



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 05:10 PM UTC

PDB ID : 2X6T / pdb_00002x6t
Title : AGME bound to ADP-B-mannose
Authors : Kowatz, T.; Morrison, J.P.; Tanner, M.E.; Naismith, J.H.
Deposited on : 2010-02-21
Resolution : 2.36 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 ⓘ symbol.

The types of validation reports are described at

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

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

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

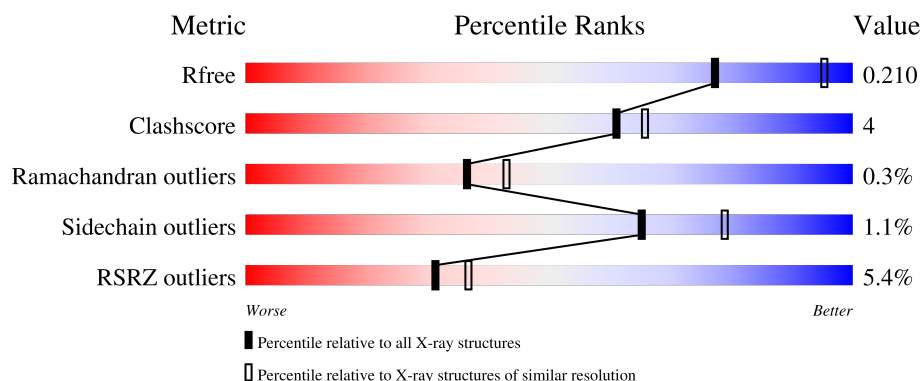
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	357	3% 80% 6% 14%
1	B	357	3% 82% . 14%
1	C	357	% 81% . 14%
1	D	357	16% 81% . 14%
1	E	357	4% 81% . 14%

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Mol	Chain	Length	Quality of chain
1	F	357	
1	G	357	
1	H	357	
1	I	357	
1	J	357	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1310	-	-	X	-
3	GOL	B	1310	-	-	X	-
3	GOL	C	1310	-	-	X	-
3	GOL	D	1310	-	-	X	-
3	GOL	E	1310	-	-	X	-
3	GOL	F	1310	-	-	X	-
3	GOL	G	1310	-	-	X	-
3	GOL	H	1310	-	-	X	-
3	GOL	I	1310	-	-	X	-
3	GOL	J	1310	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26879 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
1	A	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	B	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	C	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	D	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	E	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	F	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	G	308	Total	C	N	O	S	0	0	0
			2451	1572	400	470	9			
1	H	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	I	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			
1	J	307	Total	C	N	O	S	0	0	0
			2440	1566	396	469	9			

There are 10 discrepancies between the modelled and reference sequences:

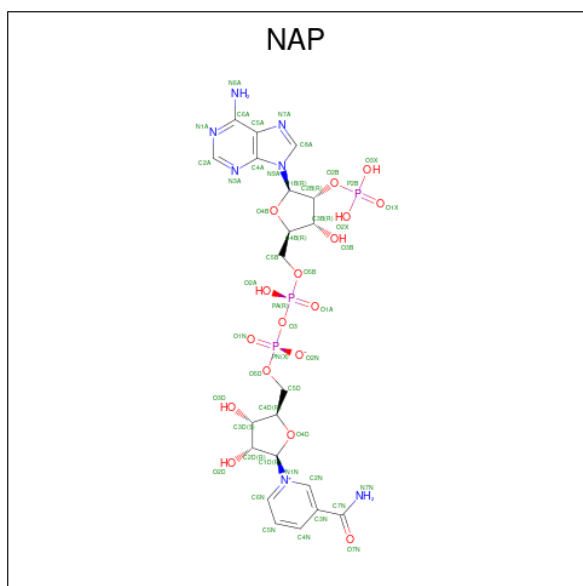
Chain	Residue	Modelled	Actual	Comment	Reference
A	140	PHE	TYR	engineered mutation	UNP P67911
B	140	PHE	TYR	engineered mutation	UNP P67911
C	140	PHE	TYR	engineered mutation	UNP P67911
D	140	PHE	TYR	engineered mutation	UNP P67911
E	140	PHE	TYR	engineered mutation	UNP P67911
F	140	PHE	TYR	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
J	140	PHE	TYR	engineered mutation	UNP P67911

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



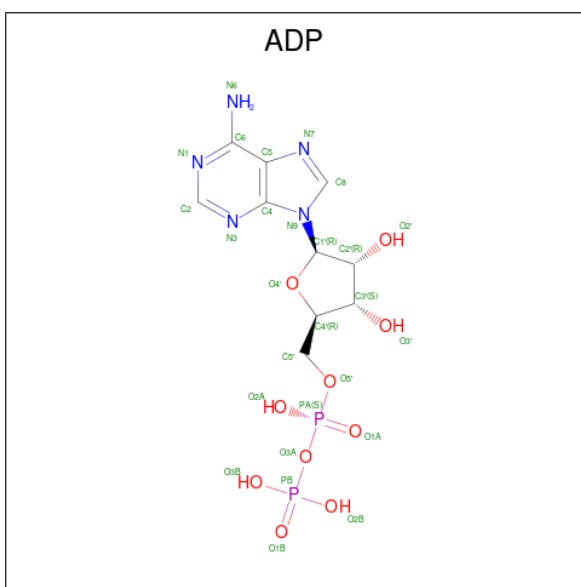
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	E	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	F	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	G	1	Total 48	C 21	N 7	O 17	P 3	0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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



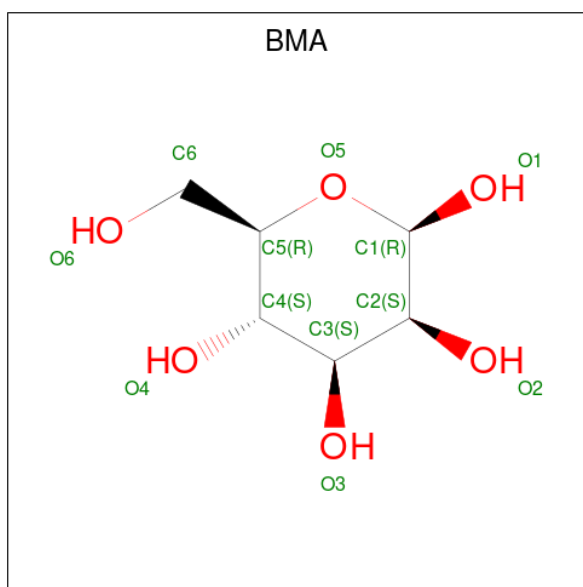
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is beta-D-mannopyranose (CCD ID: BMA) (formula: $\text{C}_6\text{H}_{12}\text{O}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	D	1	Total	C	O	0	0
			11	6	5		
5	E	1	Total	C	O	0	0
			11	6	5		
5	F	1	Total	C	O	0	0
			11	6	5		
5	G	1	Total	C	O	0	0
			11	6	5		
5	H	1	Total	C	O	0	0
			11	6	5		
5	I	1	Total	C	O	0	0
			11	6	5		
5	J	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	2	Total	Cl	0	0
			2	2		

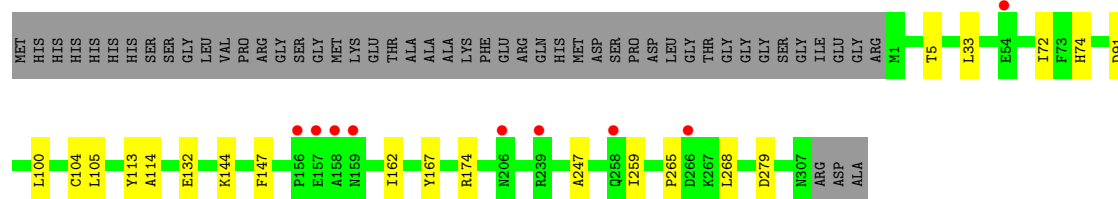
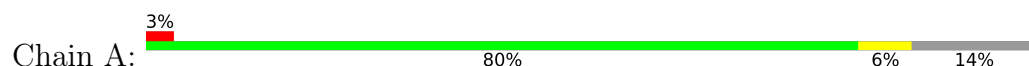
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	186	Total 186	O 186	0	0
7	B	143	Total 143	O 143	0	0
7	C	168	Total 168	O 168	0	0
7	D	115	Total 115	O 115	0	0
7	E	158	Total 158	O 158	0	0
7	F	130	Total 130	O 130	0	0
7	G	176	Total 176	O 176	0	0
7	H	169	Total 169	O 169	0	0
7	I	146	Total 146	O 146	0	0
7	J	155	Total 155	O 155	0	0

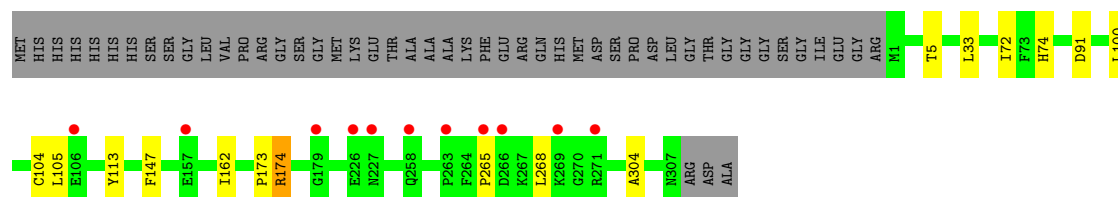
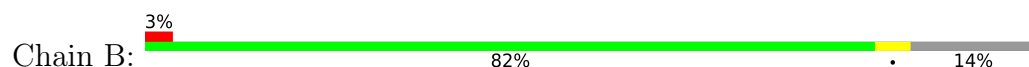
3 Residue-property plots [i](#)

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.

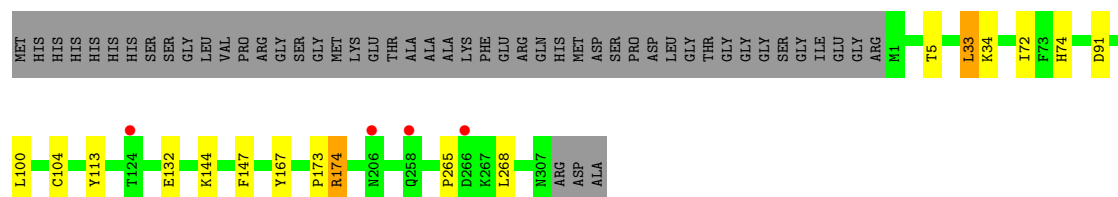
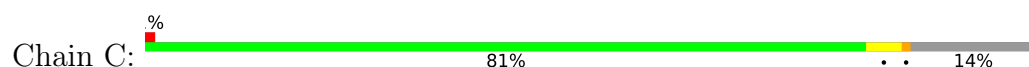
- Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE



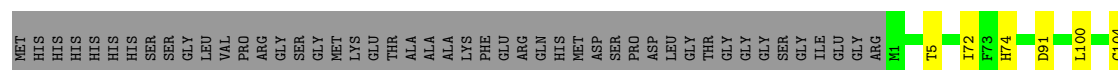
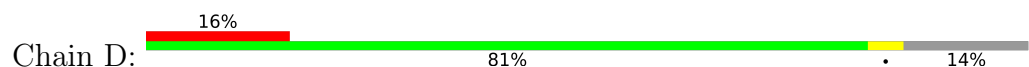
- Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

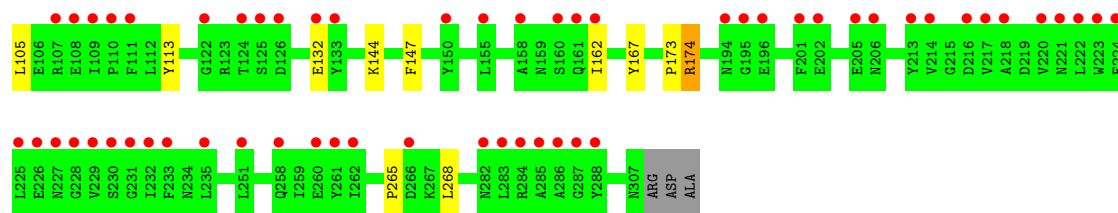


- Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

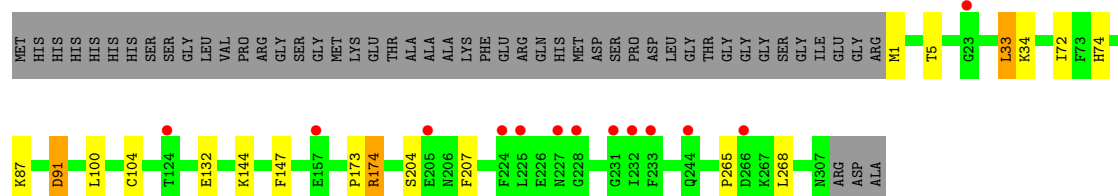
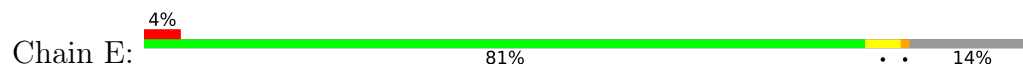


- Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

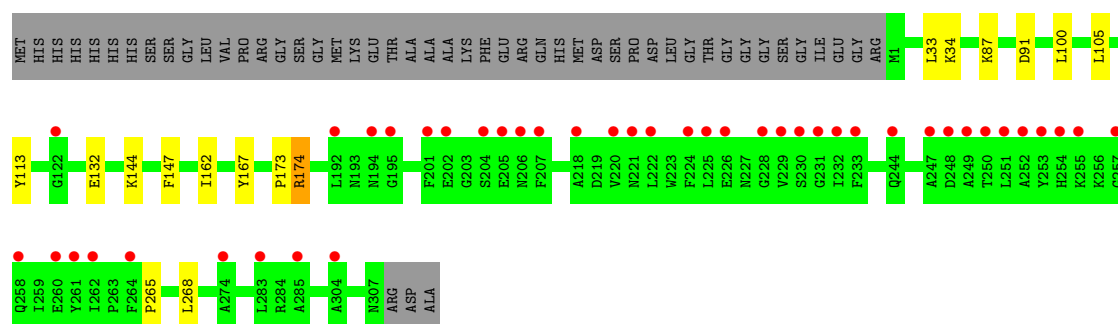
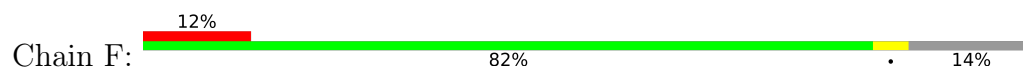




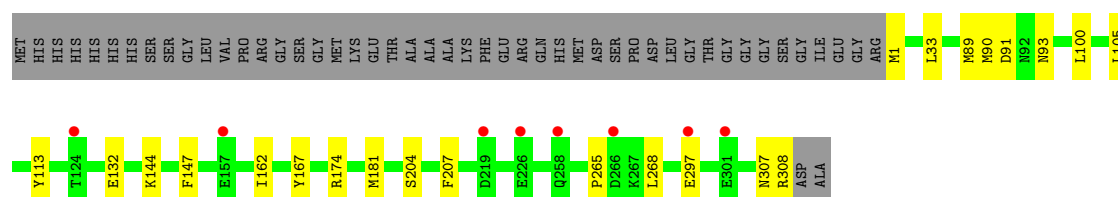
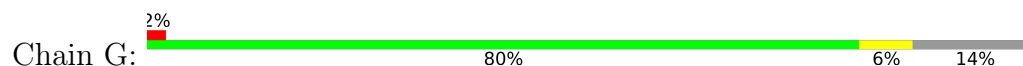
● Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE



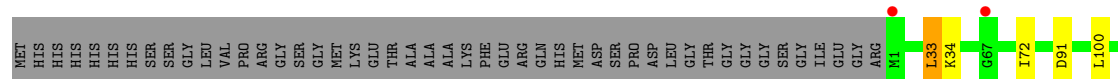
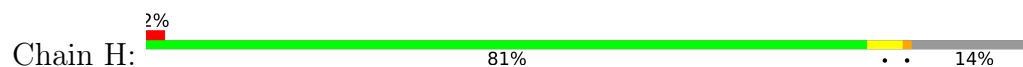
● Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE



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

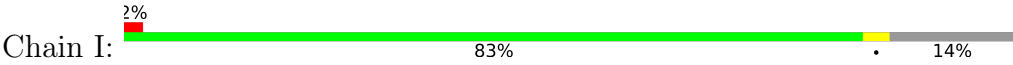


● Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE

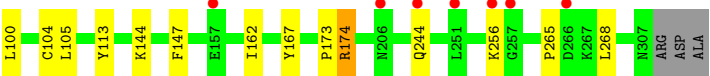
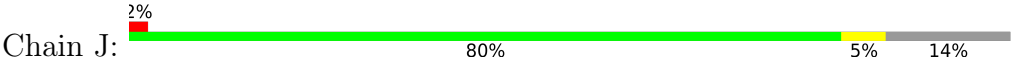




● Molecule 1: ADP-L-GLYCERO-D-MANNO-HEPTOSE-6-EPIMERASE



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	341.99Å 60.79Å 191.79Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	38.69 – 2.36 38.69 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.69-2.36) 99.3 (38.69-2.36)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.58 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.189 , 0.209 0.192 , 0.210	Depositor DCC
R_{free} test set	8157 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26879	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, ADP, NAP, CL

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	0.44	0/2498	0.70	0/3377
1	B	0.40	0/2498	0.69	0/3377
1	C	0.40	0/2498	0.68	0/3377
1	D	0.38	0/2498	0.68	0/3377
1	E	0.41	0/2498	0.69	0/3377
1	F	0.38	0/2498	0.68	0/3377
1	G	0.44	0/2509	0.70	1/3391 (0.0%)
1	H	0.40	0/2498	0.69	0/3377
1	I	0.41	0/2498	0.69	0/3377
1	J	0.41	1/2498 (0.0%)	0.68	0/3377
All	All	0.41	1/24991 (0.0%)	0.69	1/33784 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	256	LYS	CB-CG	-5.26	1.36	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	181	MET	N-CA-CB	-5.54	101.96	110.44

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	19	1
1	B	2440	0	2337	16	0
1	C	2440	0	2337	19	0
1	D	2440	0	2337	19	1
1	E	2440	0	2337	20	0
1	F	2440	0	2337	19	0
1	G	2451	0	2350	14	1
1	H	2440	0	2337	23	0
1	I	2440	0	2337	15	0
1	J	2440	0	2337	19	0
2	A	48	0	25	4	0
2	B	48	0	25	2	0
2	C	48	0	25	3	0
2	D	48	0	25	4	0
2	E	48	0	25	3	0
2	F	48	0	25	4	0
2	G	48	0	25	4	0
2	H	48	0	25	4	0
2	I	48	0	25	3	0
2	J	48	0	25	4	0
3	A	6	0	8	12	0
3	B	6	0	8	7	0
3	C	6	0	8	13	0
3	D	6	0	8	13	0
3	E	6	0	8	11	0
3	F	6	0	8	12	0
3	G	6	0	8	5	0
3	H	6	0	8	10	0
3	I	6	0	8	11	0
3	J	6	0	8	12	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
4	F	27	0	12	0	0
4	G	27	0	12	0	0
4	H	27	0	12	0	0
4	I	27	0	12	0	0
4	J	27	0	12	0	0
5	A	11	0	10	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	11	0	10	2	0
5	C	11	0	10	2	0
5	D	11	0	10	3	0
5	E	11	0	10	3	0
5	F	11	0	10	3	0
5	G	11	0	10	3	0
5	H	11	0	10	3	0
5	I	11	0	10	2	0
5	J	11	0	10	3	0
6	G	2	0	0	0	0
7	A	186	0	0	0	0
7	B	143	0	0	0	0
7	C	168	0	0	1	0
7	D	115	0	0	1	0
7	E	158	0	0	1	0
7	F	130	0	0	1	0
7	G	176	0	0	1	0
7	H	169	0	0	0	0
7	I	146	0	0	0	0
7	J	155	0	0	2	0
All	All	26879	0	23933	208	2

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 4.

All (208) 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:J:144:LYS:HA	3:J:1310:GOL:H31	1.26	1.18
1:C:144:LYS:HA	3:C:1310:GOL:H31	1.24	1.10
1:A:144:LYS:HA	3:A:1310:GOL:H31	1.33	1.08
1:I:144:LYS:HA	3:I:1310:GOL:H31	1.33	1.08
1:H:144:LYS:HA	3:H:1310:GOL:H31	1.34	1.07
1:D:144:LYS:HA	3:D:1310:GOL:H31	1.37	1.02
1:F:144:LYS:HA	3:F:1310:GOL:H31	1.45	0.95
1:B:304:ALA:CB	1:H:132:GLU:OE1	2.18	0.90
1:C:147:PHE:HB3	3:C:1310:GOL:H32	1.50	0.90
1:F:147:PHE:HB3	3:F:1310:GOL:H32	1.53	0.89
1:E:144:LYS:HA	3:E:1310:GOL:H12	1.55	0.89
1:B:147:PHE:HB3	3:B:1310:GOL:H32	1.56	0.88
1:H:147:PHE:HB3	3:H:1310:GOL:H32	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:HB3	3:A:1310:GOL:H32	1.55	0.86
1:J:147:PHE:HB3	3:J:1310:GOL:H32	1.56	0.86
1:I:147:PHE:HB3	3:I:1310:GOL:H32	1.59	0.85
1:D:147:PHE:HB3	3:D:1310:GOL:H32	1.58	0.85
1:B:304:ALA:HB1	1:H:132:GLU:OE1	1.78	0.83
2:F:1308:NAP:C4N	5:F:1321:BMA:H61	2.09	0.82
2:H:1308:NAP:C4N	5:H:1321:BMA:H61	2.09	0.82
2:J:1308:NAP:C4N	5:J:1321:BMA:H61	2.09	0.81
1:I:147:PHE:CB	3:I:1310:GOL:H32	2.12	0.80
1:H:147:PHE:CB	3:H:1310:GOL:H32	2.13	0.79
2:D:1308:NAP:C4N	5:D:1321:BMA:H61	2.12	0.78
1:J:147:PHE:CB	3:J:1310:GOL:H32	2.12	0.78
1:J:144:LYS:CD	3:J:1310:GOL:H2	2.13	0.78
1:C:147:PHE:CB	3:C:1310:GOL:H32	2.12	0.78
2:B:1308:NAP:C4N	5:B:1321:BMA:H61	2.13	0.77
2:H:1308:NAP:C5N	5:H:1321:BMA:H61	2.15	0.76
1:A:147:PHE:CB	3:A:1310:GOL:H32	2.14	0.76
1:F:147:PHE:CB	3:F:1310:GOL:H32	2.15	0.75
1:A:144:LYS:HD3	3:A:1310:GOL:H2	1.66	0.75
1:D:147:PHE:CB	3:D:1310:GOL:H32	2.15	0.75
1:A:144:LYS:CD	3:A:1310:GOL:H2	2.18	0.74
2:B:1308:NAP:C5N	5:B:1321:BMA:H61	2.18	0.74
1:C:144:LYS:HD3	3:C:1310:GOL:H2	1.70	0.73
2:G:1308:NAP:C4N	5:G:1321:BMA:H61	2.19	0.72
1:J:144:LYS:HD3	3:J:1310:GOL:H2	1.69	0.72
1:E:147:PHE:HB3	3:E:1310:GOL:H11	1.72	0.72
1:C:144:LYS:CD	3:C:1310:GOL:H2	2.20	0.71
2:A:1308:NAP:C4N	5:A:1321:BMA:H61	2.21	0.71
1:D:144:LYS:HD3	3:D:1310:GOL:H2	1.72	0.70
2:C:1308:NAP:C4N	5:C:1321:BMA:H61	2.21	0.70
1:F:144:LYS:HD3	3:F:1310:GOL:H2	1.73	0.70
2:E:1308:NAP:C4N	5:E:1321:BMA:H61	2.22	0.70
3:J:1310:GOL:O2	7:J:2155:HOH:O	2.01	0.70
1:D:265:PRO:HG2	1:D:268:LEU:HD12	1.75	0.69
1:D:144:LYS:CD	3:D:1310:GOL:H2	2.22	0.69
2:F:1308:NAP:C5N	5:F:1321:BMA:H61	2.22	0.69
1:E:147:PHE:CB	3:E:1310:GOL:H11	2.23	0.68
1:G:265:PRO:HG2	1:G:268:LEU:HD12	1.76	0.68
1:F:144:LYS:CD	3:F:1310:GOL:H2	2.25	0.67
1:H:144:LYS:CD	3:H:1310:GOL:H2	2.25	0.67
2:D:1308:NAP:C5N	5:D:1321:BMA:H61	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:265:PRO:HG2	1:J:268:LEU:HD12	1.77	0.67
1:H:265:PRO:HG2	1:H:268:LEU:HD12	1.76	0.66
1:B:265:PRO:HG2	1:B:268:LEU:HD12	1.75	0.66
1:C:265:PRO:HG2	1:C:268:LEU:HD12	1.78	0.66
1:A:265:PRO:HG2	1:A:268:LEU:HD12	1.77	0.66
1:I:265:PRO:HG2	1:I:268:LEU:HD12	1.76	0.66
1:G:147:PHE:CB	3:G:1310:GOL:H12	2.26	0.65
1:H:144:LYS:HD3	3:H:1310:GOL:H2	1.78	0.64
2:C:1308:NAP:C5N	5:C:1321:BMA:H61	2.28	0.64
1:I:144:LYS:HD3	3:I:1310:GOL:H2	1.79	0.64
1:E:144:LYS:HD3	3:E:1310:GOL:H12	1.79	0.64
1:F:265:PRO:HG2	1:F:268:LEU:HD12	1.78	0.63
1:I:144:LYS:CD	3:I:1310:GOL:H2	2.28	0.63
1:E:265:PRO:HG2	1:E:268:LEU:HD12	1.79	0.62
1:B:147:PHE:CD2	3:B:1310:GOL:H11	2.34	0.62
1:D:147:PHE:HD2	3:D:1310:GOL:H11	1.64	0.62
2:I:1308:NAP:C4N	5:I:1321:BMA:H61	2.30	0.61
1:B:304:ALA:HB2	1:H:132:GLU:CD	2.27	0.60
1:F:147:PHE:HD2	3:F:1310:GOL:H11	1.66	0.60
1:F:144:LYS:HD3	3:F:1310:GOL:H31	1.82	0.59
1:D:144:LYS:HD3	3:D:1310:GOL:H31	1.85	0.59
1:C:144:LYS:HA	3:C:1310:GOL:C3	2.16	0.59
1:B:113:TYR:CE1	3:B:1310:GOL:H31	2.38	0.59
2:G:1308:NAP:C5N	5:G:1321:BMA:H61	2.32	0.58
1:A:144:LYS:HD3	3:A:1310:GOL:C2	2.33	0.58
1:A:147:PHE:HD2	3:A:1310:GOL:H11	1.67	0.58
2:J:1308:NAP:C5N	5:J:1321:BMA:H61	2.31	0.58
1:A:144:LYS:HD3	3:A:1310:GOL:H31	1.86	0.58
1:H:144:LYS:HD3	3:H:1310:GOL:H31	1.86	0.58
1:C:144:LYS:HD3	3:C:1310:GOL:H31	1.86	0.57
1:J:147:PHE:HD2	3:J:1310:GOL:H11	1.69	0.57
1:C:147:PHE:HD2	3:C:1310:GOL:H11	1.69	0.57
1:B:304:ALA:CB	1:H:132:GLU:CD	2.78	0.57
1:C:144:LYS:HD3	3:C:1310:GOL:C2	2.35	0.56
2:E:1308:NAP:C5N	5:E:1321:BMA:H61	2.35	0.56
1:H:147:PHE:HD2	3:H:1310:GOL:H11	1.70	0.56
1:J:144:LYS:HD3	3:J:1310:GOL:C2	2.35	0.56
1:C:144:LYS:HD3	3:C:1310:GOL:C3	2.36	0.55
1:J:144:LYS:HD3	3:J:1310:GOL:C3	2.36	0.55
1:I:147:PHE:HD2	3:I:1310:GOL:H11	1.72	0.55
1:A:144:LYS:HD3	3:A:1310:GOL:C3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:LYS:HD3	3:H:1310:GOL:C3	2.37	0.54
1:I:144:LYS:HD3	3:I:1310:GOL:C3	2.39	0.53
1:D:144:LYS:HD3	3:D:1310:GOL:C3	2.39	0.53
1:G:147:PHE:HB2	3:G:1310:GOL:H12	1.89	0.53
1:H:113:TYR:CE1	3:H:1310:GOL:H11	2.43	0.53
1:F:144:LYS:HA	3:F:1310:GOL:C3	2.28	0.52
1:E:147:PHE:CD2	3:E:1310:GOL:H32	2.44	0.52
1:F:144:LYS:HD3	3:F:1310:GOL:C2	2.40	0.52
1:I:144:LYS:HD3	3:I:1310:GOL:H31	1.92	0.52
1:D:144:LYS:HD3	3:D:1310:GOL:C2	2.39	0.51
2:H:1308:NAP:C5N	5:H:1321:BMA:C6	2.88	0.51
1:A:167:TYR:HB2	2:A:1308:NAP:C5N	2.40	0.51
1:E:144:LYS:HD3	3:E:1310:GOL:C2	2.41	0.51
1:G:167:TYR:HB2	2:G:1308:NAP:C5N	2.41	0.50
1:E:144:LYS:HD3	3:E:1310:GOL:C1	2.40	0.50
1:G:113:TYR:CD1	3:G:1310:GOL:H32	2.47	0.50
1:G:147:PHE:HB3	3:G:1310:GOL:H12	1.93	0.50
1:F:144:LYS:HD3	3:F:1310:GOL:C3	2.42	0.50
1:C:113:TYR:CE1	3:C:1310:GOL:H11	2.46	0.50
1:I:144:LYS:HD3	3:I:1310:GOL:C2	2.42	0.49
1:J:113:TYR:CE1	3:J:1310:GOL:H11	2.47	0.48
1:D:113:TYR:CE1	3:D:1310:GOL:H11	2.48	0.48
1:J:144:LYS:HD2	3:J:1310:GOL:H2	1.91	0.48
1:F:144:LYS:HZ3	3:F:1310:GOL:H2	1.78	0.48
3:C:1310:GOL:O2	7:C:2168:HOH:O	2.15	0.47
1:A:144:LYS:HA	3:A:1310:GOL:C3	2.23	0.47
1:I:167:TYR:HB2	2:I:1308:NAP:C5N	2.44	0.47
1:H:144:LYS:HD3	3:H:1310:GOL:C2	2.42	0.47
1:C:167:TYR:HB2	2:C:1308:NAP:C5N	2.44	0.47
1:F:113:TYR:CE1	3:F:1310:GOL:H11	2.49	0.47
1:J:105:LEU:HD11	1:J:162:ILE:HD11	1.97	0.47
1:B:147:PHE:HD2	3:B:1310:GOL:C3	2.29	0.46
2:F:1308:NAP:C5N	5:F:1321:BMA:C6	2.93	0.46
1:E:144:LYS:HD3	3:E:1310:GOL:H2	1.98	0.46
2:D:1308:NAP:C5N	5:D:1321:BMA:C6	2.93	0.45
1:D:132:GLU:H	1:D:132:GLU:CD	2.24	0.45
2:G:1308:NAP:C5N	5:G:1321:BMA:C6	2.94	0.45
1:H:105:LEU:HD11	1:H:162:ILE:HD11	1.99	0.45
1:C:144:LYS:HZ3	3:C:1310:GOL:H2	1.81	0.45
1:G:105:LEU:HD11	1:G:162:ILE:HD11	1.99	0.45
2:J:1308:NAP:C5N	5:J:1321:BMA:C6	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:TYR:HB2	2:D:1308:NAP:C5N	2.47	0.45
1:J:167:TYR:HB2	2:J:1308:NAP:C5N	2.47	0.45
1:F:87:LYS:NZ	7:F:2040:HOH:O	2.47	0.44
1:H:132:GLU:CD	1:H:132:GLU:H	2.25	0.44
1:H:167:TYR:HB2	2:H:1308:NAP:C5N	2.47	0.44
1:F:167:TYR:HB2	2:F:1308:NAP:C5N	2.48	0.44
1:J:33:LEU:O	1:J:34:LYS:C	2.61	0.44
1:J:144:LYS:HD3	3:J:1310:GOL:H31	1.99	0.44
1:G:144:LYS:HD3	3:G:1310:GOL:H2	2.00	0.44
1:B:113:TYR:HE1	3:B:1310:GOL:H31	1.82	0.44
2:A:1308:NAP:C5N	5:A:1321:BMA:H61	2.47	0.44
1:E:1:MET:N	7:E:2001:HOH:O	2.50	0.44
1:A:132:GLU:H	1:A:132:GLU:CD	2.26	0.43
1:B:173:PRO:O	1:B:174:ARG:HB2	2.17	0.43
1:J:5:THR:OG1	1:J:74:HIS:HA	2.18	0.43
1:H:72:ILE:HD12	1:H:104:CYS:SG	2.59	0.43
2:A:1308:NAP:C5N	5:A:1321:BMA:C6	2.96	0.43
1:D:144:LYS:HA	3:D:1310:GOL:C3	2.27	0.43
1:F:173:PRO:O	1:F:174:ARG:HB2	2.18	0.43
1:G:1:MET:N	7:G:2001:HOH:O	2.52	0.43
1:I:113:TYR:CE1	3:I:1310:GOL:H11	2.53	0.43
1:E:173:PRO:O	1:E:174:ARG:HB2	2.18	0.43
1:J:173:PRO:O	1:J:174:ARG:HB2	2.19	0.43
2:E:1308:NAP:C5N	5:E:1321:BMA:C6	2.96	0.43
1:G:132:GLU:CD	1:G:132:GLU:H	2.27	0.43
1:H:33:LEU:O	1:H:34:LYS:C	2.61	0.43
1:C:72:ILE:HD12	1:C:104:CYS:SG	2.58	0.42
1:B:147:PHE:CD2	3:B:1310:GOL:C1	2.99	0.42
1:B:147:PHE:HD2	3:B:1310:GOL:H31	1.84	0.42
1:E:144:LYS:CD	3:E:1310:GOL:H2	2.50	0.42
1:A:114:ALA:O	3:A:1310:GOL:H12	2.20	0.42
1:A:247:ALA:HB1	1:A:259:ILE:HD11	2.02	0.42
1:E:147:PHE:CD2	3:E:1310:GOL:C3	3.02	0.42
1:E:33:LEU:O	1:E:34:LYS:C	2.63	0.42
1:E:132:GLU:H	1:E:132:GLU:CD	2.27	0.42
1:I:147:PHE:HB2	3:I:1310:GOL:H32	1.96	0.42
1:E:144:LYS:NZ	3:E:1310:GOL:H2	2.35	0.42
1:C:173:PRO:O	1:C:174:ARG:HB2	2.20	0.42
1:D:105:LEU:HD11	1:D:162:ILE:HD11	2.02	0.42
1:C:33:LEU:O	1:C:34:LYS:C	2.62	0.42
1:A:113:TYR:CE1	3:A:1310:GOL:H11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:173:PRO:O	1:I:174:ARG:HB2	2.21	0.41
1:J:244:GLN:NE2	7:J:2104:HOH:O	2.47	0.41
1:A:5:THR:OG1	1:A:74:HIS:HA	2.20	0.41
1:J:72:ILE:HD12	1:J:104:CYS:SG	2.60	0.41
1:D:147:PHE:HB2	3:D:1310:GOL:H32	2.00	0.41
3:D:1310:GOL:O2	7:D:2114:HOH:O	2.03	0.41
1:B:5:THR:OG1	1:B:74:HIS:HA	2.20	0.41
1:F:105:LEU:HD11	1:F:162:ILE:HD11	2.01	0.41
1:F:33:LEU:O	1:F:34:LYS:C	2.63	0.41
1:D:5:THR:OG1	1:D:74:HIS:HA	2.21	0.41
1:D:173:PRO:O	1:D:174:ARG:HB2	2.21	0.41
1:I:132:GLU:H	1:I:132:GLU:CD	2.29	0.41
1:F:132:GLU:H	1:F:132:GLU:CD	2.29	0.41
1:A:72:ILE:HD12	1:A:104:CYS:SG	2.60	0.41
1:A:105:LEU:HD11	1:A:162:ILE:HD11	2.02	0.41
1:B:72:ILE:HD12	1:B:104:CYS:SG	2.61	0.41
1:E:5:THR:OG1	1:E:74:HIS:HA	2.21	0.41
1:E:87:LYS:O	1:E:91:ASP:HB2	2.21	0.41
1:E:204:SER:HA	1:E:207:PHE:CD2	2.56	0.41
1:G:307:ASN:O	1:G:308:ARG:C	2.64	0.40
1:H:105:LEU:HD21	1:H:154:ILE:CG2	2.51	0.40
1:C:5:THR:OG1	1:C:74:HIS:HA	2.21	0.40
1:E:72:ILE:HD12	1:E:104:CYS:SG	2.61	0.40
1:C:132:GLU:CD	1:C:132:GLU:H	2.29	0.40
1:D:72:ILE:HD12	1:D:104:CYS:SG	2.62	0.40
1:G:89:MET:O	1:G:93:ASN:HB2	2.21	0.40
1:G:204:SER:HA	1:G:207:PHE:CD2	2.56	0.40
1:B:105:LEU:HD11	1:B:162:ILE:HD11	2.04	0.40
1:H:173:PRO:O	1:H:174:ARG:HB2	2.22	0.40
2:I:1308:NAP:C5N	5:I:1321:BMA:H61	2.51	0.40
1:G:90:MET:HG3	1:H:33:LEU:HD12	2.04	0.40

All (2) 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:D:132:GLU:OE1	1:D:132:GLU:OE1[2_554]	1.75	0.45
1:A:279:ASP:OD2	1:G:297:GLU:OE2[4_545]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	296 (97%)	8 (3%)	1 (0%)	36	43
1	B	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	36	43
1	C	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	36	43
1	D	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	36	43
1	E	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	36	43
1	F	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	36	43
1	G	306/357 (86%)	297 (97%)	8 (3%)	1 (0%)	36	43
1	H	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	36	43
1	I	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	36	43
1	J	305/357 (85%)	296 (97%)	8 (3%)	1 (0%)	36	43
All	All	3051/3570 (86%)	2961 (97%)	80 (3%)	10 (0%)	36	43

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	ARG
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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/292 (87%)	252 (99%)	3 (1%)	63	77
1	B	255/292 (87%)	252 (99%)	3 (1%)	63	77
1	C	255/292 (87%)	252 (99%)	3 (1%)	63	77
1	D	255/292 (87%)	253 (99%)	2 (1%)	73	84
1	E	255/292 (87%)	252 (99%)	3 (1%)	63	77
1	F	255/292 (87%)	253 (99%)	2 (1%)	73	84
1	G	256/292 (88%)	253 (99%)	3 (1%)	63	77
1	H	255/292 (87%)	252 (99%)	3 (1%)	63	77
1	I	255/292 (87%)	252 (99%)	3 (1%)	63	77
1	J	255/292 (87%)	253 (99%)	2 (1%)	73	84
All	All	2551/2920 (87%)	2524 (99%)	27 (1%)	65	79

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	91	ASP
1	A	100	LEU
1	B	33	LEU
1	B	91	ASP
1	B	100	LEU
1	C	33	LEU
1	C	91	ASP
1	C	100	LEU
1	D	91	ASP
1	D	100	LEU
1	E	33	LEU
1	E	91	ASP
1	E	100	LEU
1	F	91	ASP
1	F	100	LEU

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Mol	Chain	Res	Type
1	G	33	LEU
1	G	91	ASP
1	G	100	LEU
1	H	33	LEU
1	H	91	ASP
1	H	100	LEU
1	I	33	LEU
1	I	91	ASP
1	I	100	LEU
1	J	91	ASP
1	J	100	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	193	ASN
1	A	221	ASN
1	A	234	ASN
1	A	277	GLN
1	A	307	ASN
1	B	41	ASN
1	B	159	ASN
1	B	221	ASN
1	B	277	GLN
1	C	221	ASN
1	C	234	ASN
1	C	254	HIS
1	C	277	GLN
1	D	41	ASN
1	D	221	ASN
1	D	234	ASN
1	D	277	GLN
1	E	41	ASN
1	E	221	ASN
1	E	234	ASN
1	E	277	GLN
1	F	221	ASN
1	F	277	GLN
1	G	41	ASN
1	G	221	ASN
1	G	234	ASN

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Mol	Chain	Res	Type
1	G	277	GLN
1	H	41	ASN
1	H	221	ASN
1	H	234	ASN
1	H	277	GLN
1	H	282	ASN
1	I	41	ASN
1	I	221	ASN
1	I	234	ASN
1	I	277	GLN
1	J	41	ASN
1	J	221	ASN
1	J	234	ASN
1	J	244	GLN
1	J	254	HIS
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 2 are monoatomic - leaving 40 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	I	1308	-	50,52,52	1.72	6 (12%)	71,80,80	1.47	7 (9%)
4	ADP	D	1320	5	28,29,29	1.05	2 (7%)	43,45,45	1.81	9 (20%)
4	ADP	A	1320	5	28,29,29	1.03	2 (7%)	43,45,45	1.87	8 (18%)
4	ADP	I	1320	5	28,29,29	0.96	1 (3%)	43,45,45	1.86	10 (23%)
5	BMA	F	1321	4	11,11,12	0.46	0	15,15,17	0.79	0
5	BMA	G	1321	4	11,11,12	0.56	0	15,15,17	0.95	1 (6%)
3	GOL	J	1310	-	5,5,5	0.58	0	5,5,5	0.81	0
4	ADP	F	1320	5	28,29,29	1.02	2 (7%)	43,45,45	1.86	9 (20%)
5	BMA	A	1321	4	11,11,12	0.50	0	15,15,17	0.97	1 (6%)
2	NAP	H	1308	-	50,52,52	1.72	5 (10%)	71,80,80	1.55	9 (12%)
5	BMA	D	1321	4	11,11,12	0.48	0	15,15,17	0.62	0
4	ADP	C	1320	5	28,29,29	0.95	0	43,45,45	1.85	8 (18%)
4	ADP	E	1320	5	28,29,29	0.99	2 (7%)	43,45,45	1.86	7 (16%)
2	NAP	F	1308	-	50,52,52	1.75	7 (14%)	71,80,80	1.63	9 (12%)
3	GOL	G	1310	-	5,5,5	0.44	0	5,5,5	0.90	0
2	NAP	J	1308	-	50,52,52	1.71	5 (10%)	71,80,80	1.55	9 (12%)
2	NAP	A	1308	-	50,52,52	1.72	6 (12%)	71,80,80	1.58	10 (14%)
5	BMA	E	1321	4	11,11,12	0.49	0	15,15,17	0.65	0
5	BMA	I	1321	4	11,11,12	0.50	0	15,15,17	0.74	0
3	GOL	F	1310	-	5,5,5	0.56	0	5,5,5	1.08	0
3	GOL	E	1310	-	5,5,5	0.28	0	5,5,5	1.04	0
4	ADP	J	1320	5	28,29,29	0.89	0	43,45,45	1.81	8 (18%)
2	NAP	D	1308	-	50,52,52	1.73	6 (12%)	71,80,80	1.57	10 (14%)
3	GOL	D	1310	-	5,5,5	0.66	0	5,5,5	1.21	1 (20%)
5	BMA	J	1321	4	11,11,12	0.47	0	15,15,17	0.59	0
4	ADP	H	1320	5	28,29,29	0.99	1 (3%)	43,45,45	1.83	8 (18%)
3	GOL	C	1310	-	5,5,5	0.56	0	5,5,5	1.22	1 (20%)
3	GOL	A	1310	-	5,5,5	0.66	0	5,5,5	1.17	1 (20%)
2	NAP	E	1308	-	50,52,52	1.70	7 (14%)	71,80,80	1.51	10 (14%)
2	NAP	G	1308	-	50,52,52	1.70	6 (12%)	71,80,80	1.56	9 (12%)
2	NAP	B	1308	-	50,52,52	1.76	7 (14%)	71,80,80	1.59	10 (14%)
2	NAP	C	1308	-	50,52,52	1.73	6 (12%)	71,80,80	1.53	11 (15%)
4	ADP	G	1320	5	28,29,29	1.00	1 (3%)	43,45,45	1.79	8 (18%)
3	GOL	B	1310	-	5,5,5	0.36	0	5,5,5	1.04	0
5	BMA	B	1321	4	11,11,12	0.54	0	15,15,17	0.70	0
3	GOL	H	1310	-	5,5,5	0.55	0	5,5,5	1.25	1 (20%)
4	ADP	B	1320	5	28,29,29	0.93	1 (3%)	43,45,45	1.87	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	H	1321	4	11,11,12	0.55	0	15,15,17	0.76	0
5	BMA	C	1321	4	11,11,12	0.46	0	15,15,17	0.76	0
3	GOL	I	1310	-	5,5,5	0.59	0	5,5,5	1.16	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	I	1308	-	-	9/35/67/67	0/5/5/5
4	ADP	D	1320	5	-	0/16/32/32	0/3/3/3
4	ADP	A	1320	5	-	1/16/32/32	0/3/3/3
4	ADP	I	1320	5	-	1/16/32/32	0/3/3/3
5	BMA	F	1321	4	-	1/2/19/22	0/1/1/1
5	BMA	G	1321	4	-	0/2/19/22	0/1/1/1
3	GOL	J	1310	-	-	0/4/4/4	-
4	ADP	F	1320	5	-	0/16/32/32	0/3/3/3
5	BMA	A	1321	4	-	2/2/19/22	0/1/1/1
2	NAP	H	1308	-	-	8/35/67/67	0/5/5/5
5	BMA	D	1321	4	-	0/2/19/22	0/1/1/1
4	ADP	C	1320	5	-	1/16/32/32	0/3/3/3
4	ADP	E	1320	5	-	0/16/32/32	0/3/3/3
2	NAP	F	1308	-	-	11/35/67/67	0/5/5/5
3	GOL	G	1310	-	-	4/4/4/4	-
2	NAP	J	1308	-	-	12/35/67/67	0/5/5/5
2	NAP	A	1308	-	-	11/35/67/67	0/5/5/5
5	BMA	E	1321	4	-	0/2/19/22	0/1/1/1
5	BMA	I	1321	4	-	1/2/19/22	0/1/1/1
3	GOL	F	1310	-	-	3/4/4/4	-
3	GOL	E	1310	-	-	2/4/4/4	-
4	ADP	J	1320	5	-	0/16/32/32	0/3/3/3
2	NAP	D	1308	-	-	9/35/67/67	0/5/5/5
3	GOL	D	1310	-	-	2/4/4/4	-
5	BMA	J	1321	4	-	0/2/19/22	0/1/1/1
4	ADP	H	1320	5	-	1/16/32/32	0/3/3/3
3	GOL	C	1310	-	-	2/4/4/4	-
3	GOL	A	1310	-	-	2/4/4/4	-
2	NAP	E	1308	-	-	9/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	G	1308	-	-	10/35/67/67	0/5/5/5
2	NAP	B	1308	-	-	10/35/67/67	0/5/5/5
2	NAP	C	1308	-	-	11/35/67/67	0/5/5/5
4	ADP	G	1320	5	-	0/16/32/32	0/3/3/3
3	GOL	B	1310	-	-	4/4/4/4	-
5	BMA	B	1321	4	-	0/2/19/22	0/1/1/1
3	GOL	H	1310	-	-	2/4/4/4	-
4	ADP	B	1320	5	-	1/16/32/32	0/3/3/3
5	BMA	H	1321	4	-	0/2/19/22	0/1/1/1
5	BMA	C	1321	4	-	0/2/19/22	0/1/1/1
3	GOL	I	1310	-	-	0/4/4/4	-

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1308	NAP	O7N-C7N	9.59	1.42	1.24
2	I	1308	NAP	O7N-C7N	9.56	1.41	1.24
2	D	1308	NAP	O7N-C7N	9.55	1.41	1.24
2	A	1308	NAP	O7N-C7N	9.53	1.41	1.24
2	C	1308	NAP	O7N-C7N	9.53	1.41	1.24
2	J	1308	NAP	O7N-C7N	9.46	1.41	1.24
2	G	1308	NAP	O7N-C7N	9.43	1.41	1.24
2	H	1308	NAP	O7N-C7N	9.34	1.41	1.24
2	F	1308	NAP	O7N-C7N	9.33	1.41	1.24
2	E	1308	NAP	O7N-C7N	9.09	1.41	1.24
2	B	1308	NAP	P2B-O2B	3.67	1.66	1.59
2	E	1308	NAP	P2B-O2B	3.57	1.65	1.59
2	H	1308	NAP	P2B-O2B	3.47	1.65	1.59
2	F	1308	NAP	C2N-N1N	3.45	1.38	1.35
2	I	1308	NAP	P2B-O2B	3.44	1.65	1.59
2	F	1308	NAP	P2B-O2B	3.28	1.65	1.59
2	G	1308	NAP	P2B-O2B	3.27	1.65	1.59
2	C	1308	NAP	P2B-O2B	3.25	1.65	1.59
2	J	1308	NAP	P2B-O2B	3.02	1.64	1.59
2	A	1308	NAP	P2B-O2B	3.01	1.64	1.59
2	D	1308	NAP	P2B-O2B	2.87	1.64	1.59
2	C	1308	NAP	C2A-N1A	2.81	1.38	1.33
2	D	1308	NAP	C2A-N1A	2.76	1.38	1.33
2	C	1308	NAP	C2A-N3A	2.73	1.38	1.33
2	B	1308	NAP	C2A-N1A	2.64	1.38	1.33
2	J	1308	NAP	C2A-N3A	2.61	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1320	ADP	PA-O3A	2.59	1.62	1.59
2	A	1308	NAP	C2N-N1N	2.57	1.37	1.35
2	I	1308	NAP	C2A-N1A	2.56	1.38	1.33
2	J	1308	NAP	C2A-N1A	2.54	1.38	1.33
2	H	1308	NAP	C2A-N1A	2.54	1.38	1.33
4	A	1320	ADP	PA-O3A	2.54	1.62	1.59
4	G	1320	ADP	PA-O3A	2.54	1.62	1.59
2	E	1308	NAP	C2N-N1N	2.52	1.37	1.35
2	A	1308	NAP	C2A-N1A	2.52	1.38	1.33
2	G	1308	NAP	C2A-N1A	2.50	1.38	1.33
2	D	1308	NAP	C2N-N1N	2.49	1.37	1.35
2	H	1308	NAP	C2N-N1N	2.46	1.37	1.35
2	F	1308	NAP	C2A-N3A	2.44	1.38	1.33
4	F	1320	ADP	PA-O3A	2.43	1.62	1.59
2	E	1308	NAP	C2A-N3A	2.42	1.38	1.33
2	E	1308	NAP	C2A-N1A	2.41	1.38	1.33
2	B	1308	NAP	C2N-N1N	2.41	1.37	1.35
2	F	1308	NAP	C2A-N1A	2.40	1.38	1.33
2	B	1308	NAP	C2A-N3A	2.36	1.38	1.33
2	E	1308	NAP	C8A-N7A	2.34	1.36	1.31
2	C	1308	NAP	C2N-N1N	2.33	1.37	1.35
2	I	1308	NAP	C2N-N1N	2.32	1.37	1.35
2	I	1308	NAP	C2A-N3A	2.31	1.38	1.33
2	E	1308	NAP	C5A-N7A	-2.24	1.35	1.39
2	A	1308	NAP	C5A-N7A	-2.22	1.35	1.39
2	D	1308	NAP	C2A-N3A	2.22	1.37	1.33
2	G	1308	NAP	C2N-N1N	2.18	1.37	1.35
2	A	1308	NAP	C2A-N3A	2.15	1.37	1.33
2	B	1308	NAP	C8A-N7A	2.13	1.35	1.31
2	B	1308	NAP	C5A-N7A	-2.12	1.35	1.39
4	F	1320	ADP	PB-O3B	2.11	1.62	1.54
2	D	1308	NAP	C5A-N7A	-2.10	1.35	1.39
4	B	1320	ADP	PB-O3B	2.09	1.62	1.54
2	J	1308	NAP	C5A-N7A	-2.09	1.35	1.39
2	G	1308	NAP	C5A-N7A	-2.08	1.35	1.39
2	C	1308	NAP	C5A-N7A	-2.08	1.35	1.39
4	A	1320	ADP	PB-O3B	2.07	1.62	1.54
4	E	1320	ADP	C5-N7	-2.07	1.35	1.39
2	H	1308	NAP	C5A-N7A	-2.06	1.35	1.39
4	H	1320	ADP	PA-O3A	2.06	1.61	1.59
4	I	1320	ADP	PB-O3B	2.05	1.62	1.54
2	F	1308	NAP	C8A-N7A	2.05	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1308	NAP	C2A-N3A	2.05	1.37	1.33
2	F	1308	NAP	C5A-N7A	-2.04	1.35	1.39
4	E	1320	ADP	PB-O3B	2.04	1.62	1.54
2	I	1308	NAP	C8A-N7A	2.03	1.35	1.31
4	D	1320	ADP	PB-O3B	2.01	1.62	1.54

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1308	NAP	N3A-C2A-N1A	-5.66	120.01	128.58
2	A	1308	NAP	N3A-C2A-N1A	-5.64	120.04	128.58
2	J	1308	NAP	N3A-C2A-N1A	-5.60	120.11	128.58
4	E	1320	ADP	C5-C4-N3	-5.55	119.07	126.72
2	F	1308	NAP	N3A-C2A-N1A	-5.54	120.19	128.58
4	F	1320	ADP	C5-C4-N3	-5.48	119.17	126.72
2	I	1308	NAP	N3A-C2A-N1A	-5.47	120.30	128.58
2	H	1308	NAP	N3A-C2A-N1A	-5.44	120.34	128.58
4	H	1320	ADP	C5-C4-N3	-5.41	119.27	126.72
2	G	1308	NAP	N3A-C2A-N1A	-5.38	120.44	128.58
4	C	1320	ADP	C5-C4-N3	-5.36	119.33	126.72
4	A	1320	ADP	C5-C4-N3	-5.34	119.37	126.72
4	B	1320	ADP	C5-C4-N3	-5.21	119.55	126.72
4	I	1320	ADP	C5-C4-N3	-5.18	119.58	126.72
2	E	1308	NAP	N3A-C2A-N1A	-5.13	120.81	128.58
2	B	1308	NAP	N3A-C2A-N1A	-5.13	120.82	128.58
4	D	1320	ADP	C5-C4-N3	-5.11	119.68	126.72
4	J	1320	ADP	C5-C4-N3	-5.10	119.70	126.72
2	C	1308	NAP	N3A-C2A-N1A	-5.10	120.87	128.58
4	G	1320	ADP	C5-C4-N3	-4.93	119.93	126.72
4	F	1320	ADP	N3-C4-N9	4.81	135.35	127.17
4	A	1320	ADP	N3-C2-N1	-4.71	121.45	128.58
2	E	1308	NAP	C5A-C4A-N3A	-4.65	120.32	126.72
4	C	1320	ADP	N3-C4-N9	4.62	135.03	127.17
2	G	1308	NAP	C5A-C4A-N3A	-4.58	120.41	126.72
4	I	1320	ADP	N3-C4-N9	4.57	134.93	127.17
4	B	1320	ADP	N3-C2-N1	-4.54	121.71	128.58
4	E	1320	ADP	N3-C4-N9	4.53	134.87	127.17
4	G	1320	ADP	N3-C2-N1	-4.49	121.78	128.58
2	F	1308	NAP	C5A-C4A-N3A	-4.48	120.54	126.72
4	J	1320	ADP	N3-C2-N1	-4.47	121.81	128.58
4	D	1320	ADP	N3-C4-N9	4.47	134.77	127.17
4	A	1320	ADP	N3-C4-N9	4.46	134.75	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1320	ADP	N3-C4-N9	4.44	134.72	127.17
2	J	1308	NAP	C5A-C4A-N3A	-4.44	120.60	126.72
4	H	1320	ADP	N3-C4-N9	4.39	134.63	127.17
2	D	1308	NAP	C5A-C4A-N3A	-4.37	120.70	126.72
2	B	1308	NAP	C5A-C4A-N3A	-4.28	120.82	126.72
2	H	1308	NAP	N9A-C8A-N7A	-4.28	107.86	113.94
4	C	1320	ADP	N3-C2-N1	-4.27	122.12	128.58
4	J	1320	ADP	N3-C4-N9	4.26	134.41	127.17
4	D	1320	ADP	N3-C2-N1	-4.25	122.14	128.58
4	H	1320	ADP	N3-C2-N1	-4.23	122.18	128.58
4	G	1320	ADP	N3-C4-N9	4.22	134.35	127.17
4	F	1320	ADP	N3-C2-N1	-4.21	122.21	128.58
4	I	1320	ADP	N3-C2-N1	-4.18	122.26	128.58
4	E	1320	ADP	N3-C2-N1	-4.17	122.26	128.58
2	A	1308	NAP	C5A-C4A-N3A	-4.16	120.99	126.72
2	D	1308	NAP	N9A-C8A-N7A	-4.11	108.10	113.94
2	A	1308	NAP	N9A-C8A-N7A	-4.11	108.11	113.94
2	I	1308	NAP	C5A-C4A-N3A	-4.10	121.07	126.72
2	B	1308	NAP	N9A-C8A-N7A	-4.07	108.16	113.94
2	C	1308	NAP	C5A-C4A-N3A	-4.07	121.12	126.72
4	E	1320	ADP	C5-N7-C8	4.04	109.81	103.45
2	G	1308	NAP	N9A-C8A-N7A	-4.04	108.20	113.94
2	C	1308	NAP	N9A-C8A-N7A	-4.01	108.25	113.94
2	H	1308	NAP	C5A-C4A-N3A	-4.00	121.22	126.72
2	F	1308	NAP	N9A-C8A-N7A	-3.94	108.34	113.94
2	I	1308	NAP	N9A-C8A-N7A	-3.93	108.36	113.94
4	J	1320	ADP	C5-N7-C8	3.92	109.62	103.45
4	A	1320	ADP	C2-N3-C4	3.91	121.38	111.83
4	F	1320	ADP	C5-N7-C8	3.83	109.47	103.45
2	J	1308	NAP	N9A-C8A-N7A	-3.82	108.52	113.94
4	H	1320	ADP	C5-N7-C8	3.81	109.43	103.45
4	C	1320	ADP	C5-N7-C8	3.79	109.41	103.45
4	D	1320	ADP	C5-N7-C8	3.76	109.35	103.45
4	B	1320	ADP	C5-N7-C8	3.73	109.32	103.45
2	B	1308	NAP	C5A-N7A-C8A	3.72	109.30	103.45
4	B	1320	ADP	C2-N3-C4	3.71	120.89	111.83
4	C	1320	ADP	C2-N3-C4	3.70	120.87	111.83
2	C	1308	NAP	C5A-N7A-C8A	3.70	109.26	103.45
2	D	1308	NAP	C5A-N7A-C8A	3.69	109.26	103.45
4	G	1320	ADP	C5-N7-C8	3.68	109.24	103.45
2	A	1308	NAP	C5A-N7A-C8A	3.65	109.19	103.45
4	H	1320	ADP	C2-N3-C4	3.63	120.71	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1308	NAP	C5A-N7A-C8A	3.62	109.15	103.45
4	E	1320	ADP	C2-N3-C4	3.62	120.68	111.83
4	I	1320	ADP	C5-N7-C8	3.62	109.14	103.45
2	G	1308	NAP	C5A-N7A-C8A	3.61	109.13	103.45
4	A	1320	ADP	C5-N7-C8	3.60	109.11	103.45
4	F	1320	ADP	C2-N3-C4	3.60	120.62	111.83
4	J	1320	ADP	C2-N3-C4	3.59	120.60	111.83
2	E	1308	NAP	N9A-C8A-N7A	-3.58	108.85	113.94
4	G	1320	ADP	C2-N3-C4	3.54	120.48	111.83
2	F	1308	NAP	C5A-N7A-C8A	3.47	108.90	103.45
2	G	1308	NAP	C2A-N3A-C4A	3.46	120.29	111.83
4	I	1320	ADP	C2-N3-C4	3.46	120.27	111.83
4	D	1320	ADP	C2-N3-C4	3.45	120.27	111.83
2	I	1308	NAP	C5A-N7A-C8A	3.45	108.87	103.45
2	F	1308	NAP	C2A-N3A-C4A	3.43	120.20	111.83
2	D	1308	NAP	C2A-N3A-C4A	3.42	120.18	111.83
2	J	1308	NAP	C5A-N7A-C8A	3.41	108.81	103.45
2	J	1308	NAP	C2A-N3A-C4A	3.39	120.11	111.83
2	E	1308	NAP	C5A-N7A-C8A	3.37	108.75	103.45
2	E	1308	NAP	C2A-N3A-C4A	3.36	120.03	111.83
4	E	1320	ADP	C4-C5-N7	-3.27	106.84	110.58
2	F	1308	NAP	C3N-C7N-N7N	3.27	121.77	117.74
2	I	1308	NAP	C2A-N3A-C4A	3.24	119.75	111.83
2	A	1308	NAP	C2A-N3A-C4A	3.23	119.73	111.83
2	B	1308	NAP	C2A-N3A-C4A	3.17	119.57	111.83
2	H	1308	NAP	C2A-N3A-C4A	3.12	119.45	111.83
4	H	1320	ADP	C4-C5-N7	-3.09	107.05	110.58
4	J	1320	ADP	C4-C5-N7	-3.07	107.07	110.58
4	J	1320	ADP	N9-C8-N7	-3.05	109.60	113.94
4	F	1320	ADP	N9-C8-N7	-3.03	109.63	113.94
4	E	1320	ADP	N9-C8-N7	-3.01	109.66	113.94
2	E	1308	NAP	C4A-C5A-N7A	-2.93	107.23	110.58
2	C	1308	NAP	C2A-N3A-C4A	2.92	118.96	111.83
2	B	1308	NAP	C4A-C5A-N7A	-2.91	107.25	110.58
2	C	1308	NAP	C4A-C5A-N7A	-2.90	107.27	110.58
4	C	1320	ADP	N9-C8-N7	-2.90	109.83	113.94
2	G	1308	NAP	C4A-C5A-N7A	-2.89	107.28	110.58
4	B	1320	ADP	N9-C8-N7	-2.87	109.86	113.94
4	G	1320	ADP	N9-C8-N7	-2.86	109.87	113.94
4	D	1320	ADP	N9-C8-N7	-2.86	109.89	113.94
4	C	1320	ADP	C4-C5-N7	-2.84	107.33	110.58
2	F	1308	NAP	N3A-C4A-N9A	2.83	131.97	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1308	NAP	N3A-C4A-N9A	2.81	131.95	127.17
4	D	1320	ADP	C4-C5-N7	-2.81	107.37	110.58
2	A	1308	NAP	C4A-C5A-N7A	-2.79	107.39	110.58
4	I	1320	ADP	O3B-PB-O3A	-2.78	95.31	104.64
2	A	1308	NAP	O4B-C1B-N9A	-2.77	102.77	108.09
4	B	1320	ADP	C4-C5-N7	-2.77	107.42	110.58
2	D	1308	NAP	N3A-C4A-N9A	2.77	131.88	127.17
4	G	1320	ADP	C4-C5-N7	-2.76	107.42	110.58
2	D	1308	NAP	C4A-C5A-N7A	-2.76	107.42	110.58
4	H	1320	ADP	N9-C8-N7	-2.75	110.03	113.94
4	A	1320	ADP	C4-C5-N7	-2.72	107.47	110.58
2	G	1308	NAP	N3A-C4A-N9A	2.71	131.78	127.17
4	A	1320	ADP	N9-C8-N7	-2.71	110.09	113.94
4	F	1320	ADP	C4-C5-N7	-2.70	107.49	110.58
4	I	1320	ADP	N9-C8-N7	-2.70	110.11	113.94
2	H	1308	NAP	O3X-P2B-O2B	2.69	116.34	105.85
4	I	1320	ADP	C4-C5-N7	-2.68	107.52	110.58
2	F	1308	NAP	C4A-C5A-N7A	-2.68	107.52	110.58
2	I	1308	NAP	C4A-C5A-N7A	-2.66	107.54	110.58
2	H	1308	NAP	C4A-C5A-N7A	-2.66	107.55	110.58
2	C	1308	NAP	N3A-C4A-N9A	2.63	131.65	127.17
2	B	1308	NAP	N3A-C4A-N9A	2.57	131.53	127.17
2	A	1308	NAP	N3A-C4A-N9A	2.54	131.48	127.17
2	E	1308	NAP	N3A-C4A-N9A	2.53	131.47	127.17
2	J	1308	NAP	C4A-C5A-N7A	-2.50	107.72	110.58
2	H	1308	NAP	N3A-C4A-N9A	2.48	131.39	127.17
4	I	1320	ADP	O2B-PB-O3A	2.46	112.89	104.64
2	I	1308	NAP	N3A-C4A-N9A	2.37	131.19	127.17
5	G	1321	BMA	C1-O5-C5	2.36	115.35	112.19
2	F	1308	NAP	C2B-C1B-N9A	2.34	117.60	113.75
3	C	1310	GOL	O1-C1-C2	2.30	120.71	110.38
2	D	1308	NAP	C3N-C7N-N7N	2.29	120.56	117.74
2	B	1308	NAP	C3N-C7N-N7N	2.29	120.56	117.74
2	B	1308	NAP	O2X-P2B-O2B	2.29	114.75	105.85
2	A	1308	NAP	C2B-C1B-N9A	2.28	117.51	113.75
4	A	1320	ADP	O4'-C1'-N9	2.28	112.47	108.09
2	J	1308	NAP	C2B-C1B-N9A	2.26	117.48	113.75
3	H	1310	GOL	O1-C1-C2	2.26	120.56	110.38
4	B	1320	ADP	O2B-PB-O3A	2.25	112.19	104.64
4	G	1320	ADP	O2B-PB-O3A	2.25	112.18	104.64
2	G	1308	NAP	O3X-P2B-O2B	2.25	114.62	105.85
2	A	1308	NAP	O4B-C1B-C2B	-2.21	102.78	106.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1308	NAP	C4A-N9A-C8A	2.20	108.05	105.74
2	E	1308	NAP	C5A-C4A-N9A	2.20	108.21	105.81
4	F	1320	ADP	PA-O5'-C5'	-2.19	108.80	121.35
3	D	1310	GOL	O1-C1-C2	2.19	120.22	110.38
2	C	1308	NAP	C3N-C7N-N7N	2.16	120.40	117.74
4	B	1320	ADP	PA-O5'-C5'	-2.16	108.99	121.35
3	I	1310	GOL	O1-C1-C2	2.14	120.03	110.38
4	I	1320	ADP	PA-O5'-C5'	-2.14	109.08	121.35
2	C	1308	NAP	C4A-N9A-C8A	2.14	107.98	105.74
2	D	1308	NAP	O3X-P2B-O2B	2.12	114.12	105.85
4	D	1320	ADP	PA-O5'-C5'	-2.11	109.27	121.35
2	G	1308	NAP	O2N-PN-O1N	2.11	122.25	112.44
4	J	1320	ADP	O2B-PB-O3A	2.11	111.70	104.64
4	H	1320	ADP	PA-O5'-C5'	-2.10	109.34	121.35
4	F	1320	ADP	C4-N9-C8	2.08	107.93	105.74
2	J	1308	NAP	O4B-C1B-N9A	-2.07	104.11	108.09
4	C	1320	ADP	PA-O5'-C5'	-2.07	109.49	121.35
2	B	1308	NAP	O3B-C3B-C2B	2.07	116.97	111.19
3	A	1310	GOL	O1-C1-C2	2.07	119.68	110.38
2	D	1308	NAP	O2N-PN-O1N	2.04	121.95	112.44
2	E	1308	NAP	C6A-C5A-C4A	2.03	119.94	117.18
5	A	1321	BMA	C3-C4-C5	-2.02	106.56	110.23
4	B	1320	ADP	O3B-PB-O3A	-2.02	97.86	104.64
2	C	1308	NAP	C2B-C1B-N9A	2.02	117.08	113.75
2	C	1308	NAP	O2N-PN-O1N	2.02	121.83	112.44
2	E	1308	NAP	C2B-C1B-N9A	2.01	117.05	113.75
4	D	1320	ADP	C4-N9-C8	2.00	107.84	105.74

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1308	NAP	C2B-C1B-N9A-C8A
2	A	1308	NAP	C5D-O5D-PN-O2N
2	B	1308	NAP	C2B-C1B-N9A-C8A
2	B	1308	NAP	C5D-O5D-PN-O2N
2	C	1308	NAP	C2B-C1B-N9A-C8A
2	C	1308	NAP	C2B-C1B-N9A-C4A
2	C	1308	NAP	C5D-O5D-PN-O2N
2	D	1308	NAP	C2B-C1B-N9A-C8A
2	E	1308	NAP	C2B-C1B-N9A-C8A
2	F	1308	NAP	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
2	F	1308	NAP	C5D-O5D-PN-O2N
2	G	1308	NAP	C2B-C1B-N9A-C8A
2	G	1308	NAP	C2B-C1B-N9A-C4A
2	H	1308	NAP	C2B-C1B-N9A-C8A
2	I	1308	NAP	C2B-C1B-N9A-C8A
2	I	1308	NAP	C2B-C1B-N9A-C4A
2	J	1308	NAP	C2B-C1B-N9A-C8A
2	J	1308	NAP	C5D-O5D-PN-O2N
3	B	1310	GOL	O1-C1-C2-O2
3	B	1310	GOL	O1-C1-C2-C3
3	E	1310	GOL	C1-C2-C3-O3
3	G	1310	GOL	O1-C1-C2-O2
3	G	1310	GOL	O1-C1-C2-C3
3	G	1310	GOL	C1-C2-C3-O3
3	E	1310	GOL	O2-C2-C3-O3
2	A	1308	NAP	C2B-C1B-N9A-C4A
2	B	1308	NAP	C2B-C1B-N9A-C4A
2	D	1308	NAP	C2B-C1B-N9A-C4A
2	E	1308	NAP	C2B-C1B-N9A-C4A
2	F	1308	NAP	C2B-C1B-N9A-C4A
2	H	1308	NAP	C2B-C1B-N9A-C4A
2	J	1308	NAP	C2B-C1B-N9A-C4A
3	B	1310	GOL	C1-C2-C3-O3
3	C	1310	GOL	O1-C1-C2-C3
3	D	1310	GOL	O1-C1-C2-C3
3	F	1310	GOL	O1-C1-C2-C3
3	H	1310	GOL	O1-C1-C2-C3
3	G	1310	GOL	O2-C2-C3-O3
2	E	1308	NAP	O4B-C4B-C5B-O5B
2	I	1308	NAP	O4B-C4B-C5B-O5B
2	C	1308	NAP	O4B-C4B-C5B-O5B
2	H	1308	NAP	O4B-C4B-C5B-O5B
3	B	1310	GOL	O2-C2-C3-O3
3	C	1310	GOL	O1-C1-C2-O2
3	F	1310	GOL	O2-C2-C3-O3
2	B	1308	NAP	O4B-C4B-C5B-O5B
2	E	1308	NAP	C3B-C4B-C5B-O5B
2	F	1308	NAP	O4B-C4B-C5B-O5B
2	G	1308	NAP	O4B-C4B-C5B-O5B
2	I	1308	NAP	C3B-C4B-C5B-O5B
2	J	1308	NAP	O4B-C4B-C5B-O5B
2	F	1308	NAP	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
5	A	1321	BMA	C4-C5-C6-O6
2	C	1308	NAP	C3B-C4B-C5B-O5B
2	D	1308	NAP	O4B-C4B-C5B-O5B
2	J	1308	NAP	C3B-C4B-C5B-O5B
3	A	1310	GOL	O1-C1-C2-C3
5	I	1321	BMA	C4-C5-C6-O6
2	A	1308	NAP	O4B-C4B-C5B-O5B
2	A	1308	NAP	C2B-O2B-P2B-O1X
2	B	1308	NAP	C2B-O2B-P2B-O1X
2	D	1308	NAP	C2B-O2B-P2B-O1X
2	E	1308	NAP	C2B-O2B-P2B-O1X
2	F	1308	NAP	C2B-O2B-P2B-O1X
2	H	1308	NAP	C2B-O2B-P2B-O1X
2	I	1308	NAP	C2B-O2B-P2B-O1X
2	J	1308	NAP	C2B-O2B-P2B-O1X
2	B	1308	NAP	C3B-C4B-C5B-O5B
2	A	1308	NAP	C5D-O5D-PN-O3
2	C	1308	NAP	C5D-O5D-PN-O3
3	H	1310	GOL	O1-C1-C2-O2
2	D	1308	NAP	C3B-C4B-C5B-O5B
2	G	1308	NAP	C3B-C4B-C5B-O5B
2	H	1308	NAP	C3B-C4B-C5B-O5B
2	A	1308	NAP	C3B-C4B-C5B-O5B
3	F	1310	GOL	O1-C1-C2-O2
2	A	1308	NAP	C4B-C5B-O5B-PA
2	F	1308	NAP	C4B-C5B-O5B-PA
2	B	1308	NAP	O4D-C1D-N1N-C6N
2	C	1308	NAP	O4D-C1D-N1N-C6N
2	D	1308	NAP	O4D-C1D-N1N-C6N
2	F	1308	NAP	O4D-C1D-N1N-C6N
2	G	1308	NAP	O4D-C1D-N1N-C6N
2	I	1308	NAP	O4D-C1D-N1N-C6N
2	J	1308	NAP	O4D-C1D-N1N-C6N
2	C	1308	NAP	C2B-O2B-P2B-O1X
2	G	1308	NAP	C2B-O2B-P2B-O1X
3	A	1310	GOL	O1-C1-C2-O2
3	D	1310	GOL	O1-C1-C2-O2
5	F	1321	BMA	O5-C5-C6-O6
2	G	1308	NAP	C4B-C5B-O5B-PA
2	I	1308	NAP	C4B-C5B-O5B-PA
2	A	1308	NAP	PA-O3-PN-O2N
2	B	1308	NAP	PA-O3-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	D	1308	NAP	PA-O3-PN-O1N
2	F	1308	NAP	PA-O3-PN-O2N
2	G	1308	NAP	PA-O3-PN-O1N
2	G	1308	NAP	PA-O3-PN-O2N
2	H	1308	NAP	PA-O3-PN-O2N
2	I	1308	NAP	PA-O3-PN-O1N
2	J	1308	NAP	PA-O3-PN-O2N
4	B	1320	ADP	PB-O3A-PA-O2A
4	H	1320	ADP	PB-O3A-PA-O2A
2	B	1308	NAP	O4B-C1B-N9A-C8A
2	C	1308	NAP	O4B-C1B-N9A-C8A
2	F	1308	NAP	O4B-C1B-N9A-C8A
2	G	1308	NAP	O4B-C1B-N9A-C8A
5	A	1321	BMA	O5-C5-C6-O6
2	E	1308	NAP	C2B-O2B-P2B-O3X
2	J	1308	NAP	C2B-O2B-P2B-O3X
2	E	1308	NAP	C4B-C5B-O5B-PA
2	A	1308	NAP	O4B-C1B-N9A-C8A
2	D	1308	NAP	O4B-C1B-N9A-C8A
2	E	1308	NAP	O4B-C1B-N9A-C8A
2	J	1308	NAP	O4B-C1B-N9A-C8A
2	B	1308	NAP	C4B-C5B-O5B-PA
2	H	1308	NAP	C4B-C5B-O5B-PA
2	J	1308	NAP	C4B-C5B-O5B-PA
2	D	1308	NAP	C4B-C5B-O5B-PA
2	I	1308	NAP	O4B-C1B-N9A-C8A
2	A	1308	NAP	PA-O3-PN-O1N
2	C	1308	NAP	PA-O3-PN-O1N
2	C	1308	NAP	PA-O3-PN-O2N
2	E	1308	NAP	PA-O3-PN-O1N
2	F	1308	NAP	PA-O3-PN-O1N
2	H	1308	NAP	PA-O3-PN-O1N
2	J	1308	NAP	PA-O3-PN-O1N
4	A	1320	ADP	PB-O3A-PA-O2A
4	C	1320	ADP	PB-O3A-PA-O2A
4	I	1320	ADP	PB-O3A-PA-O2A

There are no ring outliers.

30 monomers are involved in 141 short contacts:

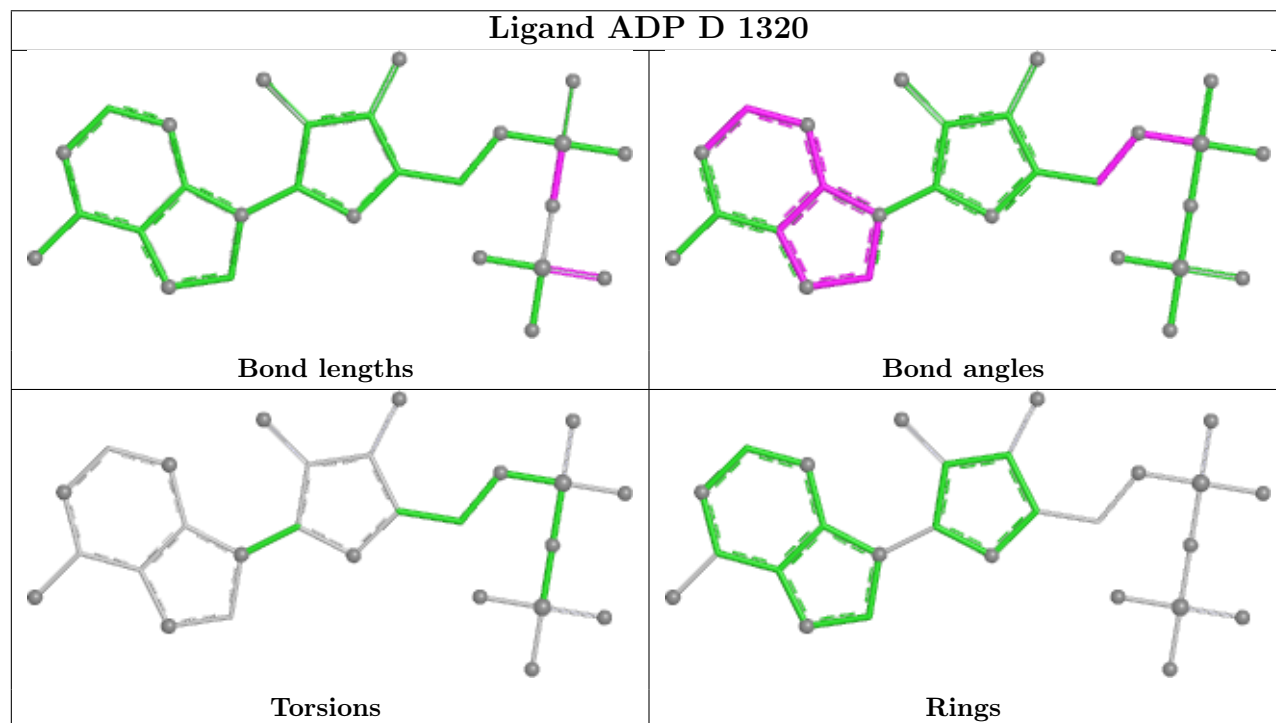
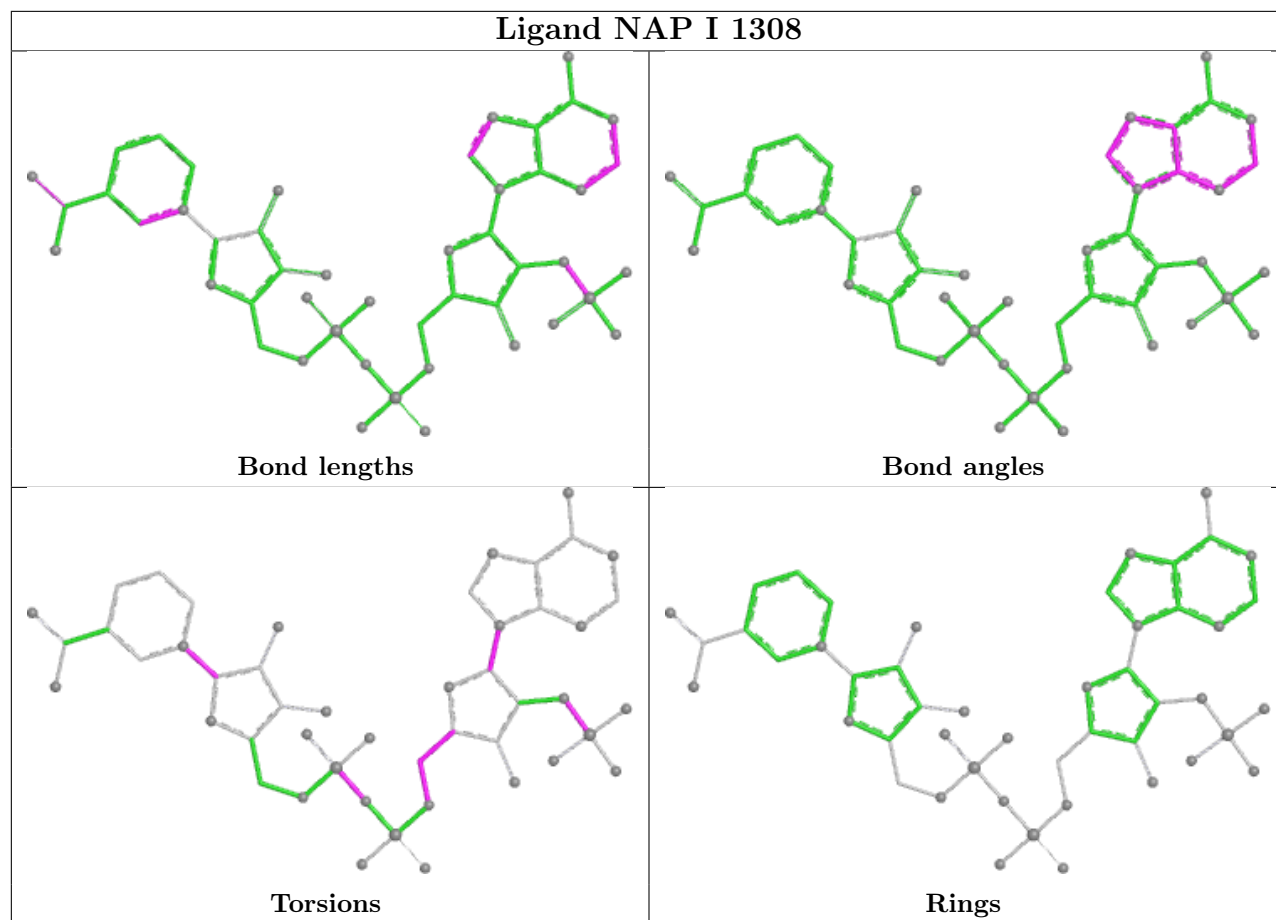
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1308	NAP	3	0

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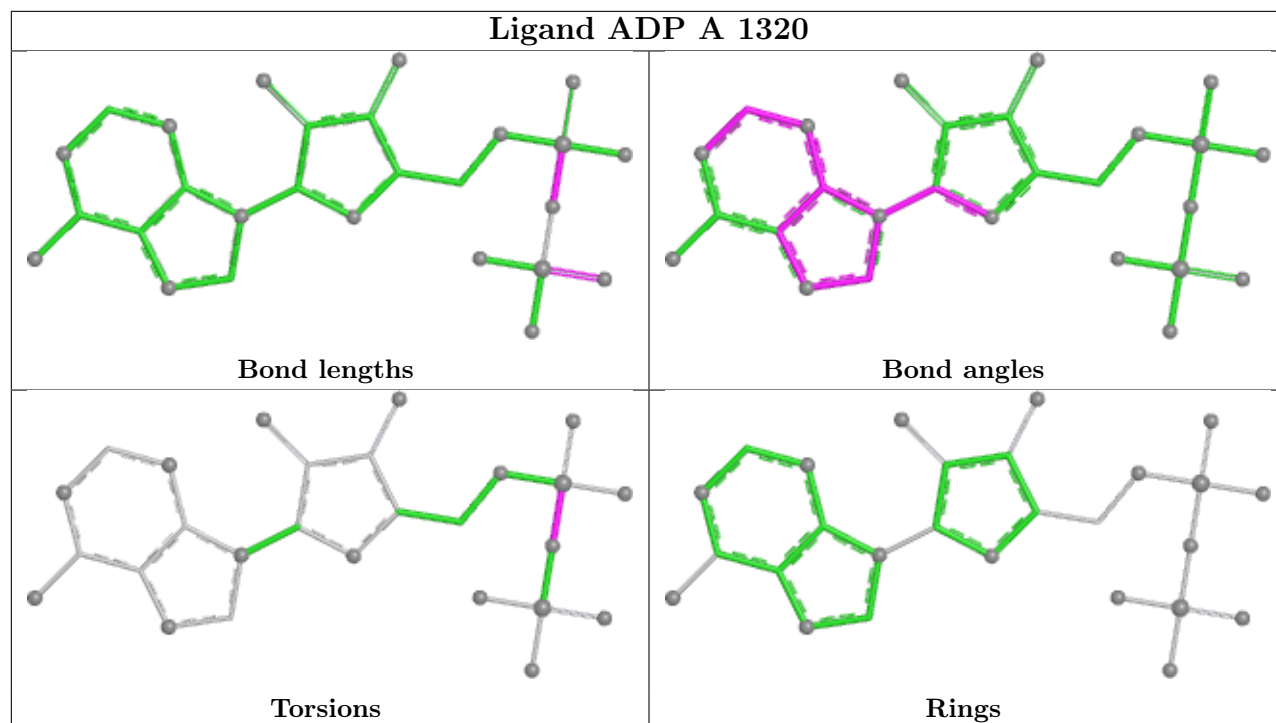
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1321	BMA	3	0
5	G	1321	BMA	3	0
3	J	1310	GOL	12	0
5	A	1321	BMA	3	0
2	H	1308	NAP	4	0
5	D	1321	BMA	3	0
2	F	1308	NAP	4	0
3	G	1310	GOL	5	0
2	J	1308	NAP	4	0
2	A	1308	NAP	4	0
5	E	1321	BMA	3	0
5	I	1321	BMA	2	0
3	F	1310	GOL	12	0
3	E	1310	GOL	11	0
2	D	1308	NAP	4	0
3	D	1310	GOL	13	0
5	J	1321	BMA	3	0
3	C	1310	GOL	13	0
3	A	1310	GOL	12	0
2	E	1308	NAP	3	0
2	G	1308	NAP	4	0
2	B	1308	NAP	2	0
2	C	1308	NAP	3	0
3	B	1310	GOL	7	0
5	B	1321	BMA	2	0
3	H	1310	GOL	10	0
5	H	1321	BMA	3	0
5	C	1321	BMA	2	0
3	I	1310	GOL	11	0

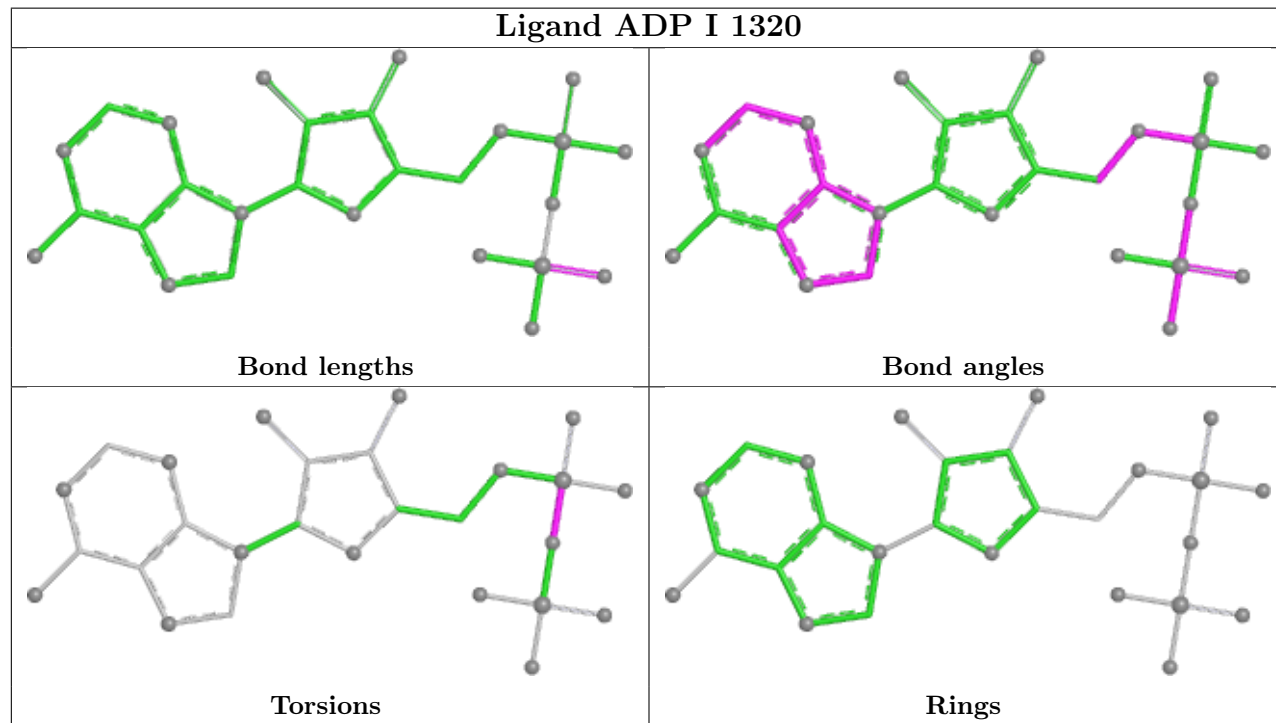
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



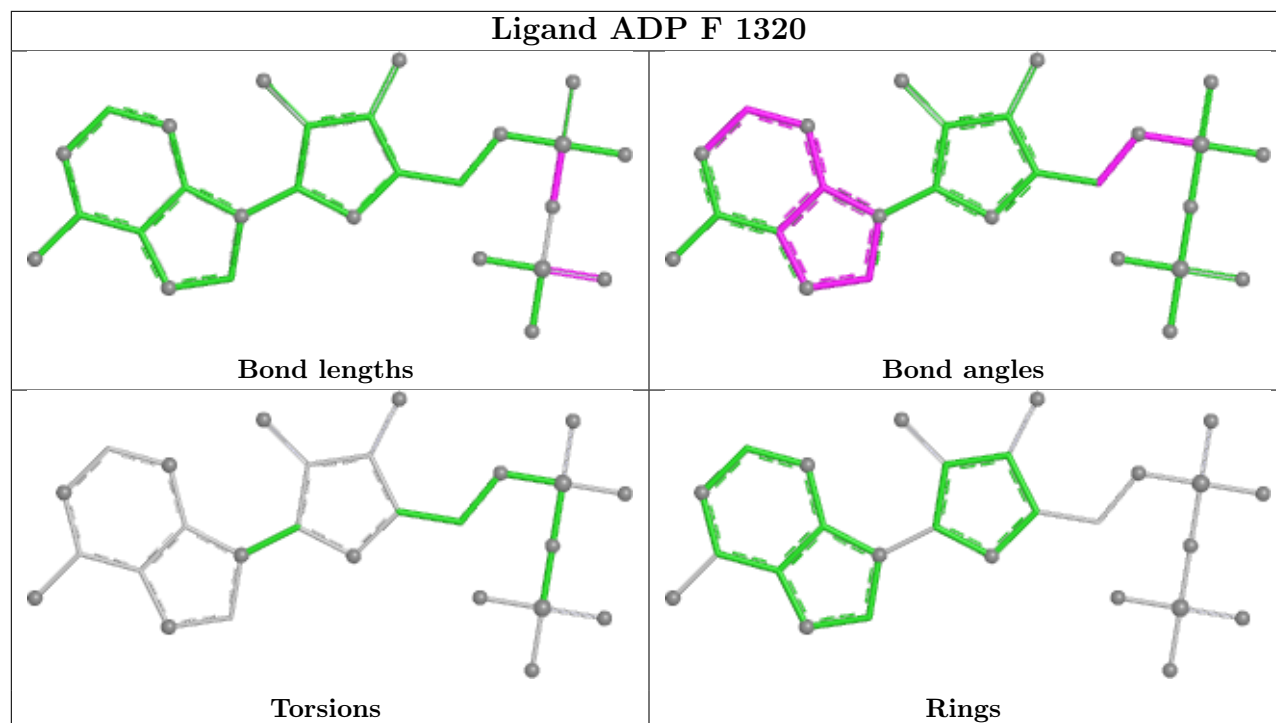
Ligand ADP A 1320



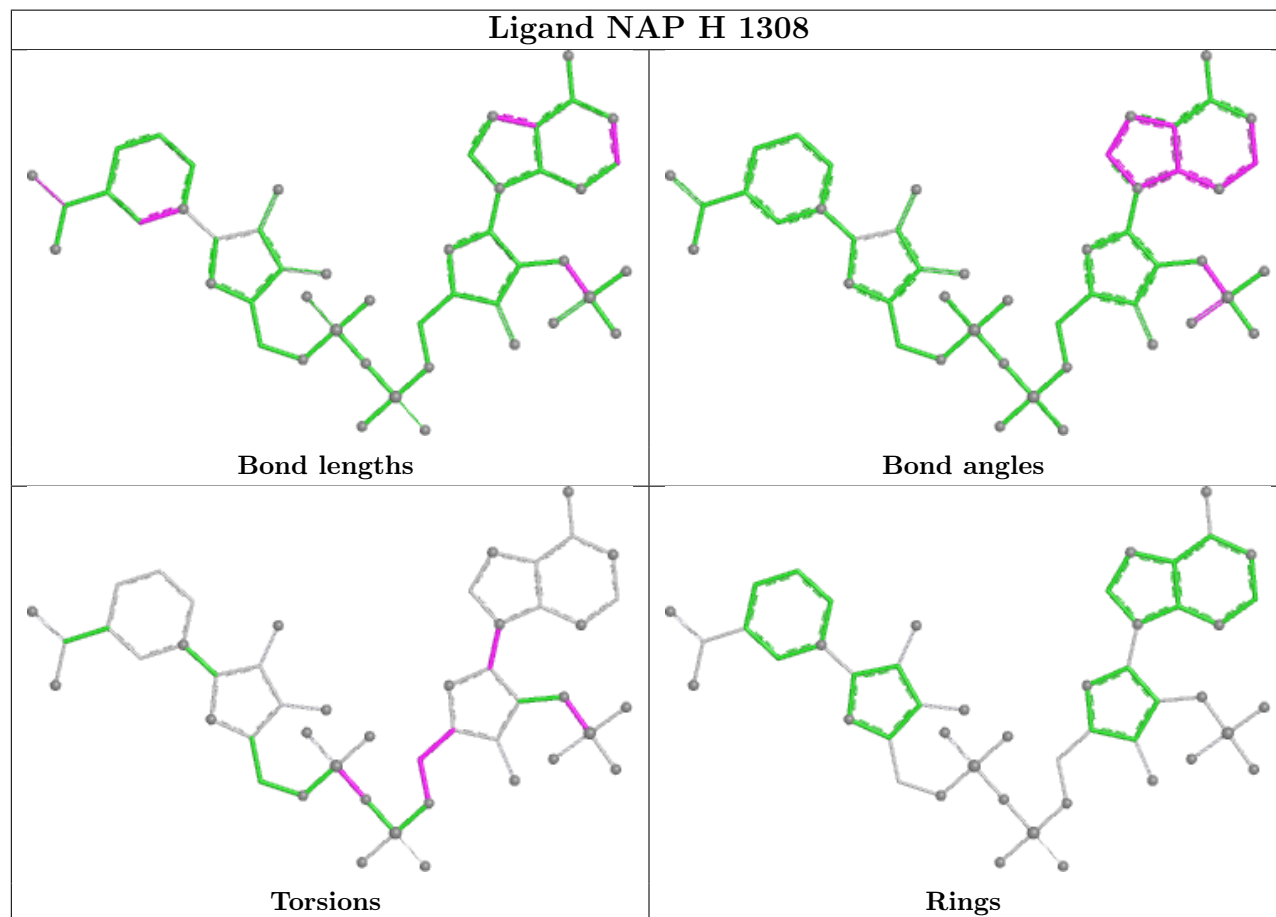
Ligand ADP I 1320

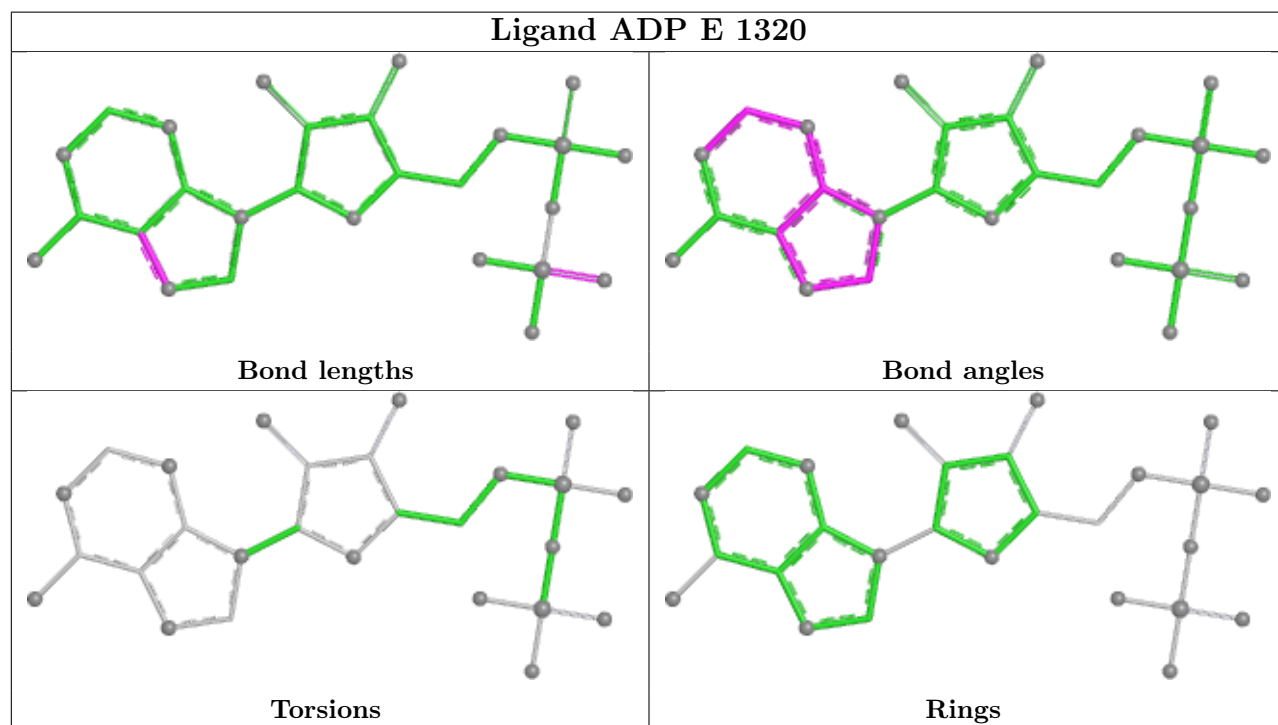
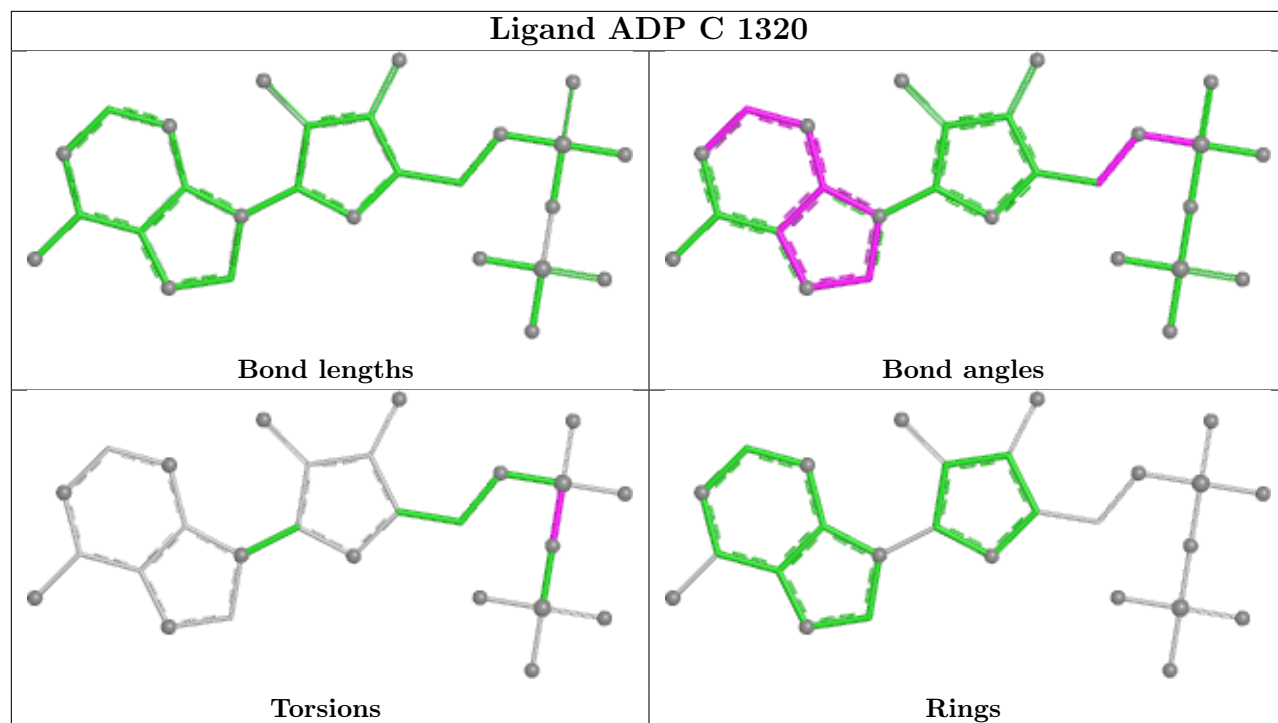


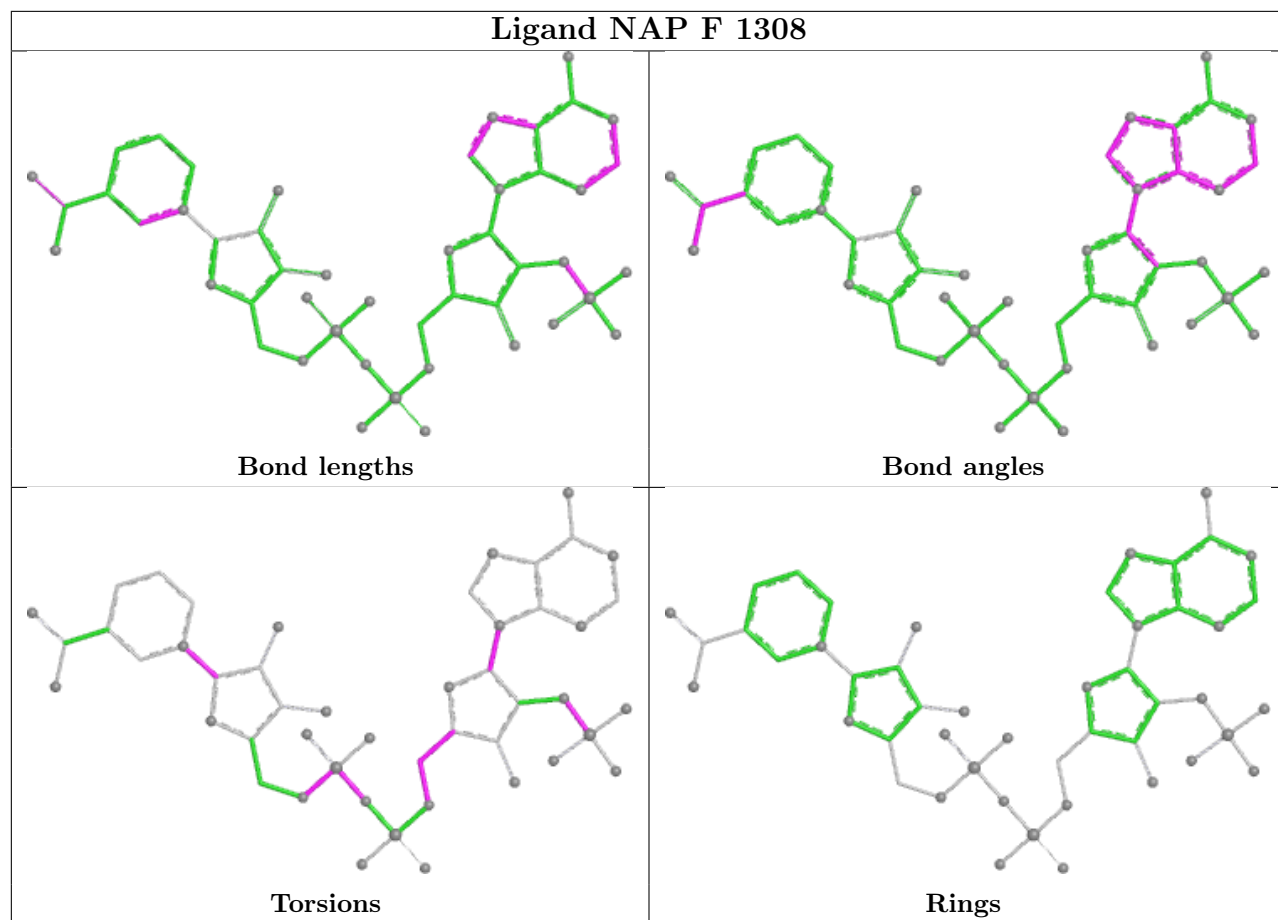
Ligand ADP F 1320

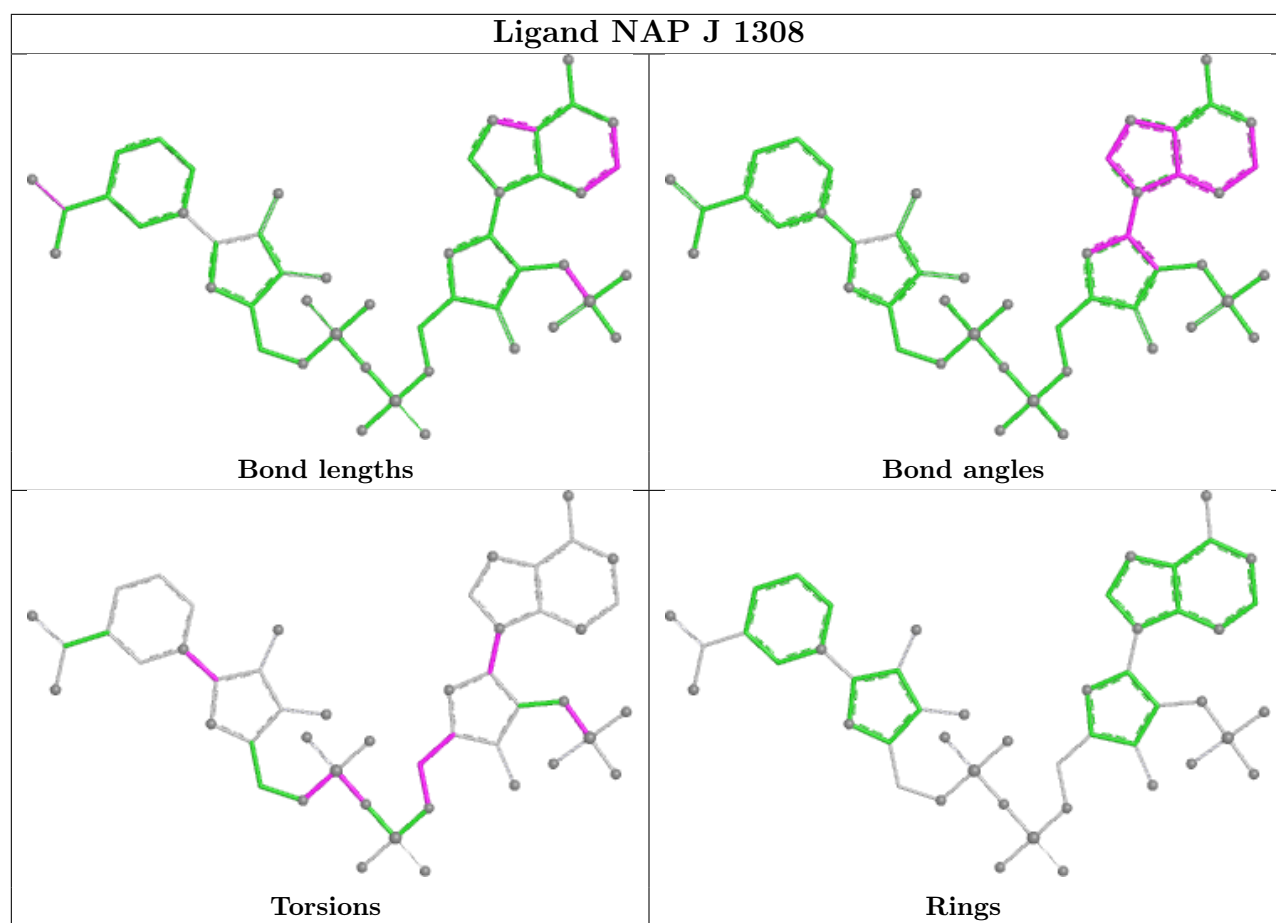


Ligand NAP H 1308

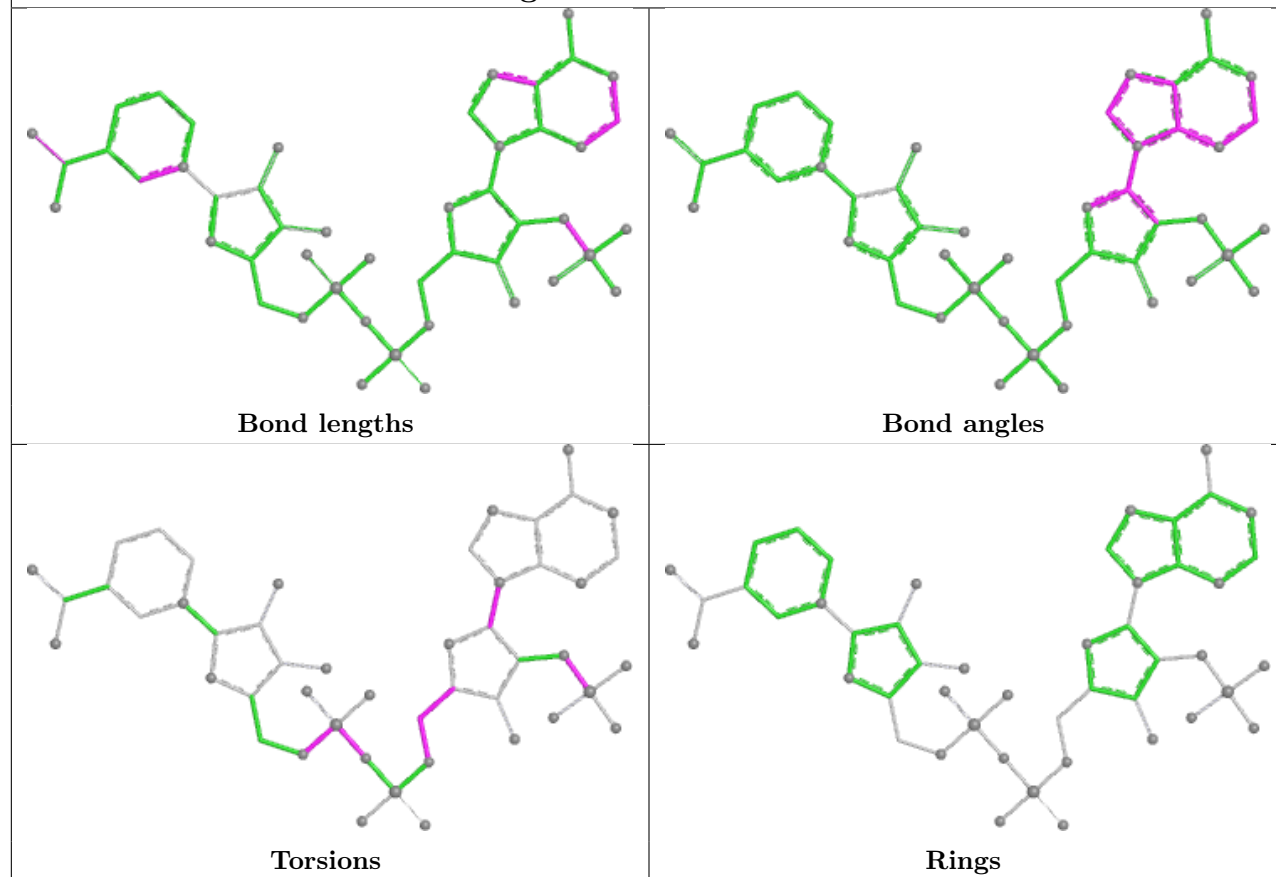




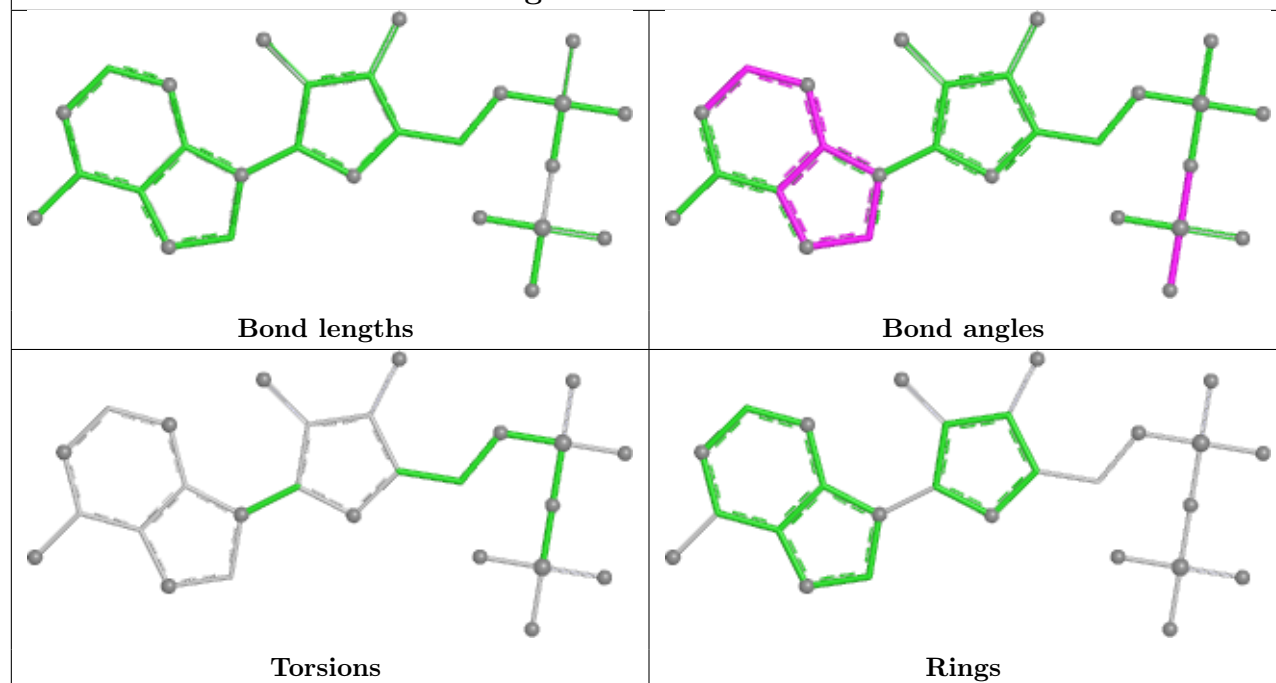




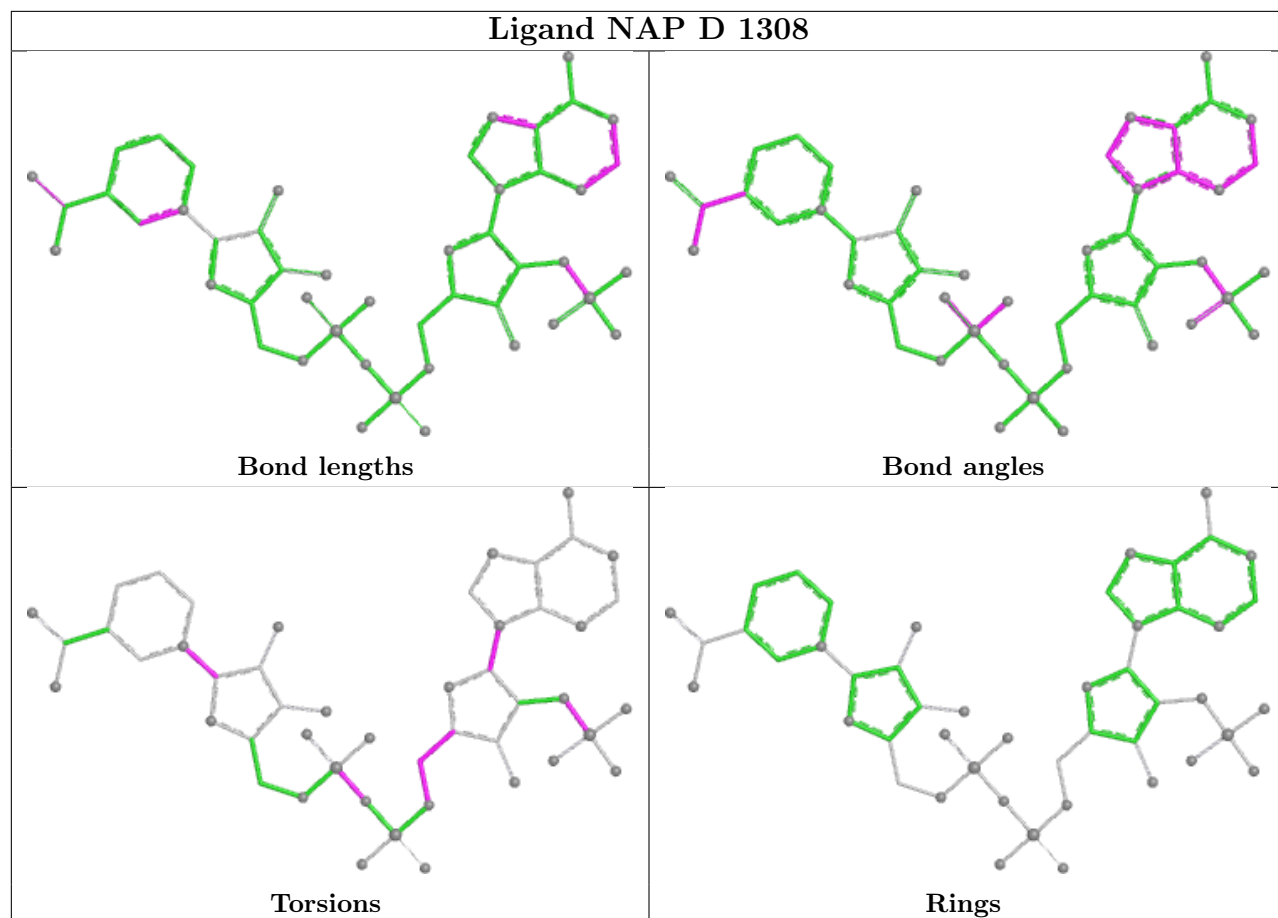
Ligand NAP A 1308



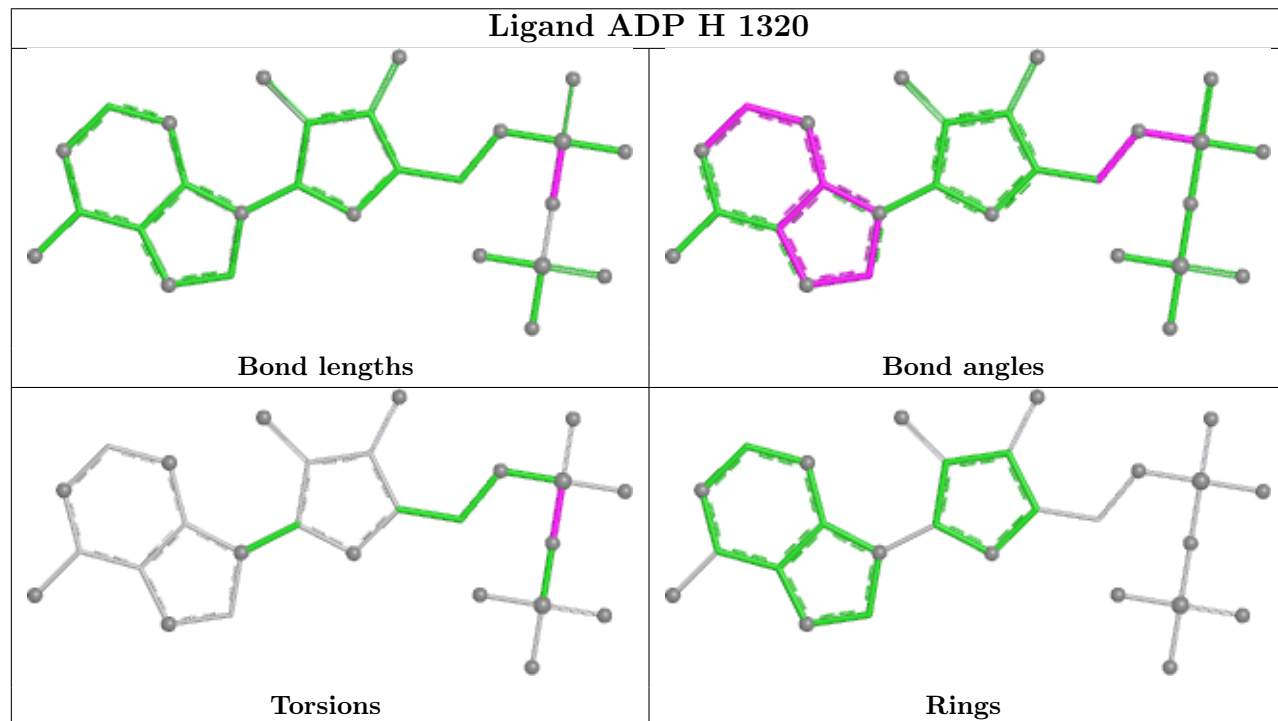
Ligand ADP J 1320

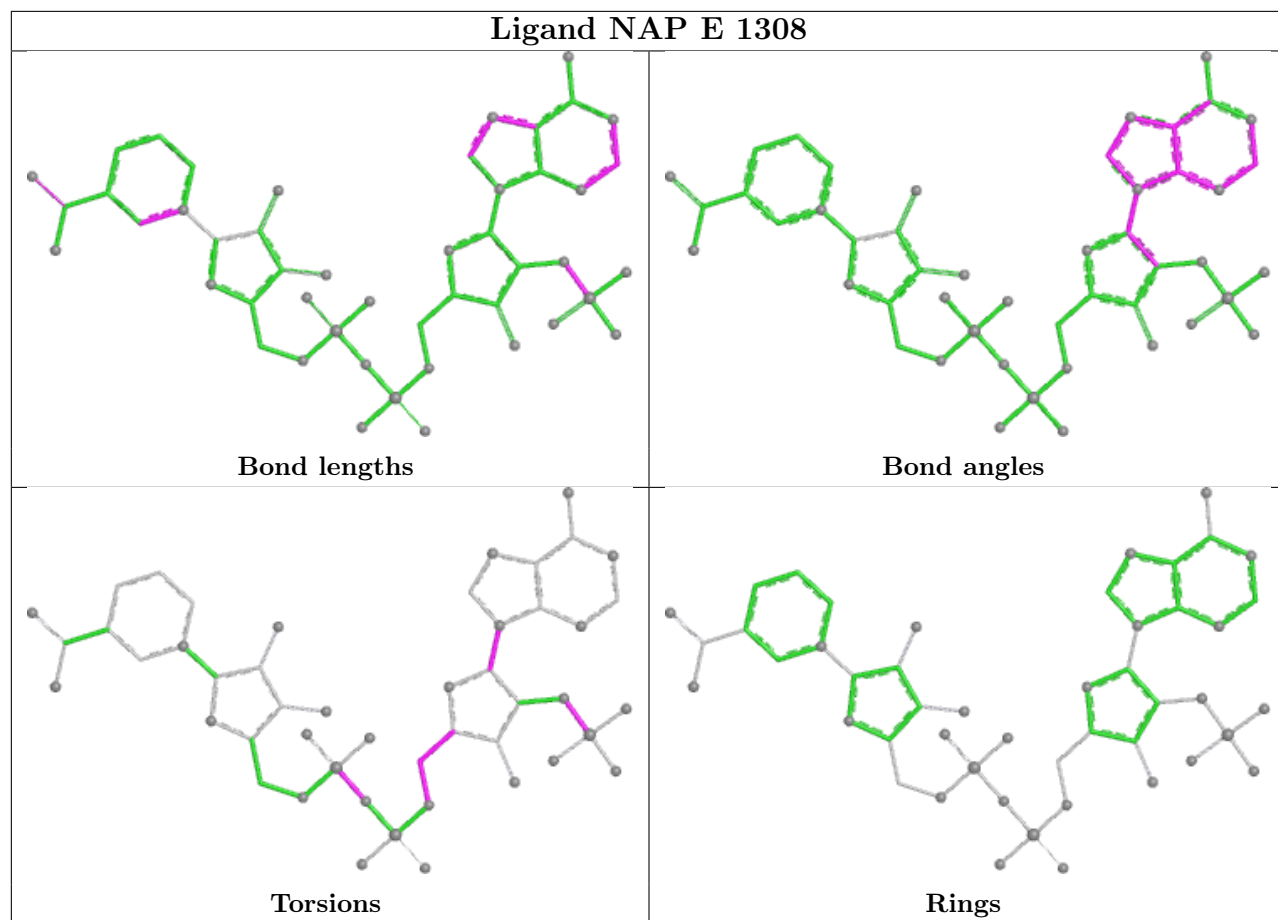


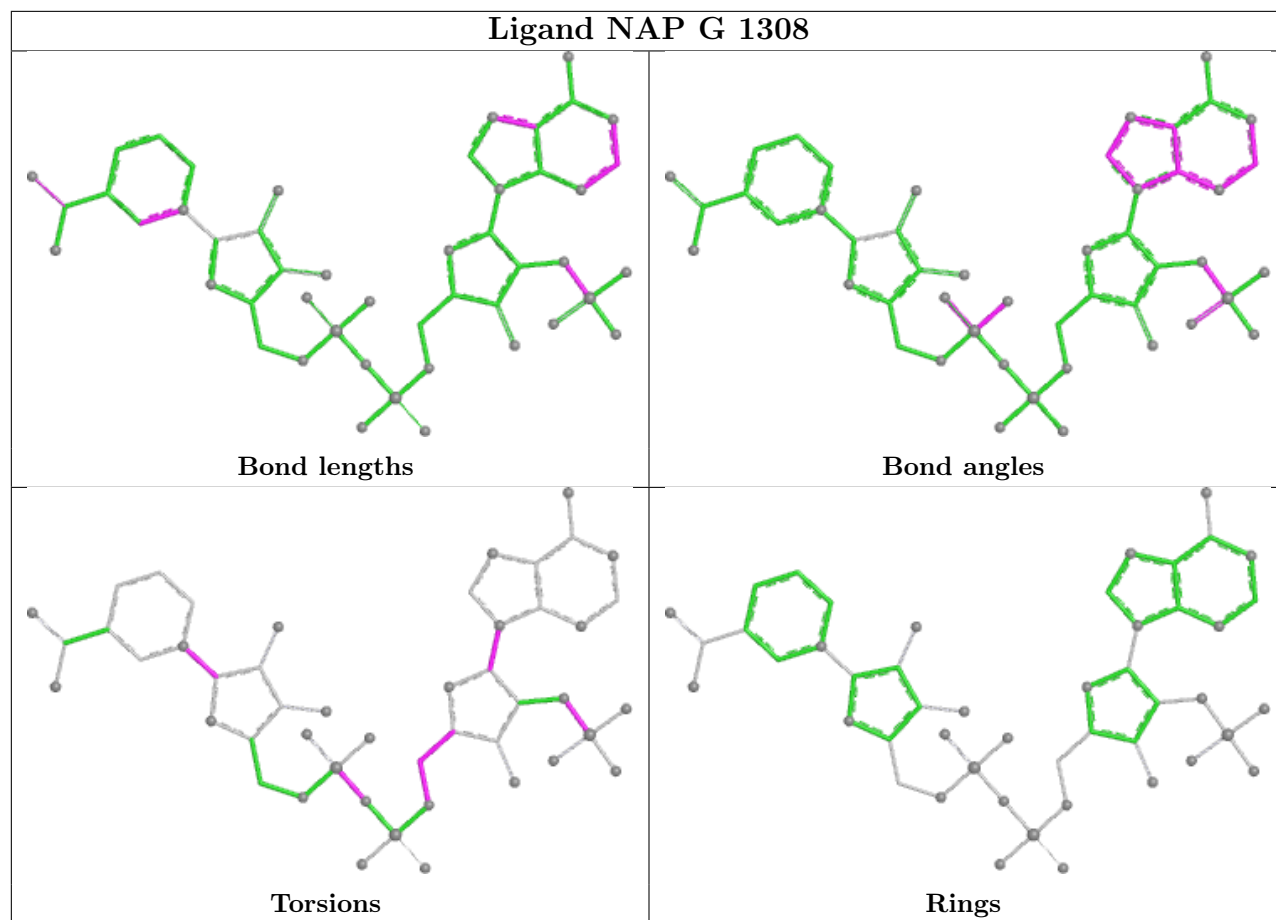
Ligand NAP D 1308

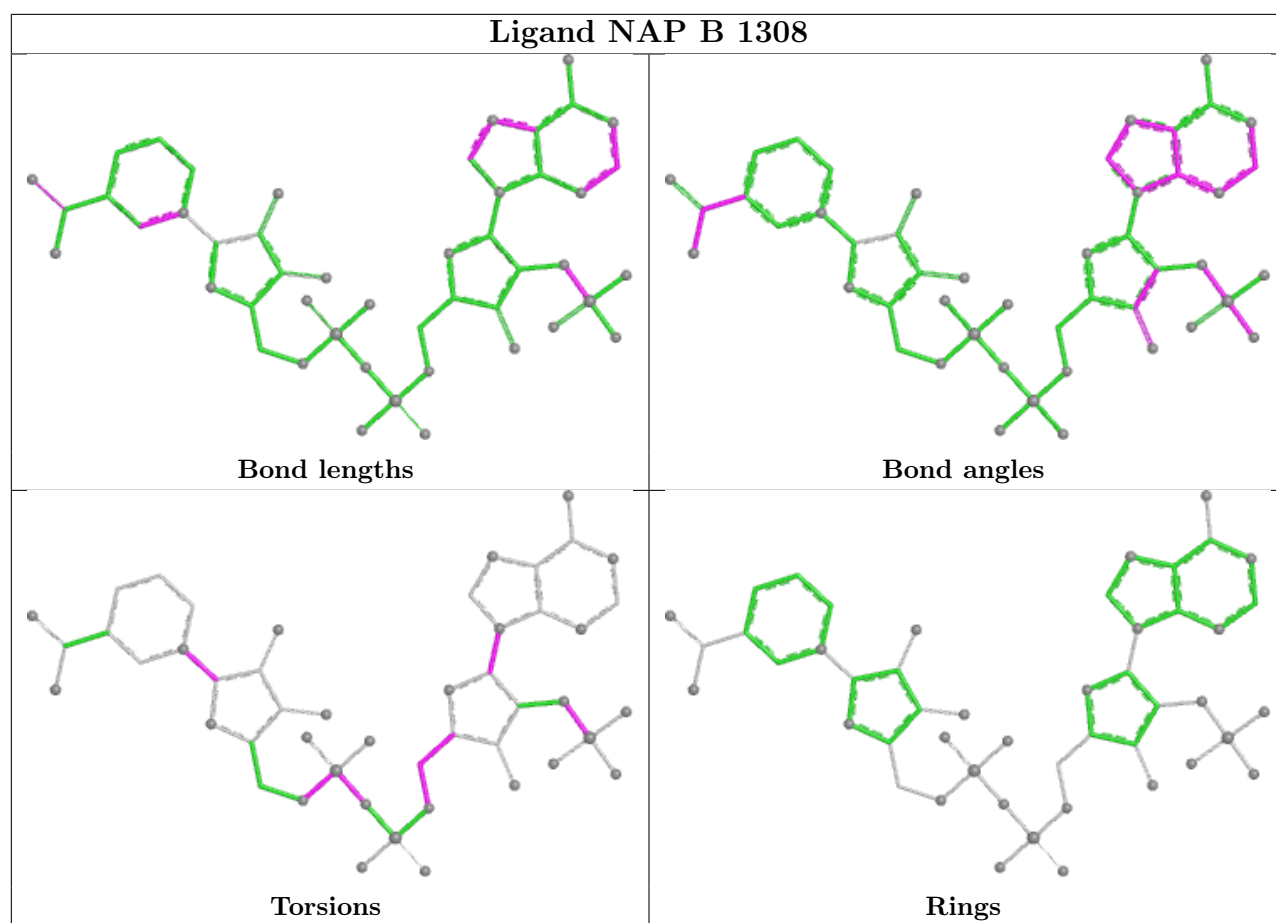


Ligand ADP H 1320

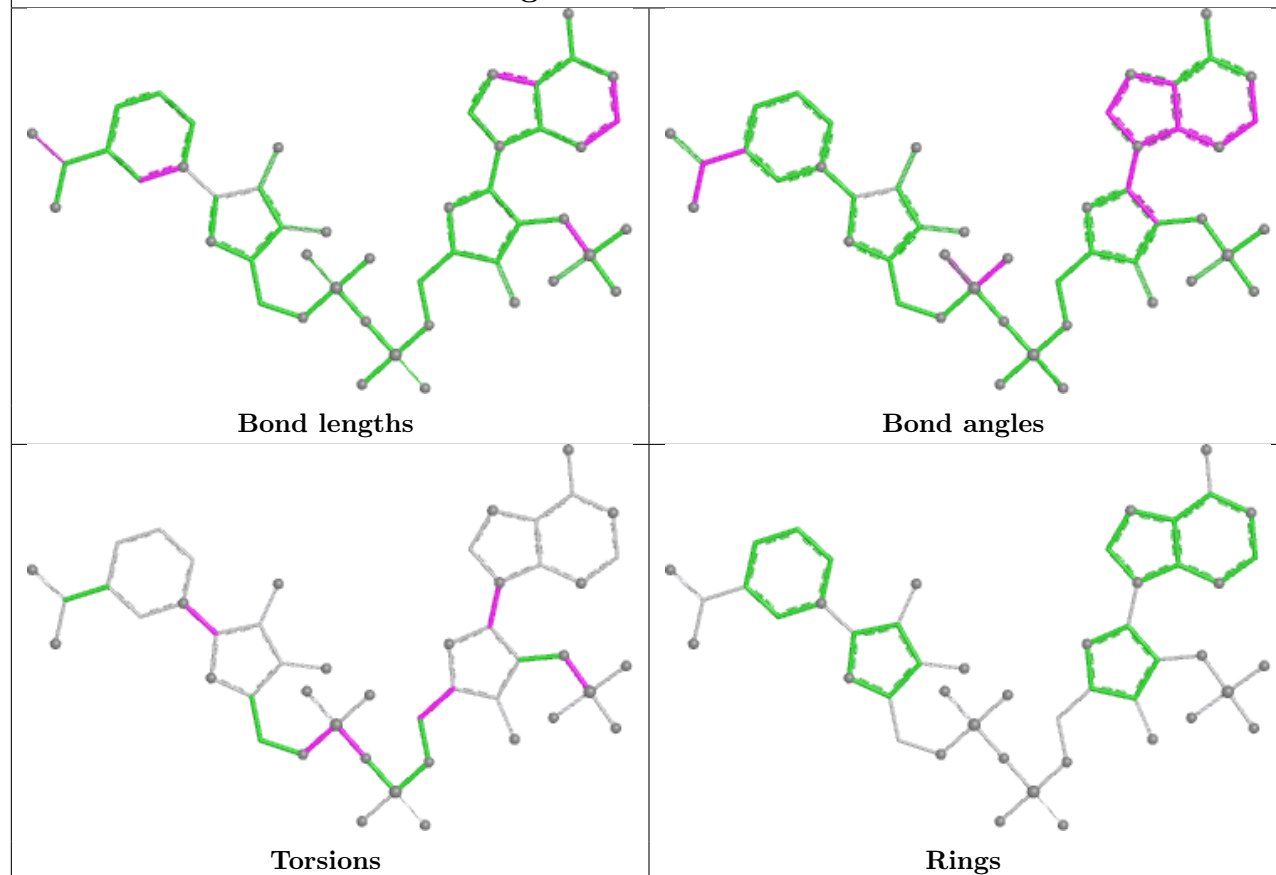




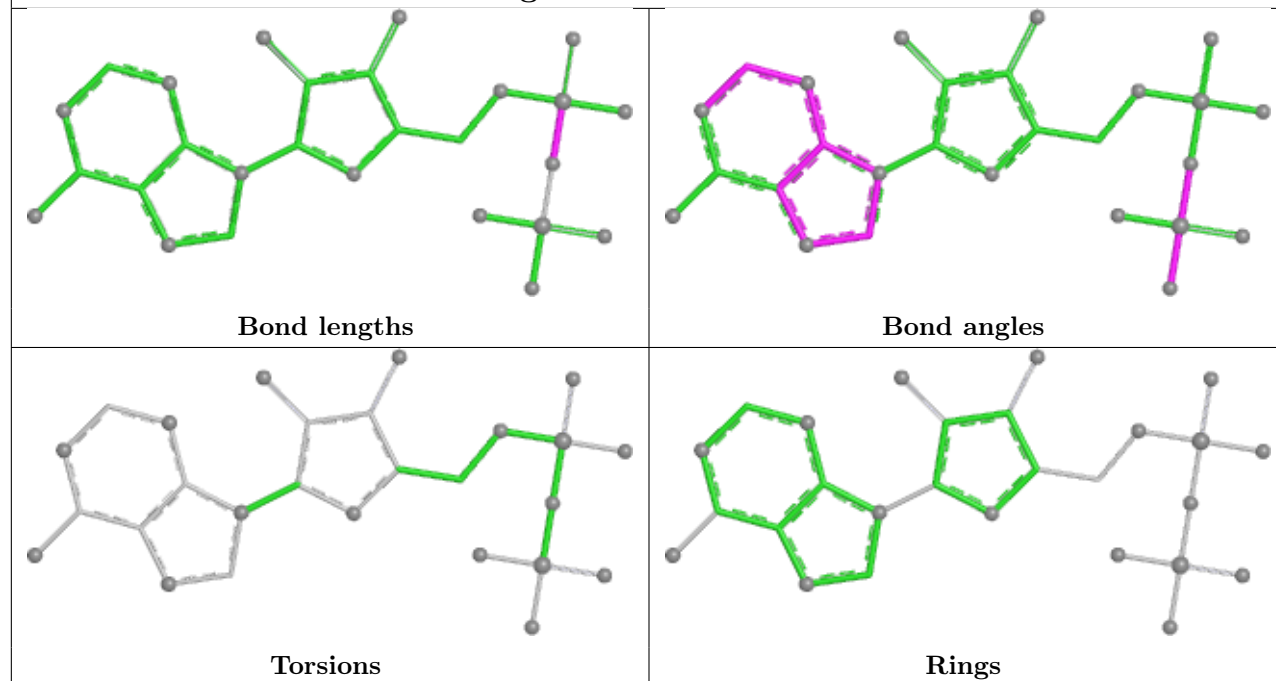


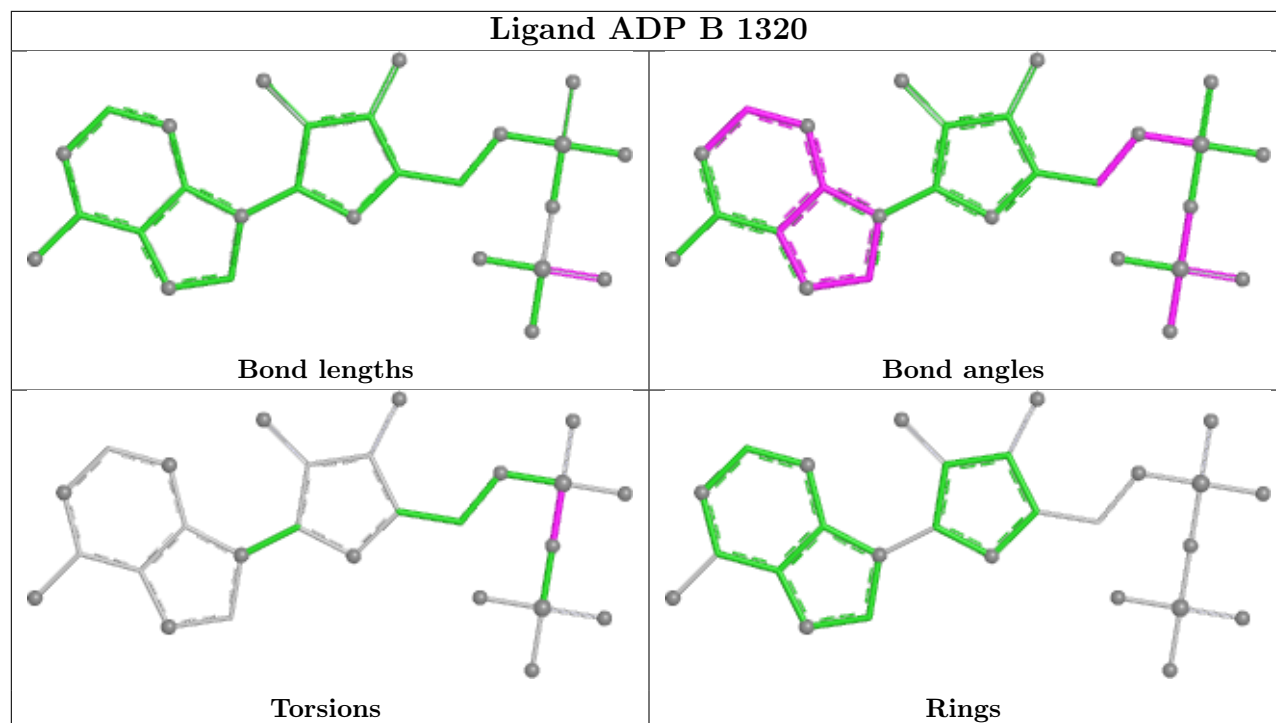


Ligand NAP C 1308



Ligand ADP G 1320





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	307/357 (85%)	0.24	9 (2%) 53 60	27, 29, 30, 32	0
1	B	307/357 (85%)	0.60	11 (3%) 46 52	27, 29, 30, 32	0
1	C	307/357 (85%)	0.29	4 (1%) 75 79	27, 29, 30, 32	0
1	D	307/357 (85%)	1.09	57 (18%) 3 3	27, 29, 30, 32	0
1	E	307/357 (85%)	0.49	13 (4%) 40 46	27, 29, 30, 32	0
1	F	307/357 (85%)	0.86	43 (14%) 6 7	27, 29, 30, 32	0
1	G	308/357 (86%)	0.24	8 (2%) 57 63	27, 29, 30, 34	0
1	H	307/357 (85%)	0.33	8 (2%) 57 63	27, 29, 30, 32	0
1	I	307/357 (85%)	0.43	6 (1%) 65 70	27, 29, 30, 32	0
1	J	307/357 (85%)	0.34	8 (2%) 57 63	27, 29, 30, 32	0
All	All	3071/3570 (86%)	0.49	167 (5%) 31 37	27, 29, 30, 34	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	258	GLN	6.1
1	D	285	ALA	6.0
1	D	225	LEU	5.9
1	D	224	PHE	5.7
1	D	230	SER	5.6
1	D	228	GLY	5.2
1	I	289	ASP	5.1
1	D	232	ILE	4.5
1	D	221	ASN	4.4
1	F	225	LEU	4.3
1	D	220	VAL	4.3
1	D	231	GLY	4.3
1	F	254	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	222	LEU	4.1
1	D	109	ILE	4.1
1	D	124	THR	3.9
1	F	206	ASN	3.9
1	D	233	PHE	3.9
1	F	195	GLY	3.9
1	D	287	GLY	3.7
1	F	122	GLY	3.7
1	D	126	ASP	3.6
1	D	206	ASN	3.6
1	D	286	ALA	3.6
1	D	132	GLU	3.5
1	F	251	LEU	3.5
1	D	218	ALA	3.5
1	D	283	LEU	3.5
1	A	239	ARG	3.5
1	D	205	GLU	3.5
1	D	194	ASN	3.4
1	D	229	VAL	3.4
1	D	288	TYR	3.4
1	F	230	SER	3.4
1	F	194	ASN	3.4
1	A	206	ASN	3.3
1	F	207	PHE	3.3
1	F	252	ALA	3.3
1	F	232	ILE	3.3
1	H	132	GLU	3.2
1	G	301	GLU	3.2
1	F	224	PHE	3.2
1	H	258	GLN	3.2
1	D	217	VAL	3.1
1	E	225	LEU	3.1
1	F	202	GLU	3.1
1	F	285	ALA	3.1
1	B	157	GLU	3.1
1	D	227	ASN	3.1
1	F	220	VAL	3.1
1	D	251	LEU	3.1
1	F	222	LEU	3.1
1	A	157	GLU	3.0
1	D	223	TRP	3.0
1	D	162	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	261	TYR	3.0
1	D	266	ASP	3.0
1	I	157	GLU	3.0
1	F	228	GLY	2.9
1	D	107	ARG	2.9
1	J	206	ASN	2.9
1	D	226	GLU	2.8
1	G	124	THR	2.8
1	A	156	PRO	2.8
1	D	258	GLN	2.8
1	G	297	GLU	2.8
1	D	150	TYR	2.8
1	F	201	PHE	2.8
1	F	205	GLU	2.7
1	D	122	GLY	2.7
1	E	224	PHE	2.7
1	A	266	ASP	2.7
1	J	157	GLU	2.6
1	D	262	ILE	2.6
1	A	158	ALA	2.6
1	J	266	ASP	2.6
1	D	284	ARG	2.6
1	E	233	PHE	2.6
1	F	262	ILE	2.6
1	J	244	GLN	2.6
1	E	23	GLY	2.6
1	F	257	GLY	2.6
1	B	266	ASP	2.5
1	F	231	GLY	2.5
1	E	232	ILE	2.5
1	D	235	LEU	2.5
1	B	227	ASN	2.5
1	F	255	LYS	2.5
1	E	157	GLU	2.5
1	F	218	ALA	2.5
1	F	250	THR	2.4
1	F	204	SER	2.4
1	F	304	ALA	2.4
1	D	125	SER	2.4
1	F	233	PHE	2.4
1	F	221	ASN	2.4
1	C	124	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	106	GLU	2.4
1	B	226	GLU	2.4
1	G	219	ASP	2.4
1	H	1	MET	2.4
1	E	231	GLY	2.3
1	D	158	ALA	2.3
1	J	1	MET	2.3
1	D	201	PHE	2.3
1	F	229	VAL	2.3
1	F	258	GLN	2.3
1	H	266	ASP	2.3
1	D	202	GLU	2.3
1	B	258	GLN	2.3
1	D	161	GLN	2.3
1	F	192	LEU	2.3
1	D	261	TYR	2.3
1	F	253	TYR	2.3
1	F	247	ALA	2.3
1	E	227	ASN	2.2
1	E	266	ASP	2.2
1	B	271	ARG	2.2
1	H	261	TYR	2.2
1	A	258	GLN	2.2
1	I	205	GLU	2.2
1	F	248	ASP	2.2
1	C	258	GLN	2.2
1	E	244	GLN	2.2
1	D	160	SER	2.2
1	D	213	TYR	2.2
1	J	251	LEU	2.2
1	D	111	PHE	2.2
1	D	282	ASN	2.2
1	F	264	PHE	2.2
1	F	226	GLU	2.2
1	G	157	GLU	2.2
1	C	266	ASP	2.1
1	H	194	ASN	2.1
1	I	40	VAL	2.1
1	B	269	LYS	2.1
1	B	265	PRO	2.1
1	D	108	GLU	2.1
1	F	260	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	179	GLY	2.1
1	D	195	GLY	2.1
1	I	290	LYS	2.1
1	J	256	LYS	2.1
1	G	226	GLU	2.1
1	D	214	VAL	2.1
1	G	258	GLN	2.1
1	H	67	GLY	2.1
1	D	260	GLU	2.1
1	A	159	ASN	2.1
1	D	133	TYR	2.1
1	D	216	ASP	2.1
1	H	159	ASN	2.1
1	F	244	GLN	2.1
1	E	205	GLU	2.1
1	C	206	ASN	2.1
1	B	263	PRO	2.1
1	E	124	THR	2.0
1	D	196	GLU	2.0
1	F	249	ALA	2.0
1	F	274	ALA	2.0
1	F	283	LEU	2.0
1	E	228	GLY	2.0
1	J	257	GLY	2.0
1	A	54	GLU	2.0
1	D	155	LEU	2.0
1	G	266	ASP	2.0
1	D	110	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	1310	6/6	0.70	0.31	45,46,48,49	0
3	GOL	H	1310	6/6	0.74	0.39	44,47,48,48	0
3	GOL	I	1310	6/6	0.74	0.40	50,51,52,52	0
3	GOL	E	1310	6/6	0.75	0.34	44,45,46,47	0
3	GOL	D	1310	6/6	0.76	0.34	42,42,43,44	0
3	GOL	F	1310	6/6	0.78	0.33	45,47,47,48	0
3	GOL	J	1310	6/6	0.78	0.37	48,49,50,50	0
3	GOL	C	1310	6/6	0.82	0.38	46,48,48,49	0
5	BMA	E	1321	11/12	0.83	0.12	34,35,37,38	0
3	GOL	G	1310	6/6	0.84	0.28	42,44,44,45	0
5	BMA	D	1321	11/12	0.85	0.12	34,35,37,38	0
3	GOL	A	1310	6/6	0.86	0.28	41,43,43,44	0
4	ADP	D	1320	27/27	0.88	0.11	28,30,31,34	0
4	ADP	F	1320	27/27	0.88	0.12	29,31,33,35	0
5	BMA	I	1321	11/12	0.88	0.12	34,35,37,39	0
5	BMA	F	1321	11/12	0.89	0.10	37,38,40,42	0
5	BMA	H	1321	11/12	0.89	0.11	32,34,37,39	0
5	BMA	B	1321	11/12	0.89	0.10	34,35,37,39	0
6	CL	G	1313	1/1	0.89	0.18	65,65,65,65	0
5	BMA	C	1321	11/12	0.90	0.10	33,35,37,39	0
5	BMA	A	1321	11/12	0.90	0.10	34,36,40,42	0
5	BMA	G	1321	11/12	0.90	0.10	32,34,37,37	0
5	BMA	J	1321	11/12	0.91	0.09	33,35,37,39	0
4	ADP	E	1320	27/27	0.91	0.10	27,30,32,34	0
2	NAP	G	1308	48/48	0.93	0.10	27,31,38,41	0
2	NAP	H	1308	48/48	0.93	0.10	28,31,36,40	0
2	NAP	J	1308	48/48	0.93	0.09	26,30,36,39	0
4	ADP	B	1320	27/27	0.93	0.11	26,29,31,33	0
2	NAP	B	1308	48/48	0.93	0.10	25,31,35,41	0
2	NAP	F	1308	48/48	0.93	0.10	27,31,38,42	0
2	NAP	A	1308	48/48	0.94	0.10	27,30,36,39	0
2	NAP	C	1308	48/48	0.94	0.09	26,30,37,40	0
2	NAP	D	1308	48/48	0.94	0.09	27,31,36,37	0
2	NAP	I	1308	48/48	0.94	0.09	26,31,37,40	0
2	NAP	E	1308	48/48	0.94	0.10	25,31,37,41	0
4	ADP	I	1320	27/27	0.95	0.09	27,30,32,34	0
6	CL	G	1312	1/1	0.95	0.30	60,60,60,60	0
4	ADP	G	1320	27/27	0.95	0.08	27,29,31,32	0
4	ADP	C	1320	27/27	0.96	0.07	27,29,31,31	0
4	ADP	H	1320	27/27	0.96	0.07	27,29,30,32	0
4	ADP	A	1320	27/27	0.96	0.08	25,30,33,34	0

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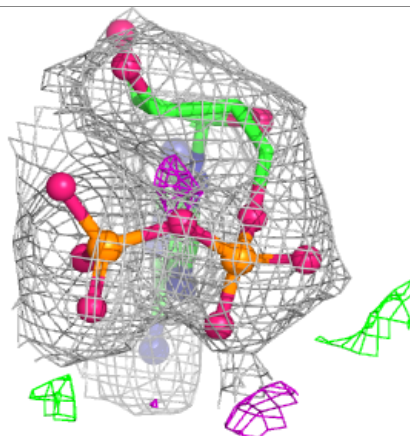
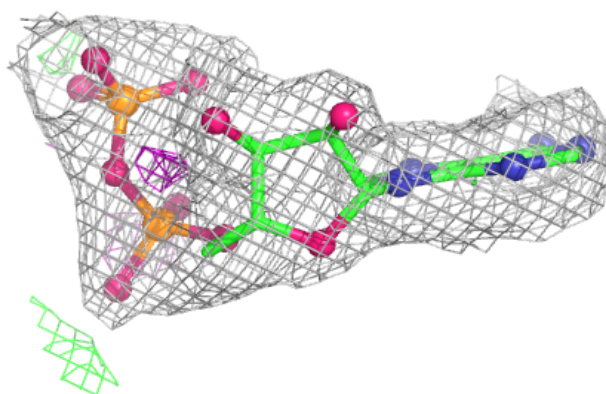
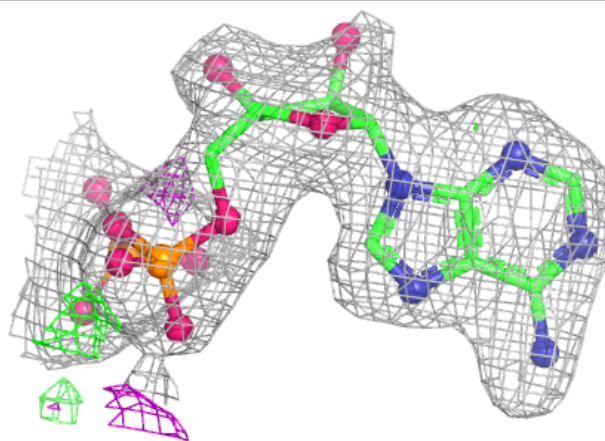
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ADP	J	1320	27/27	0.96	0.08	27,29,31,31	0

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.

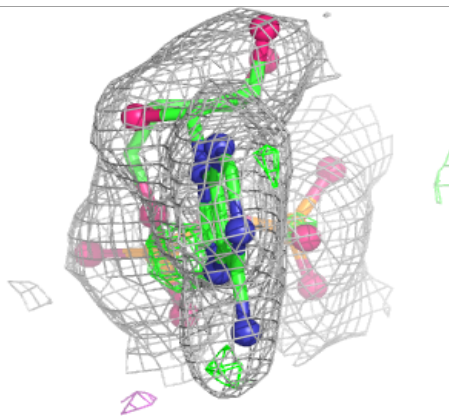
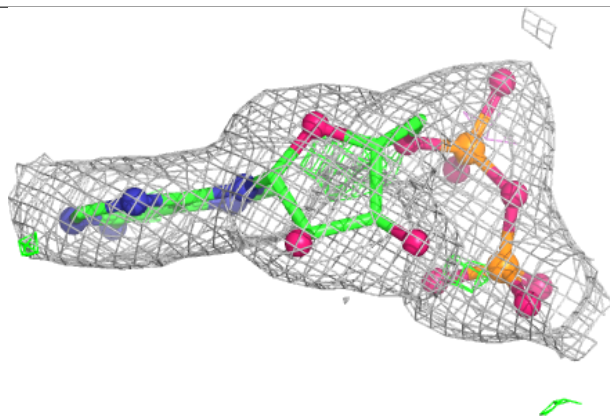
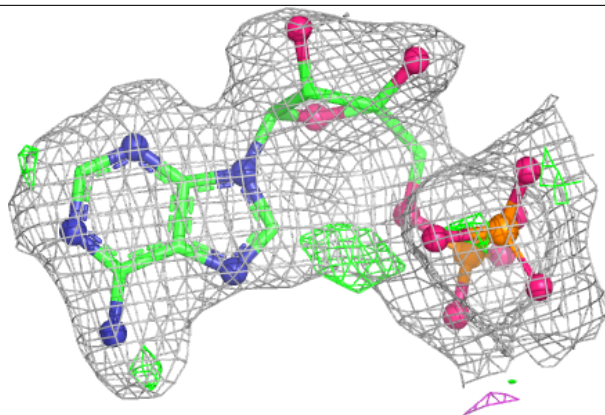
Electron density around ADP D 1320:

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



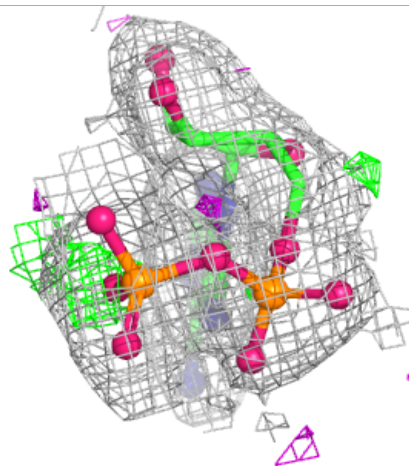
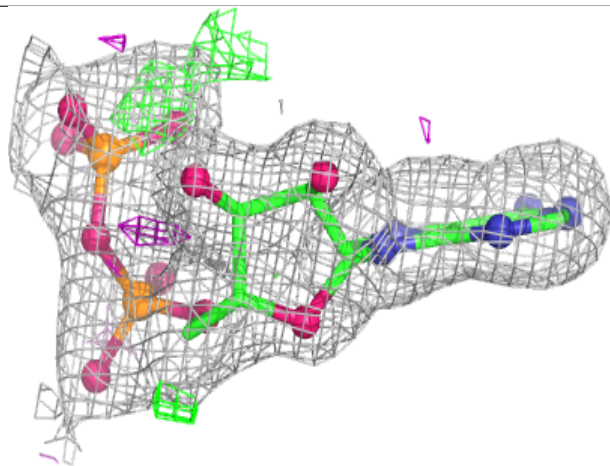
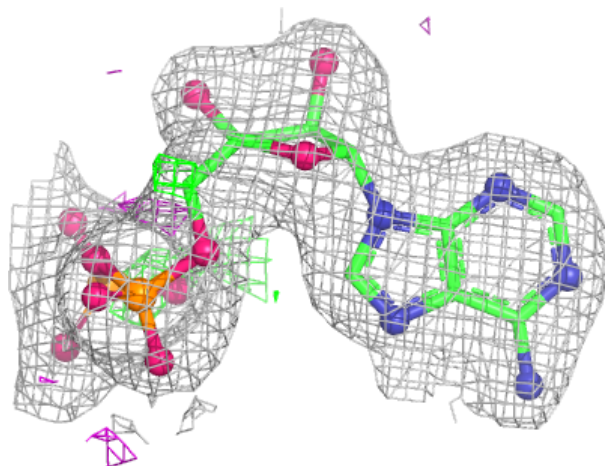
Electron density around ADP F 1320:

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



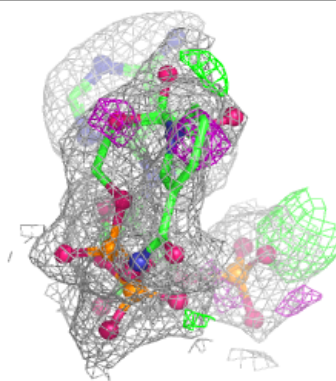
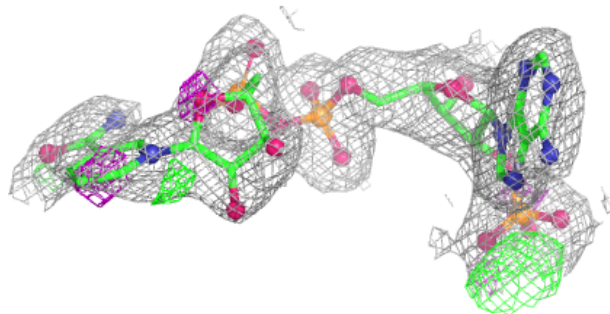
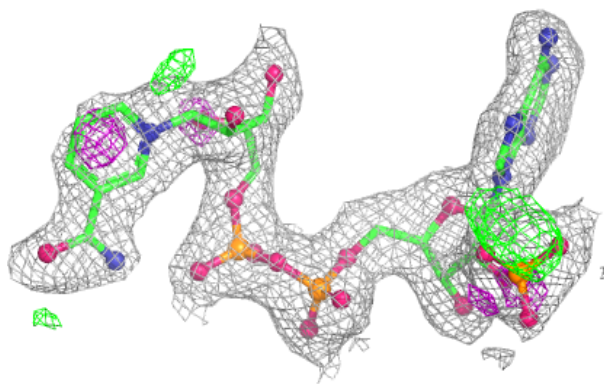
Electron density around ADP E 1320:

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

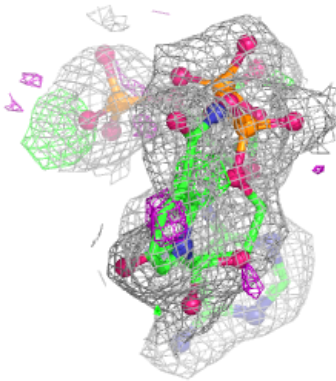
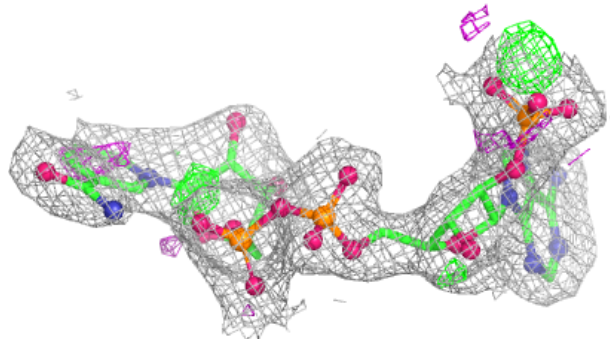
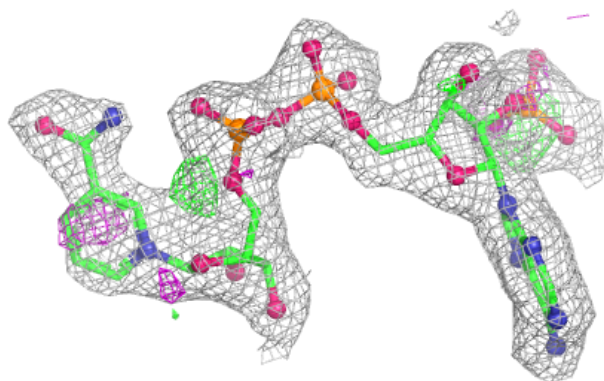


Electron density around NAP G 1308:

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

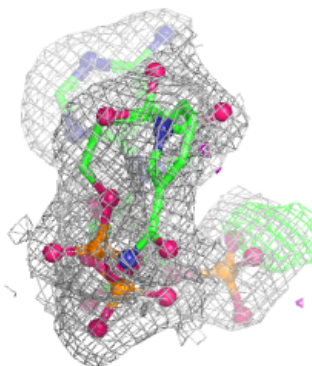
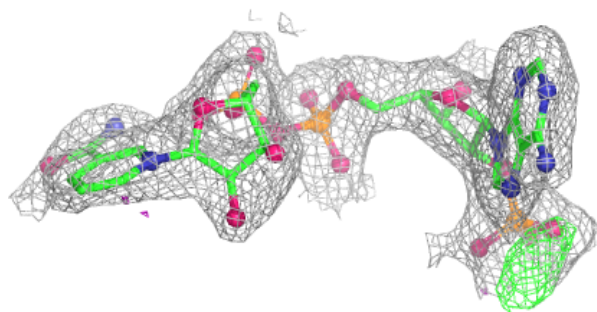
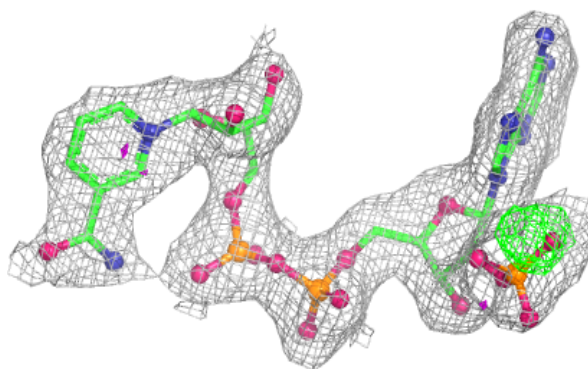
**Electron density around NAP H 1308:**

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

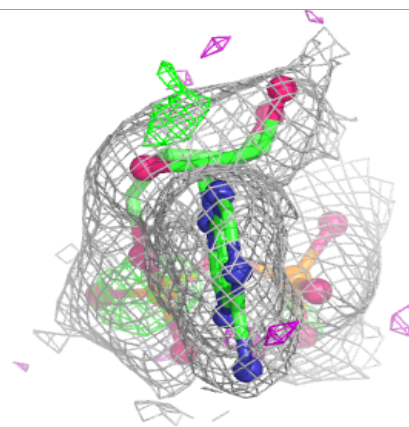
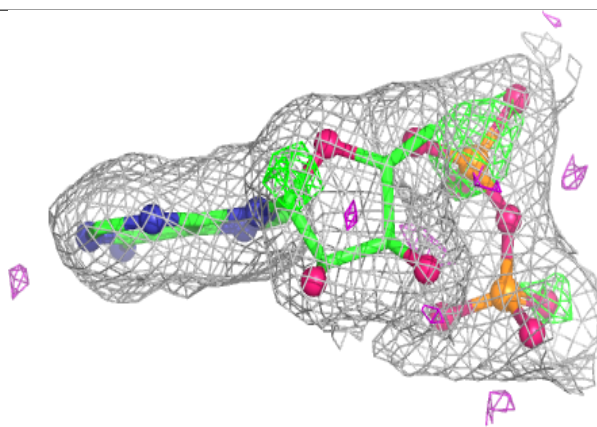
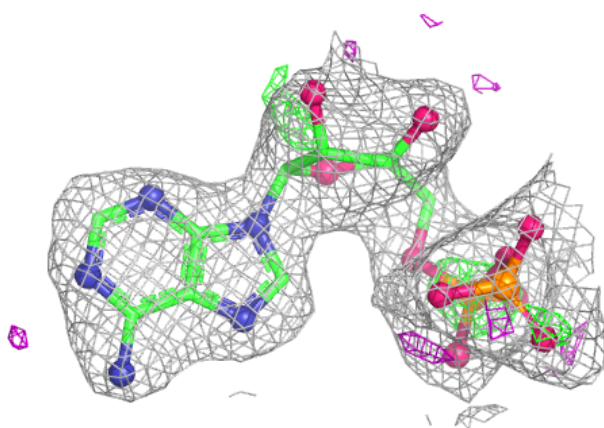


Electron density around NAP J 1308:

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

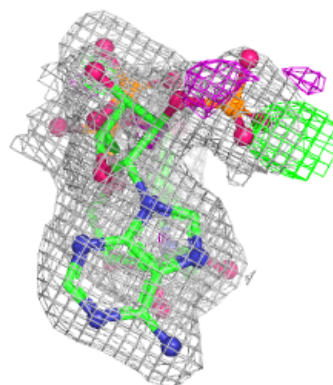
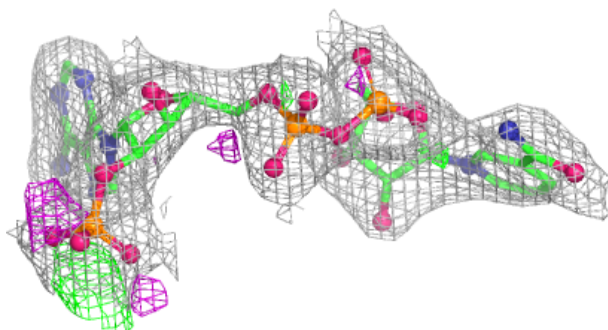
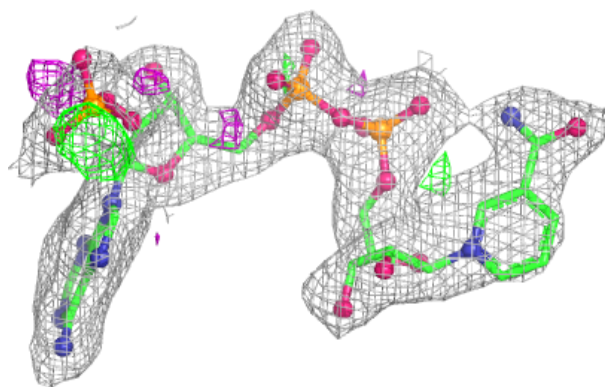
**Electron density around ADP B 1320:**

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

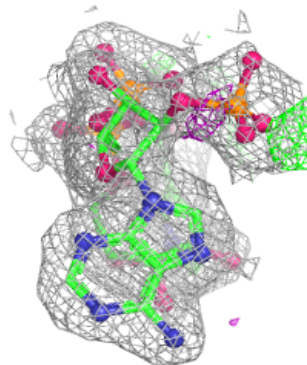
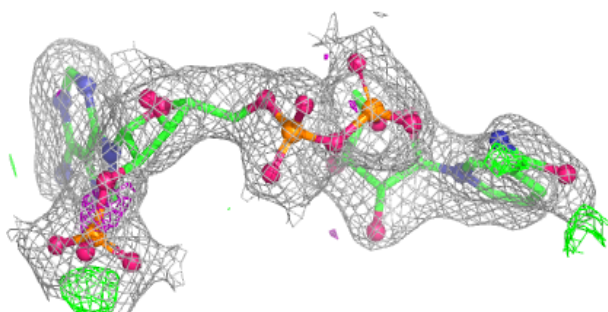
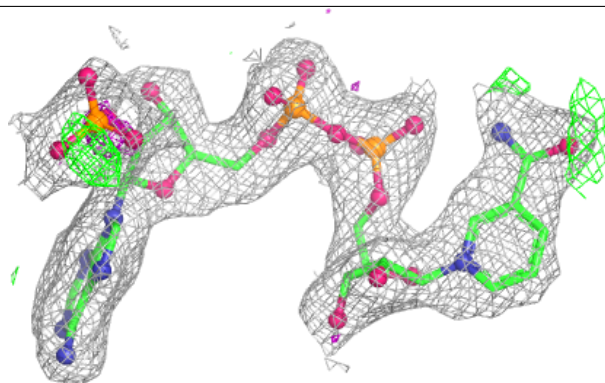


Electron density around NAP B 1308:

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

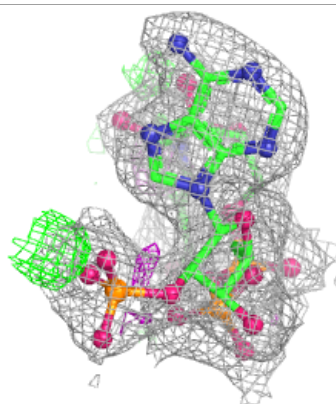
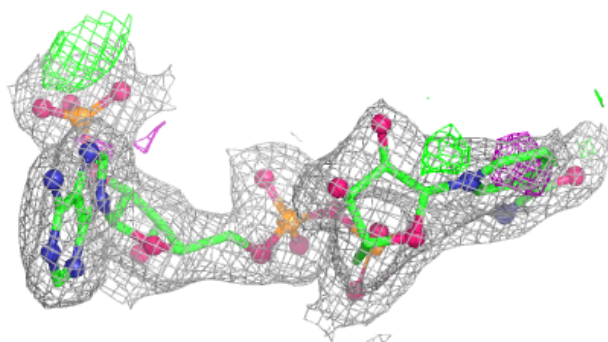
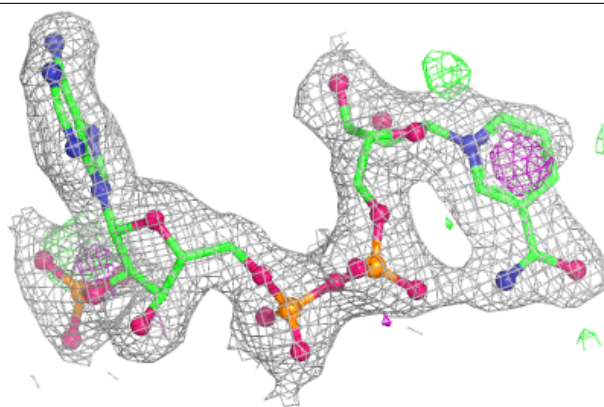
**Electron density around NAP F 1308:**

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

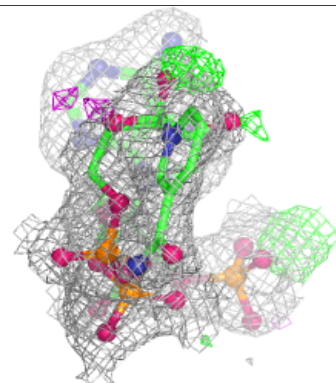
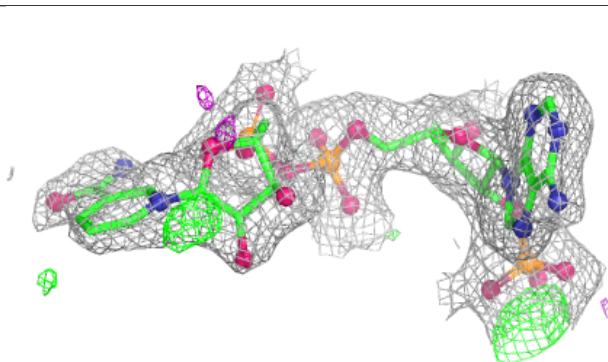
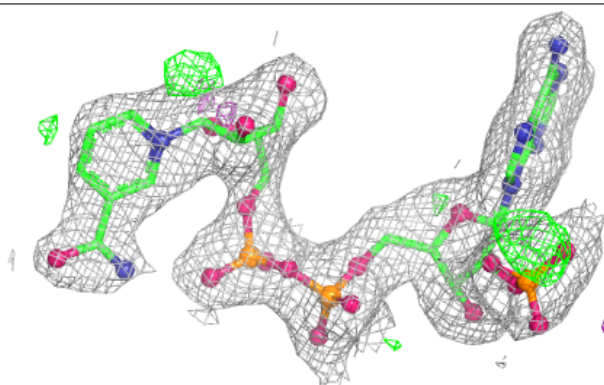


Electron density around NAP A 1308:

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

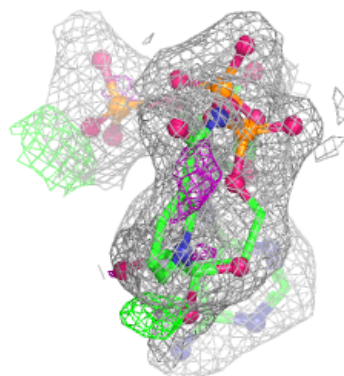
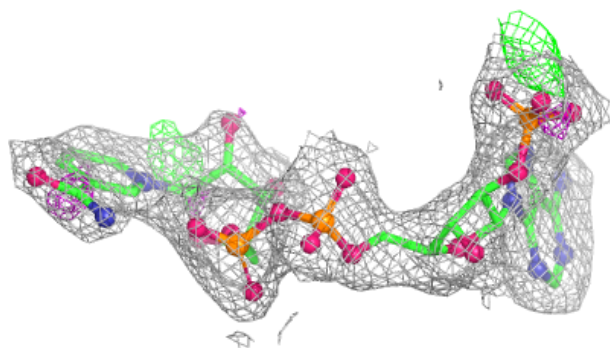
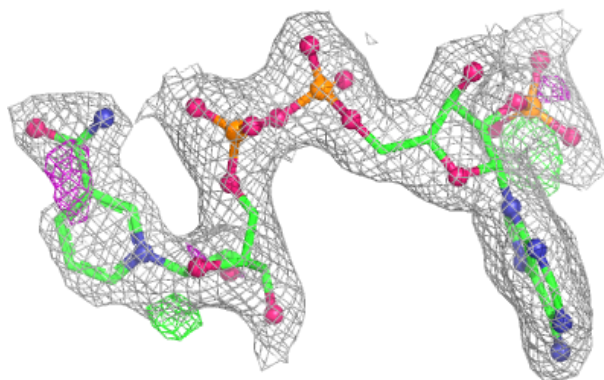
**Electron density around NAP C 1308:**

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

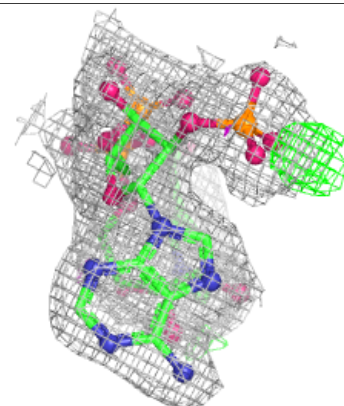
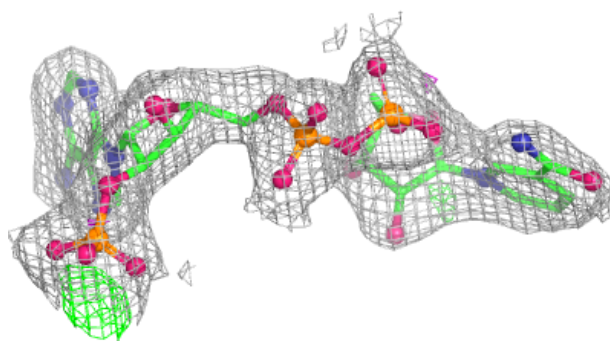
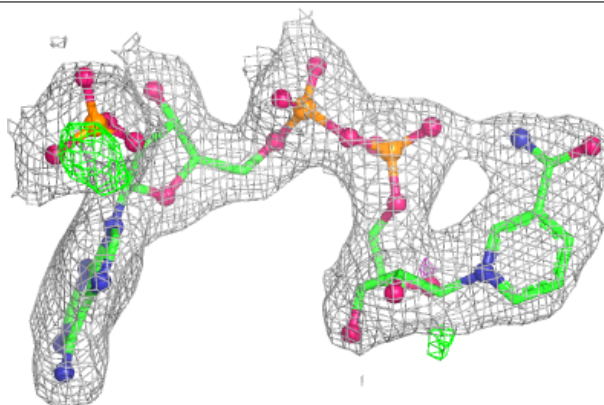


Electron density around NAP D 1308:

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

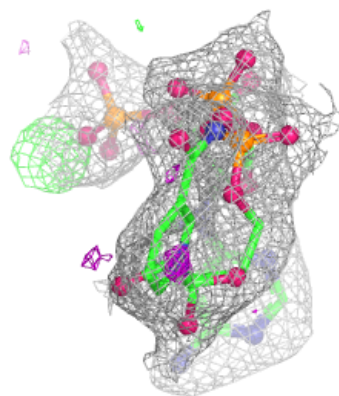
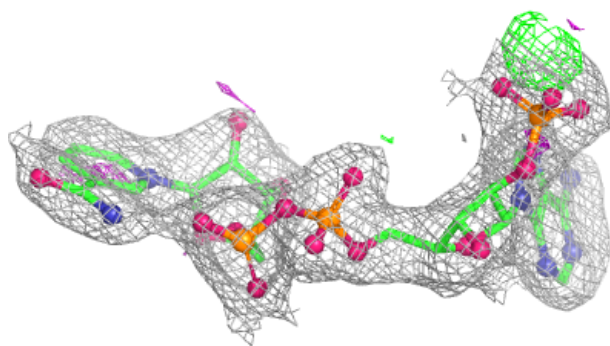
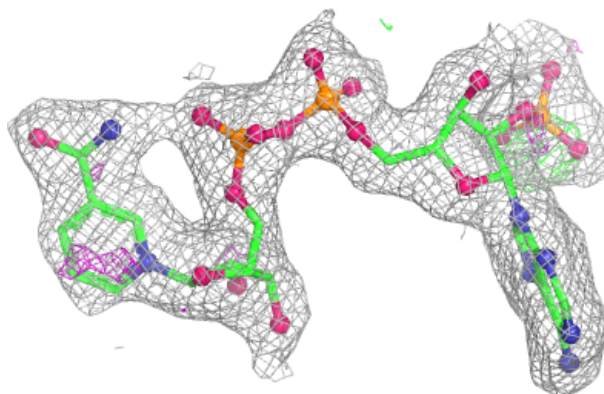
**Electron density around NAP I 1308:**

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

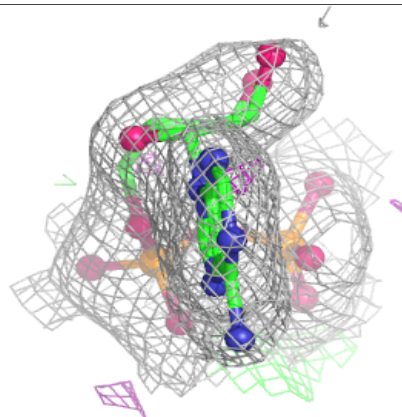
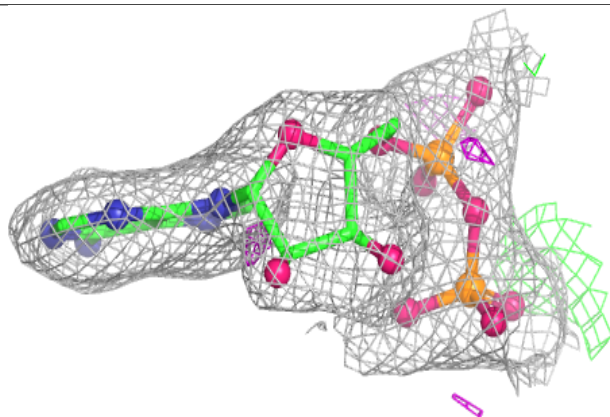
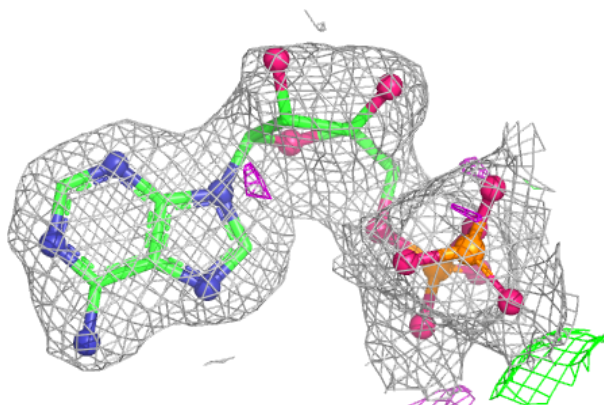


Electron density around NAP E 1308:

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

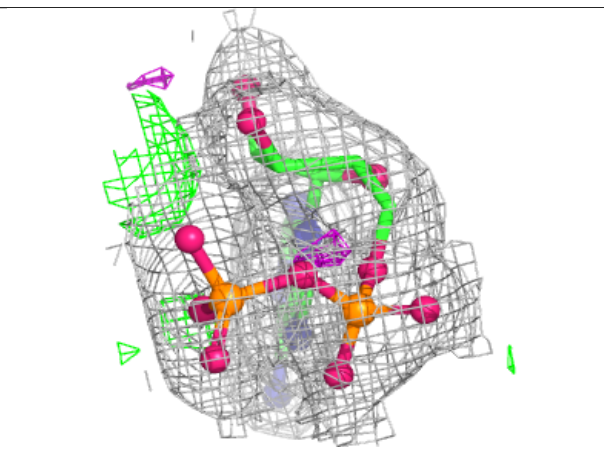
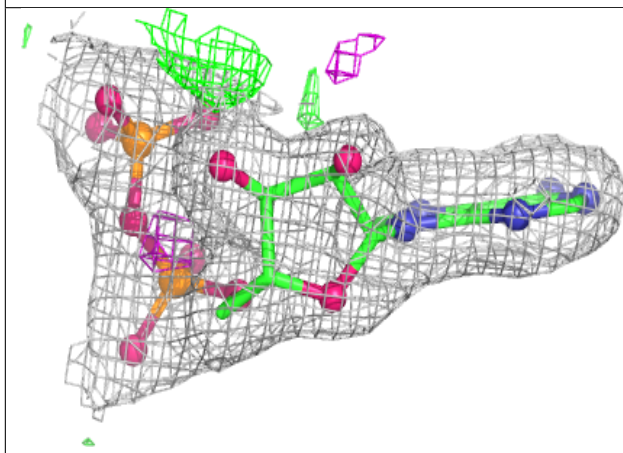
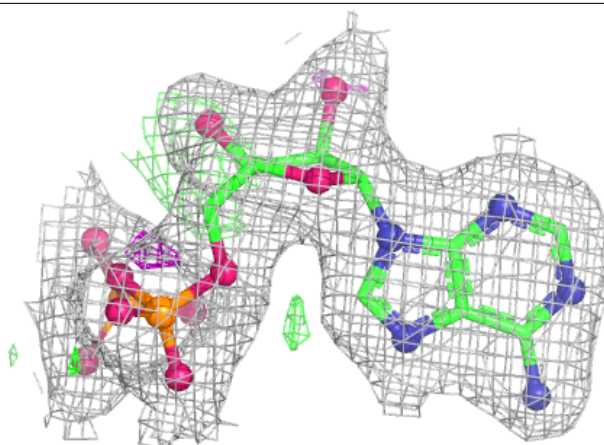
**Electron density around ADP I 1320:**

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

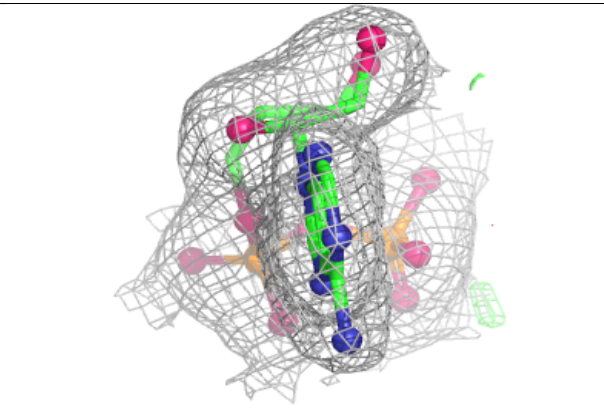
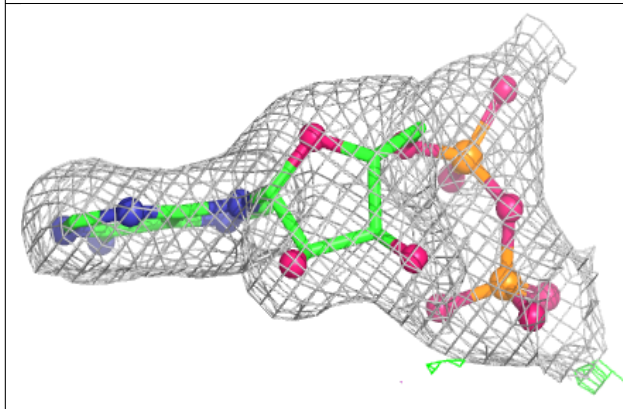
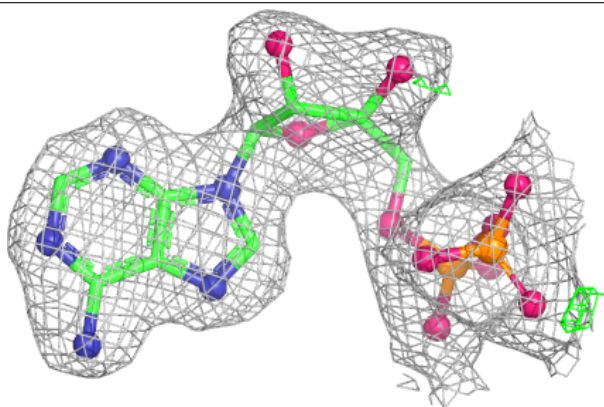


Electron density around ADP G 1320:

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

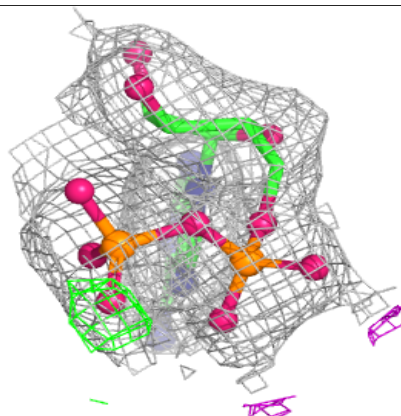
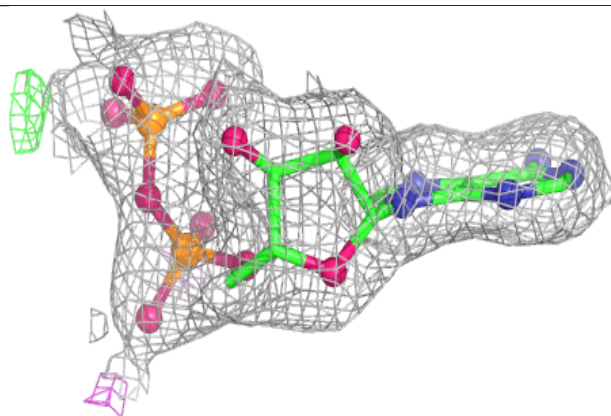
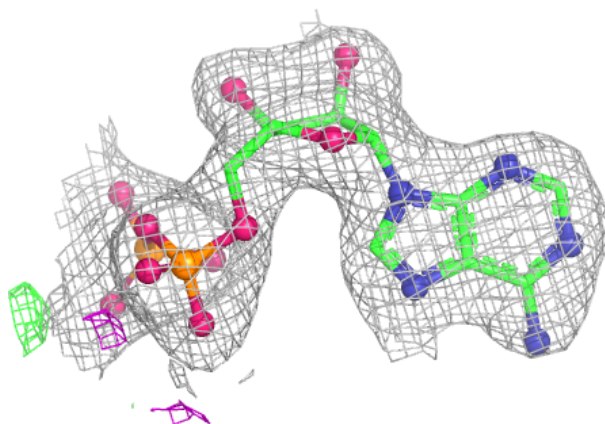
**Electron density around ADP C 1320:**

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

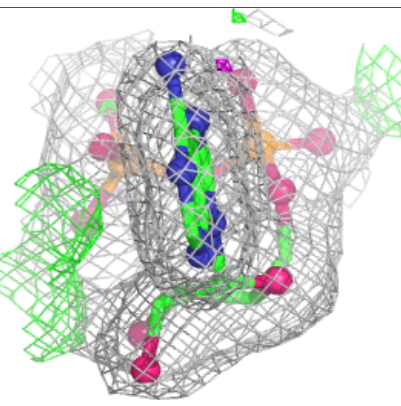
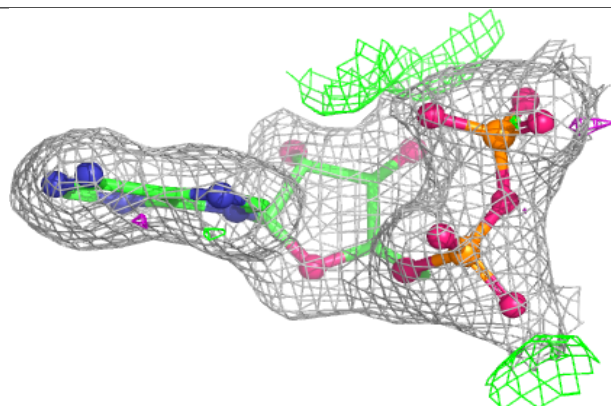
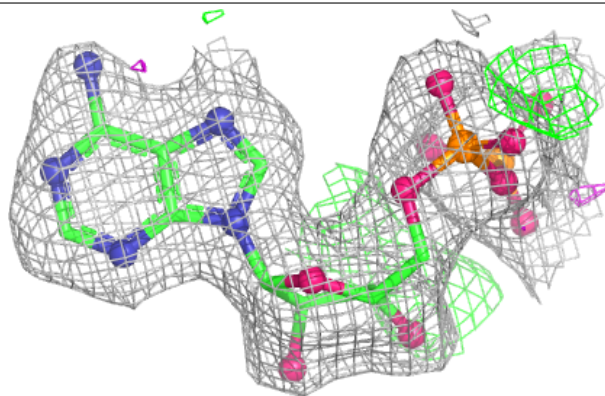


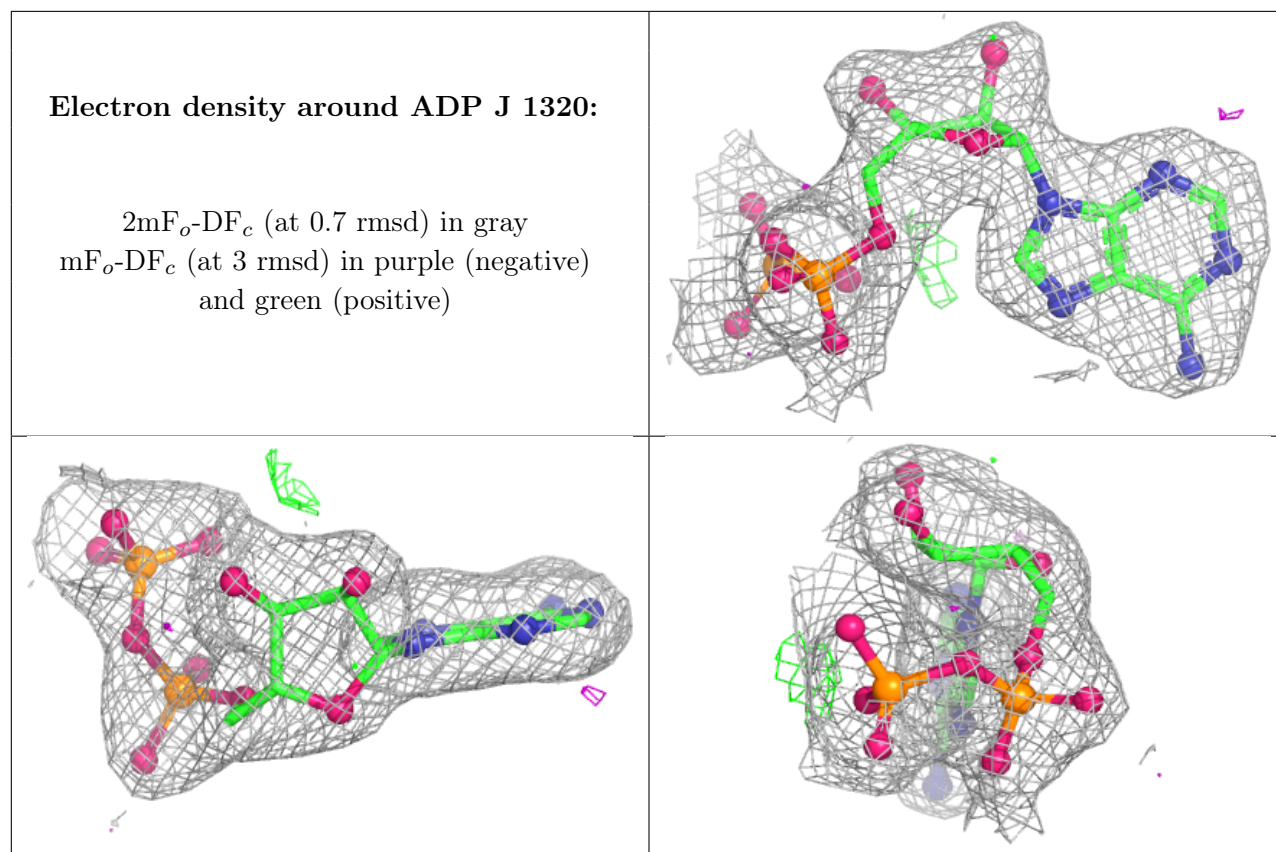
Electron density around ADP H 1320:

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

**Electron density around ADP A 1320:**

$2mF_o-DF_c$ (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.