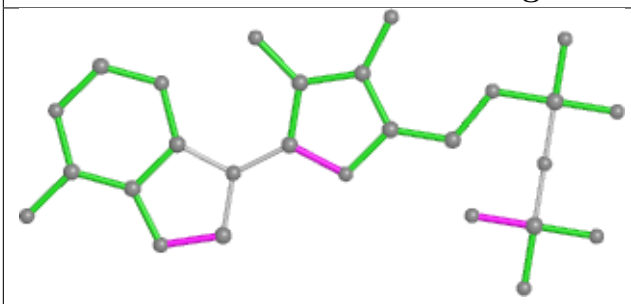


Torsions

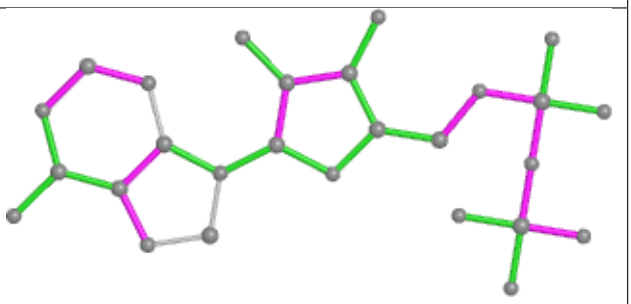


Rings

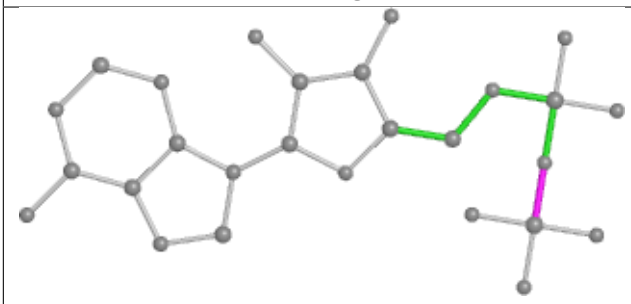
Ligand ADP T 401



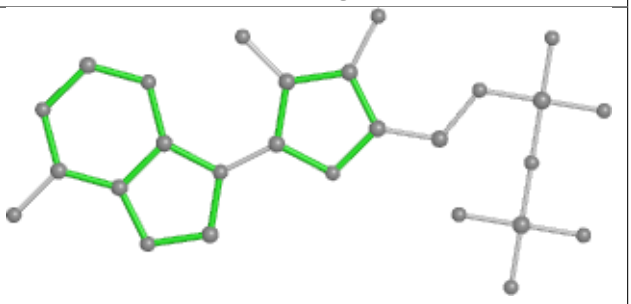
Bond lengths



Bond angles

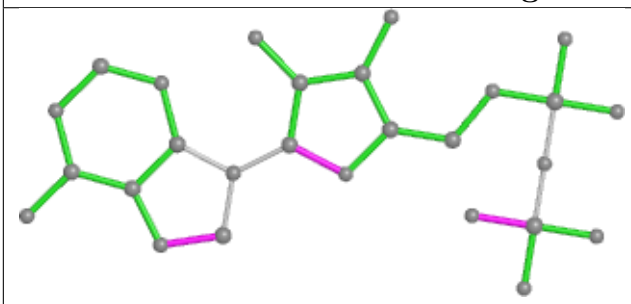


Torsions

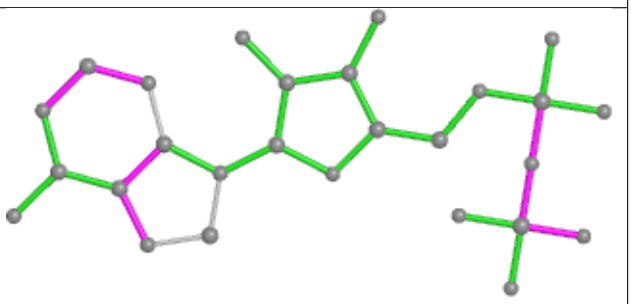


Rings

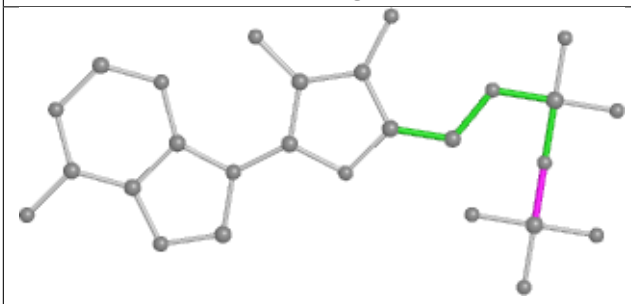
Ligand ADP O 401



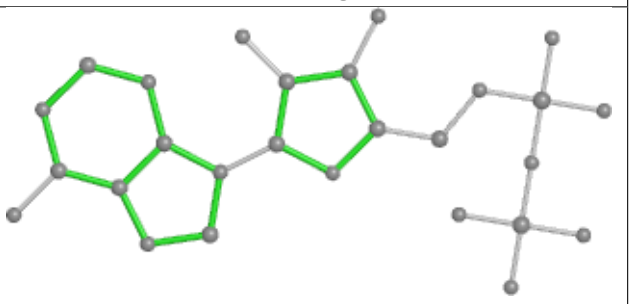
Bond lengths



Bond angles

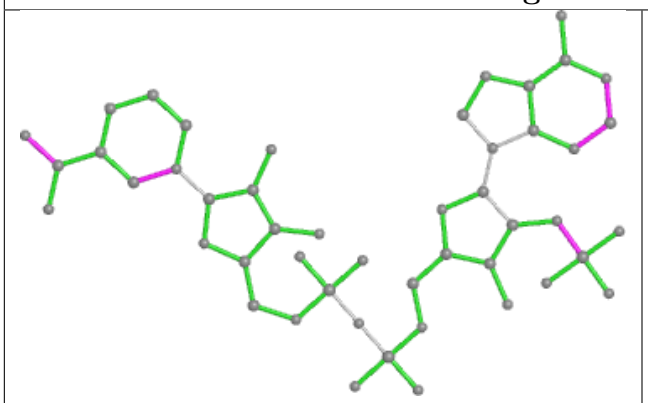


Torsions

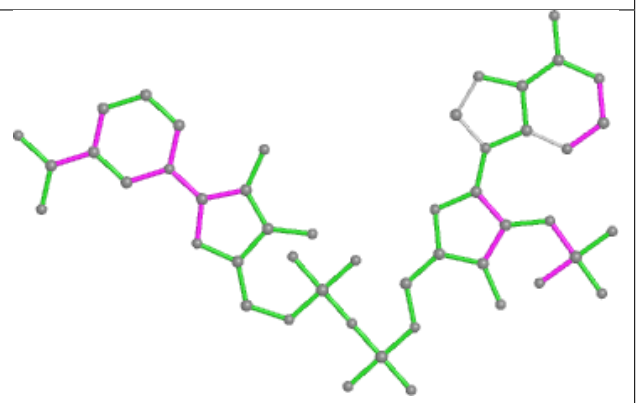


Rings

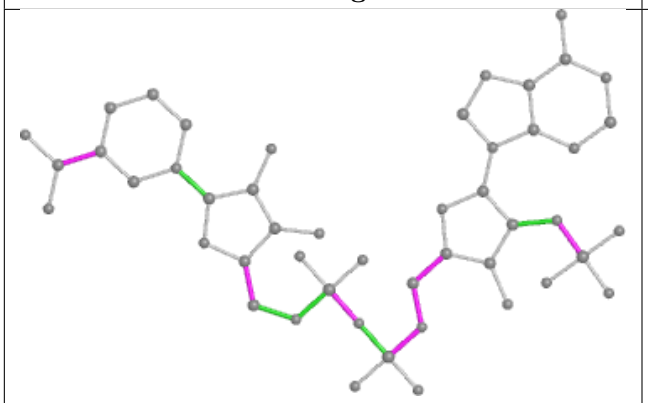
Ligand NAP B 400



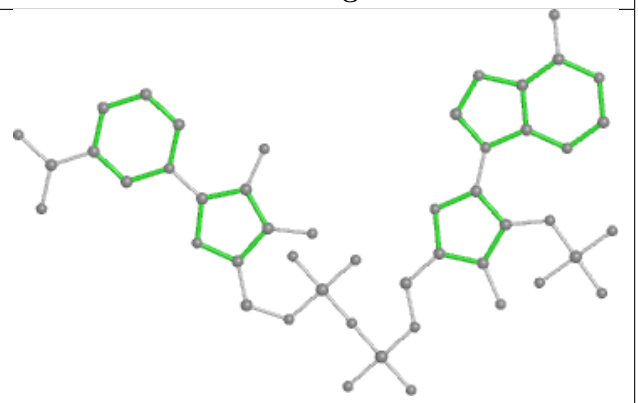
Bond lengths



Bond angles

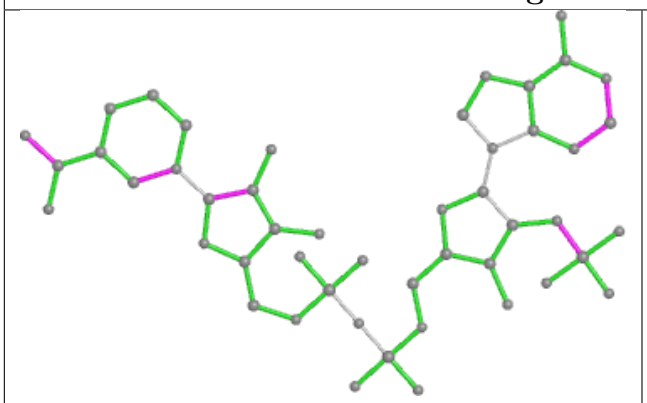


Torsions

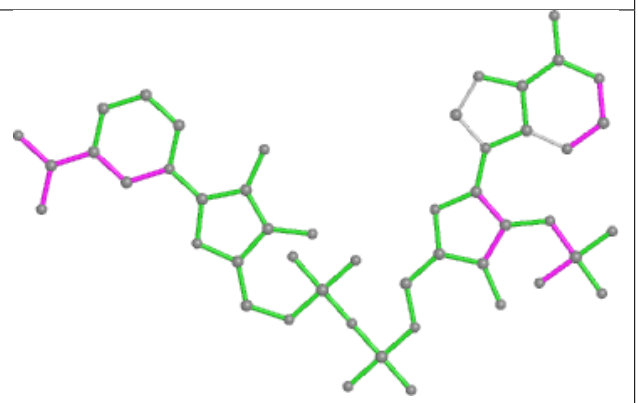


Rings

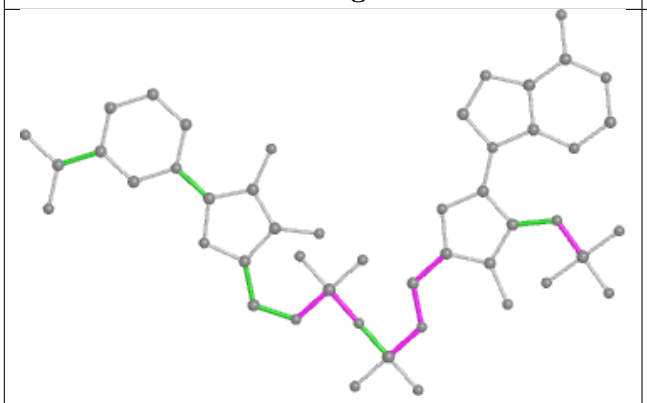
Ligand NAP J 400



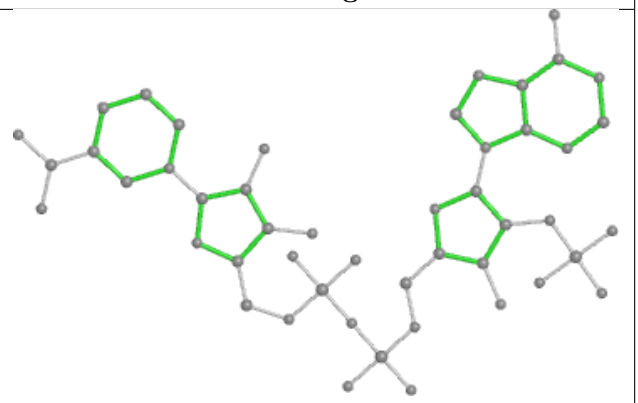
Bond lengths



Bond angles

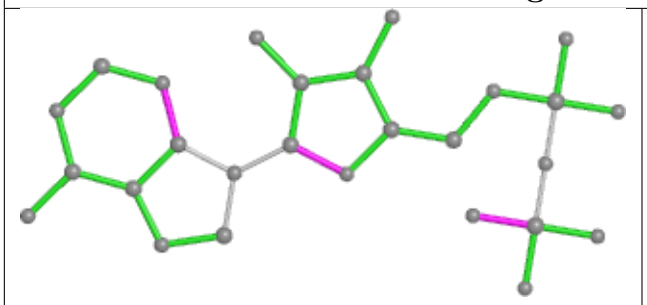


Torsions

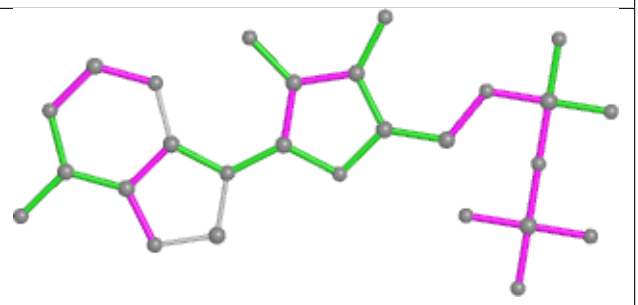


Rings

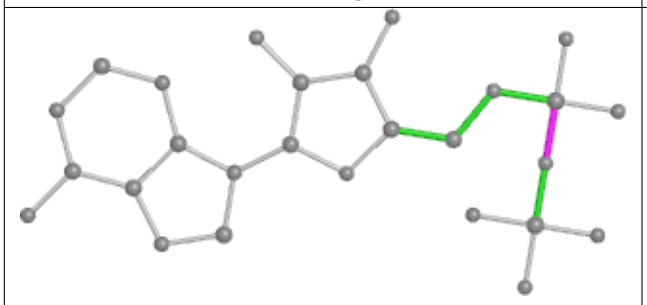
Ligand ADP J 401



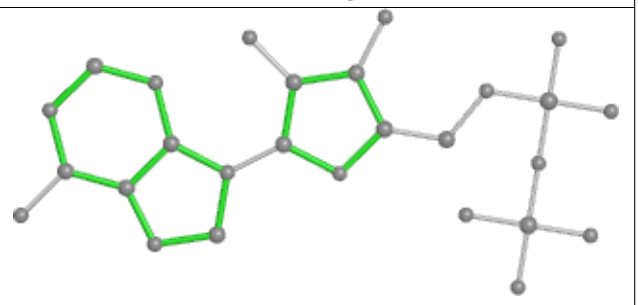
Bond lengths



Bond angles

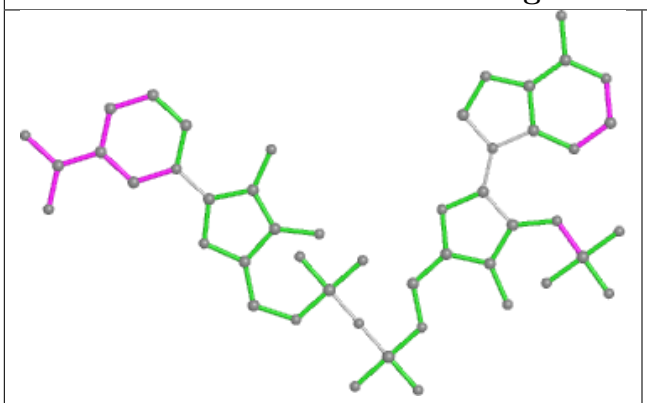


Torsions

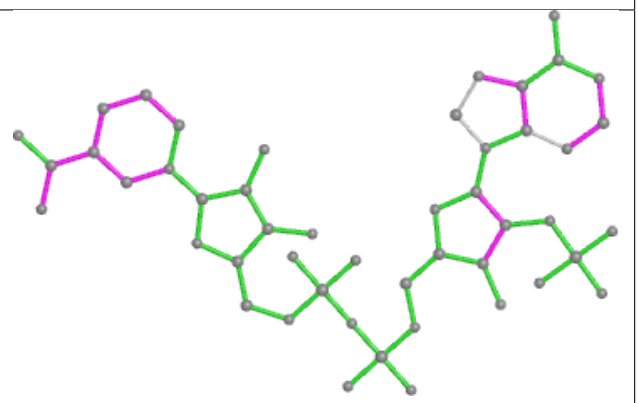


Rings

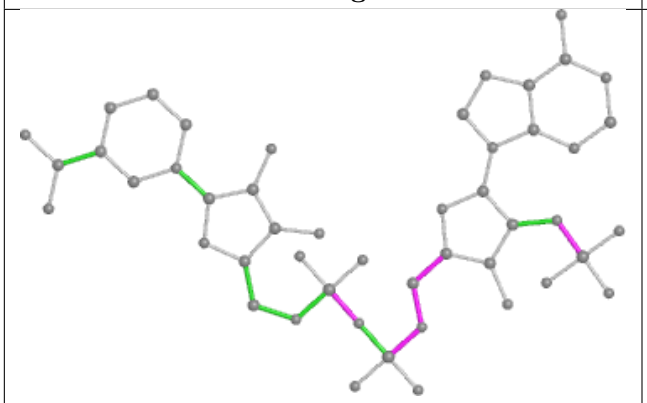
Ligand NAP P 400



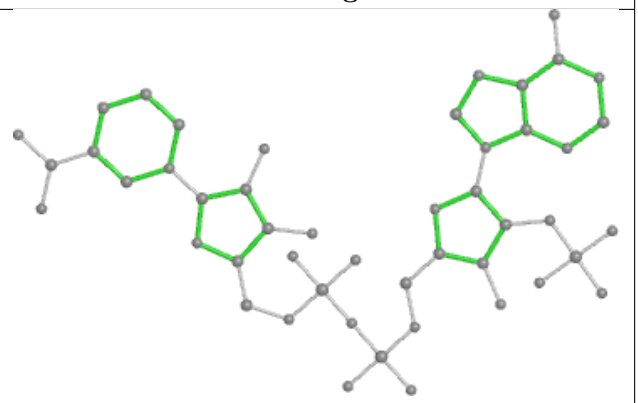
Bond lengths



Bond angles

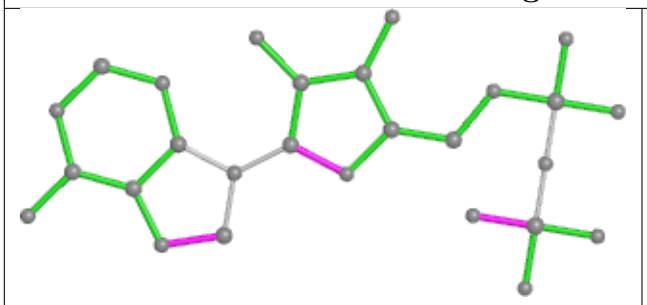


Torsions

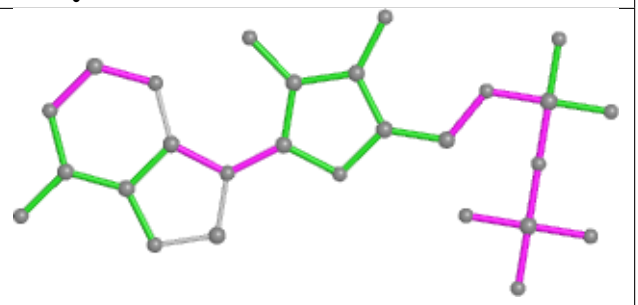


Rings

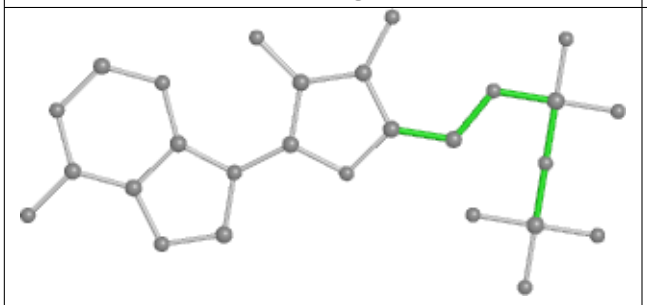
Ligand ADP Q 401



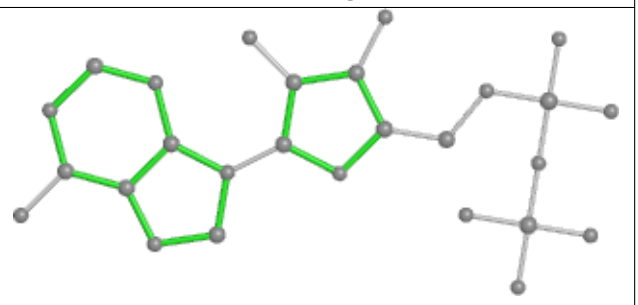
Bond lengths



Bond angles

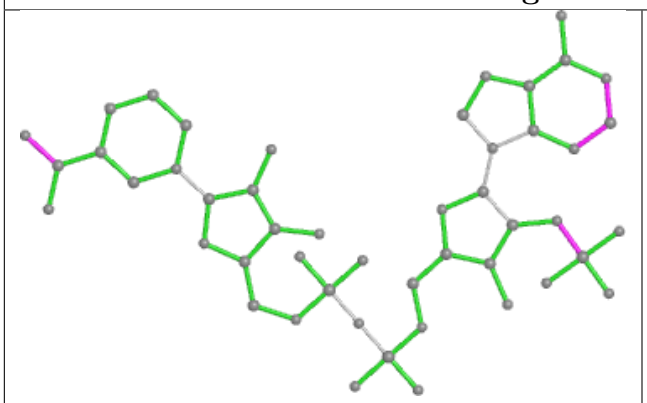


Torsions

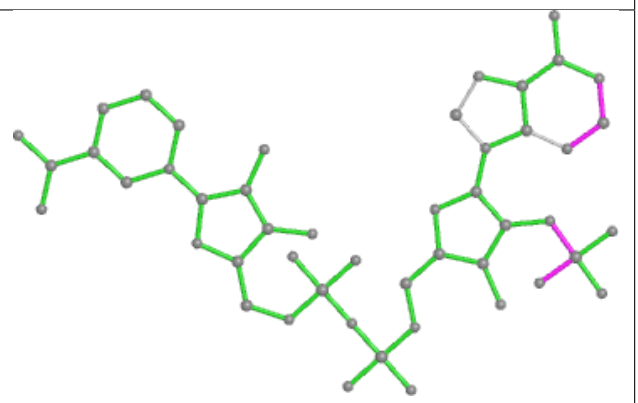


Rings

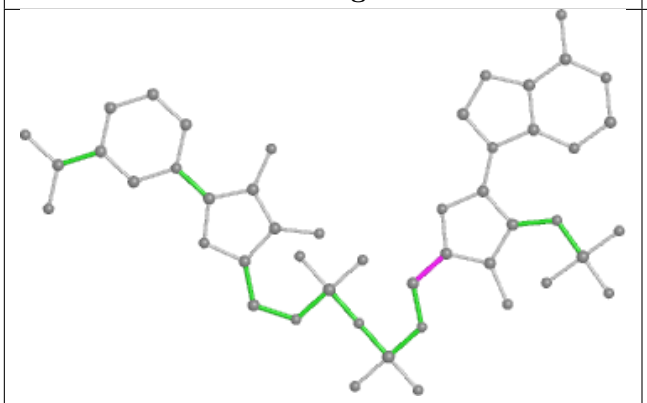
Ligand NAP D 400



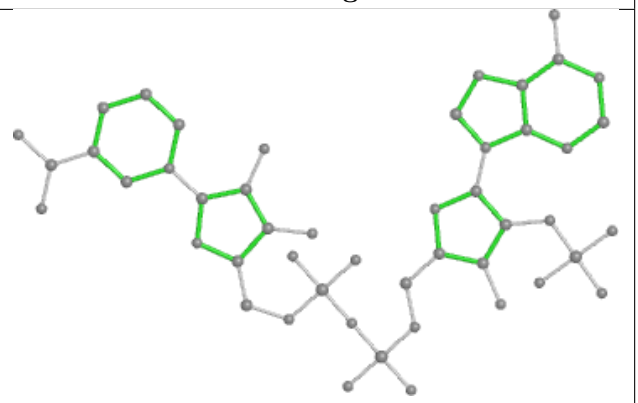
Bond lengths



Bond angles

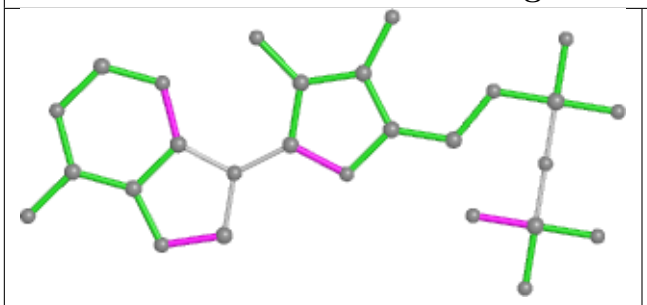


Torsions

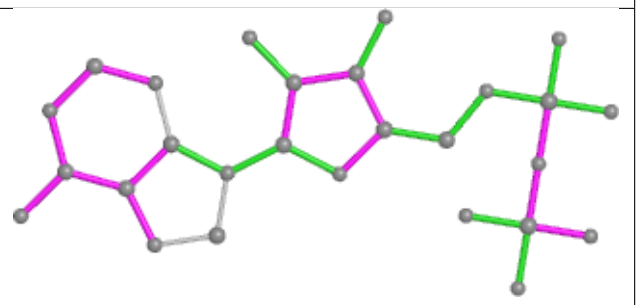


Rings

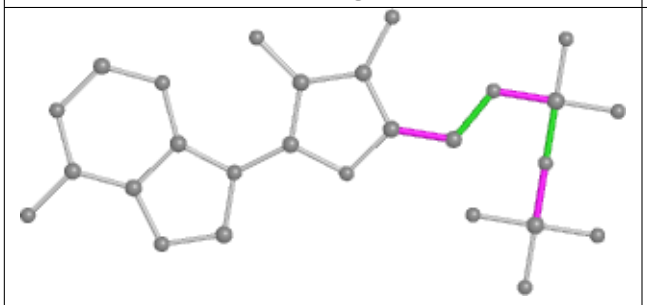
Ligand ADP E 401



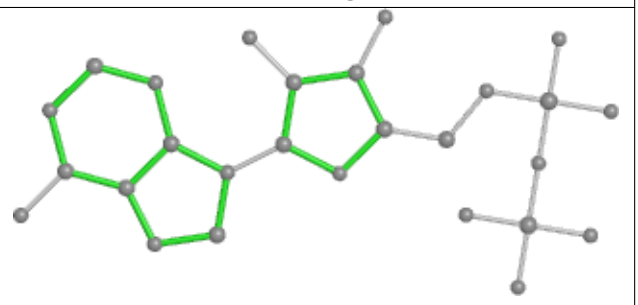
Bond lengths



Bond angles

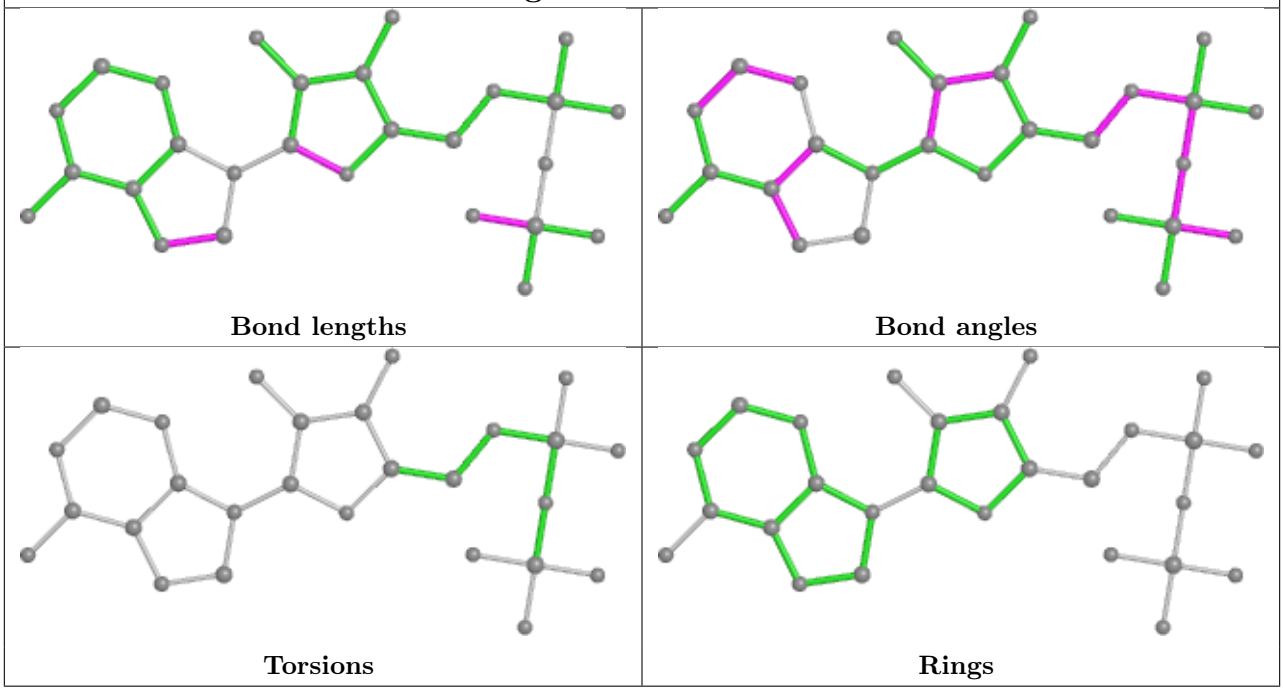


Torsions

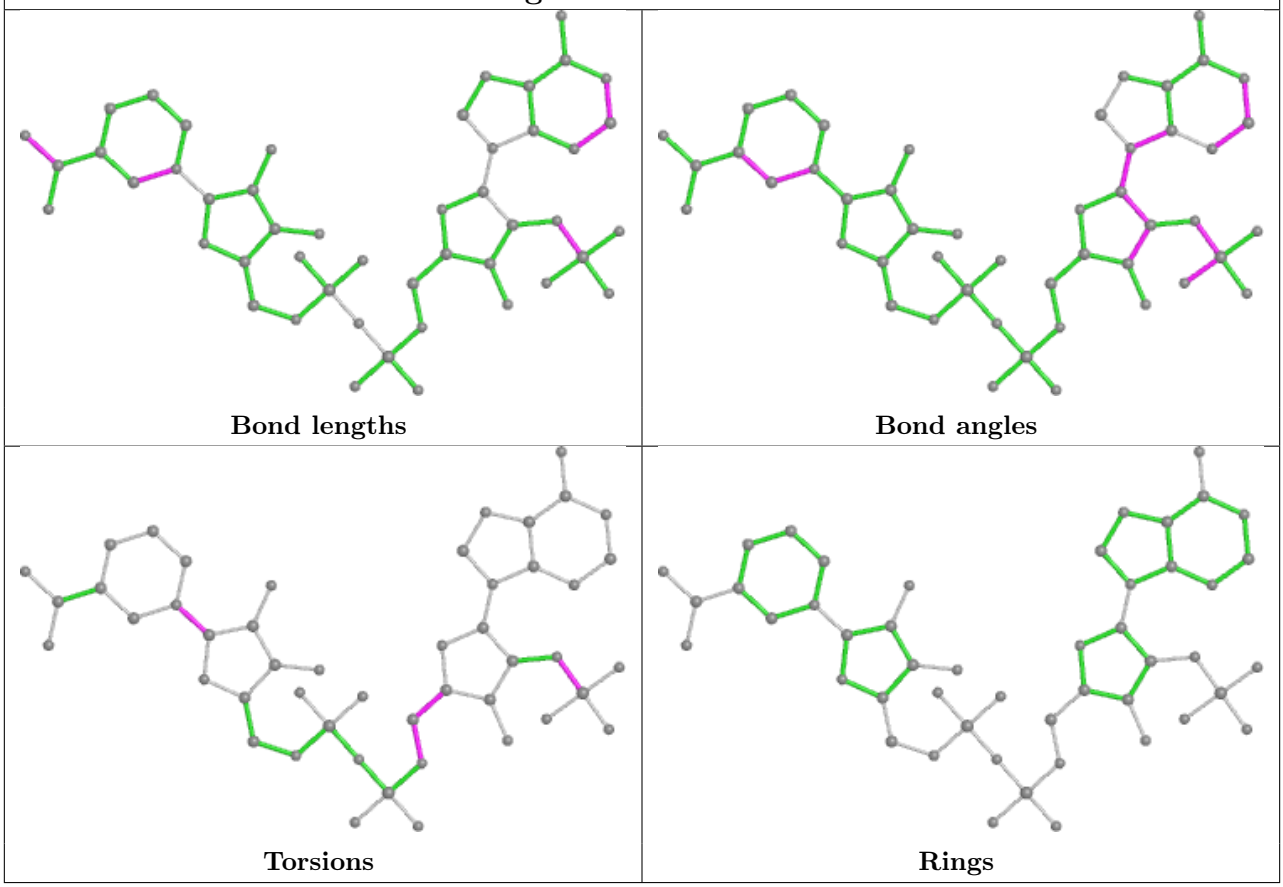


Rings

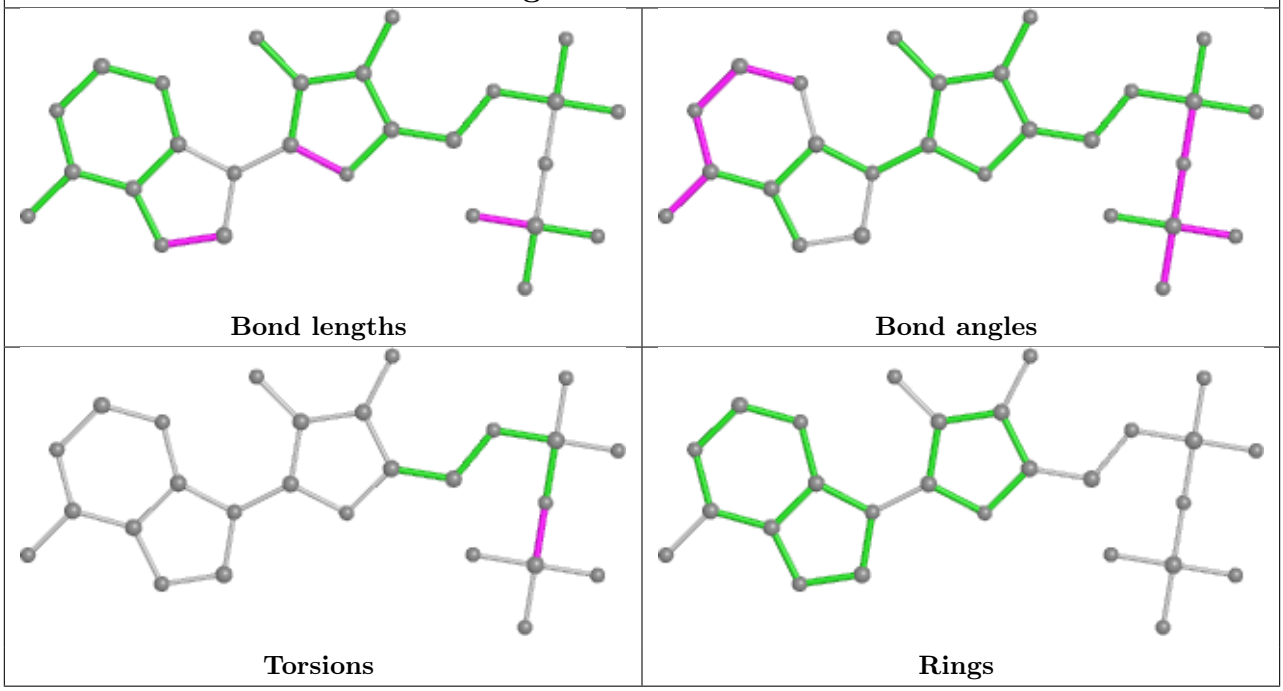
Ligand ADP F 401



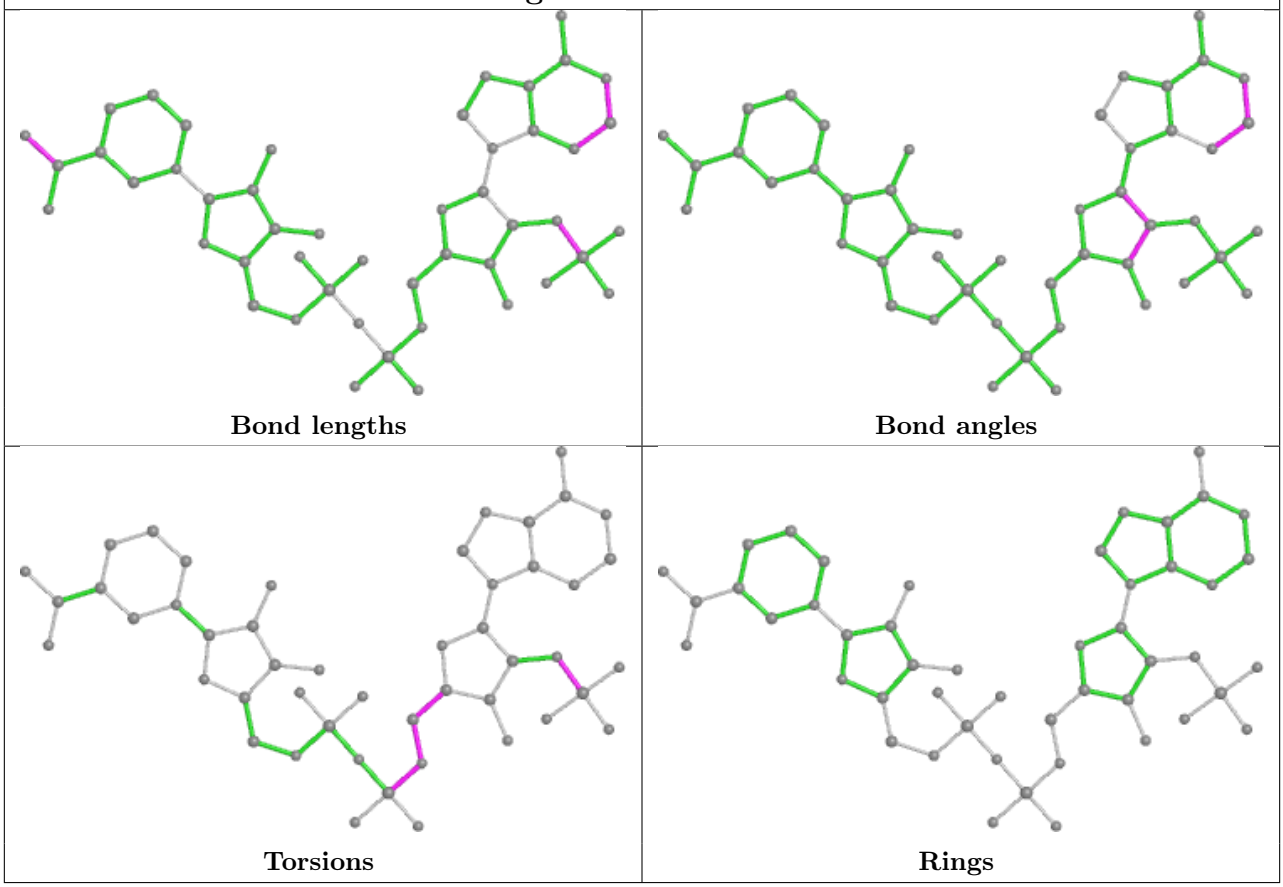
Ligand NAP L 400



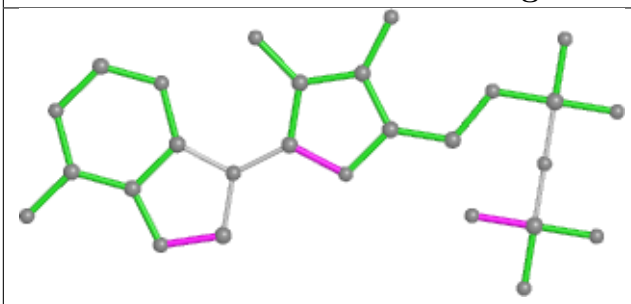
Ligand ADP C 401



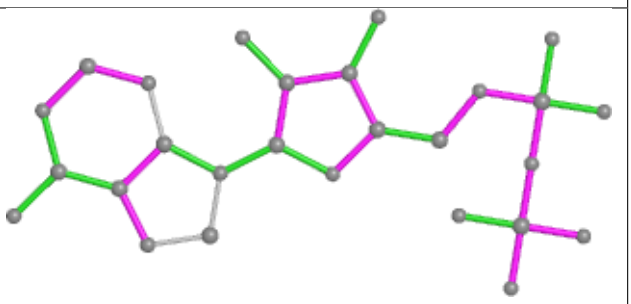
Ligand NAP S 400



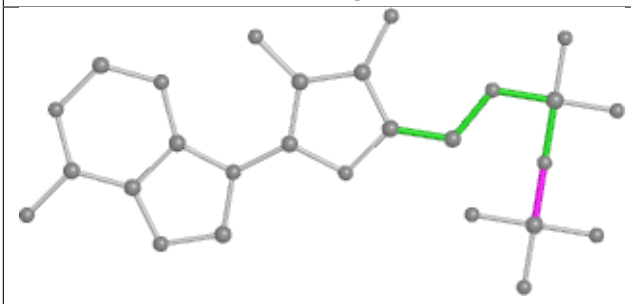
Ligand ADP A 401



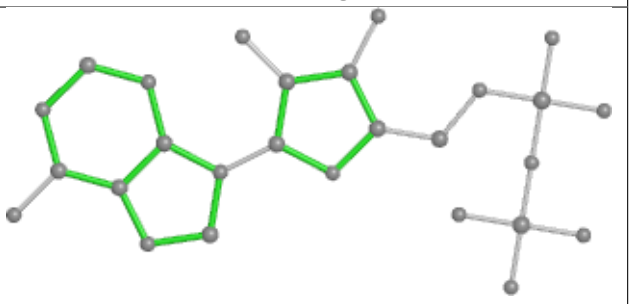
Bond lengths



Bond angles

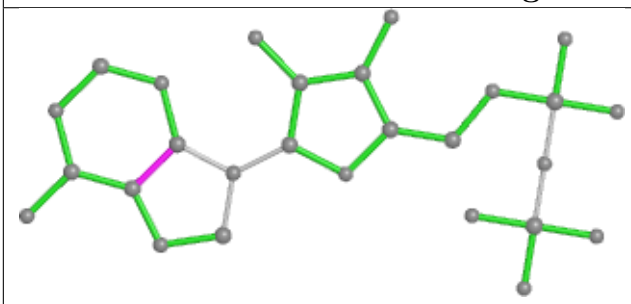


Torsions

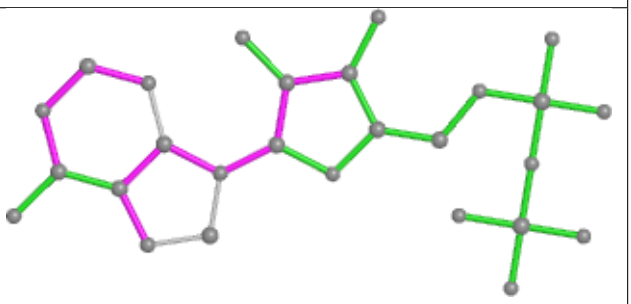


Rings

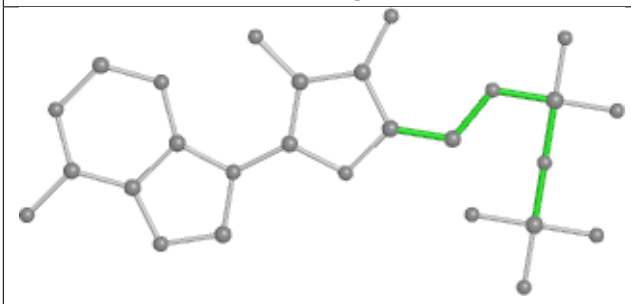
Ligand ADP B 401



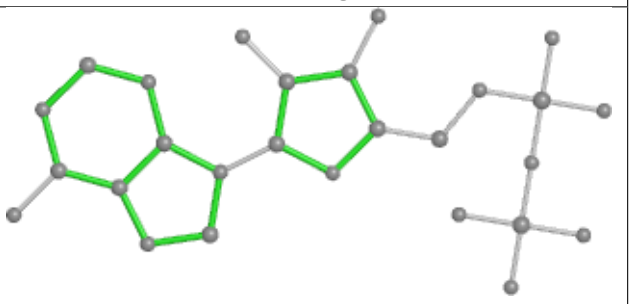
Bond lengths



Bond angles

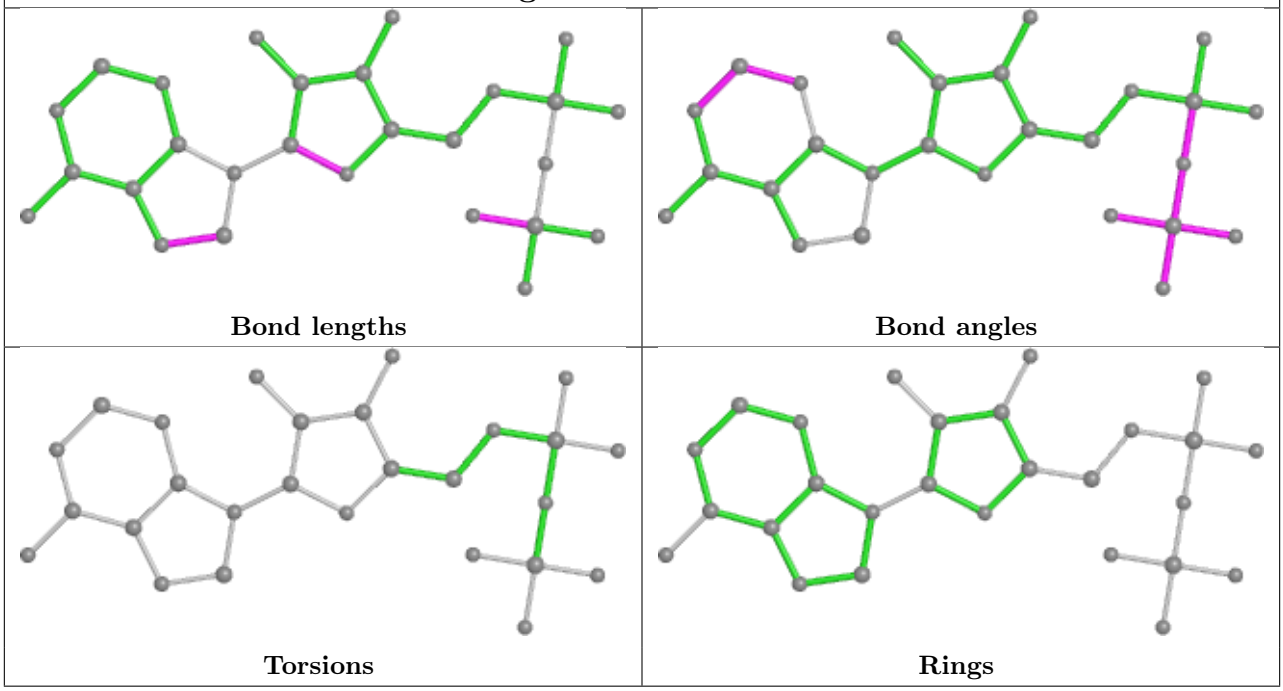


Torsions

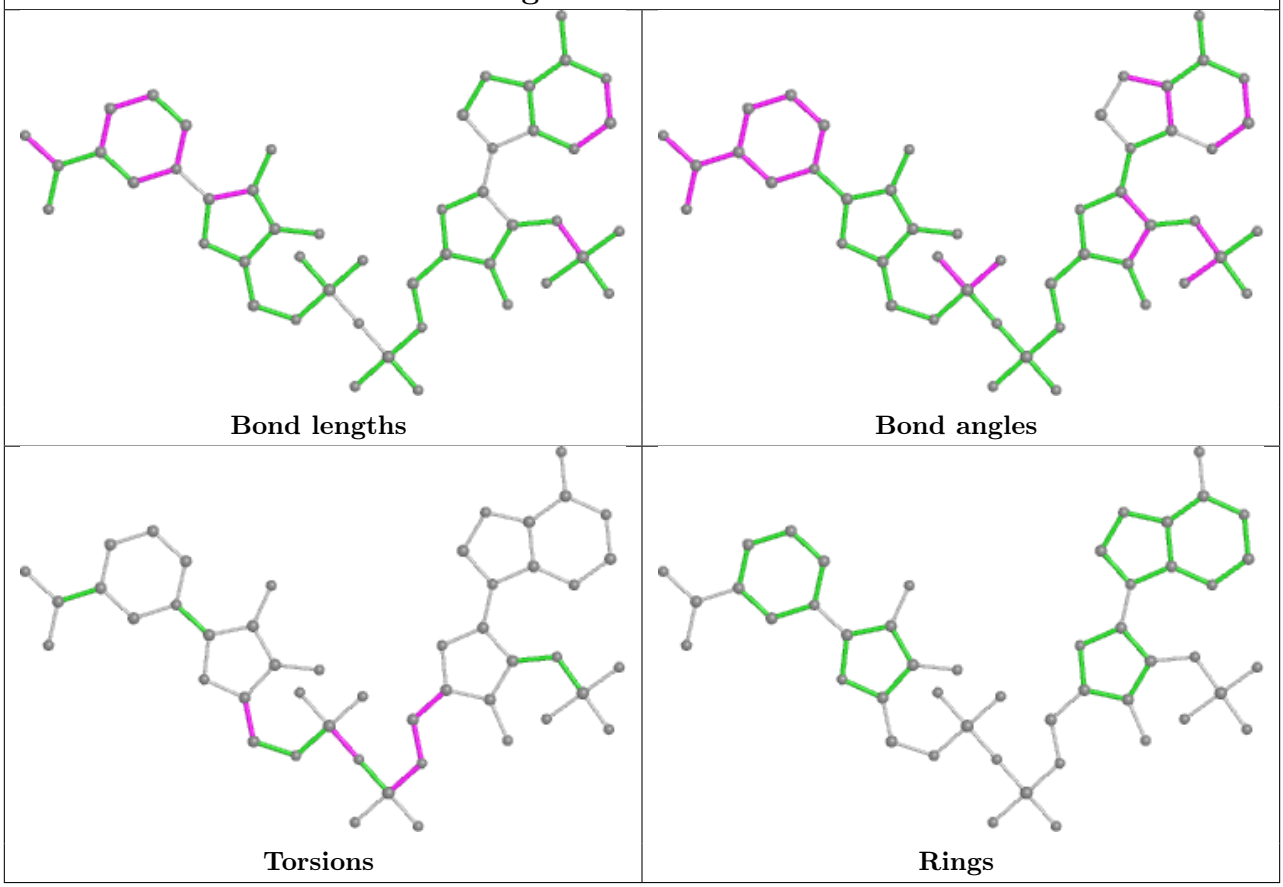


Rings

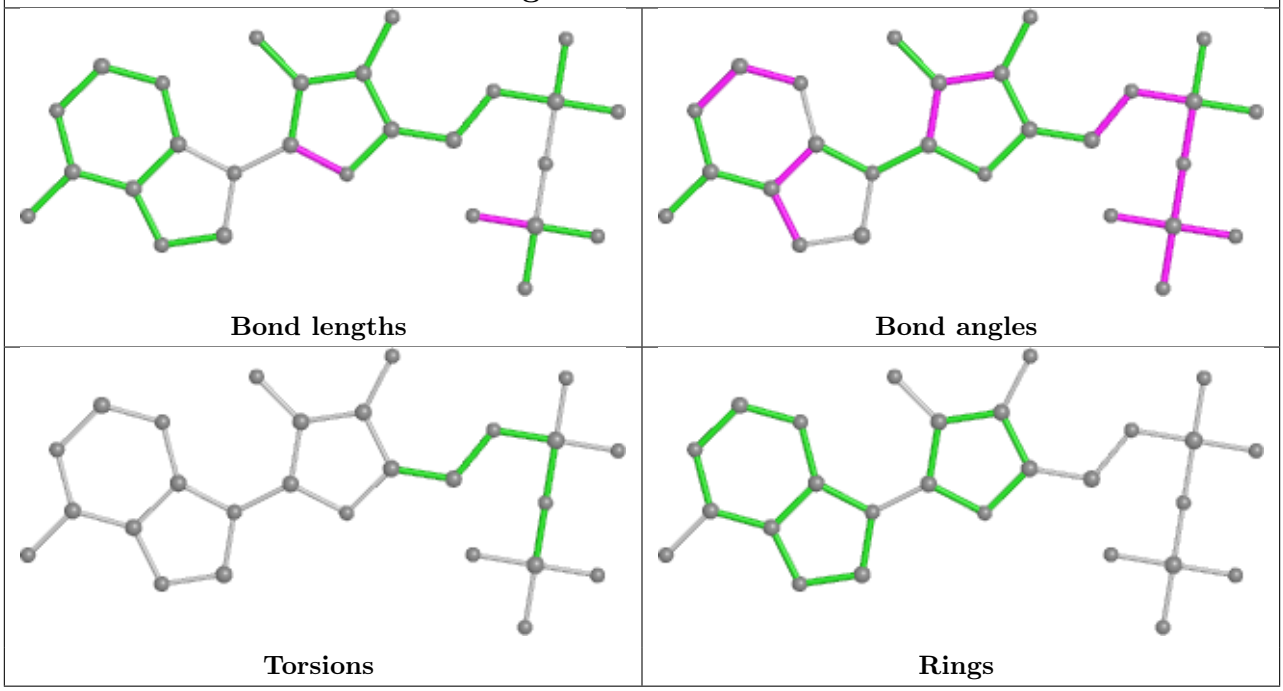
Ligand ADP M 401



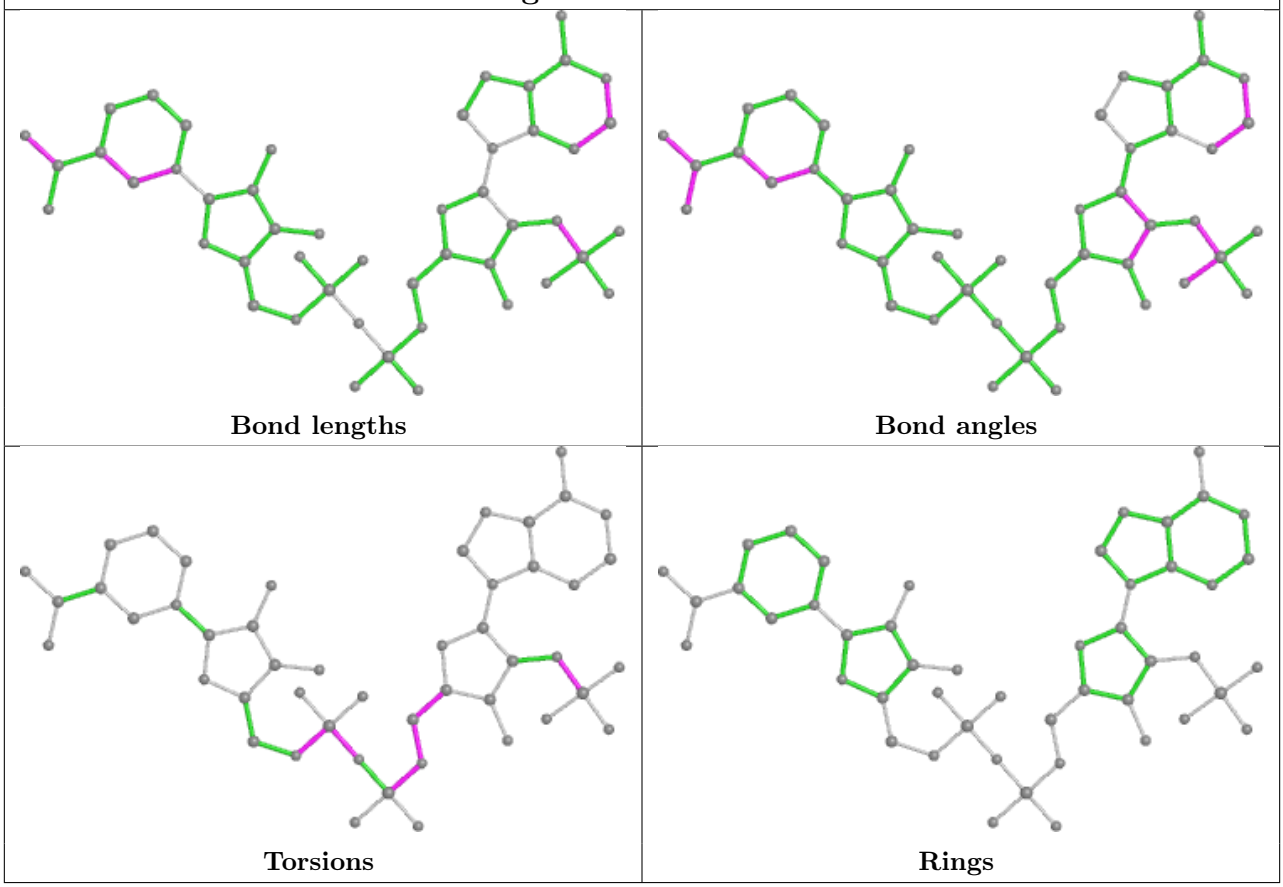
Ligand NAP K 400



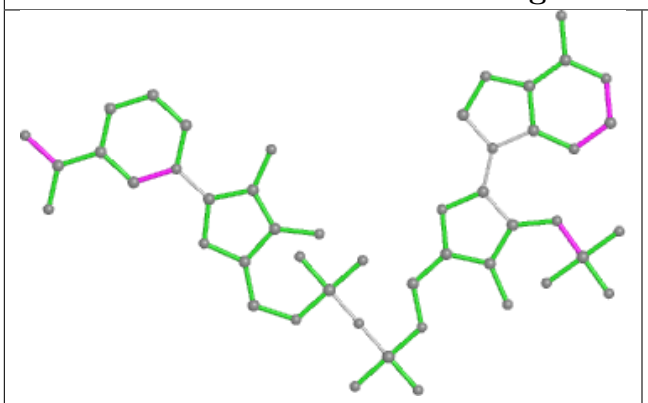
Ligand ADP D 401



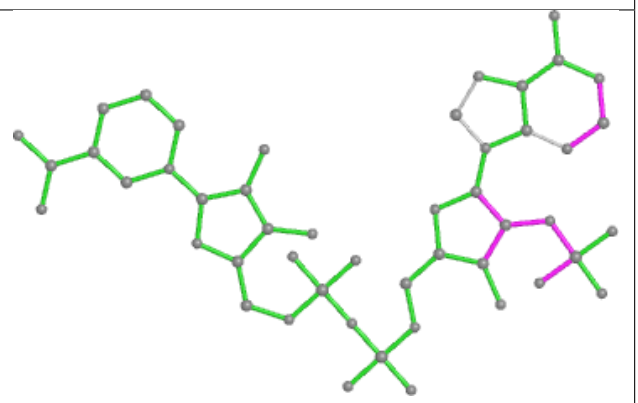
Ligand NAP H 400



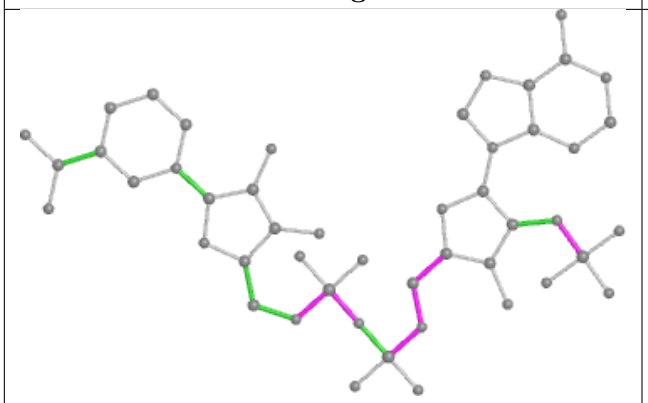
Ligand NAP I 400



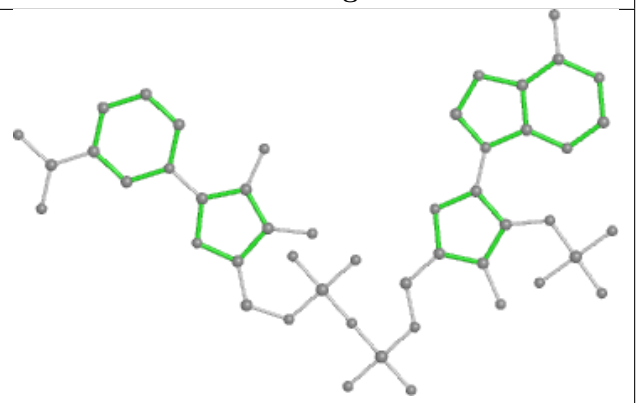
Bond lengths



Bond angles

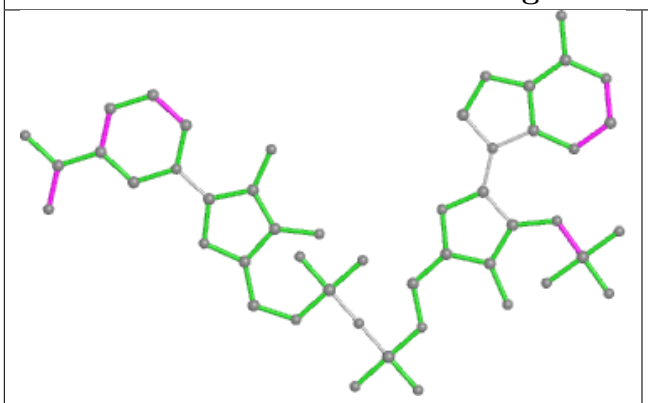


Torsions

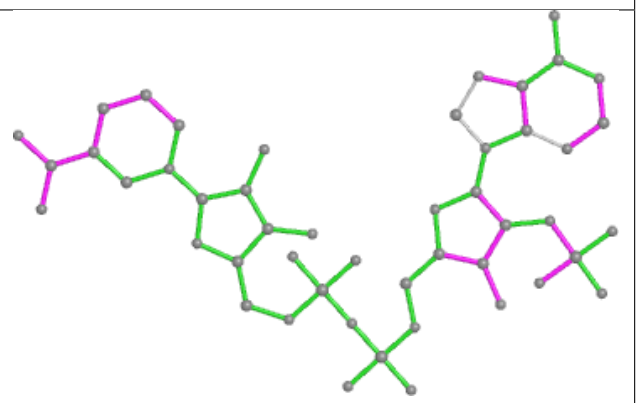


Rings

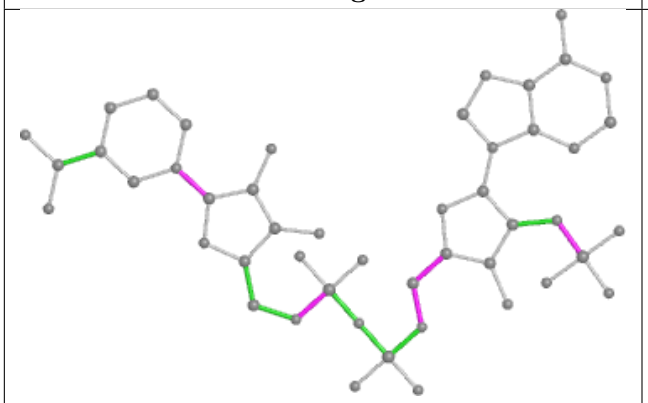
Ligand NAP A 400



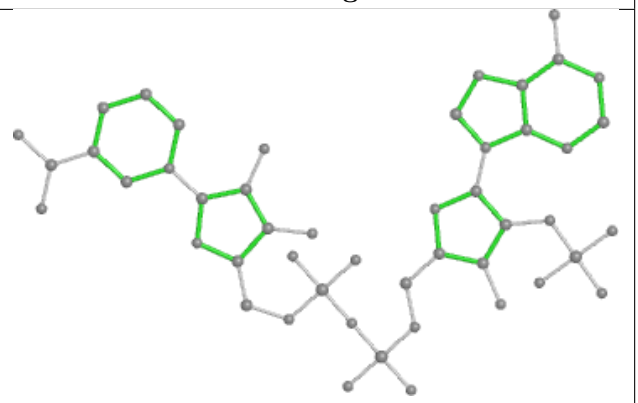
Bond lengths



Bond angles

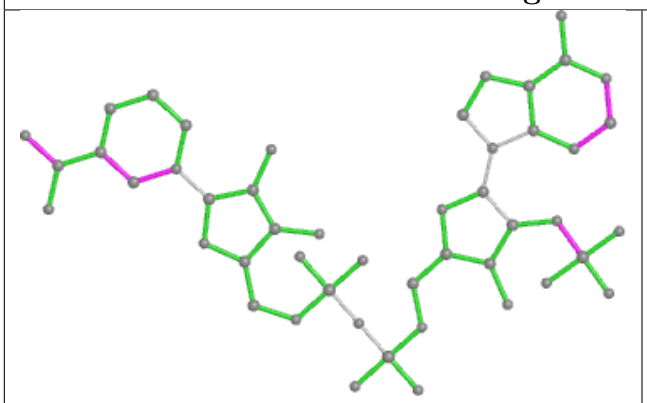


Torsions

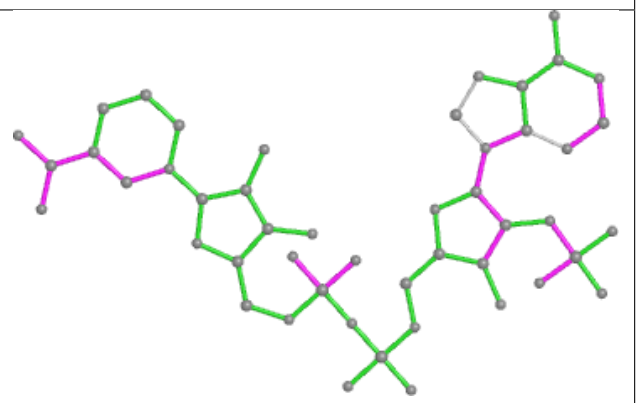


Rings

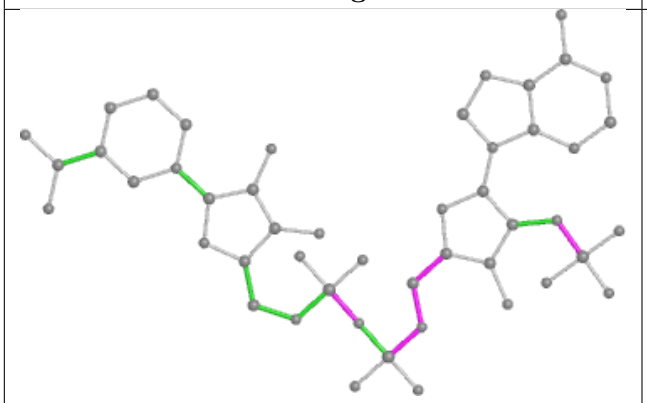
Ligand NAP T 400



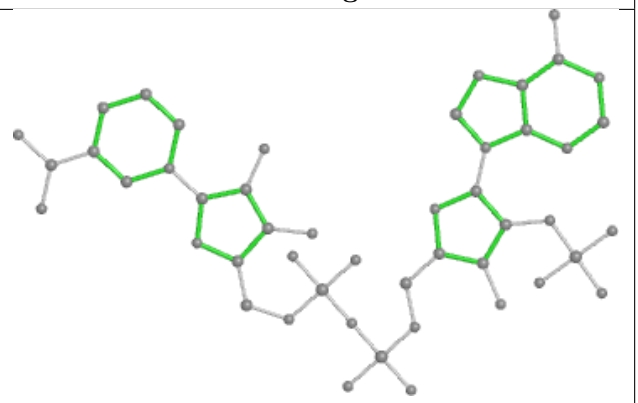
Bond lengths



Bond angles

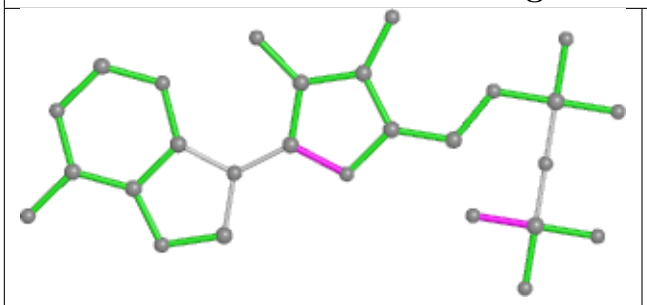


Torsions

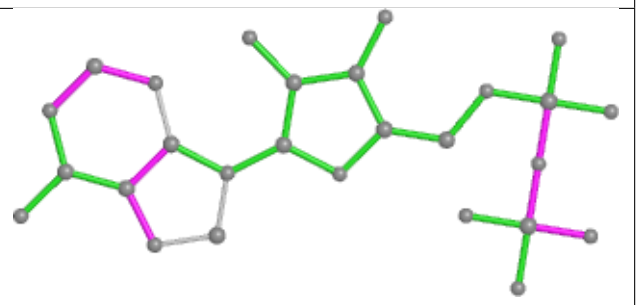


Rings

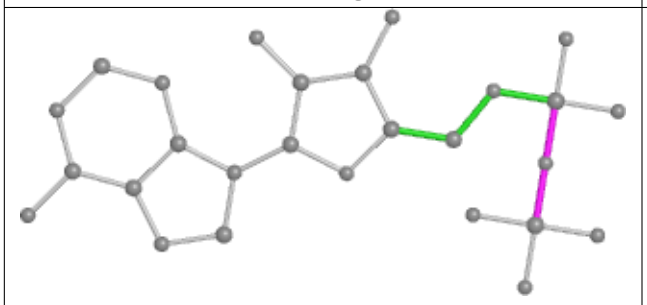
Ligand ADP S 401



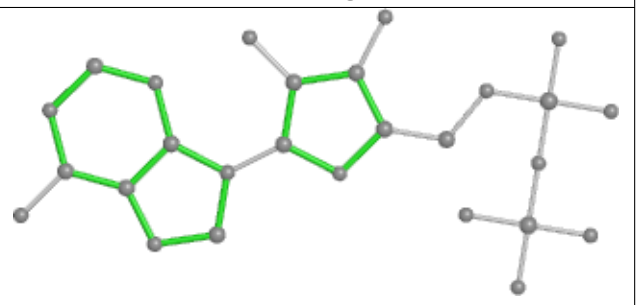
Bond lengths



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	307/357 (85%)	-0.02	8 (2%)	56	46	6, 11, 26, 36	0
1	B	307/357 (85%)	0.26	22 (7%)	15	8	4, 12, 24, 36	0
1	C	307/357 (85%)	0.16	11 (3%)	42	32	6, 12, 20, 30	0
1	D	307/357 (85%)	-0.02	2 (0%)	87	84	6, 11, 20, 30	0
1	E	307/357 (85%)	-0.15	4 (1%)	77	72	4, 10, 19, 26	0
1	F	307/357 (85%)	-0.05	9 (2%)	51	41	5, 11, 25, 36	0
1	G	307/357 (85%)	0.34	27 (8%)	10	5	4, 11, 32, 48	0
1	H	307/357 (85%)	-0.08	6 (1%)	65	56	6, 11, 20, 28	0
1	I	307/357 (85%)	-0.14	2 (0%)	87	84	6, 11, 19, 27	0
1	J	307/357 (85%)	-0.07	4 (1%)	77	72	5, 11, 20, 27	0
1	K	307/357 (85%)	0.03	6 (1%)	65	56	6, 12, 19, 31	0
1	L	307/357 (85%)	-0.07	4 (1%)	77	72	5, 11, 20, 27	0
1	M	307/357 (85%)	-0.10	4 (1%)	77	72	5, 11, 22, 30	0
1	N	307/357 (85%)	0.14	17 (5%)	25	16	5, 11, 26, 32	0
1	O	307/357 (85%)	0.34	20 (6%)	18	11	6, 12, 22, 34	0
1	P	307/357 (85%)	-0.04	7 (2%)	60	51	5, 11, 20, 33	0
1	Q	307/357 (85%)	-0.03	3 (0%)	82	77	5, 11, 19, 30	0
1	R	307/357 (85%)	0.02	7 (2%)	60	51	6, 11, 18, 32	0
1	S	307/357 (85%)	0.41	19 (6%)	20	13	4, 12, 22, 36	0
1	T	307/357 (85%)	0.09	10 (3%)	46	36	5, 11, 20, 27	0
All	All	6140/7140 (85%)	0.05	192 (3%)	49	39	4, 11, 22, 48	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	PRO	5.9
1	O	254	HIS	5.8
1	G	206	ASN	5.5
1	O	194	ASN	5.4
1	G	263	PRO	5.4
1	B	266	ASP	4.8
1	B	268	LEU	4.5
1	G	266	ASP	4.3
1	G	204	SER	4.3
1	G	262	ILE	4.1
1	B	202	GLU	4.1
1	G	202	GLU	4.1
1	S	300	THR	4.1
1	S	254	HIS	4.0
1	S	257	GLY	4.0
1	G	265	PRO	3.9
1	O	202	GLU	3.8
1	T	206	ASN	3.8
1	O	197	SER	3.8
1	K	195	GLY	3.7
1	G	254	HIS	3.6
1	S	274	ALA	3.6
1	B	262	ILE	3.6
1	J	255	LYS	3.6
1	G	205	GLU	3.6
1	S	255	LYS	3.6
1	S	243	PHE	3.6
1	F	206	ASN	3.5
1	P	259	ILE	3.5
1	O	257	GLY	3.5
1	O	259	ILE	3.4
1	P	195	GLY	3.4
1	N	206	ASN	3.3
1	G	193	ASN	3.3
1	G	201	PHE	3.3
1	R	206	ASN	3.3
1	B	206	ASN	3.2
1	O	262	ILE	3.2
1	F	194	ASN	3.1
1	G	259	ILE	3.1
1	N	250	THR	3.1
1	O	201	PHE	3.1
1	S	252	ALA	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	255	LYS	3.1
1	O	256	LYS	3.1
1	C	196	GLU	3.1
1	B	201	PHE	3.0
1	N	254	HIS	3.0
1	C	266	ASP	3.0
1	B	254	HIS	3.0
1	G	271	ARG	3.0
1	S	266	ASP	3.0
1	C	203	GLY	3.0
1	P	258	GLN	3.0
1	G	261	TYR	2.9
1	C	260	GLU	2.9
1	C	202	GLU	2.9
1	O	255	LYS	2.9
1	N	255	LYS	2.9
1	A	265	PRO	2.9
1	B	264	PHE	2.9
1	O	228	GLY	2.9
1	S	263	PRO	2.8
1	F	260	GLU	2.8
1	A	194	ASN	2.8
1	O	229	VAL	2.8
1	A	262	ILE	2.8
1	G	264	PHE	2.8
1	Q	258	GLN	2.8
1	T	194	ASN	2.8
1	P	255	LYS	2.8
1	R	260	GLU	2.8
1	R	261	TYR	2.8
1	K	259	ILE	2.7
1	L	157	GLU	2.7
1	S	262	ILE	2.7
1	T	251	LEU	2.7
1	F	202	GLU	2.7
1	G	196	GLU	2.7
1	T	255	LYS	2.7
1	E	304	ALA	2.7
1	O	253	TYR	2.6
1	O	248	ASP	2.6
1	C	194	ASN	2.6
1	S	195	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	271	ARG	2.6
1	P	202	GLU	2.6
1	B	250	THR	2.6
1	N	258	GLN	2.6
1	S	250	THR	2.6
1	O	260	GLU	2.6
1	A	259	ILE	2.5
1	G	258	GLN	2.5
1	H	157	GLU	2.5
1	P	199	LYS	2.5
1	B	261	TYR	2.5
1	K	197	SER	2.5
1	B	263	PRO	2.5
1	A	261	TYR	2.5
1	R	304	ALA	2.5
1	I	255	LYS	2.5
1	G	304	ALA	2.5
1	M	159	ASN	2.5
1	N	133	TYR	2.5
1	Q	261	TYR	2.5
1	G	194	ASN	2.5
1	N	261	TYR	2.4
1	B	267	LYS	2.4
1	O	199	LYS	2.4
1	O	206	ASN	2.4
1	B	194	ASN	2.4
1	F	157	GLU	2.4
1	C	201	PHE	2.4
1	T	289	ASP	2.4
1	E	255	LYS	2.4
1	N	239	ARG	2.4
1	B	256	LYS	2.4
1	J	157	GLU	2.4
1	S	124	THR	2.4
1	N	262	ILE	2.3
1	O	263	PRO	2.3
1	G	268	LEU	2.3
1	L	258	GLN	2.3
1	N	259	ILE	2.3
1	T	307	ASN	2.3
1	E	258	GLN	2.3
1	B	304	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	201	PHE	2.3
1	G	248	ASP	2.3
1	Q	157	GLU	2.3
1	T	256	LYS	2.3
1	B	270	GLY	2.3
1	K	196	GLU	2.3
1	N	244	GLN	2.3
1	R	157	GLU	2.3
1	K	206	ASN	2.2
1	H	263	PRO	2.2
1	J	206	ASN	2.2
1	C	306	LEU	2.2
1	D	259	ILE	2.2
1	C	254	HIS	2.2
1	N	265	PRO	2.2
1	G	208	LYS	2.2
1	L	194	ASN	2.2
1	G	251	LEU	2.2
1	H	196	GLU	2.2
1	T	257	GLY	2.2
1	F	205	GLU	2.2
1	J	264	PHE	2.2
1	S	205	GLU	2.2
1	F	262	ILE	2.2
1	N	304	ALA	2.2
1	S	201	PHE	2.2
1	A	205	GLU	2.2
1	C	157	GLU	2.2
1	O	261	TYR	2.2
1	S	228	GLY	2.1
1	T	266	ASP	2.1
1	P	262	ILE	2.1
1	L	263	PRO	2.1
1	N	205	GLU	2.1
1	F	266	ASP	2.1
1	C	262	ILE	2.1
1	M	261	TYR	2.1
1	N	264	PHE	2.1
1	H	206	ASN	2.1
1	R	200	LEU	2.1
1	R	202	GLU	2.1
1	H	266	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	266	ASP	2.1
1	G	203	GLY	2.1
1	E	157	GLU	2.1
1	H	202	GLU	2.1
1	M	260	GLU	2.1
1	G	246	VAL	2.1
1	G	253	TYR	2.0
1	N	253	TYR	2.0
1	S	261	TYR	2.0
1	B	199	LYS	2.0
1	S	198	PRO	2.0
1	G	199	LYS	2.0
1	S	202	GLU	2.0
1	I	258	GLN	2.0
1	T	254	HIS	2.0
1	B	157	GLU	2.0
1	B	205	GLU	2.0
1	D	260	GLU	2.0
1	A	258	GLN	2.0
1	A	266	ASP	2.0
1	N	204	SER	2.0
1	F	199	LYS	2.0
1	M	200	LEU	2.0

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 monosaccharides 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	G	402	11/12	0.81	0.33	29,31,32,32	0
4	BMA	S	402	11/12	0.81	0.26	22,23,24,24	0
3	ADP	G	401	27/27	0.83	0.27	30,32,34,35	0
4	BMA	C	402	11/12	0.83	0.25	20,20,21,22	0
4	BMA	A	402	11/12	0.84	0.25	33,35,41,44	0
3	ADP	S	401	27/27	0.84	0.31	17,19,19,21	0
3	ADP	O	401	27/27	0.85	0.30	14,16,17,18	0
3	ADP	B	401	27/27	0.85	0.31	15,19,20,20	0
4	BMA	H	402	11/12	0.86	0.23	22,23,23,23	0
4	BMA	N	402	11/12	0.88	0.22	27,28,31,34	0
4	BMA	J	402	11/12	0.88	0.22	22,23,26,27	0
4	BMA	E	402	11/12	0.89	0.19	19,20,23,23	0
3	ADP	F	401	27/27	0.89	0.20	13,14,19,21	0
3	ADP	N	401	27/27	0.89	0.23	10,12,20,25	0
3	ADP	T	401	27/27	0.90	0.21	10,11,18,21	0
3	ADP	C	401	27/27	0.90	0.24	14,15,17,19	0
4	BMA	P	402	11/12	0.90	0.19	24,25,28,29	0
3	ADP	A	401	27/27	0.90	0.20	14,17,23,28	0
4	BMA	Q	402	11/12	0.91	0.17	18,18,19,21	0
4	BMA	R	402	11/12	0.91	0.22	21,23,26,26	0
3	ADP	K	401	27/27	0.91	0.23	14,14,21,23	0
4	BMA	F	402	11/12	0.92	0.18	24,25,28,30	0
4	BMA	O	402	11/12	0.92	0.22	18,18,19,19	0
4	BMA	K	402	11/12	0.92	0.20	25,27,30,32	0
4	BMA	D	402	11/12	0.93	0.16	20,21,22,24	0
3	ADP	L	401	27/27	0.93	0.17	10,12,14,16	0
3	ADP	R	401	27/27	0.93	0.19	14,14,16,18	0
4	BMA	L	402	11/12	0.93	0.15	15,17,19,20	0
3	ADP	H	401	27/27	0.93	0.17	15,16,20,22	0
3	ADP	D	401	27/27	0.94	0.18	12,13,17,19	0
3	ADP	P	401	27/27	0.94	0.18	8,10,19,22	0
4	BMA	I	402	11/12	0.94	0.17	16,17,17,18	0
3	ADP	Q	401	27/27	0.94	0.17	12,12,14,16	0
2	NAP	R	400	48/48	0.94	0.14	9,14,37,37	0
2	NAP	S	400	48/48	0.94	0.16	12,14,23,23	0
2	NAP	T	400	48/48	0.94	0.16	9,12,25,26	0
3	ADP	J	401	27/27	0.94	0.15	10,11,16,20	0
2	NAP	B	400	48/48	0.94	0.16	10,14,27,28	0
2	NAP	G	400	48/48	0.94	0.16	10,13,29,30	0
3	ADP	M	401	27/27	0.94	0.16	12,12,16,16	0
2	NAP	O	400	48/48	0.94	0.15	10,12,26,27	0

Continued on next page...

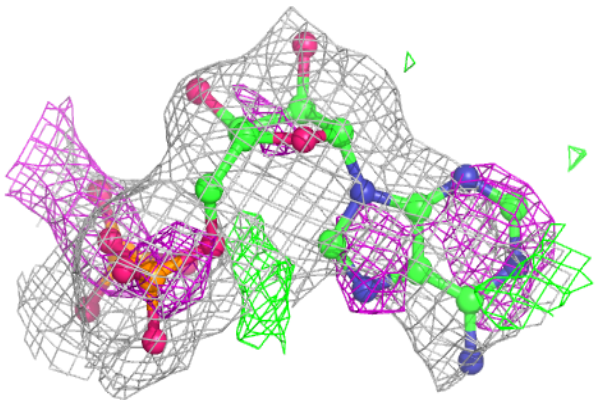
Continued from previous page...

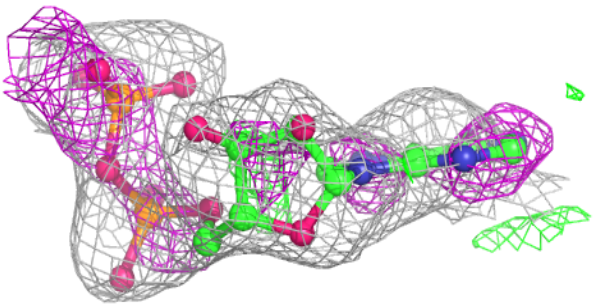
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAP	I	400	48/48	0.95	0.15	10,13,26,27	0
2	NAP	J	400	48/48	0.95	0.16	9,13,21,23	0
2	NAP	K	400	48/48	0.95	0.14	9,13,21,22	0
2	NAP	L	400	48/48	0.95	0.14	8,16,29,30	0
3	ADP	E	401	27/27	0.95	0.12	8,10,15,18	0
2	NAP	N	400	48/48	0.95	0.14	9,12,26,27	0
4	BMA	M	402	11/12	0.95	0.15	17,19,19,20	0
2	NAP	C	400	48/48	0.95	0.15	10,14,36,37	0
2	NAP	P	400	48/48	0.95	0.14	9,12,22,24	0
2	NAP	Q	400	48/48	0.95	0.13	11,14,28,29	0
2	NAP	D	400	48/48	0.95	0.15	13,18,34,35	0
2	NAP	E	400	48/48	0.95	0.15	8,11,28,30	0
2	NAP	A	400	48/48	0.95	0.14	9,15,27,29	0
4	BMA	T	402	11/12	0.95	0.13	24,27,29,30	0
2	NAP	M	400	48/48	0.96	0.14	10,15,26,26	0
3	ADP	I	401	27/27	0.96	0.13	12,12,15,16	0
2	NAP	F	400	48/48	0.96	0.12	8,13,24,25	0
2	NAP	H	400	48/48	0.96	0.12	10,12,25,26	0

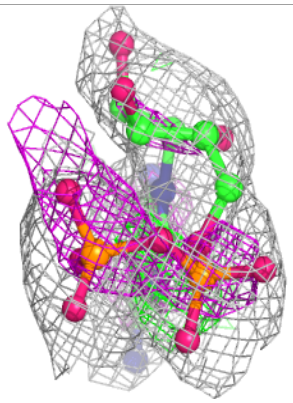
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP G 401:

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

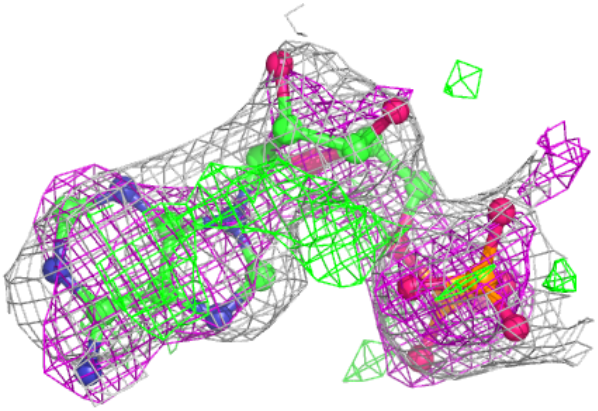


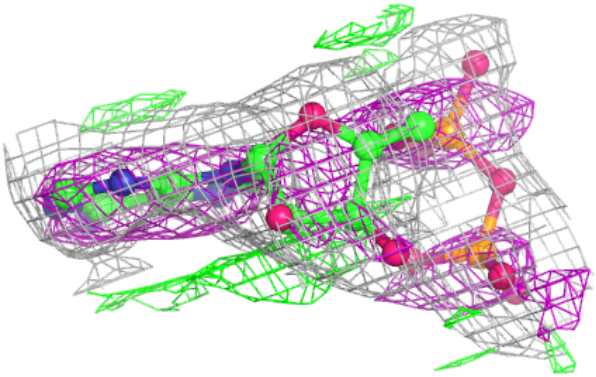


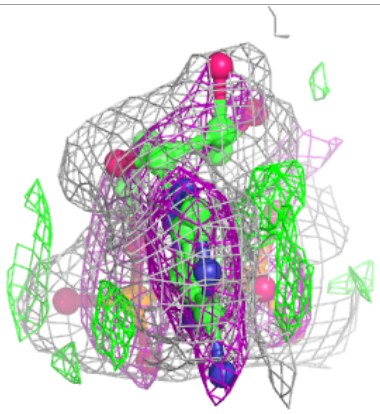


Electron density around ADP S 401:

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

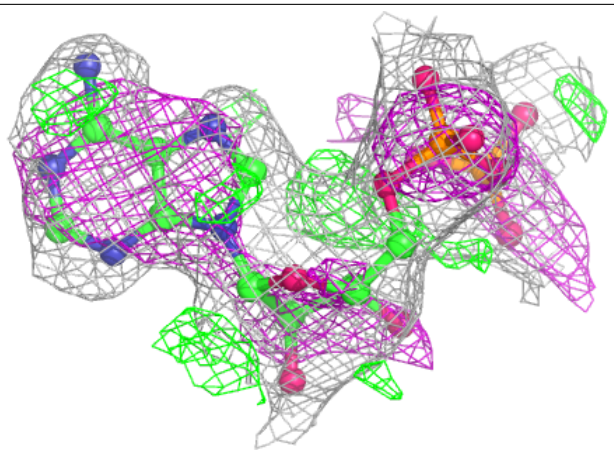


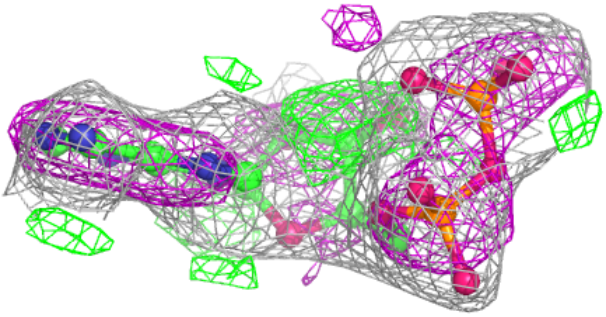


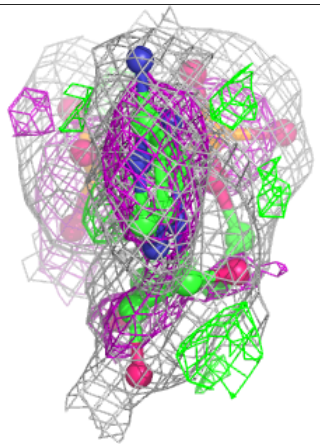


Electron density around ADP O 401:

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

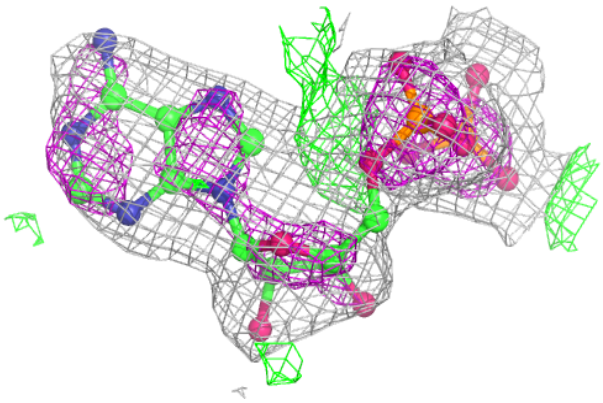


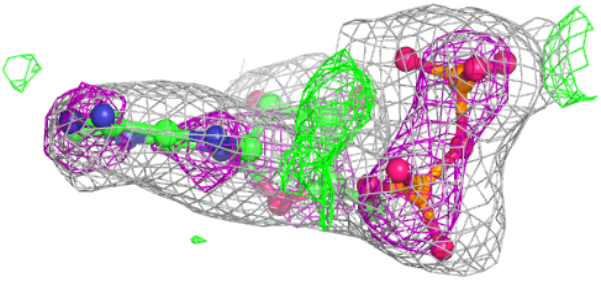


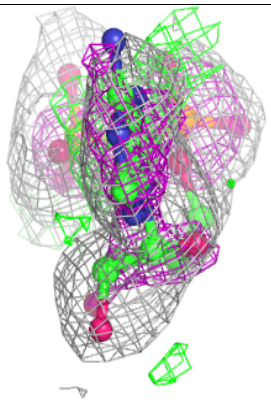


Electron density around ADP B 401:

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

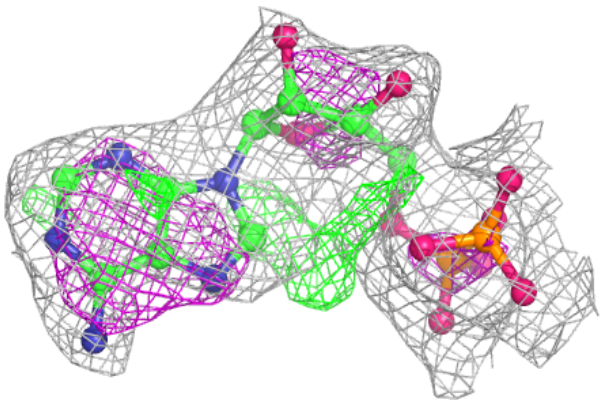


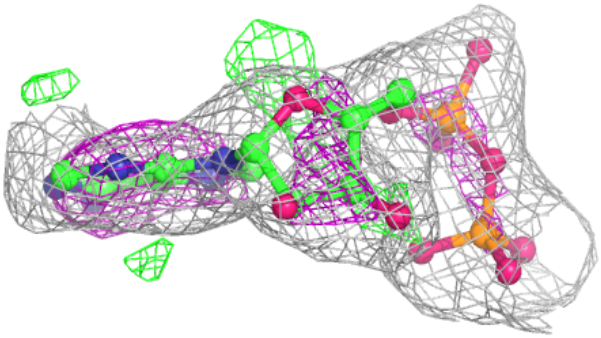


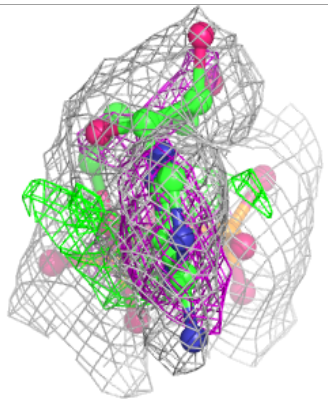


Electron density around ADP F 401:

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

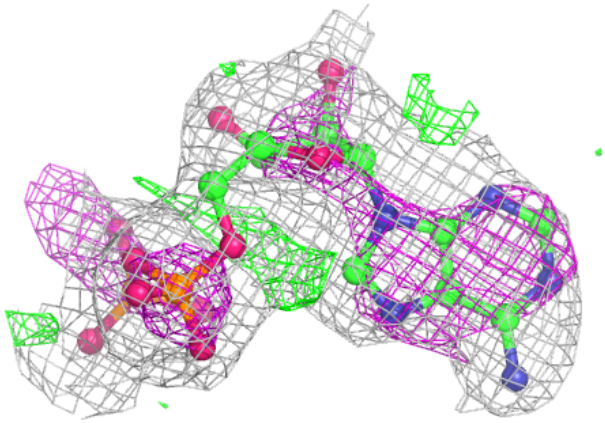


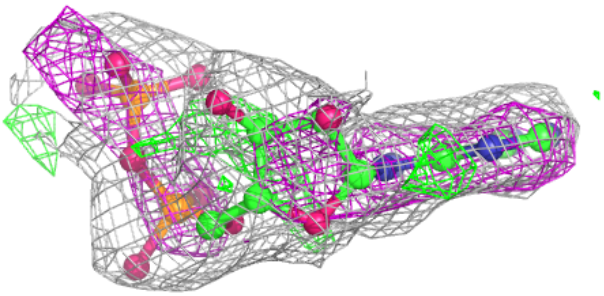


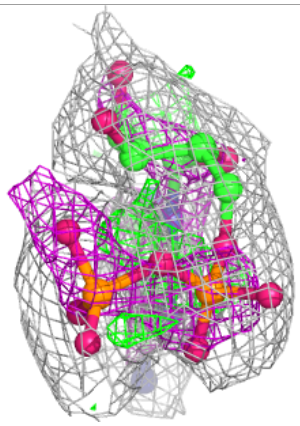


Electron density around ADP N 401:

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

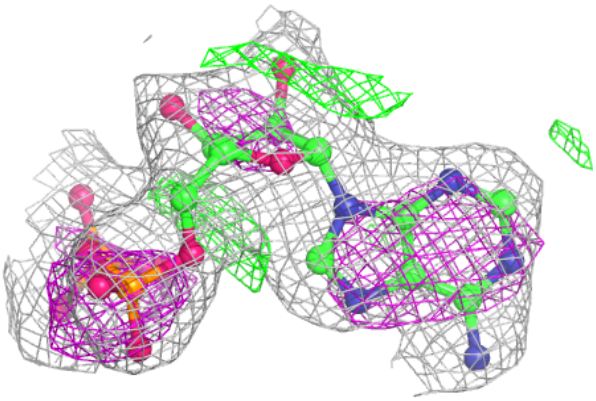


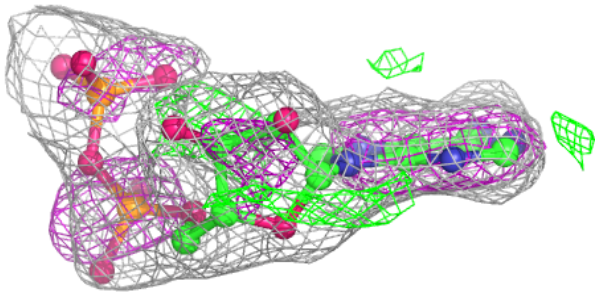


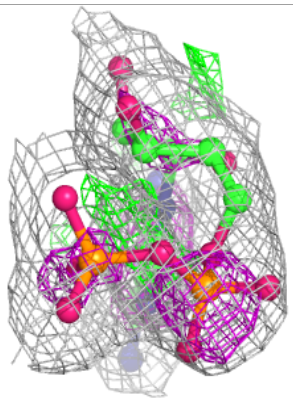


Electron density around ADP T 401:

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

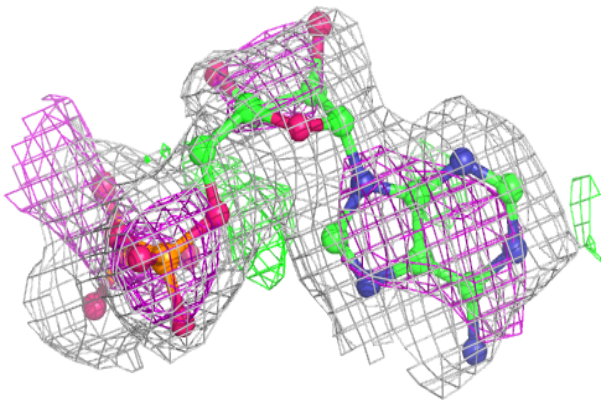


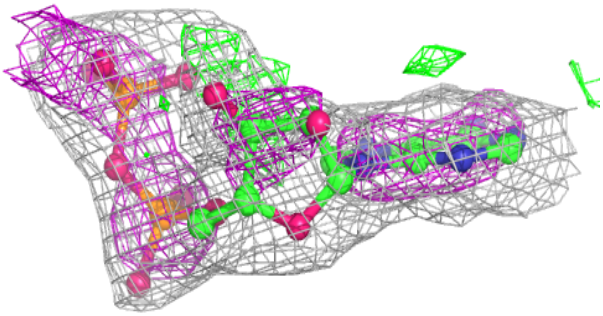


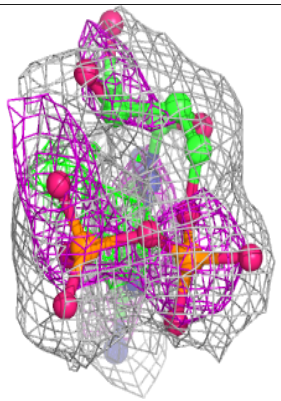


Electron density around ADP C 401:

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

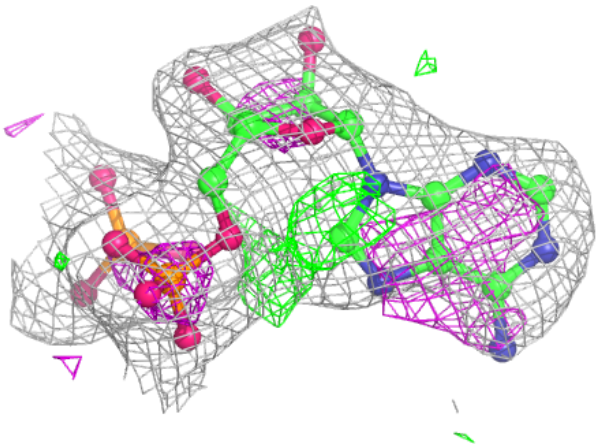


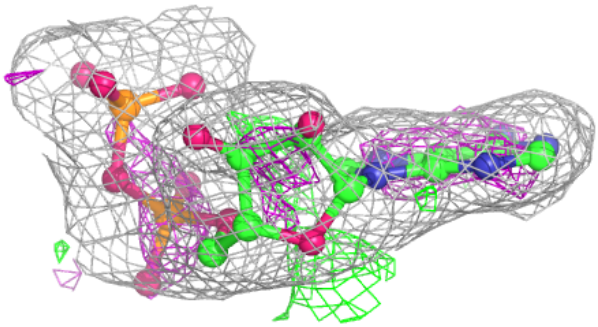


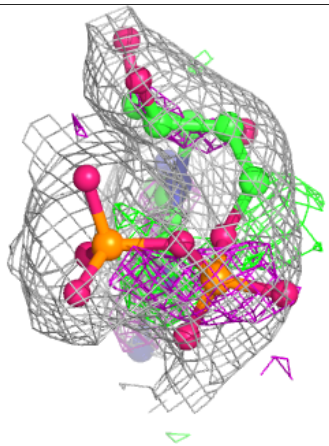


Electron density around ADP A 401:

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

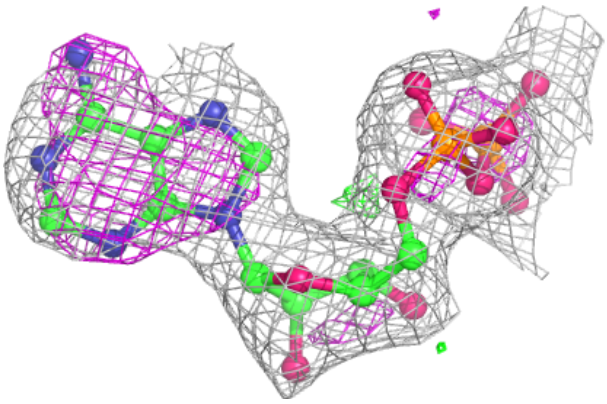


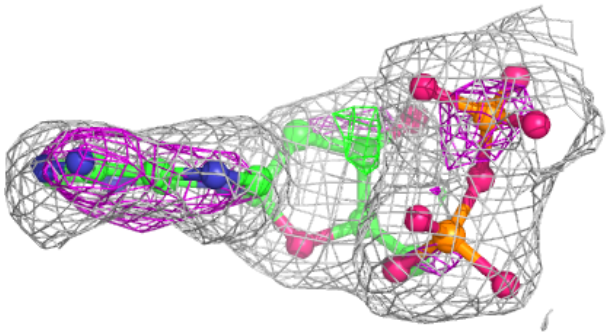


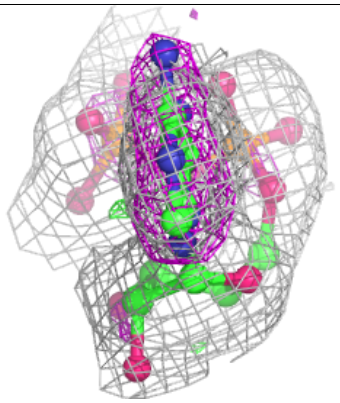


Electron density around ADP K 401:

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

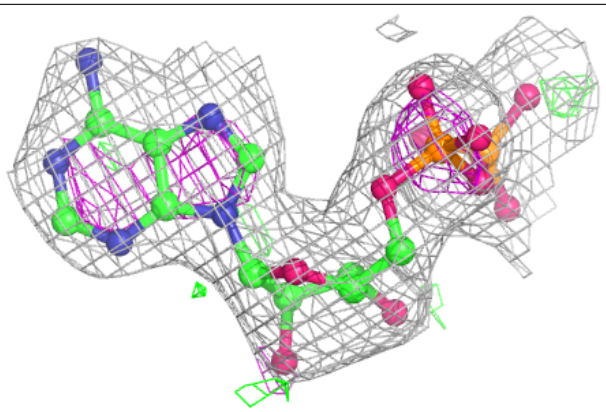


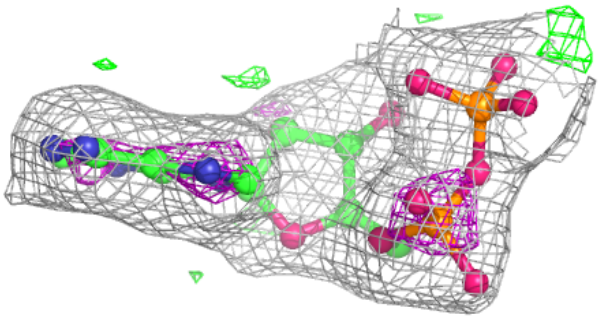


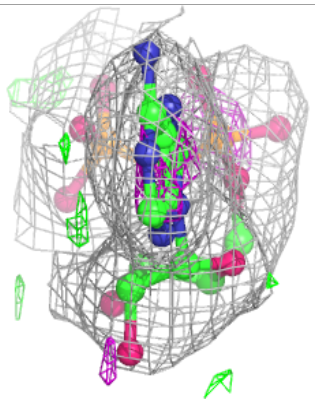


Electron density around ADP L 401:

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

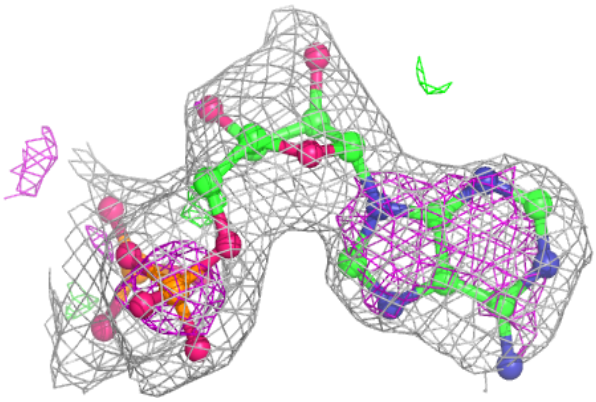


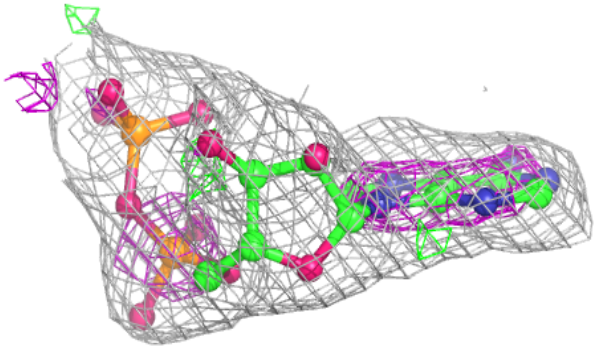


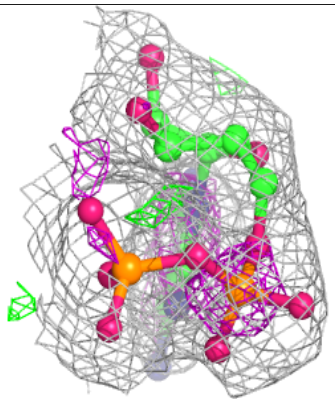


Electron density around ADP R 401:

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

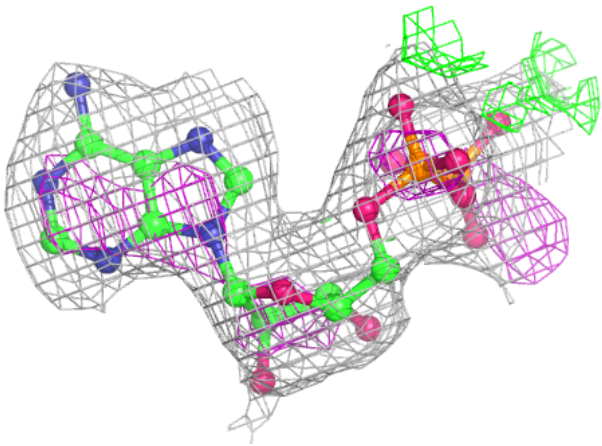


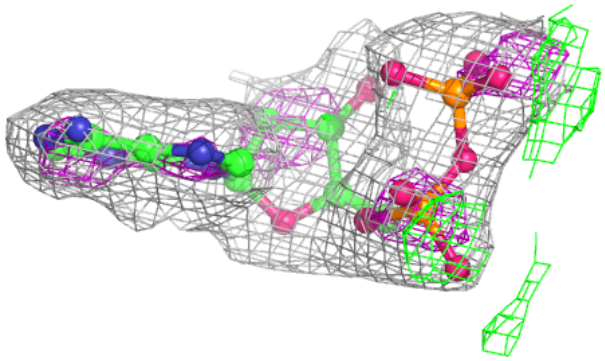


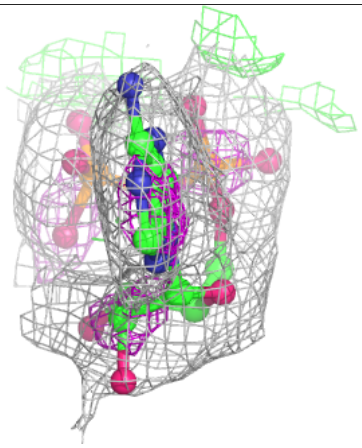


Electron density around ADP H 401:

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

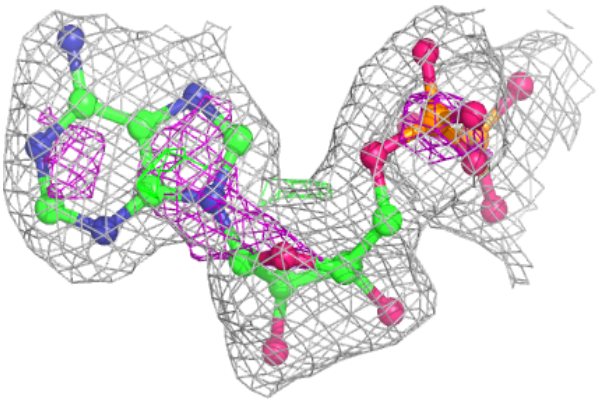


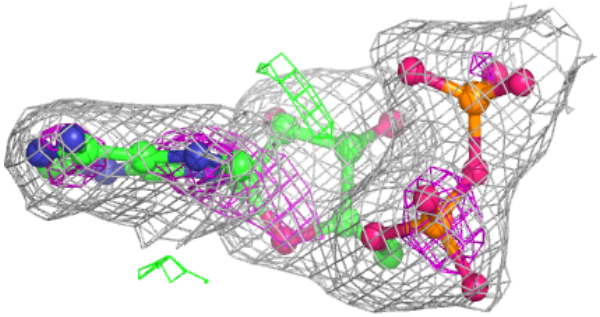


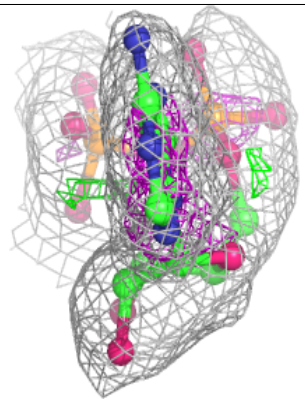


Electron density around ADP D 401:

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

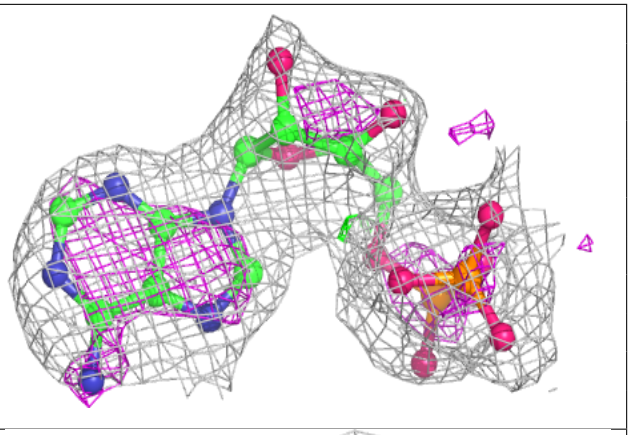


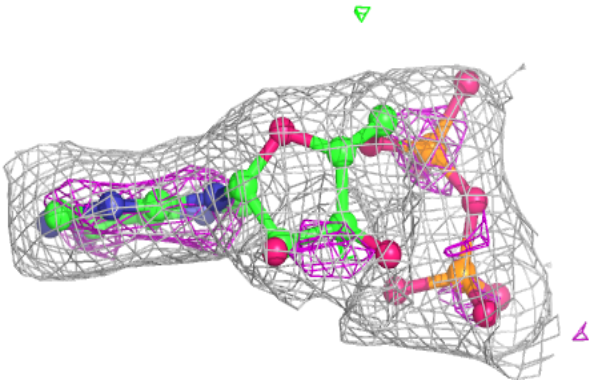


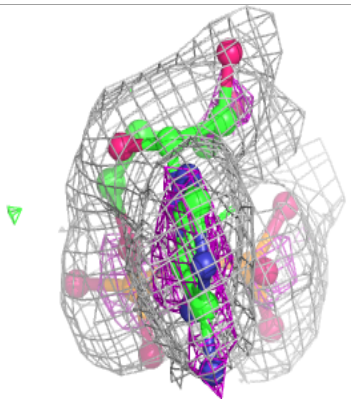


Electron density around ADP P 401:

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

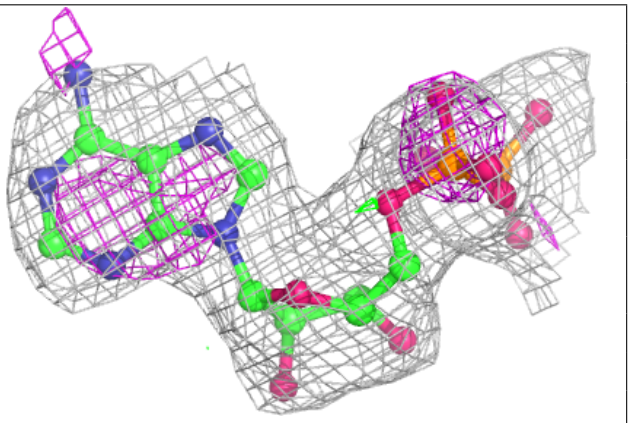


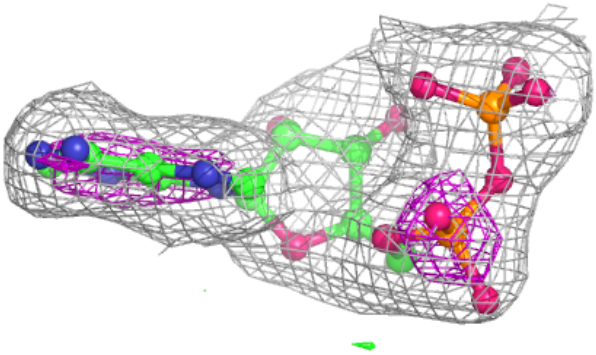


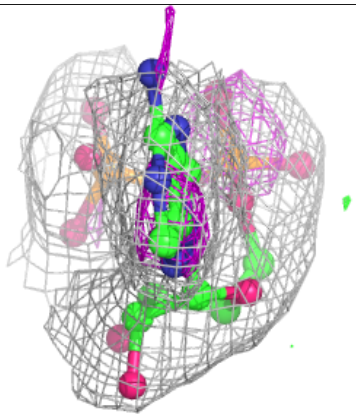


Electron density around ADP Q 401:

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

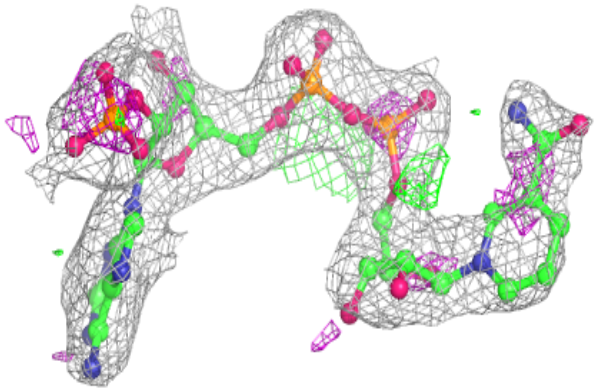


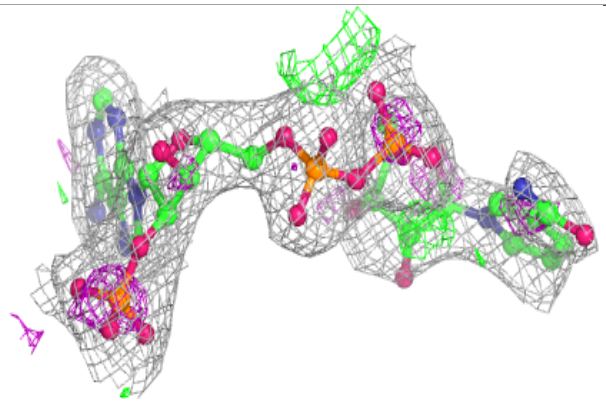


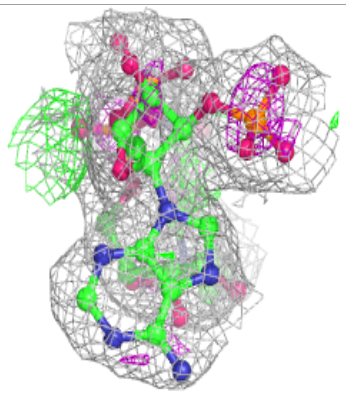


Electron density around NAP R 400:

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

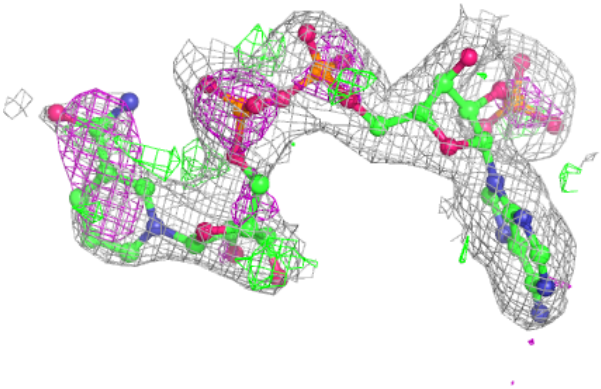


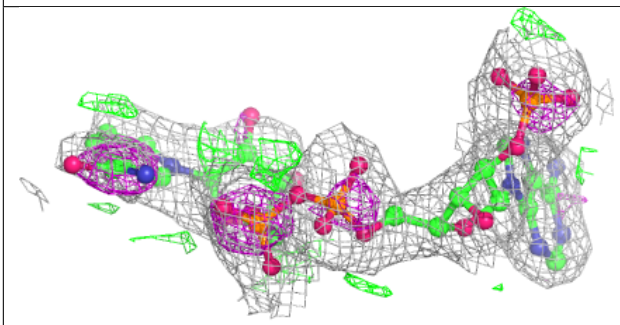


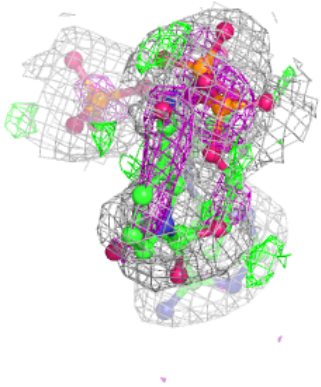


Electron density around NAP S 400:

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

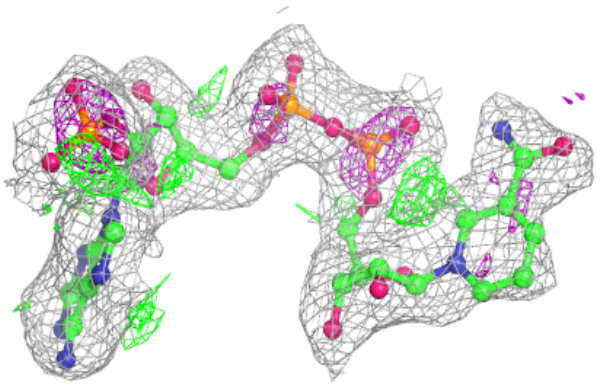


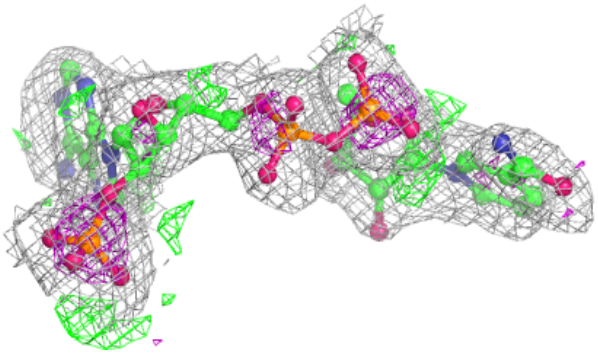


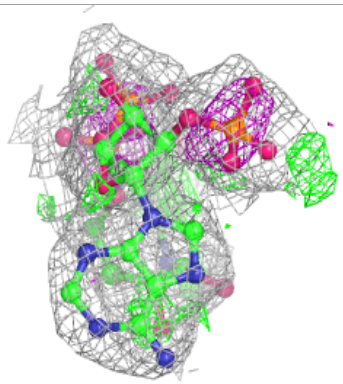


Electron density around NAP T 400:

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

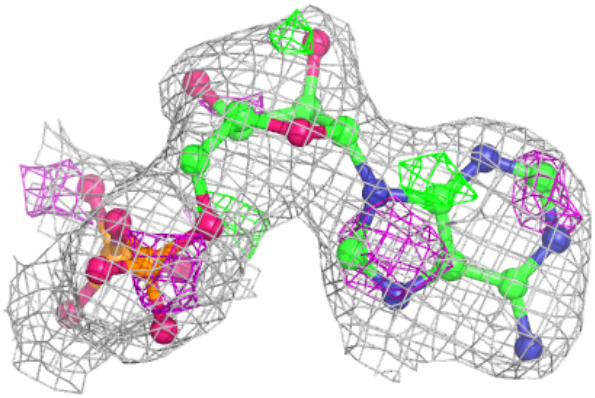


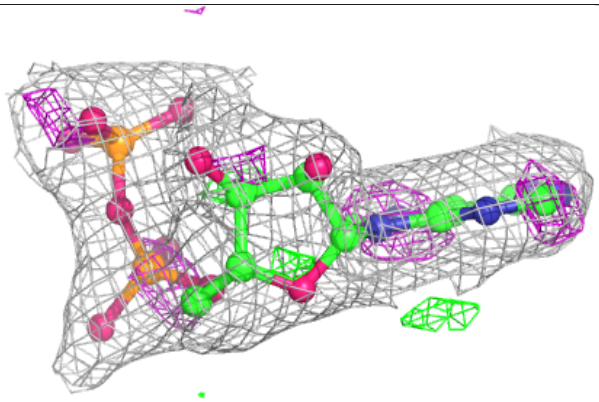


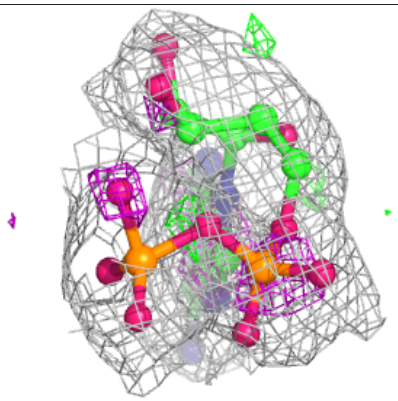


Electron density around ADP J 401:

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

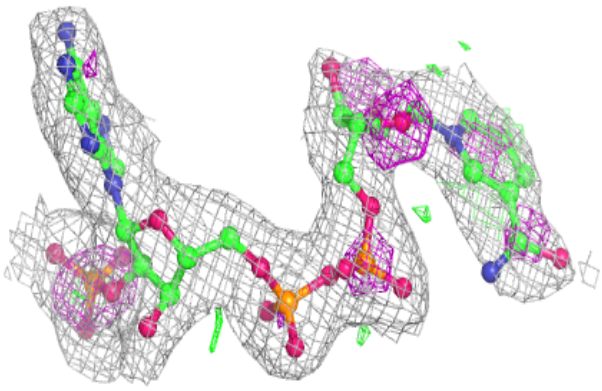


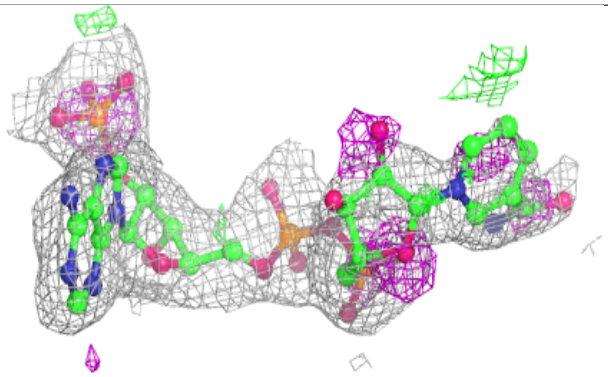


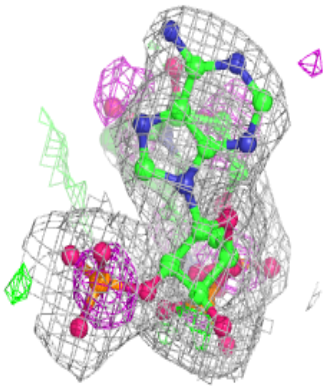


Electron density around NAP B 400:

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

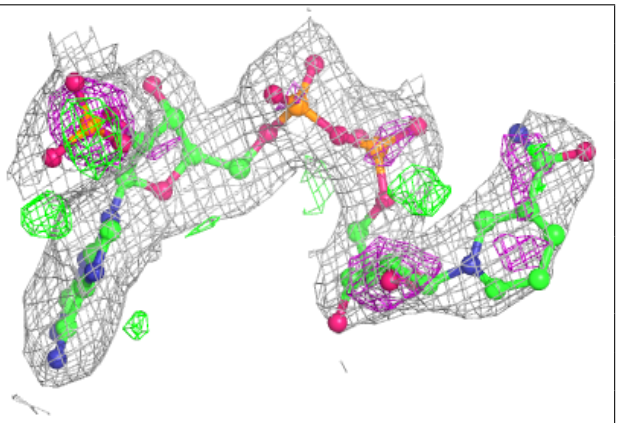


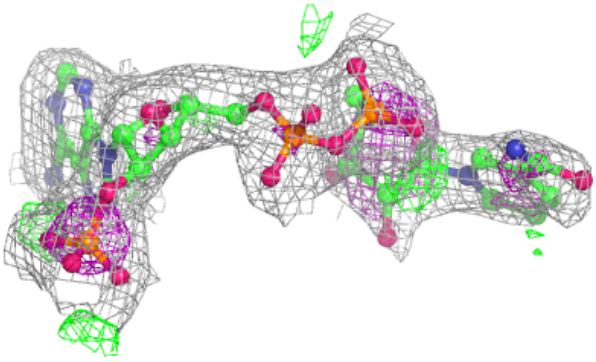


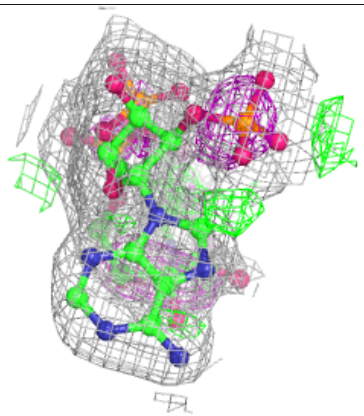


Electron density around NAP G 400:

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

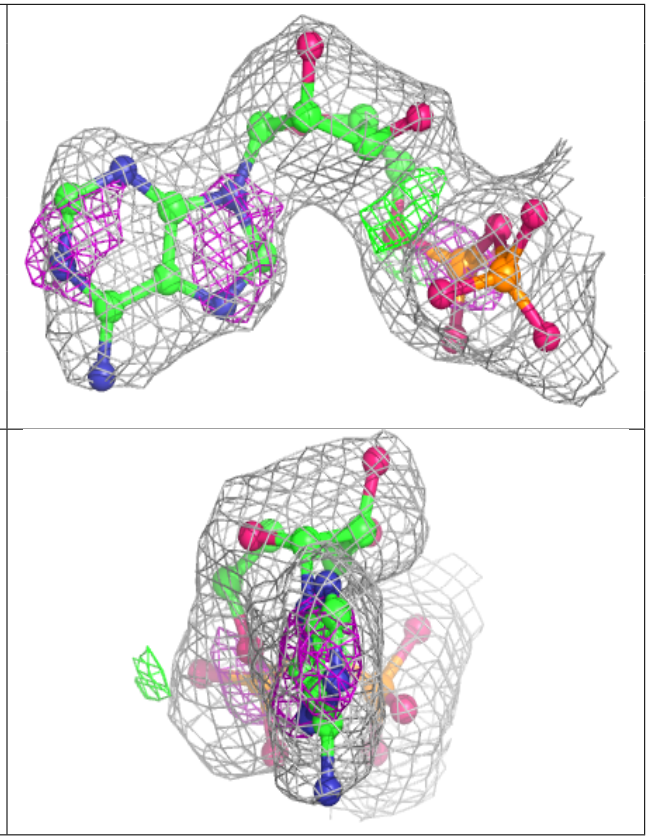






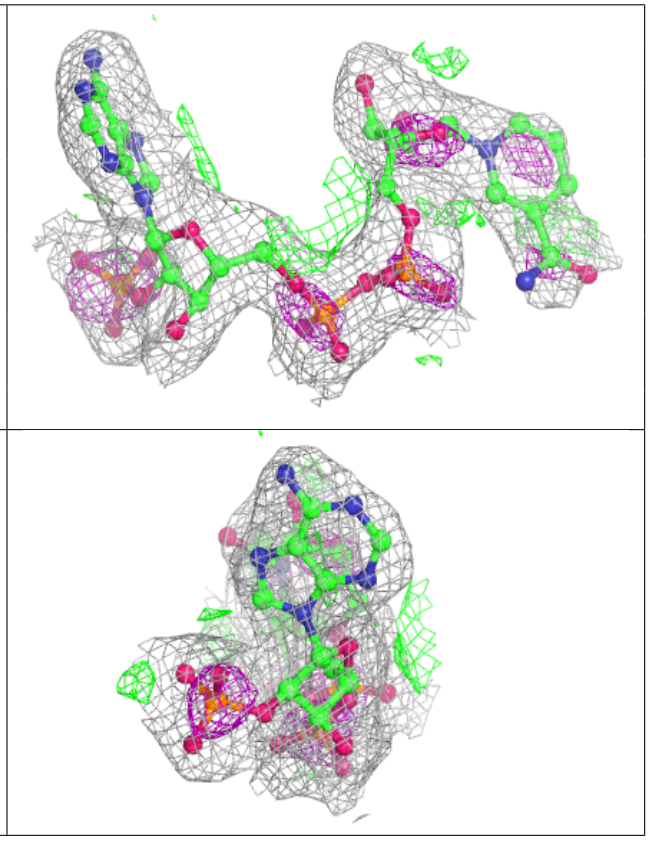
Electron density around ADP M 401:

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



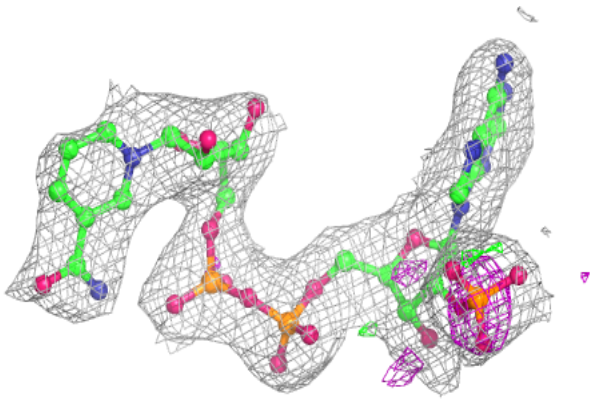
Electron density around NAP O 400:

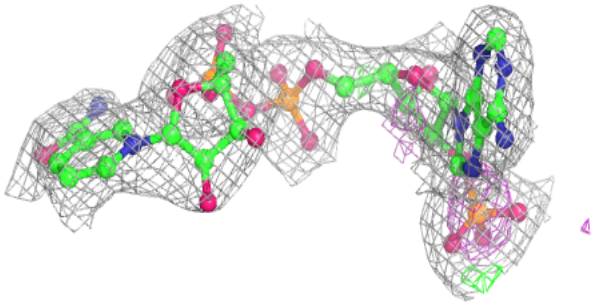
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

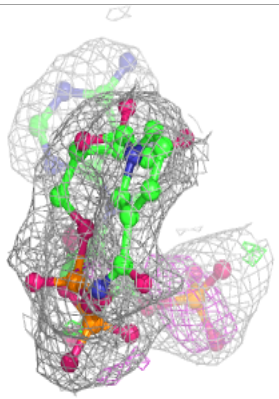


Electron density around NAP I 400:

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

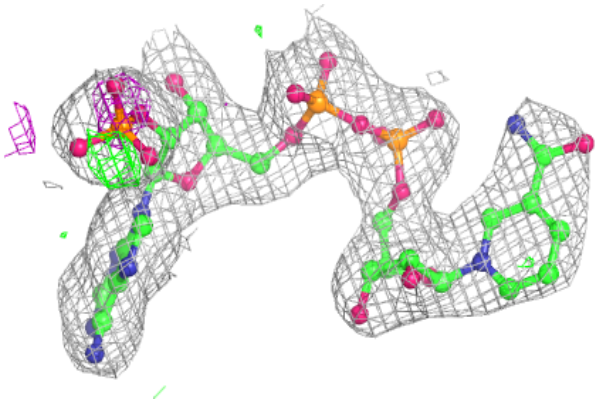


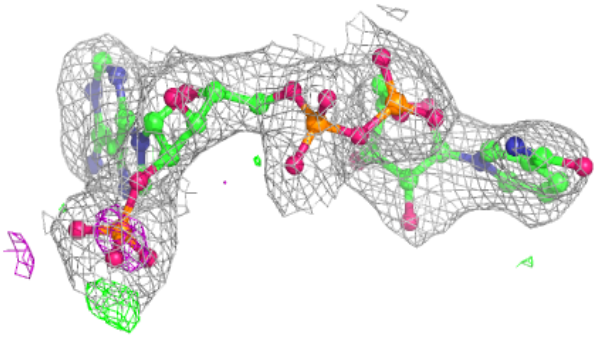


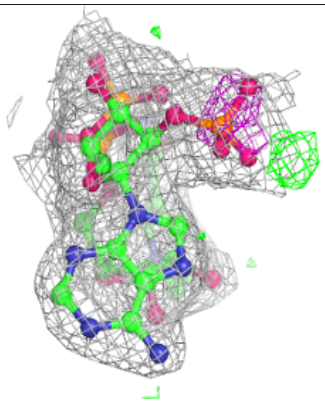


Electron density around NAP J 400:

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

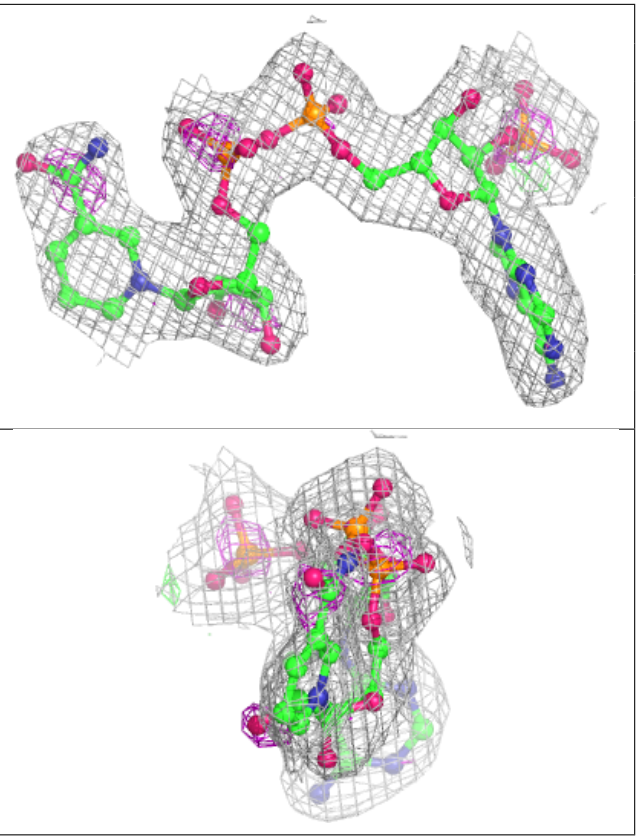






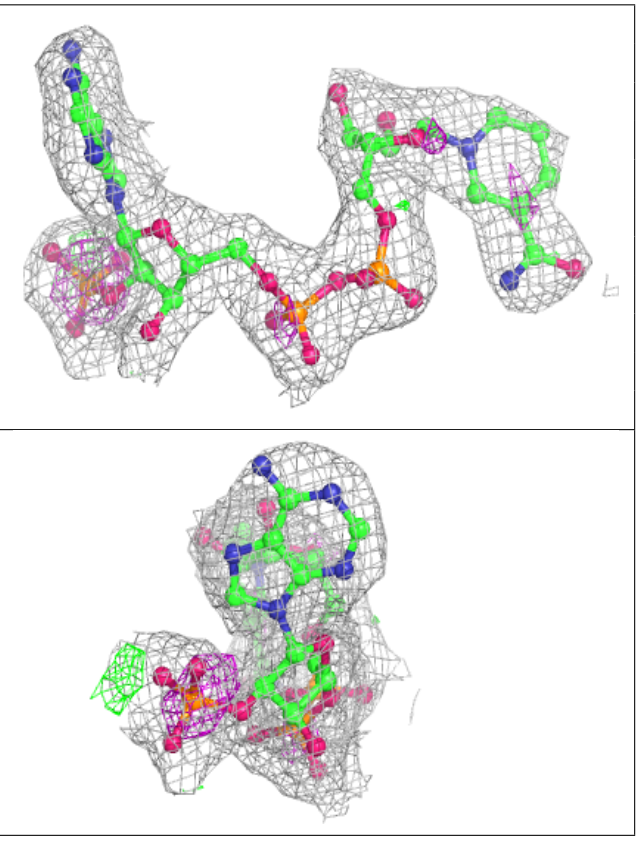
Electron density around NAP K 400:

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



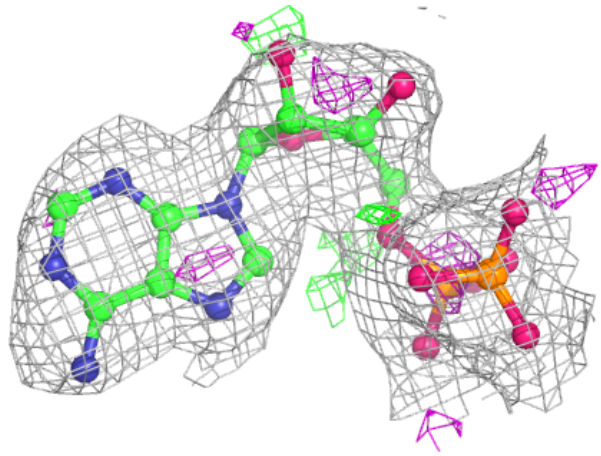
Electron density around NAP L 400:

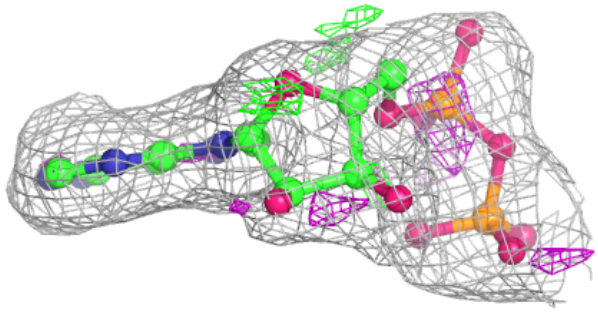
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

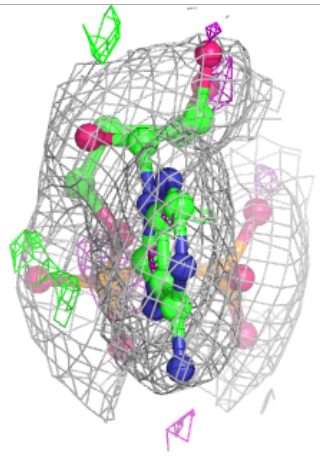


Electron density around ADP E 401:

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

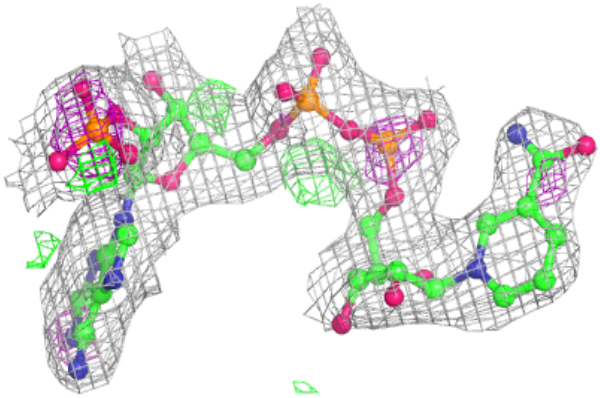


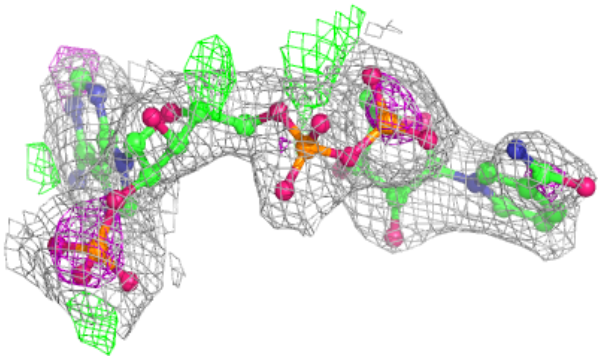


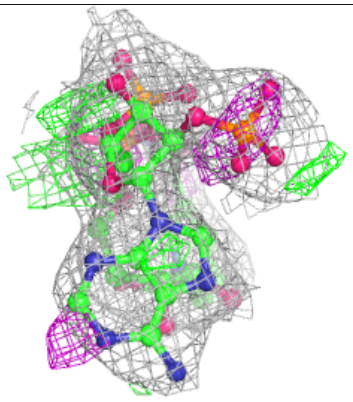


Electron density around NAP N 400:

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

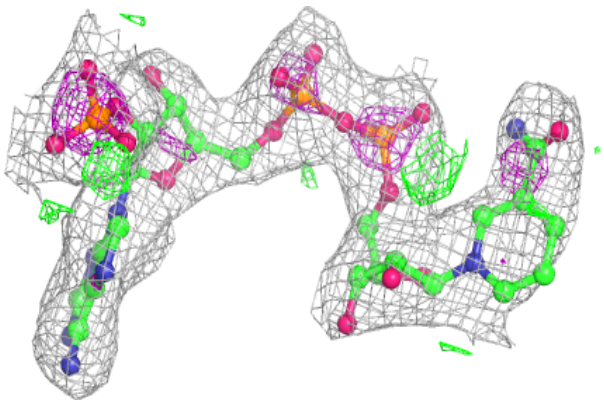


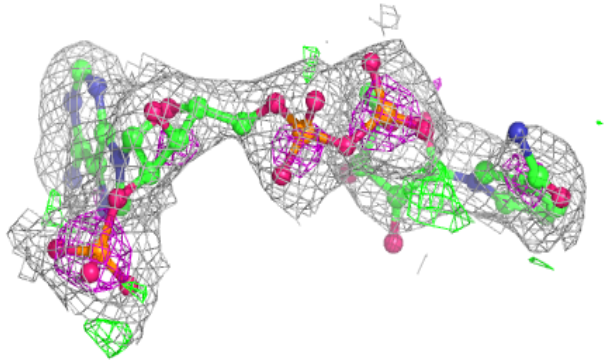


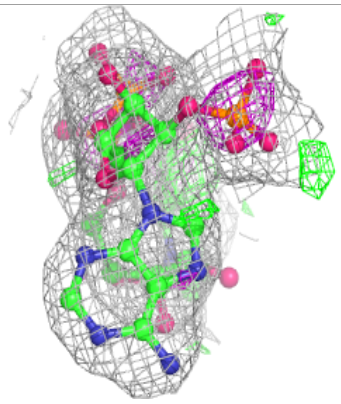


Electron density around NAP C 400:

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

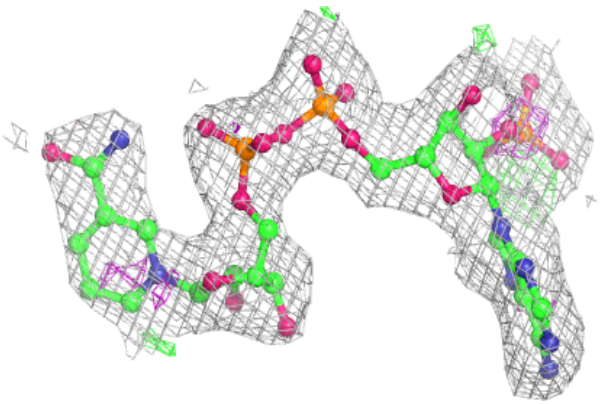


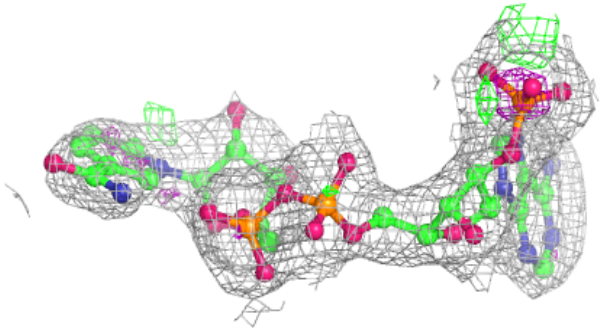


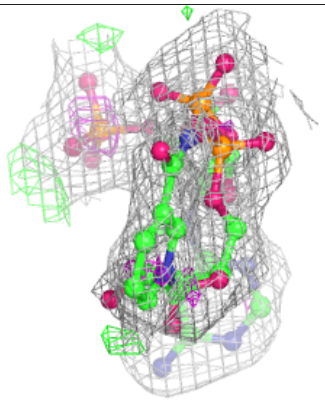


Electron density around NAP P 400:

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

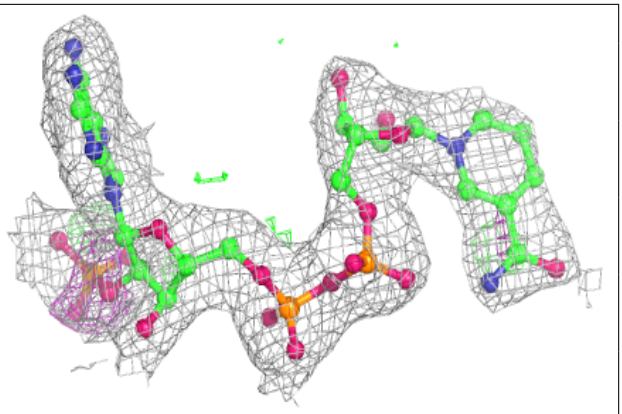


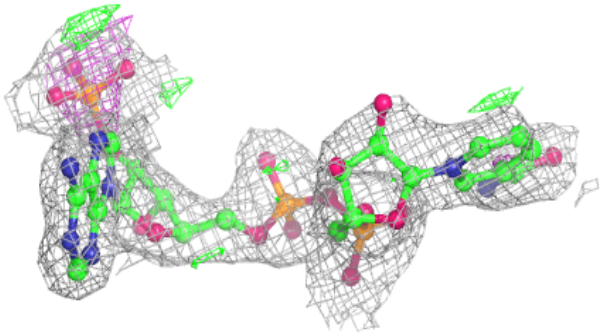


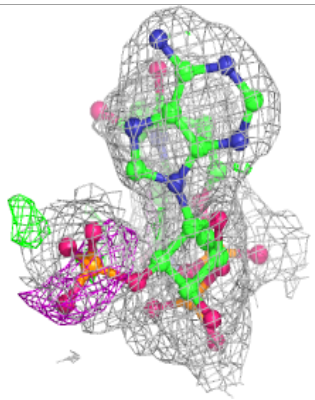


Electron density around NAP Q 400:

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

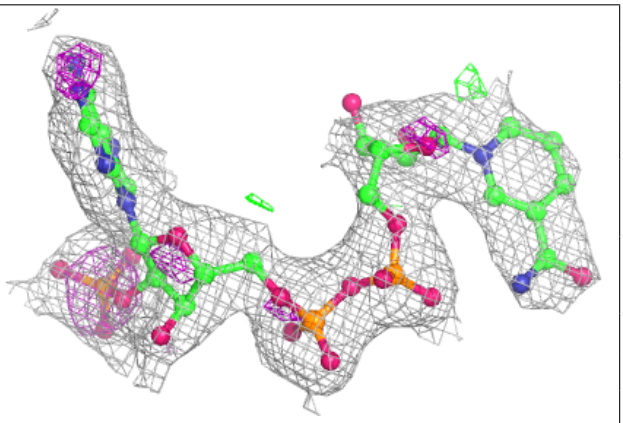


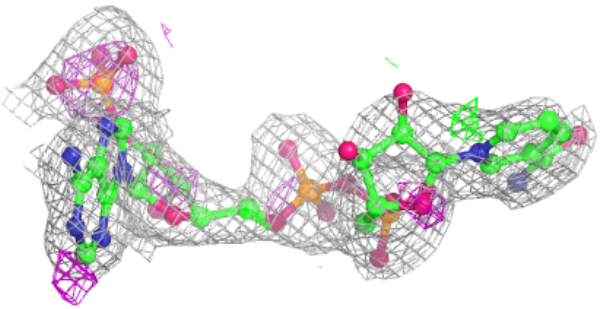


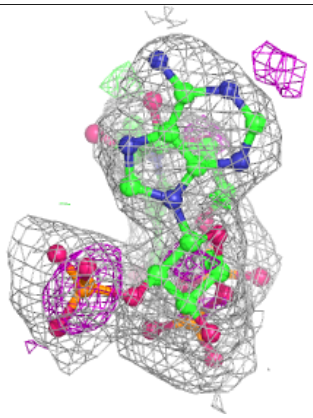


Electron density around NAP D 400:

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

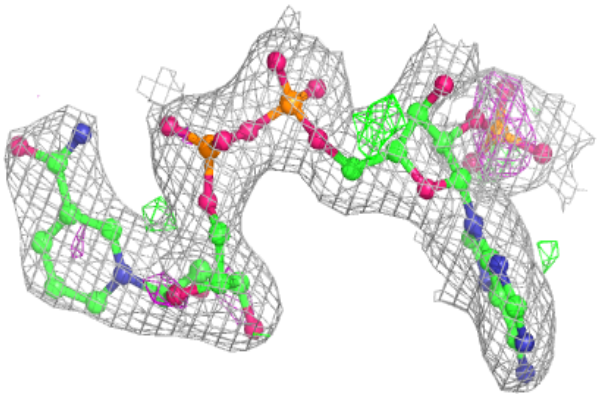


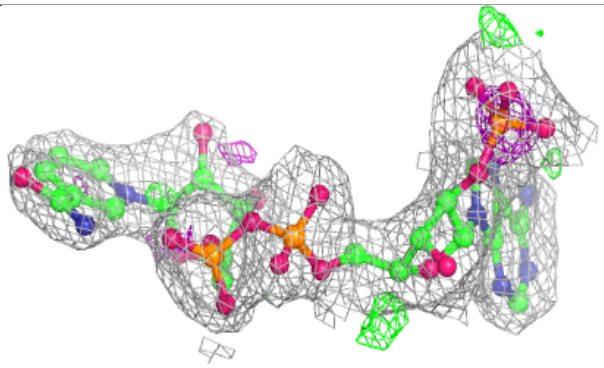


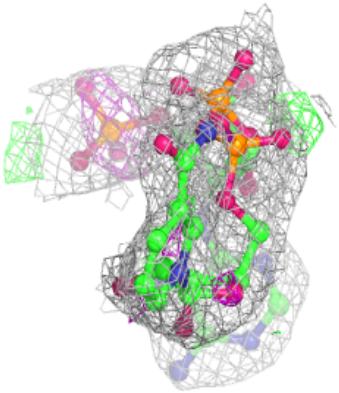


Electron density around NAP E 400:

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

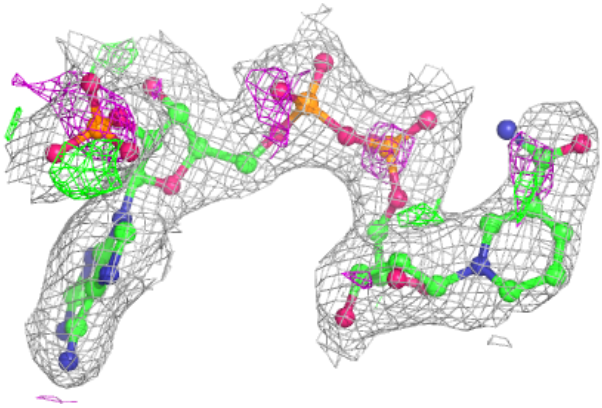


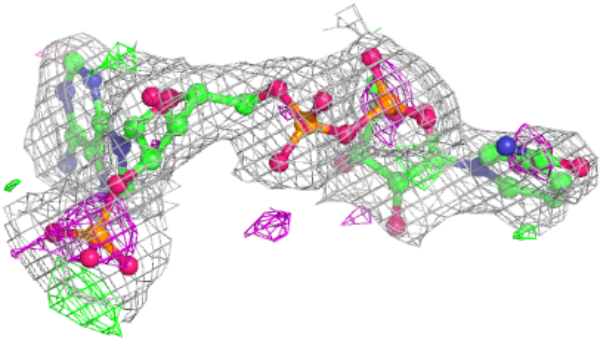


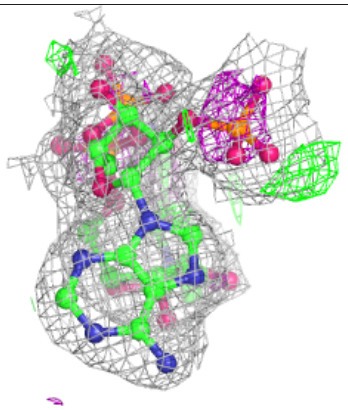


Electron density around NAP A 400:

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

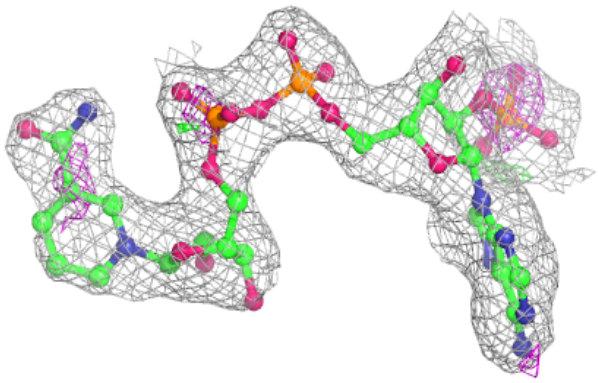


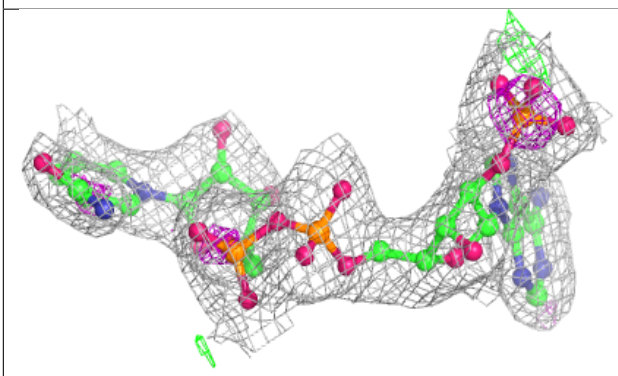


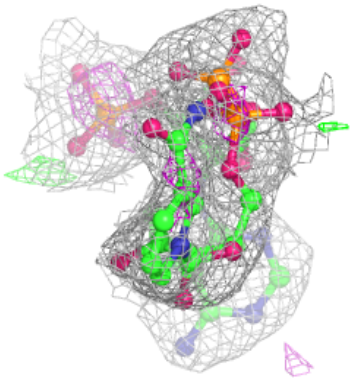


Electron density around NAP M 400:

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

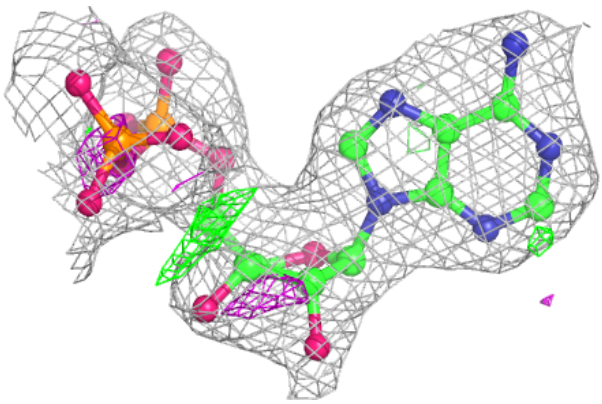


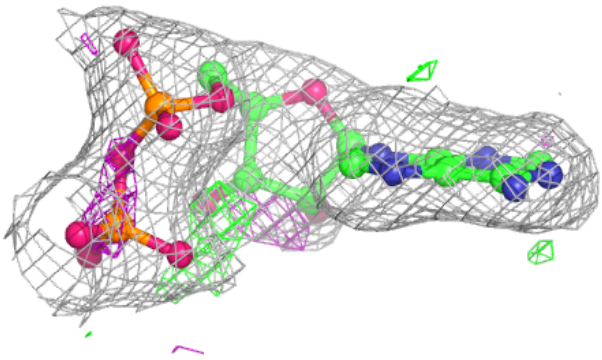


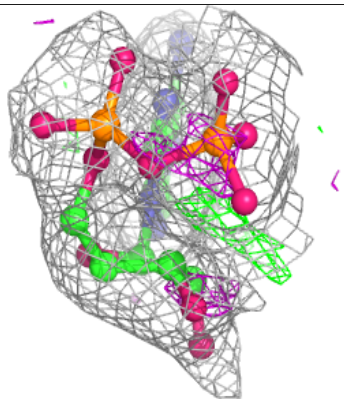


Electron density around ADP I 401:

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

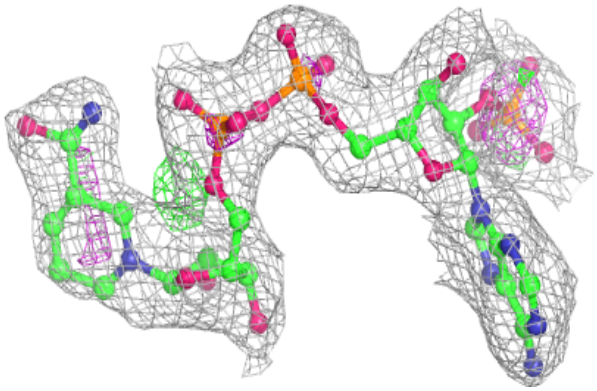


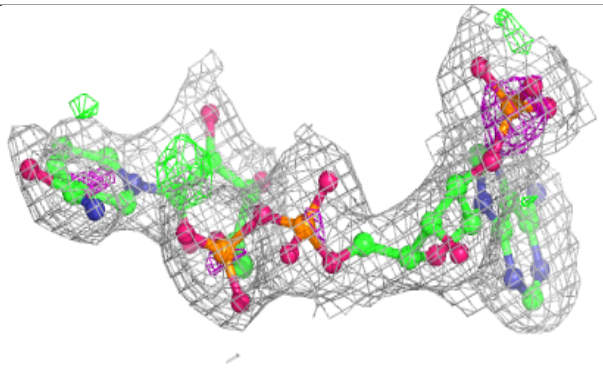


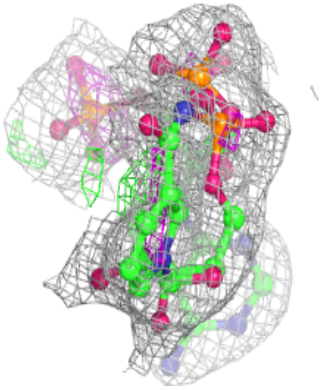


Electron density around NAP F 400:

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

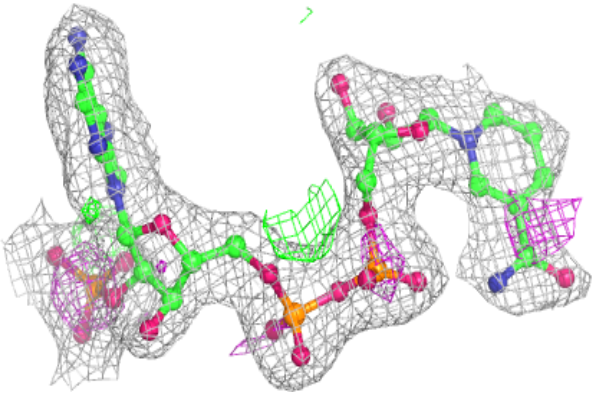


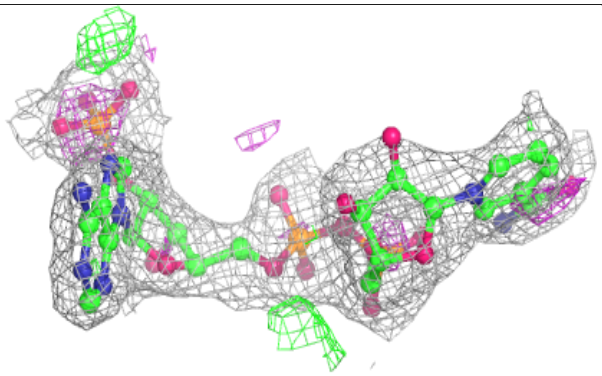


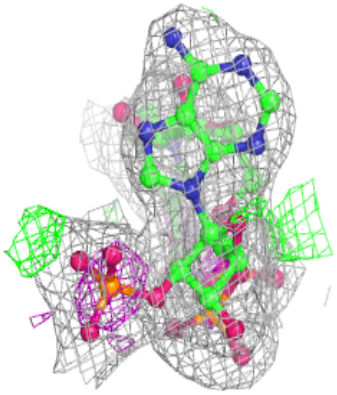


Electron density around NAP H 400:

$2mF_o$-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.