



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:32 am BST

PDB ID : 3N83
Title : T244A mutant of human mitochondrial aldehyde dehydrogenase, NAD complex
Authors : Gonzalez-Segura, L.; Hurley, T.D.
Deposited on : 2010-05-27
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

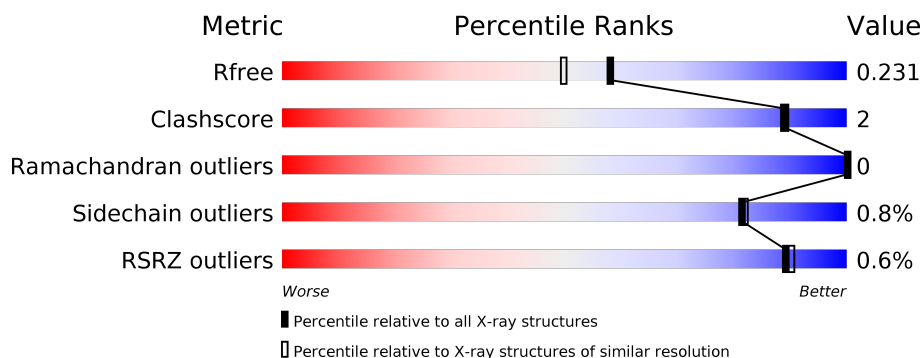
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	500	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	500	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>.</div> </div> </div>
1	C	500	<div> <div></div> <div> <div></div> <div>92%</div> <div>7%</div> <div>.</div> </div> </div>
1	D	500	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
1	E	500	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>5%</div> <div>.</div> </div> </div>
1	F	500	<div> <div></div> <div> <div></div> <div>95%</div> <div>.</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	500	<div><div></div><div>93%</div><div>6%</div></div>
1	H	500	<div>%<div><div></div><div>94%</div><div>5%</div></div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34066 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 Aldehyde dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	5	0
			3836	2437	657	722	20			
1	B	494	Total	C	N	O	S	0	6	0
			3843	2441	658	724	20			
1	C	494	Total	C	N	O	S	0	4	0
			3827	2432	655	720	20			
1	D	494	Total	C	N	O	S	0	6	0
			3840	2441	657	722	20			
1	E	494	Total	C	N	O	S	0	5	0
			3836	2437	657	722	20			
1	F	494	Total	C	N	O	S	0	5	0
			3833	2436	656	721	20			
1	G	494	Total	C	N	O	S	0	5	0
			3832	2435	655	722	20			
1	H	494	Total	C	N	O	S	0	6	0
			3842	2440	658	724	20			

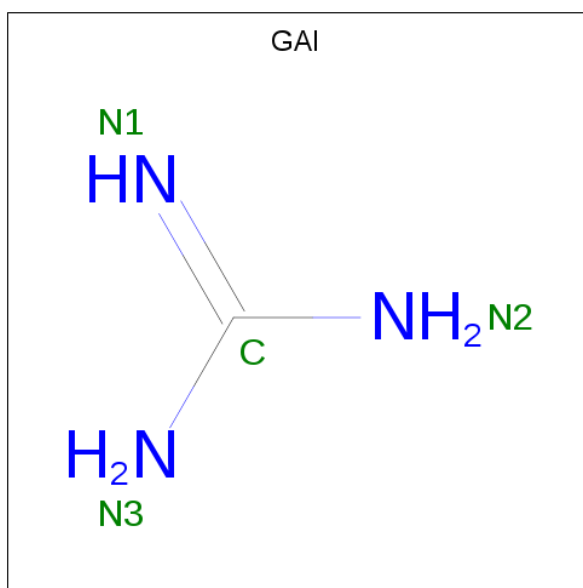
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
B	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
C	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
D	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
E	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
F	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
G	244	ALA	THR	ENGINEERED MUTATION	UNP P05091
H	244	ALA	THR	ENGINEERED MUTATION	UNP P05091

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	A	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0

- Molecule 3 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



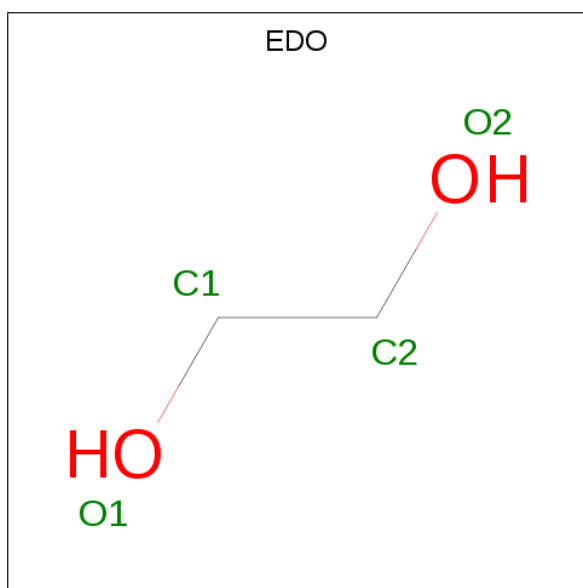
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 4 1 3	0	0
3	B	1	Total C N 4 1 3	0	0
3	B	1	Total C N 4 1 3	0	0
3	C	1	Total C N 4 1 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	N	0	0
			4	1	3		
3	D	1	Total	C	N	0	0
			4	1	3		
3	D	1	Total	C	N	0	0
			4	1	3		
3	E	1	Total	C	N	0	0
			4	1	3		
3	E	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	F	1	Total	C	N	0	0
			4	1	3		
3	G	1	Total	C	N	0	0
			4	1	3		
3	G	1	Total	C	N	0	0
			4	1	3		
3	G	1	Total	C	N	0	0
			4	1	3		
3	H	1	Total	C	N	0	0
			4	1	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



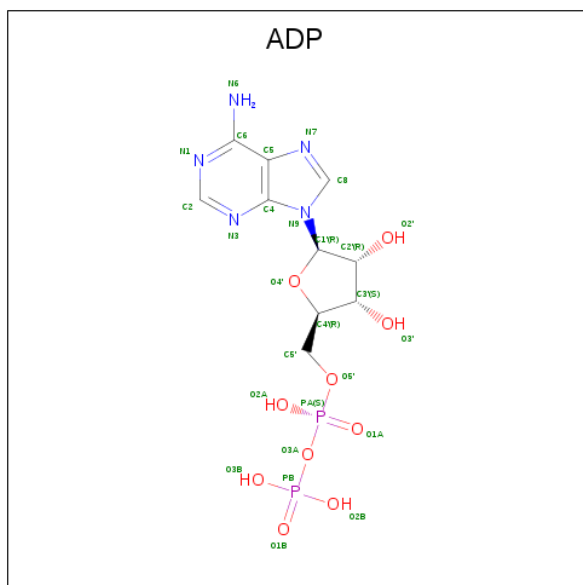
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			35	10	5	16	4		
5	B	1	Total	C	N	O	P	0	1
			35	10	5	16	4		
5	C	1	Total	C	N	O	P	0	1
			35	10	5	16	4		
5	D	1	Total	C	N	O	P	0	1
			35	10	5	16	4		
5	E	1	Total	C	N	O	P	0	1
			35	10	5	16	4		
5	F	1	Total	C	N	O	P	0	1
			35	10	5	16	4		
5	G	1	Total	C	N	O	P	0	1
			35	10	5	16	4		
5	H	1	Total	C	N	O	P	0	1
			35	10	5	16	4		

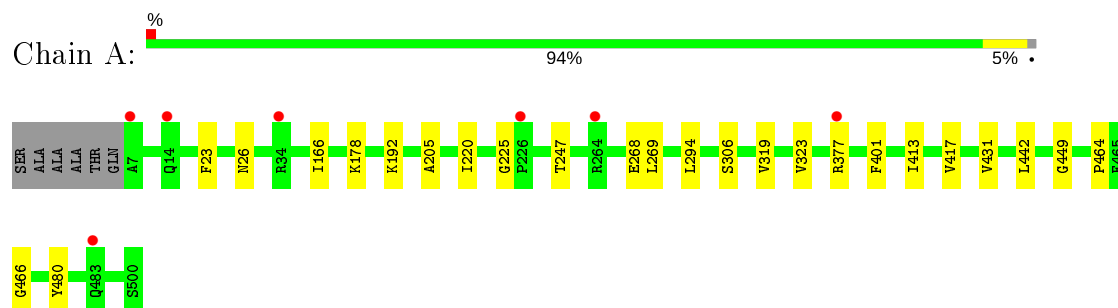
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	327	Total 327	O 327	0	0
6	B	340	Total 340	O 340	0	0
6	C	387	Total 387	O 387	0	0
6	D	356	Total 356	O 356	0	0
6	E	373	Total 373	O 373	0	0
6	F	390	Total 390	O 390	0	0
6	G	372	Total 372	O 372	0	0
6	H	388	Total 388	O 388	0	0

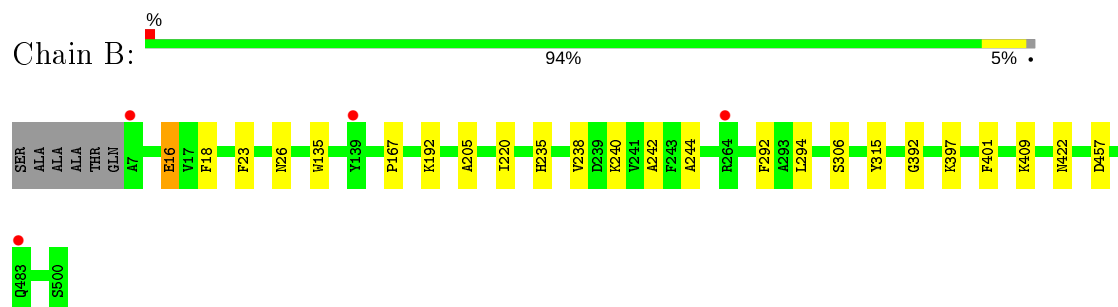
3 Residue-property plots [i](#)

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

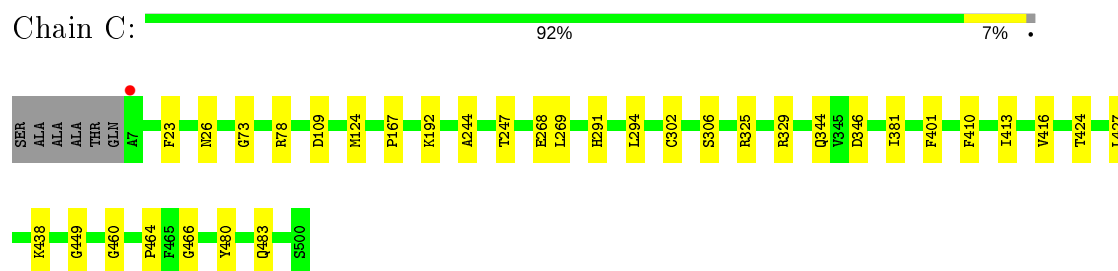
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



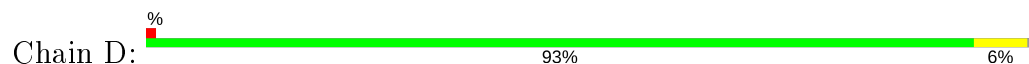
- Molecule 1: Aldehyde dehydrogenase, mitochondrial

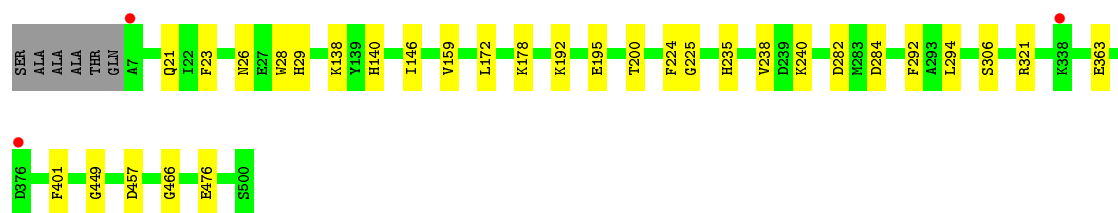


- Molecule 1: Aldehyde dehydrogenase, mitochondrial

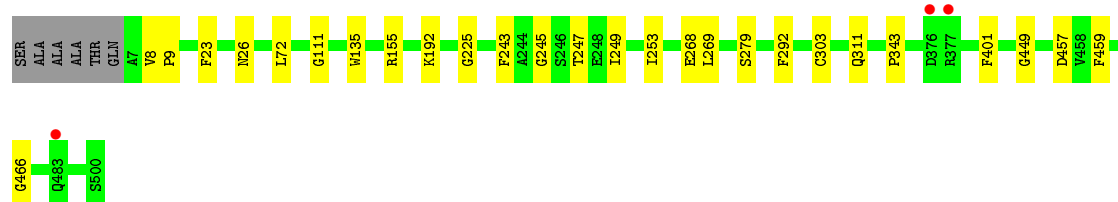
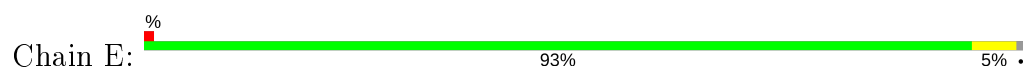


- Molecule 1: Aldehyde dehydrogenase, mitochondrial





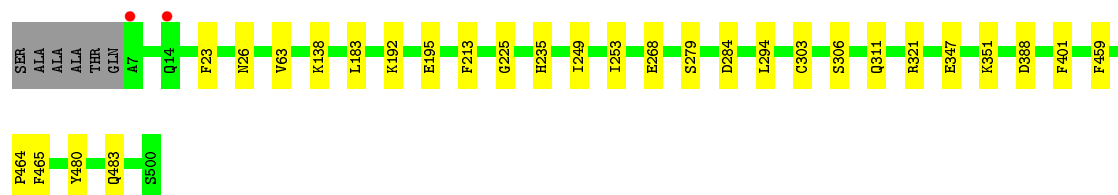
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



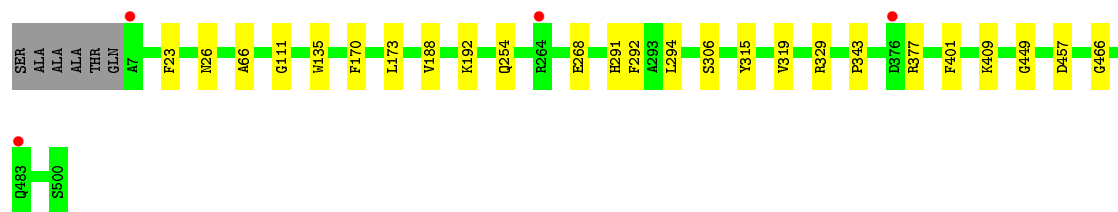
- Molecule 1: Aldehyde dehydrogenase, mitochondrial



- Molecule 1: Aldehyde dehydrogenase, mitochondrial



- Molecule 1: Aldehyde dehydrogenase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.13Å 150.99Å 177.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.06 – 1.90 43.79 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.06-1.90) 99.5 (43.79-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.189 , 0.232 0.188 , 0.231	Depositor DCC
R_{free} test set	15253 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	20.3	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34066	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 37.09 % 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 4.5245e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: NA, EDO, ADP, GAI

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	0.54	0/3923	0.58	0/5320
1	B	0.54	0/3930	0.59	0/5330
1	C	0.57	0/3914	0.61	2/5308 (0.0%)
1	D	0.55	0/3930	0.59	1/5330 (0.0%)
1	E	0.57	0/3923	0.60	0/5320
1	F	0.58	0/3923	0.62	0/5320
1	G	0.56	0/3922	0.60	0/5319
1	H	0.57	0/3929	0.59	0/5328
All	All	0.56	0/31394	0.60	3/42575 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	ASP	CB-CG-OD1	6.70	124.33	118.30
1	C	109	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	282	ASP	CB-CG-OD2	5.02	122.82	118.30

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	3836	0	3782	11	0
1	B	3843	0	3788	13	0
1	C	3827	0	3775	21	0
1	D	3840	0	3791	22	0
1	E	3836	0	3782	17	0
1	F	3833	0	3783	10	0
1	G	3832	0	3779	16	0
1	H	3842	0	3786	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	4	0	4	0	0
3	B	8	0	8	0	0
3	C	4	0	4	0	0
3	D	12	0	12	0	0
3	E	8	0	8	0	0
3	F	12	0	12	0	0
3	G	12	0	12	0	0
3	H	4	0	4	0	0
4	A	12	0	18	0	0
4	B	8	0	12	0	0
4	C	16	0	24	0	0
4	D	8	0	12	0	0
4	E	8	0	12	1	0
4	F	20	0	30	2	0
4	G	12	0	18	0	0
4	H	8	0	12	0	0
5	A	35	0	0	0	0
5	B	35	0	0	0	0
5	C	35	0	0	1	0
5	D	35	0	0	0	0
5	E	35	0	0	0	0
5	F	35	0	0	0	0
5	G	35	0	0	1	0
5	H	35	0	0	0	0
6	A	327	0	0	0	0
6	B	340	0	0	2	0
6	C	387	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	356	0	0	1	0
6	E	373	0	0	0	0
6	F	390	0	0	1	0
6	G	372	0	0	2	0
6	H	388	0	0	1	0
All	All	34066	0	30468	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (120) 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:G:195:GLU:HG3	6:G:1591:HOH:O	1.75	0.85
1:D:159[A]:VAL:HG11	1:D:240:LYS:HB2	1.63	0.81
1:C:291:HIS:HE1	1:C:329:ARG:HH11	1.29	0.80
1:E:279:SER:H	1:E:311[B]:GLN:HE21	1.34	0.75
1:G:279:SER:H	1:G:311[B]:GLN:HE21	1.40	0.70
1:E:279:SER:H	1:E:311[B]:GLN:NE2	1.91	0.68
1:E:155:ARG:HD2	4:E:905:EDO:H11	1.75	0.68
1:E:72:LEU:HD21	4:F:946:EDO:H11	1.76	0.65
1:C:291:HIS:CE1	1:C:329:ARG:HH11	2.14	0.64
1:D:195:GLU:OE2	1:D:224:PHE:HD2	1.81	0.63
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.33	0.63
1:D:195:GLU:OE2	1:D:224:PHE:CD2	2.53	0.62
1:G:63:VAL:HG11	1:G:235:HIS:CE1	2.36	0.60
1:B:167:PRO:HD3	1:B:244:ALA:HB3	1.84	0.59
1:G:279:SER:H	1:G:311[B]:GLN:NE2	1.99	0.59
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.38	0.59
6:B:915:HOH:O	1:D:140:HIS:HD2	1.86	0.59
1:H:291:HIS:HE1	1:H:329:ARG:HH11	1.50	0.57
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.38	0.57
1:B:392:GLY:O	1:B:397:LYS:HE2	2.05	0.57
1:H:291:HIS:HD2	6:H:555:HOH:O	1.88	0.56
1:F:167:PRO:HD3	1:F:244:ALA:HB3	1.87	0.56
1:D:292:PHE:HE1	1:D:457:ASP:HB2	1.72	0.54
1:A:449:GLY:HA3	1:A:466:GLY:O	2.08	0.54
1:F:464:PRO:HG3	1:F:480:TYR:CD1	2.44	0.53
1:H:294:LEU:HD23	1:H:306:SER:HA	1.91	0.53
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.45	0.52
1:E:249:ILE:O	1:E:253:ILE:HG12	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:GLU:HG2	1:B:18:PHE:CZ	2.46	0.51
1:D:21:GLN:HB3	1:D:29:HIS:O	2.10	0.51
1:D:159[A]:VAL:CG1	1:D:240:LYS:HB2	2.38	0.51
1:C:73:GLY:O	1:C:78:ARG:HD3	2.11	0.50
1:B:16:GLU:CG	1:B:18:PHE:CZ	2.94	0.50
1:C:344:GLN:HG3	1:C:381:ILE:HD12	1.93	0.50
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.46	0.50
1:E:279:SER:N	1:E:311[B]:GLN:HE21	2.07	0.50
1:G:388[A]:ASP:HB2	6:G:2563:HOH:O	2.11	0.50
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.47	0.50
1:F:358:ASN:O	1:F:362:GLN:HG2	2.13	0.49
1:D:449:GLY:HA3	1:D:466:GLY:O	2.13	0.49
1:C:247:THR:HA	1:C:269:LEU:HD13	1.94	0.48
1:C:464:PRO:HG3	1:C:480:TYR:CD1	2.49	0.48
1:C:413:ILE:HD12	1:C:438:LYS:HG2	1.96	0.48
1:A:413:ILE:O	1:A:417:VAL:HG23	2.14	0.47
1:B:235:HIS:HB3	1:B:238:VAL:HG23	1.96	0.47
1:A:294:LEU:HD23	1:A:306:SER:HA	1.95	0.47
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.50	0.46
1:H:449:GLY:HA3	1:H:466:GLY:O	2.16	0.46
1:A:205:ALA:HB2	1:A:220:ILE:HD12	1.97	0.46
1:D:294:LEU:HD23	1:D:306:SER:HA	1.97	0.46
1:G:303:CYS:SG	1:G:459:PHE:HZ	2.38	0.45
1:D:159[A]:VAL:HG11	1:D:240:LYS:CB	2.39	0.45
1:C:424:THR:HG23	6:C:2757:HOH:O	2.17	0.45
1:G:464:PRO:HG3	1:G:480:TYR:CD1	2.52	0.45
1:B:294:LEU:HD23	1:B:306:SER:HA	1.98	0.45
1:C:291:HIS:CE1	1:C:329:ARG:NH1	2.83	0.45
1:H:170:PHE:HB3	1:H:173:LEU:HB3	1.99	0.45
1:D:363:GLU:HB2	6:D:2778:HOH:O	2.16	0.45
1:E:135:TRP:CE2	1:G:138:LYS:HD3	2.53	0.44
1:E:449:GLY:HA3	1:E:466:GLY:O	2.16	0.44
1:E:245:GLY:O	1:E:269:LEU:HA	2.18	0.44
1:F:170:PHE:HZ	1:F:301[B]:CYS:HG	1.64	0.44
1:B:16:GLU:HG3	1:B:18:PHE:CZ	2.53	0.44
1:B:205:ALA:HB2	1:B:220:ILE:HD12	2.00	0.44
1:F:138:LYS:HD3	1:H:135:TRP:CE2	2.53	0.43
1:F:154:THR:HA	1:F:489:LYS:O	2.18	0.43
1:A:247:THR:HA	1:A:269:LEU:HD13	2.00	0.43
1:E:111:GLY:O	1:E:343:PRO:HD2	2.19	0.43
1:H:292:PHE:CE2	1:H:457:ASP:HB2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:THR:HA	1:E:269:LEU:HD13	2.01	0.43
1:G:294:LEU:HD23	1:G:306:SER:HA	2.00	0.43
1:C:291:HIS:HE1	1:C:329:ARG:NH1	2.07	0.42
1:D:178:LYS:NZ	1:D:476:GLU:OE2	2.52	0.42
1:G:284:ASP:OD1	1:G:321:ARG:NH1	2.51	0.42
1:D:172:LEU:HD21	1:D:200:THR:HB	2.01	0.42
1:D:235:HIS:HB3	1:D:238:VAL:HG23	2.00	0.42
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.54	0.42
1:C:410:PHE:CD1	1:C:416:VAL:HB	2.54	0.42
1:A:319:VAL:O	1:A:323:VAL:HG23	2.20	0.42
1:C:167:PRO:HD3	1:C:244:ALA:HB3	2.01	0.42
1:A:431:VAL:HG21	1:A:442:LEU:HB3	2.01	0.42
1:C:294:LEU:HD23	1:C:306:SER:HA	2.01	0.42
1:G:249:ILE:O	1:G:253:ILE:HG12	2.19	0.42
1:A:464:PRO:HG3	1:A:480:TYR:CD1	2.54	0.42
1:G:459:PHE:HE2	1:G:465:PHE:CE1	2.38	0.42
6:B:501:HOH:O	1:D:140:HIS:HE1	2.03	0.42
1:D:23:PHE:HB2	1:D:28:TRP:CZ3	2.55	0.42
1:C:449:GLY:HA3	1:C:466:GLY:O	2.20	0.42
1:G:183:LEU:HD13	1:G:213:PHE:CE2	2.55	0.42
1:H:111:GLY:O	1:H:343:PRO:HD2	2.19	0.42
1:H:66:ALA:O	1:H:188:VAL:HG21	2.21	0.41
1:B:292:PHE:CE1	1:B:457:ASP:HB2	2.55	0.41
1:C:294:LEU:C	1:C:294:LEU:HD13	2.41	0.41
1:E:292:PHE:HE1	1:E:457:ASP:HB2	1.85	0.41
1:F:294:LEU:HD23	1:F:306:SER:HA	2.02	0.41
1:B:315:TYR:CD1	1:B:409:LYS:HE2	2.55	0.41
1:C:124[B]:MET:HE3	6:C:502:HOH:O	2.21	0.41
1:F:441:TYR:CE1	4:F:946:EDO:H12	2.56	0.41
1:D:284:ASP:OD1	1:D:321:ARG:NH1	2.54	0.41
1:B:135:TRP:CE2	1:D:138:LYS:HD3	2.56	0.41
1:H:315:TYR:CG	1:H:409:LYS:HE2	2.56	0.41
1:C:483:GLN:HB3	6:C:2502:HOH:O	2.21	0.40
1:C:460:GLY:HA3	1:D:146:ILE:HG13	2.02	0.40
1:D:292:PHE:CE1	1:D:457:ASP:HB2	2.54	0.40
1:E:303:CYS:SG	1:E:459:PHE:HZ	2.44	0.40
1:G:347:GLU:HG2	1:G:351:LYS:HE2	2.03	0.40
1:B:240:LYS:HE3	1:B:242:ALA:HB2	2.03	0.40
1:C:291:HIS:CD2	1:C:325:ARG:HG3	2.57	0.40
1:H:315:TYR:CE1	1:H:319:VAL:HG21	2.56	0.40
1:A:166:ILE:HG22	1:A:178:LYS:HE2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:CYS:SG	1:C:427:LEU:HD21	2.62	0.40
1:E:8:VAL:HA	1:E:9:PRO:HD3	1.94	0.40
1:F:14:GLN:HG2	6:F:942:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/500 (99%)	484 (97%)	13 (3%)	0	100	100
1	B	498/500 (100%)	485 (97%)	13 (3%)	0	100	100
1	C	496/500 (99%)	483 (97%)	13 (3%)	0	100	100
1	D	498/500 (100%)	483 (97%)	15 (3%)	0	100	100
1	E	497/500 (99%)	485 (98%)	12 (2%)	0	100	100
1	F	497/500 (99%)	480 (97%)	17 (3%)	0	100	100
1	G	497/500 (99%)	481 (97%)	16 (3%)	0	100	100
1	H	498/500 (100%)	484 (97%)	14 (3%)	0	100	100
All	All	3978/4000 (100%)	3865 (97%)	113 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	403/401 (100%)	399 (99%)	4 (1%)	76	76
1	B	404/401 (101%)	400 (99%)	4 (1%)	76	76
1	C	402/401 (100%)	399 (99%)	3 (1%)	84	84
1	D	404/401 (101%)	402 (100%)	2 (0%)	88	89
1	E	403/401 (100%)	400 (99%)	3 (1%)	84	84
1	F	403/401 (100%)	401 (100%)	2 (0%)	88	89
1	G	403/401 (100%)	399 (99%)	4 (1%)	76	76
1	H	404/401 (101%)	399 (99%)	5 (1%)	71	70
All	All	3226/3208 (101%)	3199 (99%)	27 (1%)	81	82

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

Mol	Chain	Res	Type
1	A	192	LYS
1	A	268	GLU
1	A	377	ARG
1	A	401	PHE
1	B	16	GLU
1	B	192	LYS
1	B	401	PHE
1	B	422	ASN
1	C	192	LYS
1	C	268	GLU
1	C	401	PHE
1	D	192	LYS
1	D	401	PHE
1	E	192	LYS
1	E	268	GLU
1	E	401	PHE
1	F	192	LYS
1	F	401	PHE
1	G	192	LYS
1	G	268	GLU
1	G	401	PHE
1	G	483	GLN
1	H	192	LYS
1	H	254	GLN
1	H	268	GLU
1	H	377	ARG
1	H	401	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	GLN
1	A	440	ASN
1	B	422	ASN
1	B	440	ASN
1	C	291	HIS
1	C	358	ASN
1	D	29	HIS
1	D	140	HIS
1	D	300	GLN
1	D	362	GLN
1	D	390	GLN
1	F	358	ASN
1	G	254	GLN
1	H	291	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 63 ligands modelled in this entry, 8 are monoatomic - leaving 55 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
4	EDO	G	917	-	3,3,3	0.44	0	2,2,2	0.20	0
4	EDO	F	926	-	3,3,3	0.32	0	2,2,2	0.50	0
5	ADP	B	502[B]	-	24,29,29	0.84	1 (4%)	29,45,45	1.25	3 (10%)
4	EDO	F	916	-	3,3,3	0.40	0	2,2,2	0.36	0
4	EDO	A	921	-	3,3,3	0.36	0	2,2,2	0.43	0
4	EDO	B	902	-	3,3,3	0.44	0	2,2,2	0.19	0
3	GAI	E	815	-	3,3,3	1.68	0	3,3,3	1.13	0
4	EDO	H	908	-	3,3,3	0.36	0	2,2,2	0.49	0
4	EDO	A	911	-	3,3,3	0.39	0	2,2,2	0.23	0
5	ADP	D	504[B]	-	24,29,29	0.82	1 (4%)	29,45,45	1.29	2 (6%)
4	EDO	F	966	-	3,3,3	0.44	0	2,2,2	0.10	0
3	GAI	B	802	-	3,3,3	1.37	0	3,3,3	0.81	0
5	ADP	F	506[A]	-	24,29,29	0.75	0	29,45,45	1.32	2 (6%)
5	ADP	H	508[A]	-	24,29,29	0.74	0	29,45,45	1.35	1 (3%)
4	EDO	C	963	-	3,3,3	0.34	0	2,2,2	0.40	0
5	ADP	A	501[A]	-	24,29,29	0.80	1 (4%)	29,45,45	1.29	2 (6%)
5	ADP	F	506[B]	-	24,29,29	0.75	0	29,45,45	1.31	2 (6%)
3	GAI	F	826	-	3,3,3	1.49	1 (33%)	3,3,3	1.38	1 (33%)
5	ADP	A	501[B]	-	24,29,29	0.79	1 (4%)	29,45,45	1.32	3 (10%)
4	EDO	F	906	-	3,3,3	0.46	0	2,2,2	0.14	0
4	EDO	E	915	-	3,3,3	0.34	0	2,2,2	0.51	0
5	ADP	C	503[A]	-	24,29,29	0.76	0	29,45,45	1.35	2 (6%)
4	EDO	C	903	-	3,3,3	0.42	0	2,2,2	0.20	0
3	GAI	D	833	-	3,3,3	1.58	1 (33%)	3,3,3	1.15	0
3	GAI	F	806	-	3,3,3	1.09	0	3,3,3	0.84	0
3	GAI	G	838	-	3,3,3	1.41	0	3,3,3	1.02	0
5	ADP	C	503[B]	-	24,29,29	0.75	0	29,45,45	1.29	2 (6%)
4	EDO	D	904	-	3,3,3	0.43	0	2,2,2	0.29	0
5	ADP	D	504[A]	-	24,29,29	0.82	1 (4%)	29,45,45	1.31	1 (3%)
3	GAI	B	812	-	3,3,3	1.78	1 (33%)	3,3,3	0.88	0
3	GAI	C	803	-	3,3,3	1.25	0	3,3,3	1.22	0
5	ADP	E	505[A]	-	24,29,29	0.76	0	29,45,45	1.38	3 (10%)
4	EDO	A	901	-	3,3,3	0.43	0	2,2,2	0.51	0
4	EDO	F	946	-	3,3,3	0.42	0	2,2,2	0.31	0
3	GAI	D	804	-	3,3,3	1.50	0	3,3,3	1.00	0
5	ADP	E	505[B]	-	24,29,29	0.75	0	29,45,45	1.30	2 (6%)
3	GAI	A	801	-	3,3,3	1.53	1 (33%)	3,3,3	1.41	1 (33%)
3	GAI	H	808	-	3,3,3	1.12	0	3,3,3	0.92	0
5	ADP	G	507[A]	-	24,29,29	0.79	0	29,45,45	1.26	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	H	508[B]	-	24,29,29	0.73	0	29,45,45	1.36	2 (6%)
4	EDO	G	907	-	3,3,3	0.42	0	2,2,2	0.38	0
3	GAI	F	816	-	3,3,3	1.43	0	3,3,3	1.09	0
4	EDO	C	923	-	3,3,3	0.32	0	2,2,2	0.62	0
5	ADP	G	507[B]	-	24,29,29	0.79	0	29,45,45	1.22	3 (10%)
5	ADP	B	502[A]	-	24,29,29	0.84	1 (4%)	29,45,45	1.22	2 (6%)
3	GAI	G	807	-	3,3,3	1.20	0	3,3,3	1.00	0
4	EDO	C	913	-	3,3,3	0.40	0	2,2,2	0.21	0
4	EDO	E	905	-	3,3,3	0.41	0	2,2,2	0.41	0
3	GAI	D	814	-	3,3,3	1.54	0	3,3,3	1.19	0
4	EDO	B	912	-	3,3,3	0.39	0	2,2,2	0.47	0
3	GAI	E	805	-	3,3,3	1.10	0	3,3,3	1.06	0
4	EDO	H	928	-	3,3,3	0.37	0	2,2,2	0.47	0
4	EDO	D	944	-	3,3,3	0.34	0	2,2,2	0.51	0
4	EDO	G	927	-	3,3,3	0.33	0	2,2,2	0.50	0
3	GAI	G	817	-	3,3,3	1.51	0	3,3,3	0.89	0

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
4	EDO	G	917	-	-	0/1/1/1	-
4	EDO	F	926	-	-	0/1/1/1	-
5	ADP	B	502[B]	-	-	0/12/32/32	0/3/3/3
4	EDO	F	916	-	-	0/1/1/1	-
4	EDO	A	921	-	-	1/1/1/1	-
4	EDO	B	902	-	-	0/1/1/1	-
4	EDO	H	928	-	-	1/1/1/1	-
4	EDO	H	908	-	-	0/1/1/1	-
4	EDO	A	911	-	-	0/1/1/1	-
5	ADP	D	504[B]	-	-	0/12/32/32	0/3/3/3
4	EDO	F	966	-	-	0/1/1/1	-
5	ADP	F	506[A]	-	-	7/12/32/32	0/3/3/3
5	ADP	H	508[A]	-	-	6/12/32/32	0/3/3/3
4	EDO	C	963	-	-	1/1/1/1	-
5	ADP	A	501[A]	-	-	4/12/32/32	0/3/3/3
5	ADP	F	506[B]	-	-	0/12/32/32	0/3/3/3
5	ADP	A	501[B]	-	-	0/12/32/32	0/3/3/3
4	EDO	F	906	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	E	915	-	-	0/1/1/1	-
5	ADP	C	503[A]	-	-	4/12/32/32	0/3/3/3
4	EDO	C	903	-	-	1/1/1/1	-
5	ADP	C	503[B]	-	-	1/12/32/32	0/3/3/3
4	EDO	D	904	-	-	0/1/1/1	-
5	ADP	D	504[A]	-	-	5/12/32/32	0/3/3/3
4	EDO	F	946	-	-	0/1/1/1	-
5	ADP	E	505[A]	-	-	6/12/32/32	0/3/3/3
4	EDO	A	901	-	-	0/1/1/1	-
5	ADP	E	505[B]	-	-	0/12/32/32	0/3/3/3
4	EDO	D	944	-	-	0/1/1/1	-
5	ADP	G	507[A]	-	-	6/12/32/32	0/3/3/3
5	ADP	H	508[B]	-	-	1/12/32/32	0/3/3/3
4	EDO	G	907	-	-	0/1/1/1	-
4	EDO	C	923	-	-	0/1/1/1	-
5	ADP	G	507[B]	-	-	1/12/32/32	0/3/3/3
5	ADP	B	502[A]	-	-	6/12/32/32	0/3/3/3
4	EDO	C	913	-	-	0/1/1/1	-
4	EDO	E	905	-	-	1/1/1/1	-
4	EDO	B	912	-	-	0/1/1/1	-
4	EDO	G	927	-	-	0/1/1/1	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502[B]	ADP	O4'-C1'	2.30	1.44	1.41
5	B	502[A]	ADP	O4'-C1'	2.30	1.44	1.41
5	A	501[A]	ADP	O4'-C1'	2.23	1.44	1.41
5	A	501[B]	ADP	O4'-C1'	2.23	1.44	1.41
5	D	504[B]	ADP	O4'-C1'	2.13	1.44	1.41
5	D	504[A]	ADP	O4'-C1'	2.13	1.44	1.41
3	B	812	GAI	C-N2	-2.12	1.32	1.36
3	D	833	GAI	C-N1	-2.08	1.26	1.30
3	F	826	GAI	C-N1	-2.02	1.26	1.30
3	A	801	GAI	C-N1	-2.02	1.26	1.30

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	508[A]	ADP	N3-C2-N1	-5.17	120.59	128.68
5	H	508[B]	ADP	N3-C2-N1	-5.17	120.59	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	505[A]	ADP	N3-C2-N1	-5.15	120.63	128.68
5	E	505[B]	ADP	N3-C2-N1	-5.15	120.63	128.68
5	A	501[A]	ADP	N3-C2-N1	-4.81	121.16	128.68
5	A	501[B]	ADP	N3-C2-N1	-4.81	121.16	128.68
5	D	504[B]	ADP	N3-C2-N1	-4.72	121.30	128.68
5	D	504[A]	ADP	N3-C2-N1	-4.72	121.30	128.68
5	F	506[A]	ADP	N3-C2-N1	-4.57	121.53	128.68
5	F	506[B]	ADP	N3-C2-N1	-4.57	121.53	128.68
5	B	502[B]	ADP	N3-C2-N1	-4.55	121.56	128.68
5	B	502[A]	ADP	N3-C2-N1	-4.55	121.56	128.68
5	C	503[A]	ADP	N3-C2-N1	-4.39	121.82	128.68
5	C	503[B]	ADP	N3-C2-N1	-4.39	121.82	128.68
5	G	507[B]	ADP	N3-C2-N1	-4.34	121.90	128.68
5	G	507[A]	ADP	N3-C2-N1	-4.34	121.90	128.68
5	C	503[A]	ADP	C4-C5-N7	-2.68	106.61	109.40
5	C	503[B]	ADP	C4-C5-N7	-2.68	106.61	109.40
5	F	506[A]	ADP	C4-C5-N7	-2.48	106.81	109.40
5	F	506[B]	ADP	C4-C5-N7	-2.48	106.81	109.40
5	D	504[B]	ADP	PA-O3A-PB	-2.48	124.32	132.83
5	B	502[B]	ADP	PA-O3A-PB	-2.30	124.94	132.83
5	H	508[B]	ADP	PA-O3A-PB	-2.27	125.02	132.83
5	A	501[B]	ADP	PA-O3A-PB	-2.26	125.06	132.83
5	E	505[A]	ADP	C4-C5-N7	-2.18	107.13	109.40
5	E	505[B]	ADP	C4-C5-N7	-2.18	107.13	109.40
5	G	507[B]	ADP	PA-O3A-PB	-2.17	125.39	132.83
5	B	502[B]	ADP	C4-C5-N7	-2.15	107.16	109.40
5	B	502[A]	ADP	C4-C5-N7	-2.15	107.16	109.40
5	A	501[A]	ADP	C4-C5-N7	-2.10	107.21	109.40
5	A	501[B]	ADP	C4-C5-N7	-2.10	107.21	109.40
5	E	505[A]	ADP	O3B-PB-O2B	2.06	115.53	107.64
3	A	801	GAI	N3-C-N2	2.04	120.98	116.13
3	F	826	GAI	N3-C-N2	2.03	120.97	116.13
5	G	507[B]	ADP	C1'-N9-C4	-2.01	123.12	126.64
5	G	507[A]	ADP	C1'-N9-C4	-2.01	123.12	126.64

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	506[A]	ADP	PA-O3A-PB-O2B
5	F	506[A]	ADP	PA-O3A-PB-O3B
5	F	506[A]	ADP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	501[A]	ADP	C5'-O5'-PA-O1A
5	A	501[A]	ADP	C5'-O5'-PA-O2A
5	C	503[A]	ADP	C5'-O5'-PA-O2A
5	D	504[A]	ADP	PA-O3A-PB-O2B
5	E	505[A]	ADP	PA-O3A-PB-O2B
5	E	505[A]	ADP	C5'-O5'-PA-O2A
5	H	508[A]	ADP	PA-O3A-PB-O2B
5	H	508[A]	ADP	C5'-O5'-PA-O2A
5	B	502[A]	ADP	PA-O3A-PB-O2B
5	B	502[A]	ADP	C5'-O5'-PA-O2A
5	C	503[B]	ADP	PB-O3A-PA-O5'
5	G	507[A]	ADP	PA-O3A-PB-O2B
5	G	507[A]	ADP	PA-O3A-PB-O3B
5	G	507[A]	ADP	C5'-O5'-PA-O2A
4	C	963	EDO	O1-C1-C2-O2
5	H	508[B]	ADP	PB-O3A-PA-O5'
5	H	508[A]	ADP	PA-O3A-PB-O3B
5	F	506[A]	ADP	C5'-O5'-PA-O3A
5	C	503[A]	ADP	C5'-O5'-PA-O3A
5	E	505[A]	ADP	C5'-O5'-PA-O3A
5	H	508[A]	ADP	C5'-O5'-PA-O3A
5	B	502[A]	ADP	C5'-O5'-PA-O3A
5	G	507[A]	ADP	C5'-O5'-PA-O3A
5	F	506[A]	ADP	C5'-O5'-PA-O1A
5	C	503[A]	ADP	C5'-O5'-PA-O1A
5	E	505[A]	ADP	C5'-O5'-PA-O1A
5	H	508[A]	ADP	C5'-O5'-PA-O1A
5	B	502[A]	ADP	C5'-O5'-PA-O1A
5	G	507[A]	ADP	C5'-O5'-PA-O1A
4	A	921	EDO	O1-C1-C2-O2
4	E	905	EDO	O1-C1-C2-O2
4	H	928	EDO	O1-C1-C2-O2
5	F	506[A]	ADP	PB-O3A-PA-O1A
5	A	501[A]	ADP	PB-O3A-PA-O1A
5	G	507[B]	ADP	PB-O3A-PA-O5'
5	E	505[A]	ADP	PA-O3A-PB-O1B
5	H	508[A]	ADP	PA-O3A-PB-O1B
5	B	502[A]	ADP	PA-O3A-PB-O1B
5	G	507[A]	ADP	PA-O3A-PB-O1B
5	C	503[A]	ADP	PA-O3A-PB-O3B
5	D	504[A]	ADP	PA-O3A-PB-O3B
5	E	505[A]	ADP	PA-O3A-PB-O3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	502[A]	ADP	PA-O3A-PB-O3B
5	A	501[A]	ADP	C5'-O5'-PA-O3A
5	D	504[A]	ADP	C5'-O5'-PA-O3A
5	F	506[A]	ADP	PB-O3A-PA-O2A
5	D	504[A]	ADP	PB-O3A-PA-O1A
5	D	504[A]	ADP	C5'-O5'-PA-O1A
4	C	903	EDO	O1-C1-C2-O2

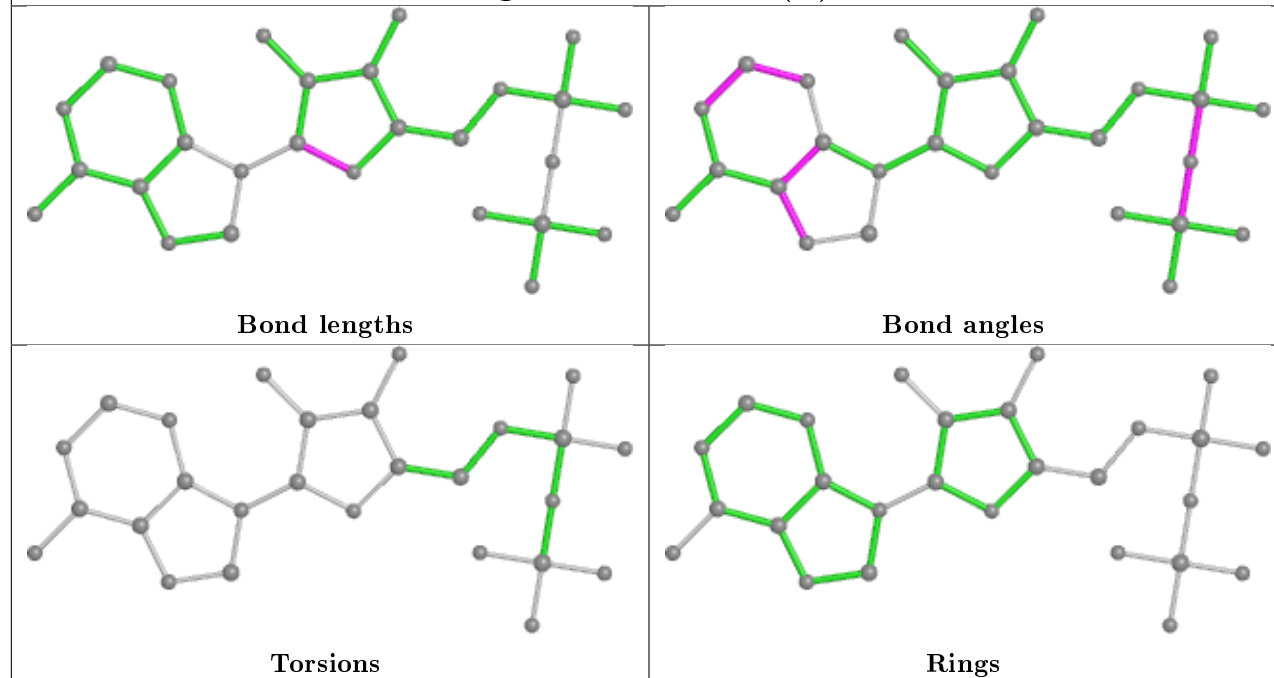
There are no ring outliers.

4 monomers are involved in 5 short contacts:

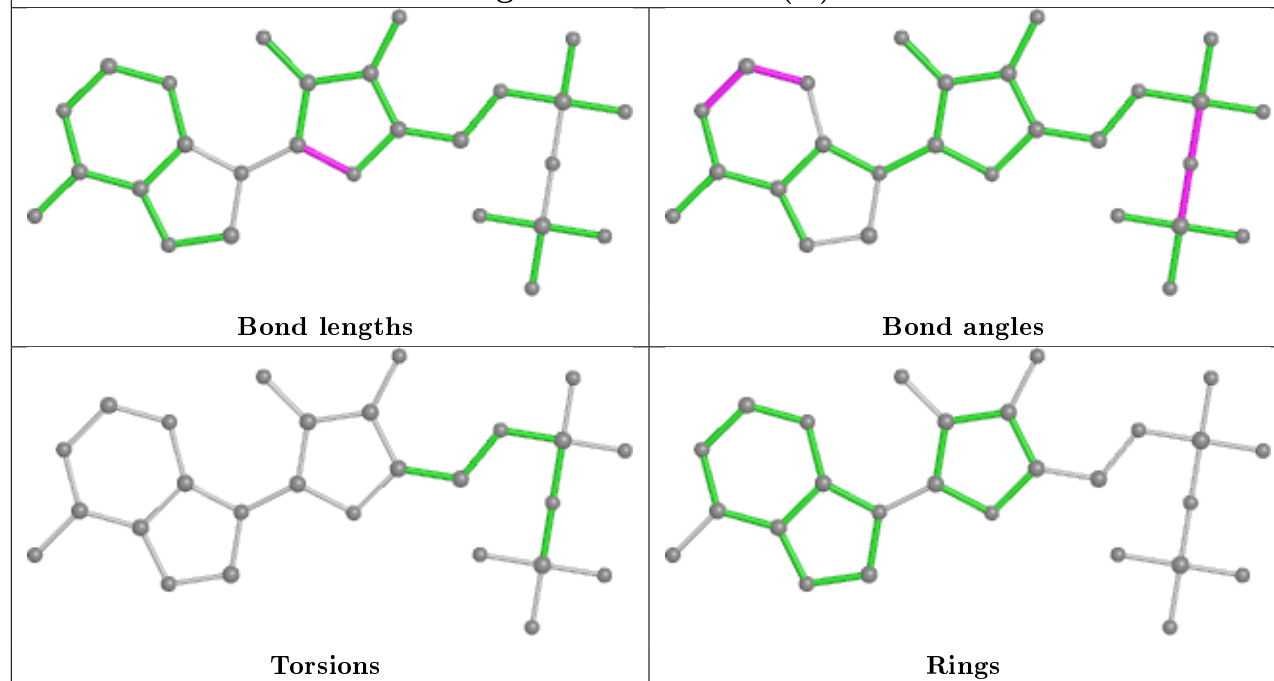
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	503[B]	ADP	1	0
4	F	946	EDO	2	0
5	G	507[B]	ADP	1	0
4	E	905	EDO	1	0

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

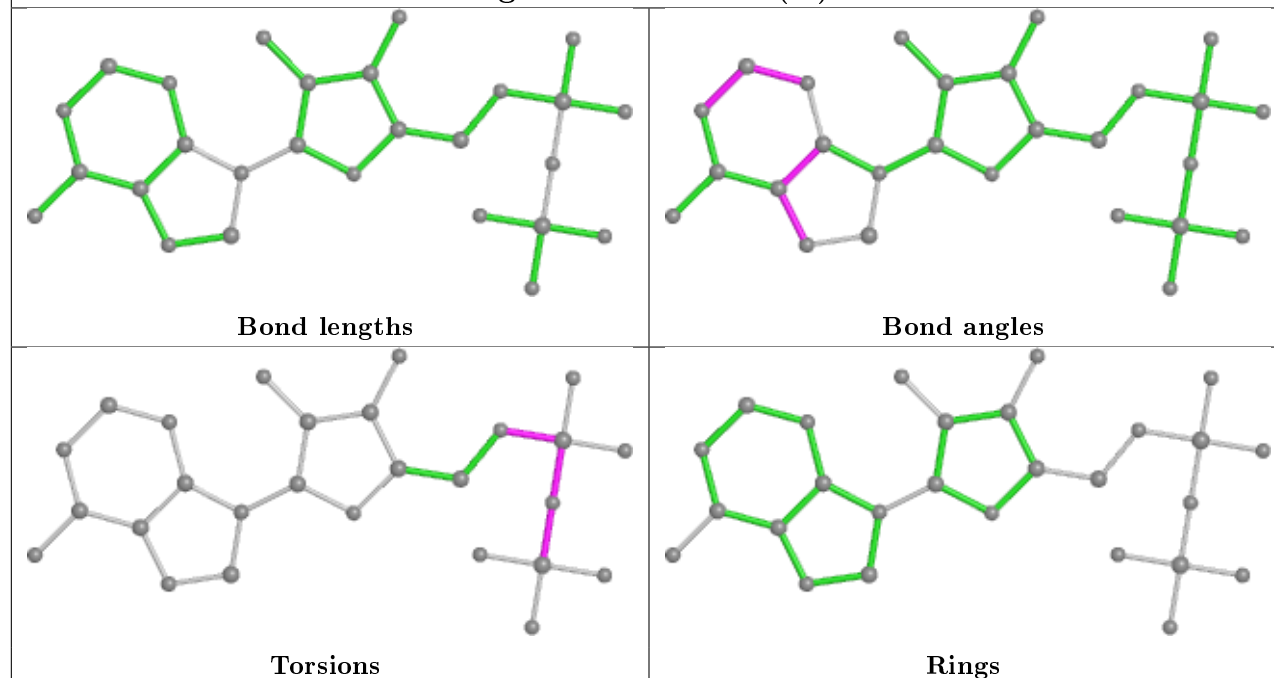
Ligand ADP B 502 (B)



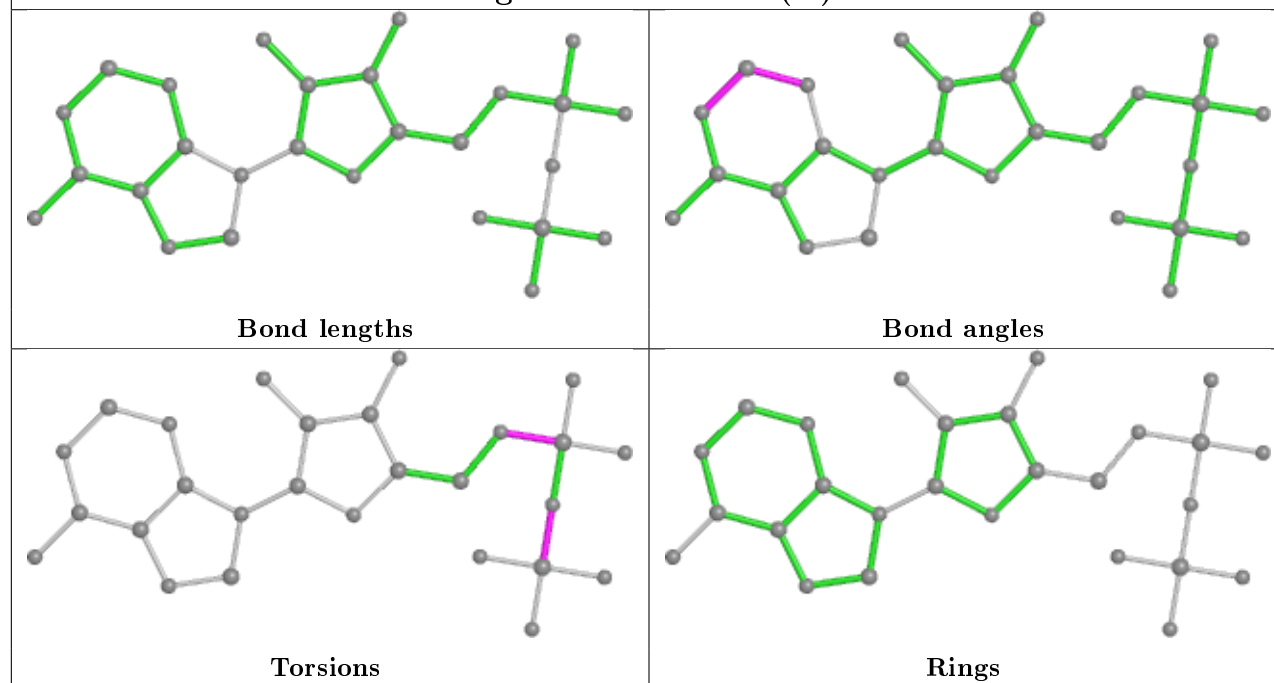
Ligand ADP D 504 (B)



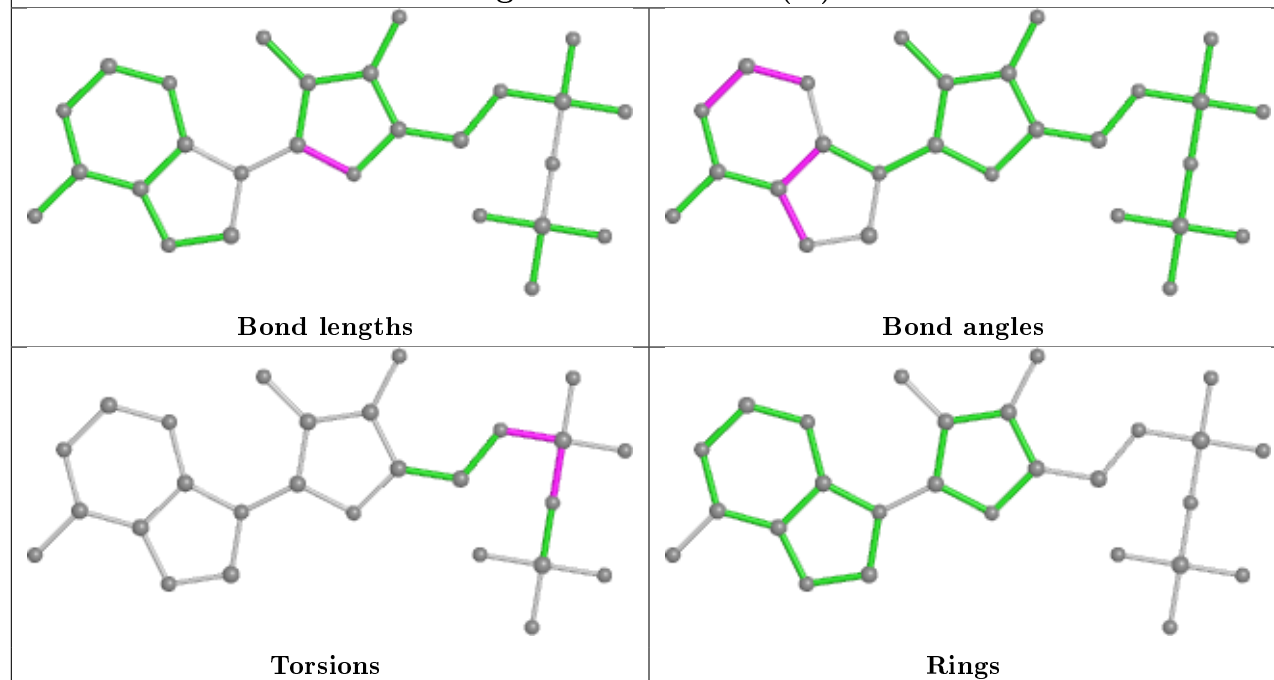
Ligand ADP F 506 (A)



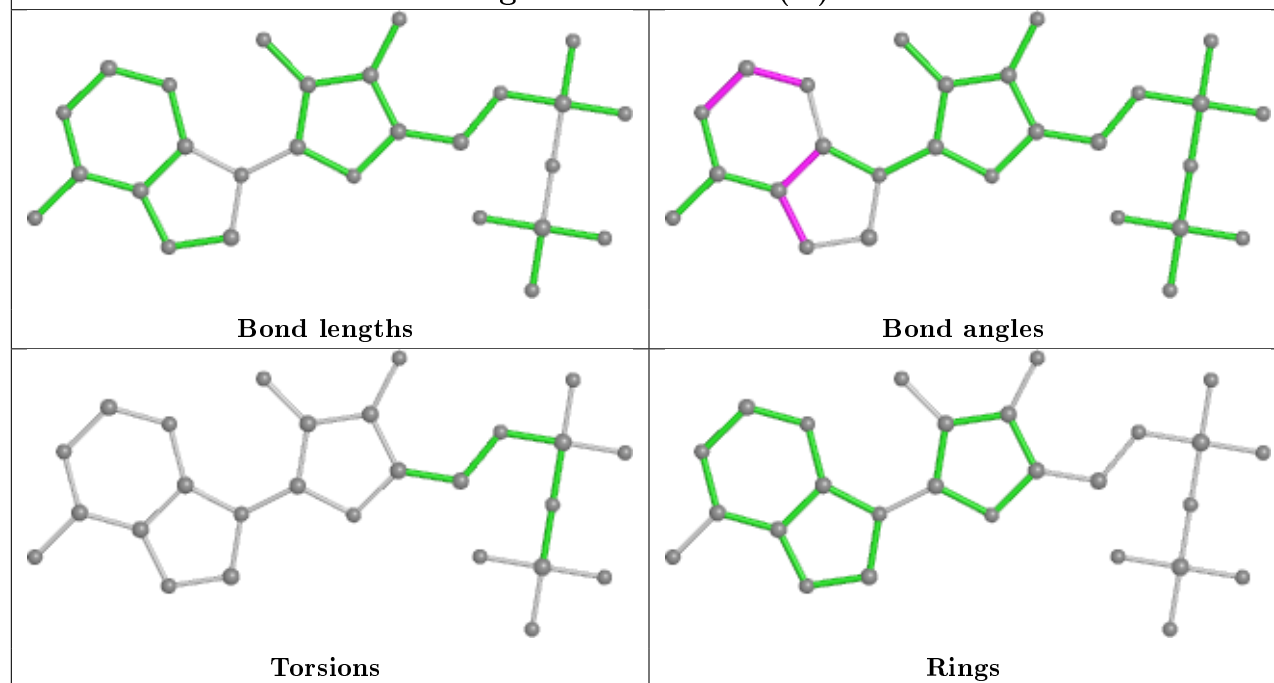
Ligand ADP H 508 (A)



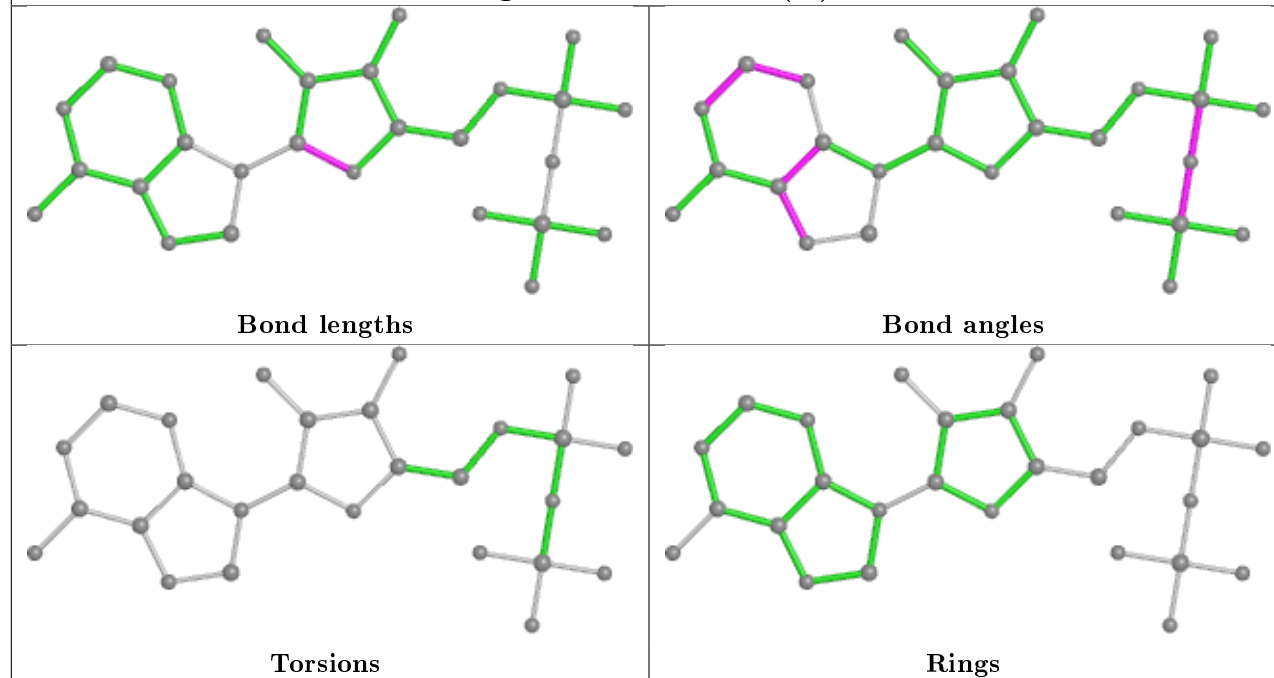
Ligand ADP A 501 (A)



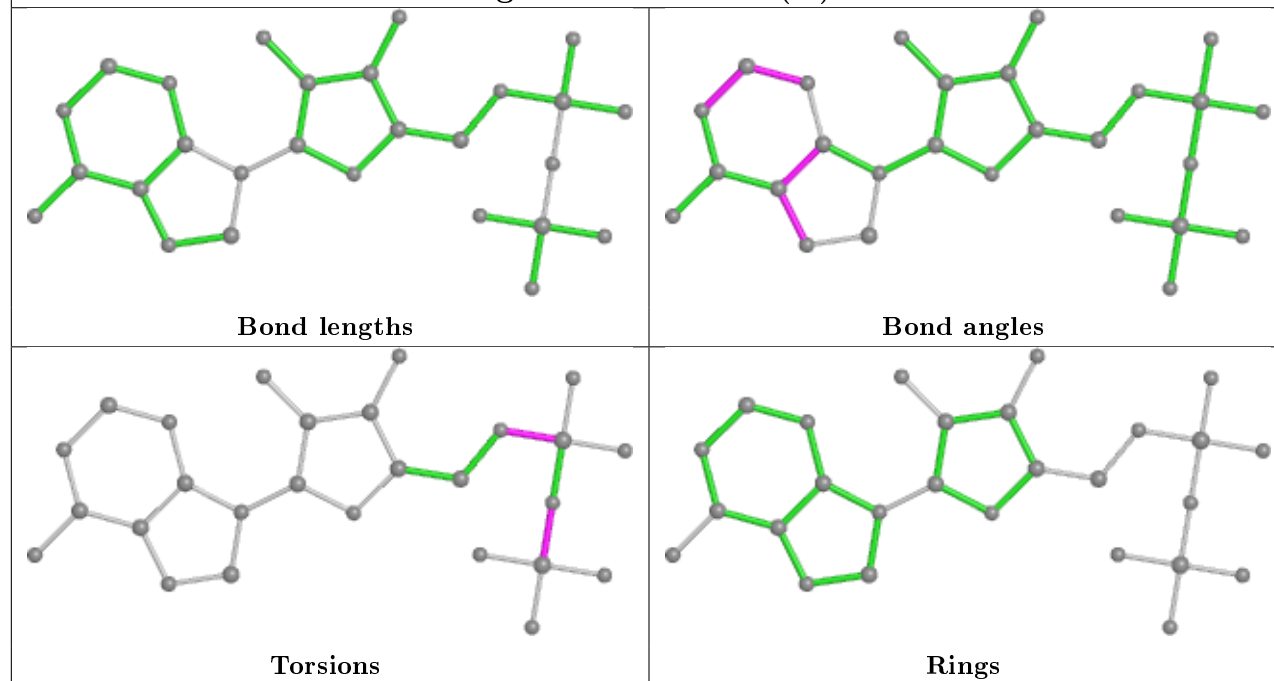
Ligand ADP F 506 (B)



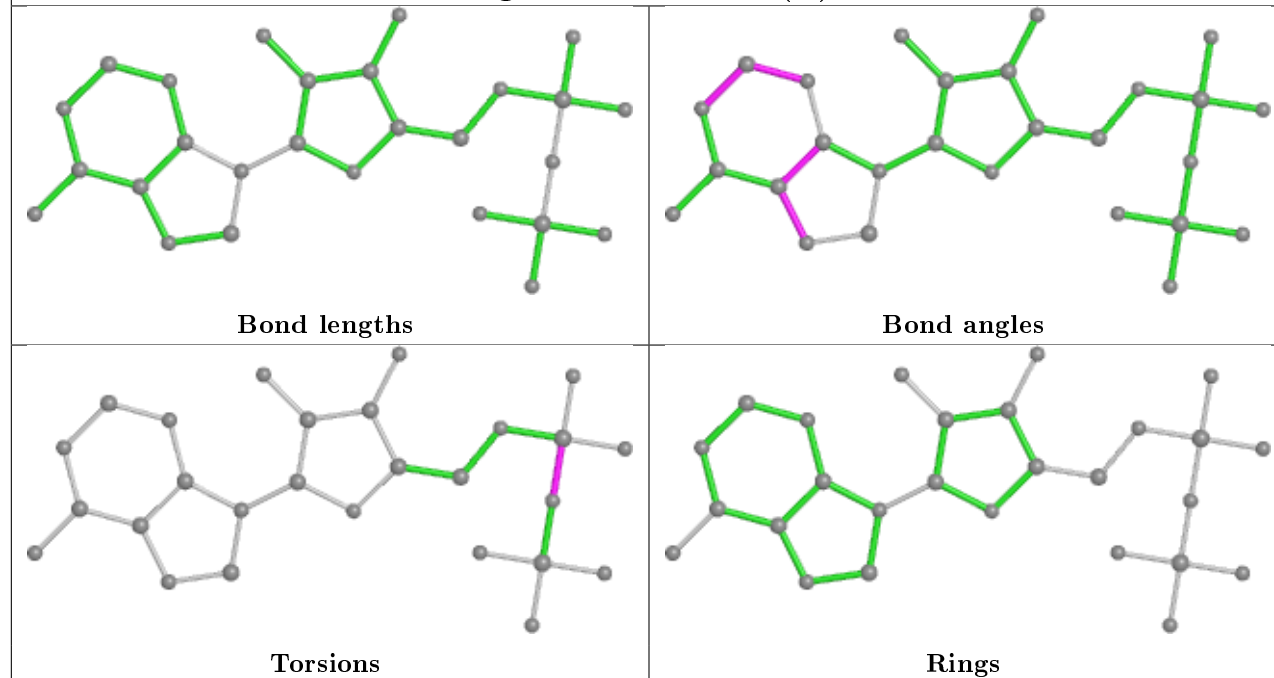
Ligand ADP A 501 (B)



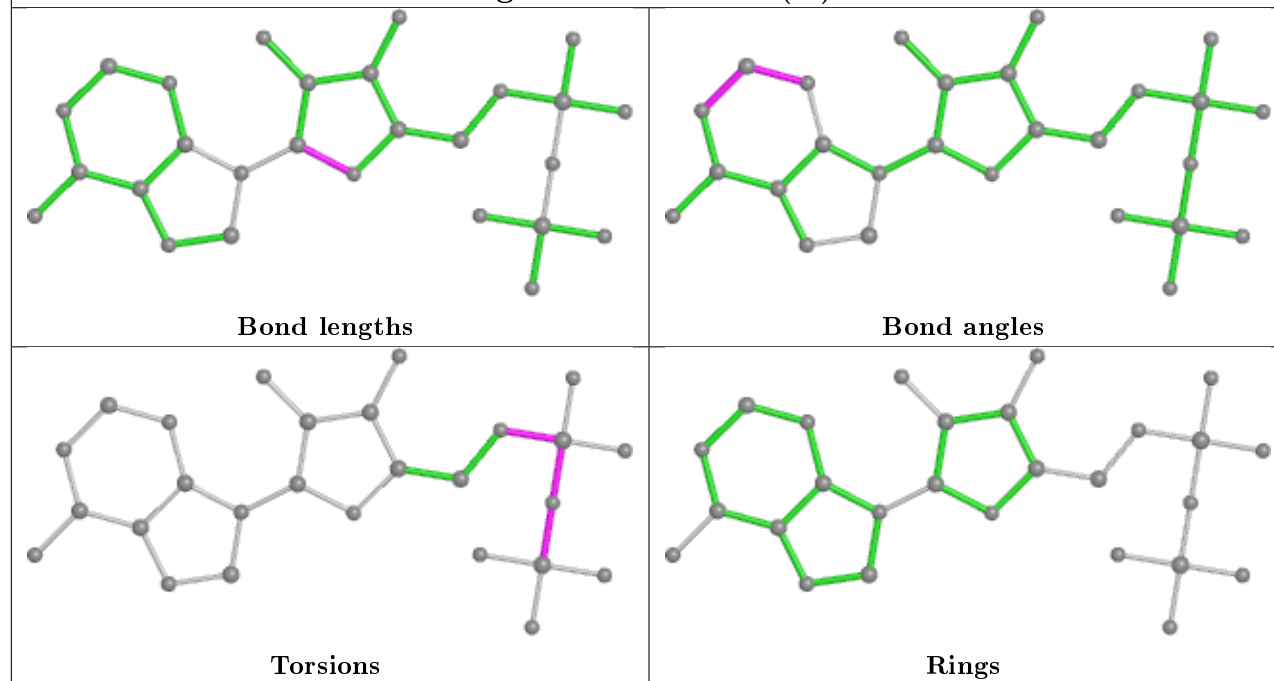
Ligand ADP C 503 (A)



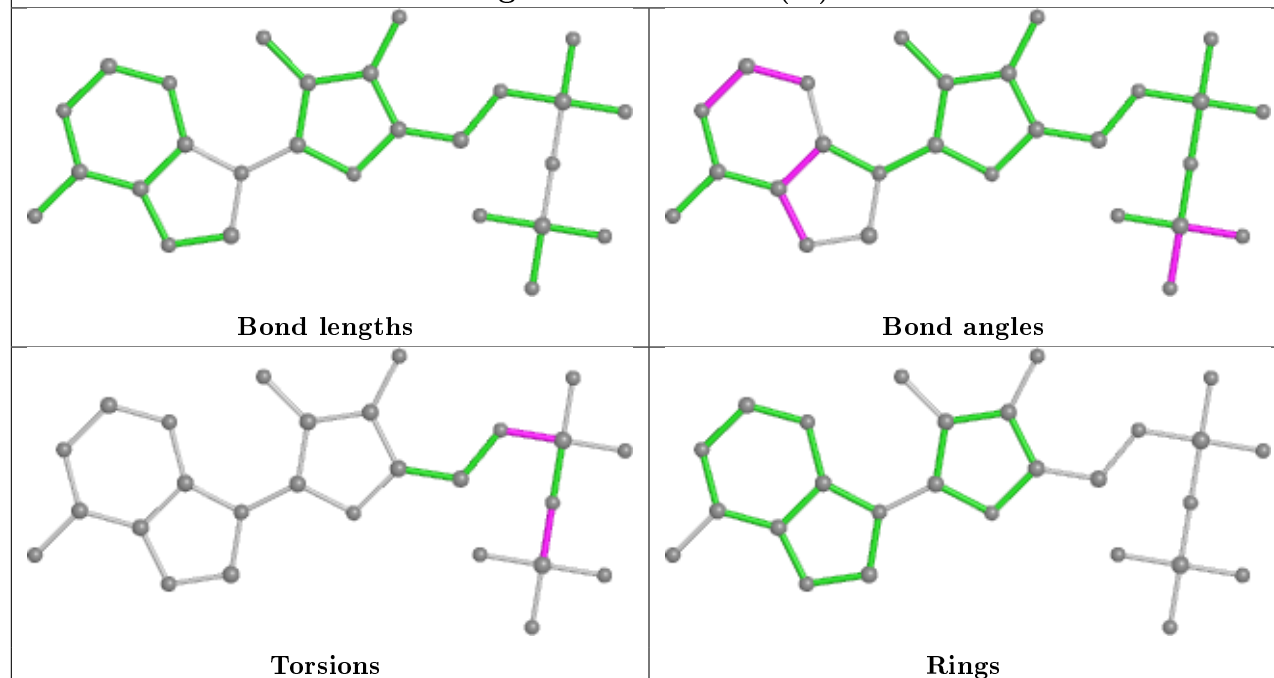
Ligand ADP C 503 (B)



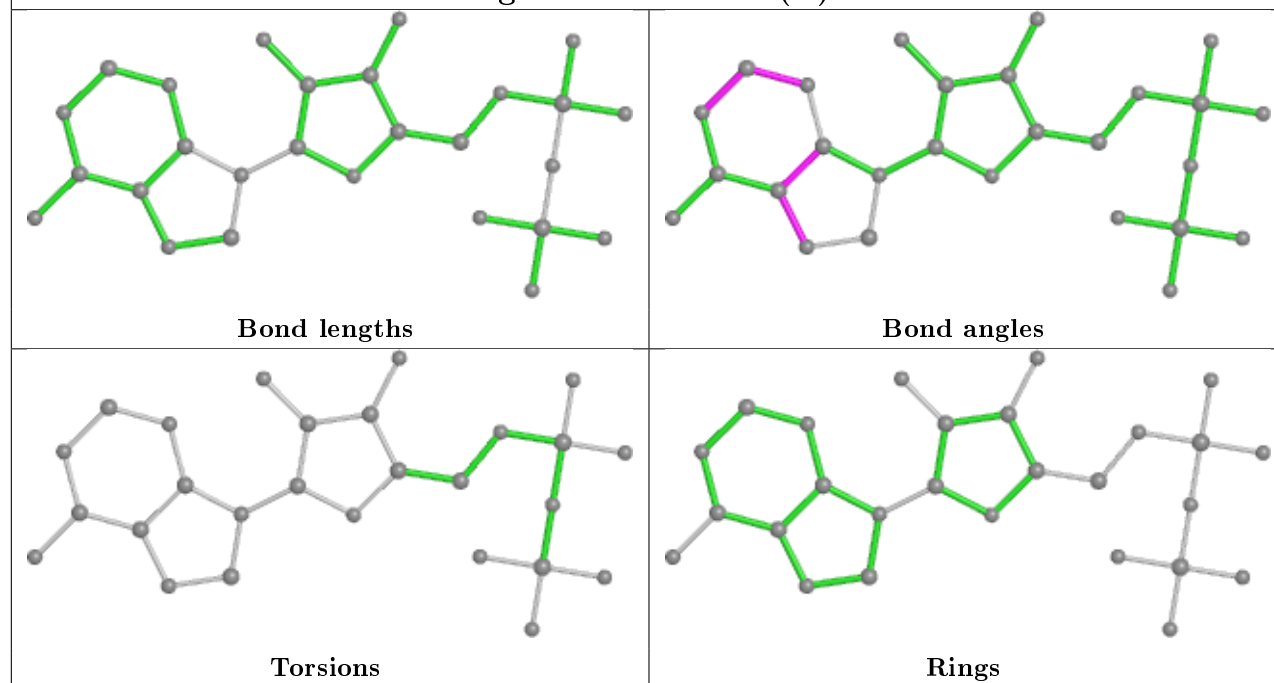
Ligand ADP D 504 (A)



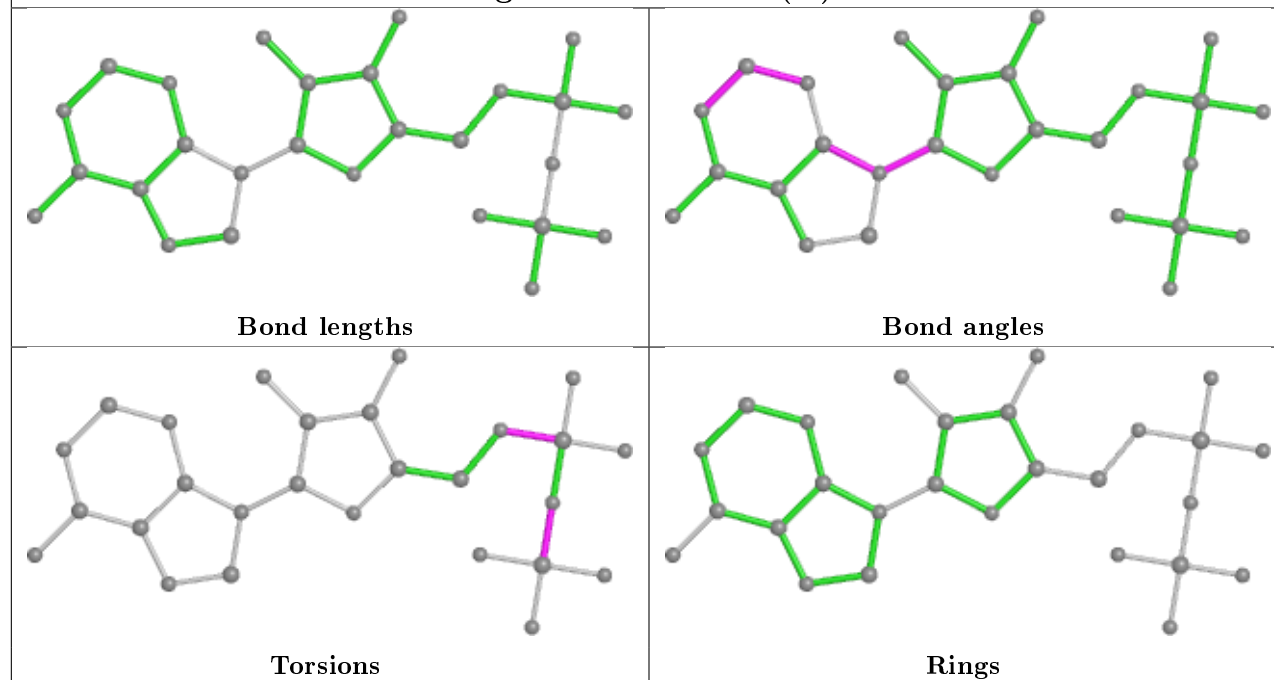
Ligand ADP E 505 (A)



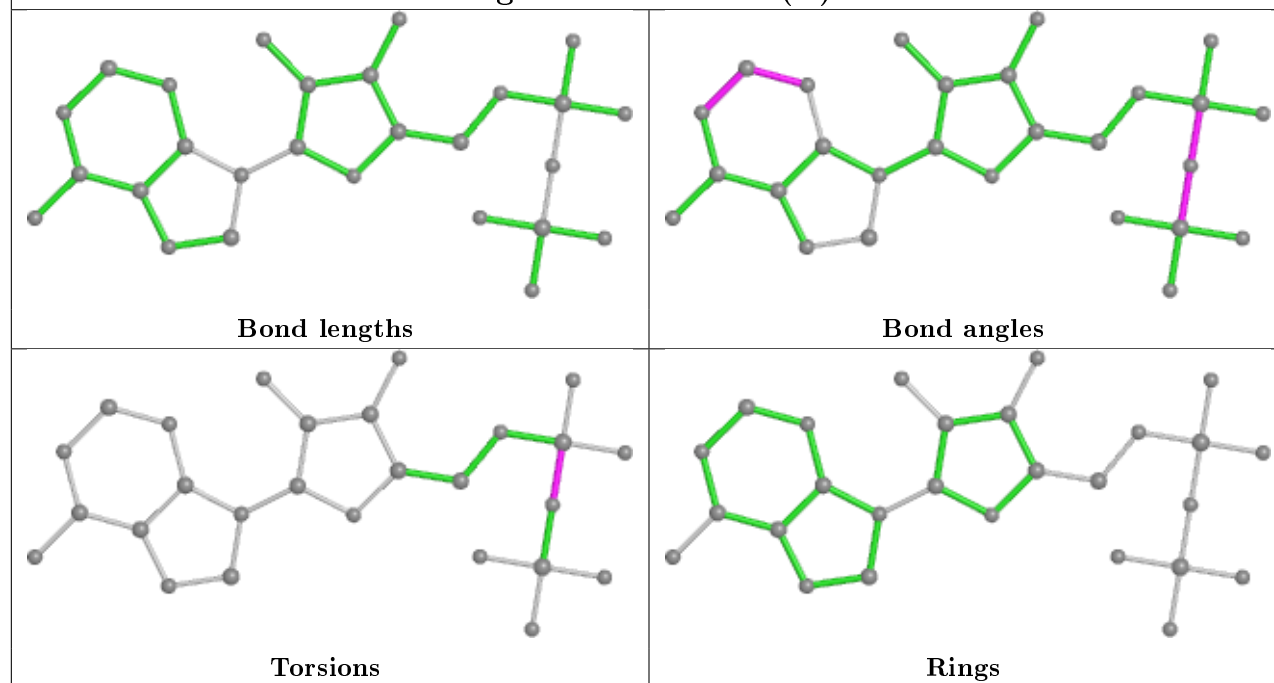
Ligand ADP E 505 (B)

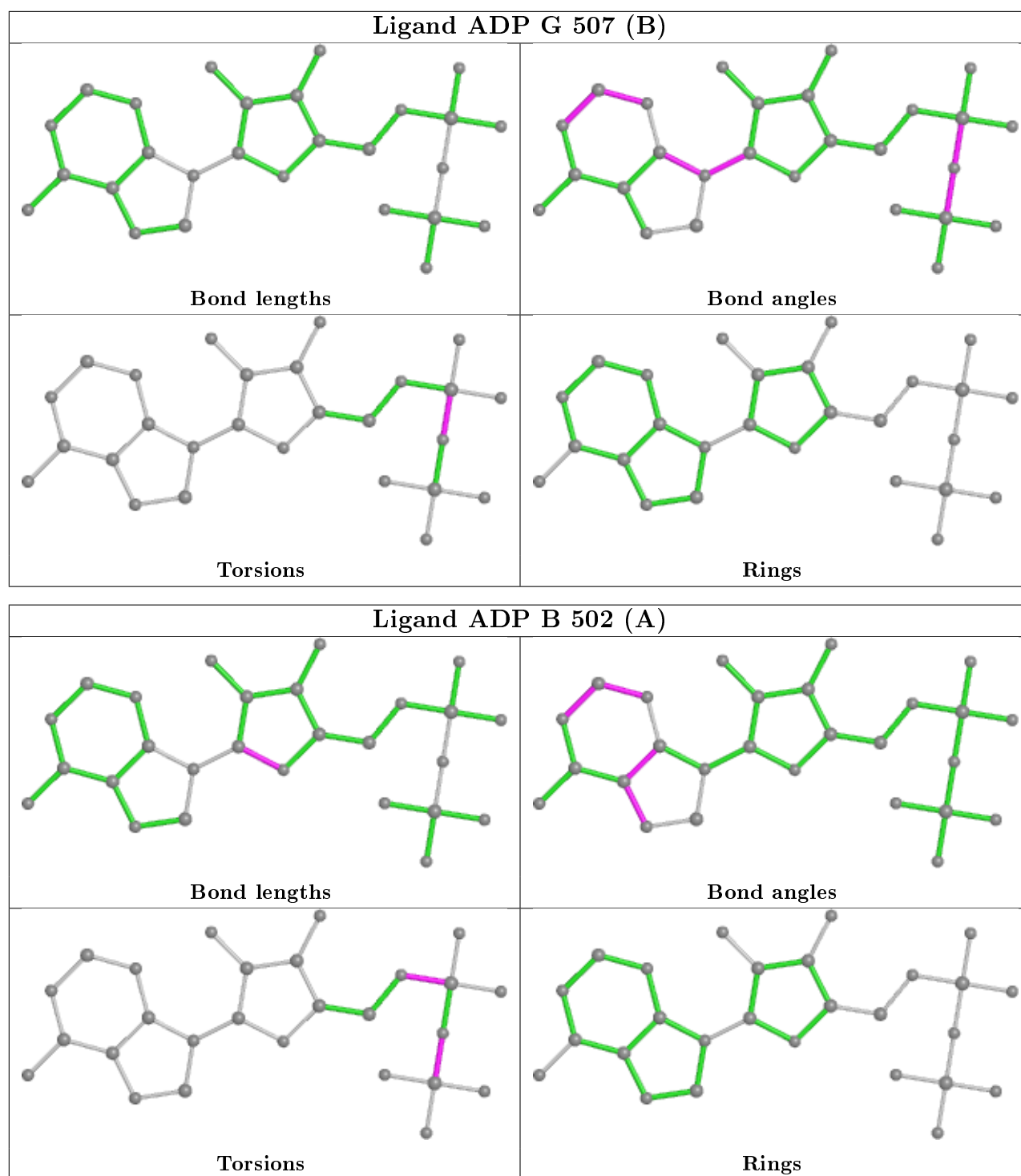


Ligand ADP G 507 (A)



Ligand ADP H 508 (B)





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	494/500 (98%)	-0.03	7 (1%) 75 77	15, 23, 32, 40	0
1	B	494/500 (98%)	-0.13	4 (0%) 86 87	15, 21, 31, 39	0
1	C	494/500 (98%)	-0.29	1 (0%) 95 95	12, 18, 26, 34	0
1	D	494/500 (98%)	-0.18	3 (0%) 89 90	14, 21, 30, 38	0
1	E	494/500 (98%)	-0.24	3 (0%) 89 90	13, 19, 29, 44	0
1	F	494/500 (98%)	-0.33	1 (0%) 95 95	12, 17, 24, 33	0
1	G	494/500 (98%)	-0.17	2 (0%) 92 93	13, 19, 28, 36	0
1	H	494/500 (98%)	-0.14	4 (0%) 86 87	13, 20, 28, 39	0
All	All	3952/4000 (98%)	-0.19	25 (0%) 89 90	12, 20, 29, 44	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ALA	7.6
1	A	7	ALA	4.8
1	H	7	ALA	4.5
1	G	7	ALA	4.3
1	H	483[A]	GLN	3.4
1	E	376	ASP	3.2
1	D	7	ALA	3.0
1	D	376	ASP	2.9
1	A	226	PRO	2.8
1	A	483[A]	GLN	2.7
1	H	376	ASP	2.7
1	H	264[A]	ARG	2.6
1	B	139	TYR	2.4
1	A	264[A]	ARG	2.4
1	B	483[A]	GLN	2.4
1	B	264[A]	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	377	ARG	2.3
1	G	14	GLN	2.3
1	C	7	ALA	2.2
1	D	338	LYS	2.2
1	A	14	GLN	2.1
1	F	7	ALA	2.1
1	A	34	ARG	2.0
1	A	377	ARG	2.0
1	E	483[A]	GLN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	EDO	F	946	4/4	0.82	0.31	26,32,33,39	0
5	ADP	A	501[A]	27/27	0.83	0.18	40,42,43,44	8
5	ADP	A	501[B]	27/27	0.83	0.18	40,42,43,44	8
3	GAI	D	814	4/4	0.83	0.16	34,35,35,36	0
4	EDO	H	928	4/4	0.84	0.17	39,40,41,41	0
5	ADP	B	502[A]	27/27	0.85	0.16	32,35,39,40	8
5	ADP	B	502[B]	27/27	0.85	0.16	32,35,38,39	8
3	GAI	B	812	4/4	0.85	0.19	29,30,30,31	0
4	EDO	A	911	4/4	0.86	0.15	44,44,45,45	0
4	EDO	C	963	4/4	0.87	0.14	40,41,41,42	0
4	EDO	A	921	4/4	0.88	0.13	43,43,43,44	0
5	ADP	F	506[B]	27/27	0.89	0.16	21,24,30,31	8
5	ADP	F	506[A]	27/27	0.89	0.16	21,24,28,28	8
3	GAI	G	817	4/4	0.89	0.19	37,38,38,38	0

Continued on next page...

Continued from previous page...

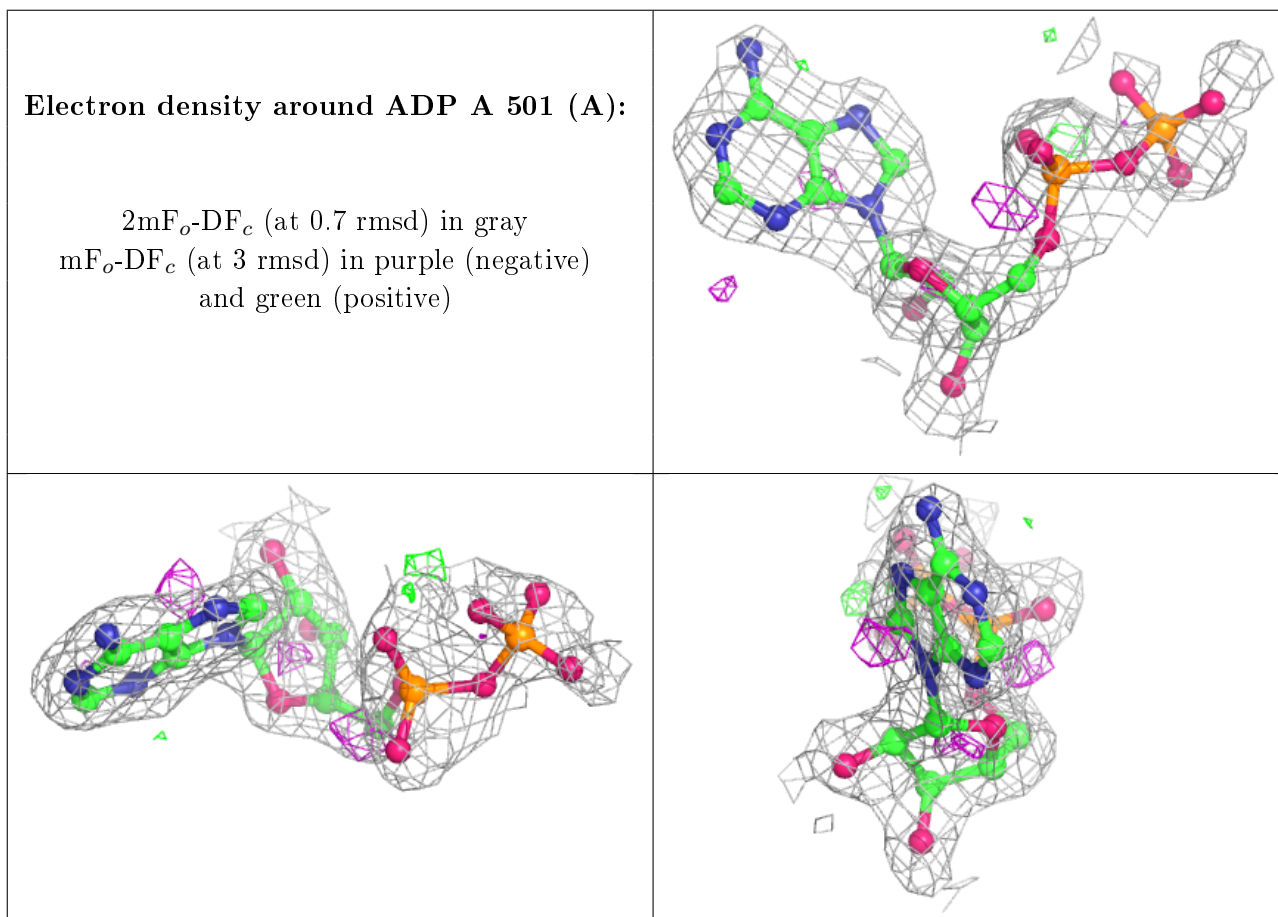
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ADP	H	508[B]	27/27	0.90	0.15	27,29,34,34	8
3	GAI	F	816	4/4	0.90	0.15	38,39,39,40	0
5	ADP	G	507[B]	27/27	0.90	0.14	26,31,35,35	8
5	ADP	D	504[B]	27/27	0.90	0.15	29,31,32,33	8
4	EDO	E	905	4/4	0.90	0.16	25,27,28,29	0
3	GAI	F	826	4/4	0.90	0.17	31,31,32,32	0
4	EDO	F	926	4/4	0.90	0.16	41,41,42,42	0
5	ADP	G	507[A]	27/27	0.90	0.14	26,31,39,39	8
5	ADP	D	504[A]	27/27	0.90	0.15	30,32,36,37	8
5	ADP	H	508[A]	27/27	0.90	0.15	27,29,35,35	8
4	EDO	D	904	4/4	0.91	0.11	26,26,27,28	0
4	EDO	G	917	4/4	0.91	0.19	33,35,36,37	0
5	ADP	C	503[B]	27/27	0.91	0.14	22,25,29,30	8
5	ADP	E	505[A]	27/27	0.91	0.15	23,25,34,35	8
5	ADP	E	505[B]	27/27	0.91	0.15	23,25,28,28	8
4	EDO	F	966	4/4	0.91	0.16	27,27,28,31	0
4	EDO	B	912	4/4	0.91	0.20	29,29,30,31	0
3	GAI	E	815	4/4	0.91	0.15	30,31,31,31	0
5	ADP	C	503[A]	27/27	0.91	0.14	22,25,31,31	8
4	EDO	D	944	4/4	0.91	0.15	26,31,31,34	0
4	EDO	C	923	4/4	0.91	0.16	43,43,43,45	0
4	EDO	C	913	4/4	0.92	0.12	24,28,29,29	0
4	EDO	A	901	4/4	0.92	0.14	27,27,28,29	0
4	EDO	E	915	4/4	0.93	0.14	28,28,28,29	0
3	GAI	H	808	4/4	0.93	0.11	19,20,20,20	0
3	GAI	E	805	4/4	0.93	0.10	21,21,22,23	0
2	NA	A	701	1/1	0.94	0.06	26,26,26,26	0
4	EDO	C	903	4/4	0.94	0.10	22,23,24,25	0
3	GAI	A	801	4/4	0.94	0.10	22,24,24,24	0
2	NA	G	707	1/1	0.94	0.07	20,20,20,20	0
3	GAI	C	803	4/4	0.95	0.12	19,20,20,20	0
3	GAI	G	838	4/4	0.95	0.19	27,27,27,28	0
3	GAI	G	807	4/4	0.95	0.10	18,18,19,20	0
3	GAI	D	833	4/4	0.95	0.18	26,27,27,27	0
3	GAI	D	804	4/4	0.95	0.10	18,20,20,21	0
4	EDO	H	908	4/4	0.95	0.10	21,23,23,25	0
4	EDO	G	927	4/4	0.95	0.13	40,42,43,45	0
3	GAI	F	806	4/4	0.95	0.09	17,18,19,20	0
2	NA	B	702	1/1	0.96	0.10	25,25,25,25	0
4	EDO	F	906	4/4	0.96	0.09	22,26,27,27	0
4	EDO	G	907	4/4	0.96	0.09	24,25,25,25	0
4	EDO	B	902	4/4	0.96	0.09	21,21,22,23	0

Continued on next page...

Continued from previous page...

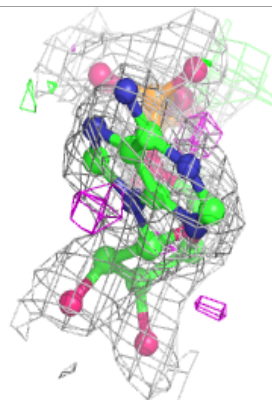
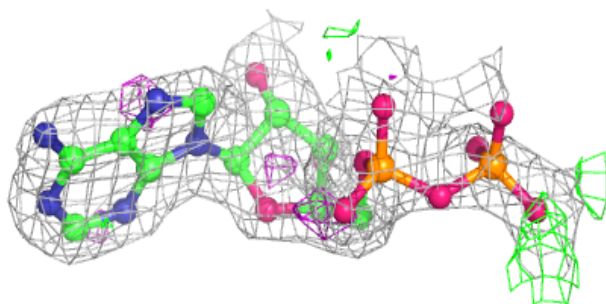
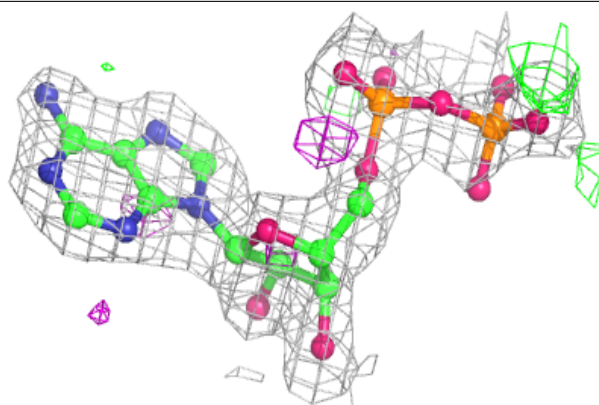
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GAI	B	802	4/4	0.96	0.07	23,23,23,23	0
2	NA	F	706	1/1	0.97	0.08	21,21,21,21	0
4	EDO	F	916	4/4	0.97	0.10	23,23,24,25	0
2	NA	C	703	1/1	0.97	0.14	26,26,26,26	0
2	NA	D	704	1/1	0.98	0.10	24,24,24,24	0
2	NA	H	708	1/1	0.98	0.07	20,20,20,20	0
2	NA	E	705	1/1	0.98	0.07	26,26,26,26	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.



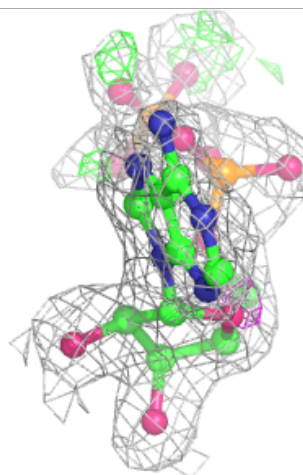
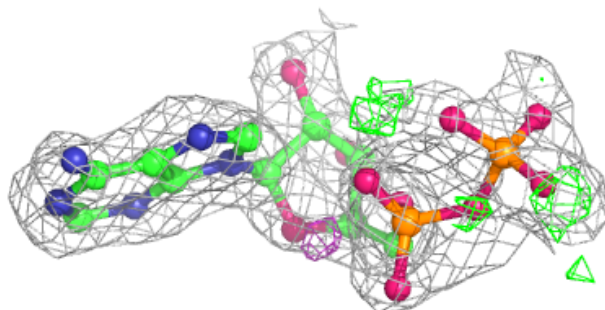
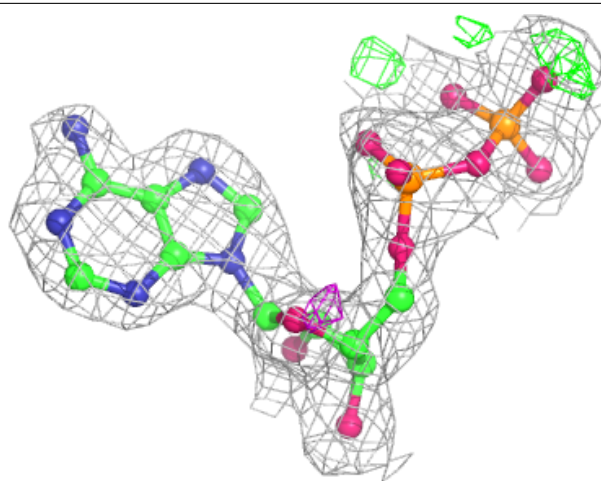
Electron density around ADP A 501 (B):

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



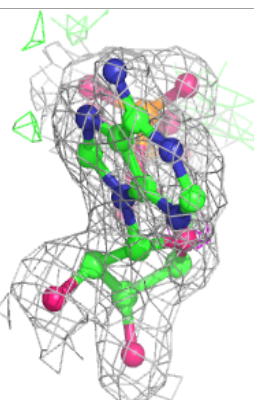
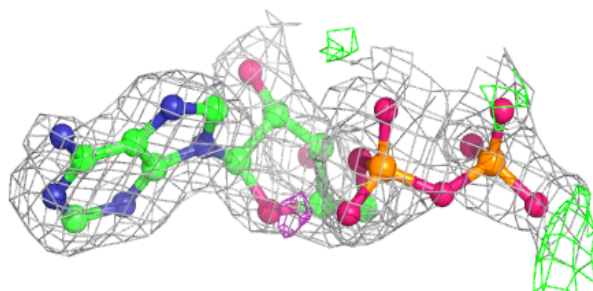
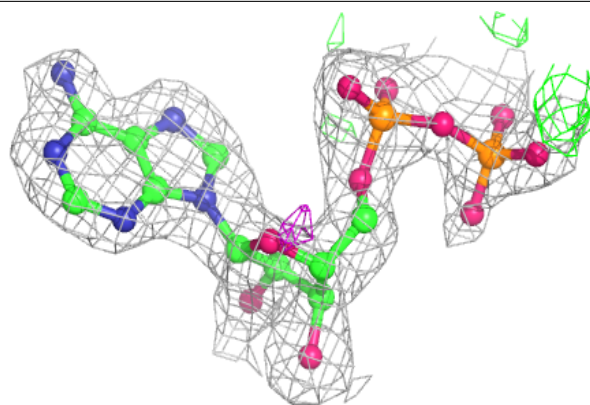
Electron density around ADP B 502 (A):

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

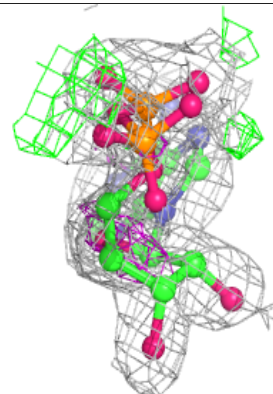
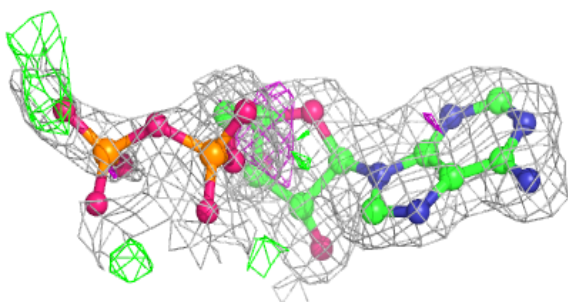
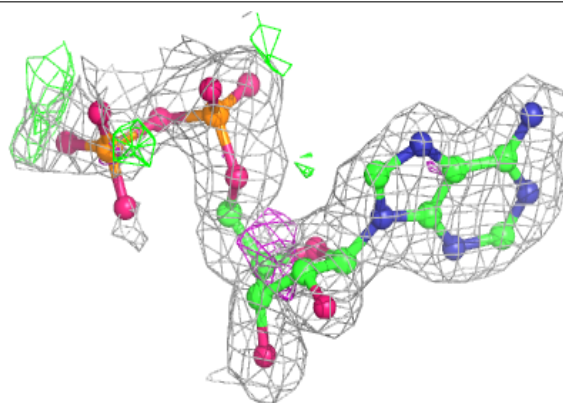


Electron density around ADP B 502 (B):

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

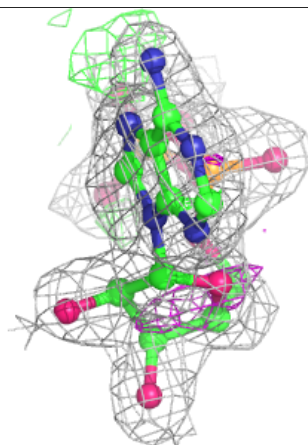
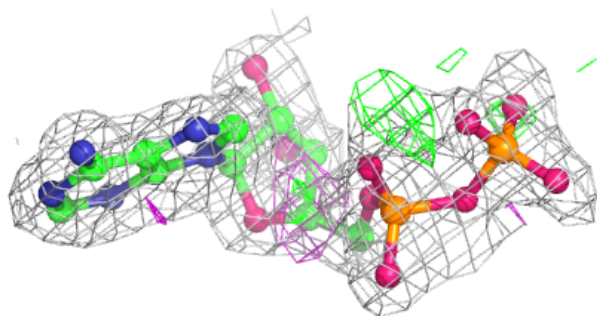
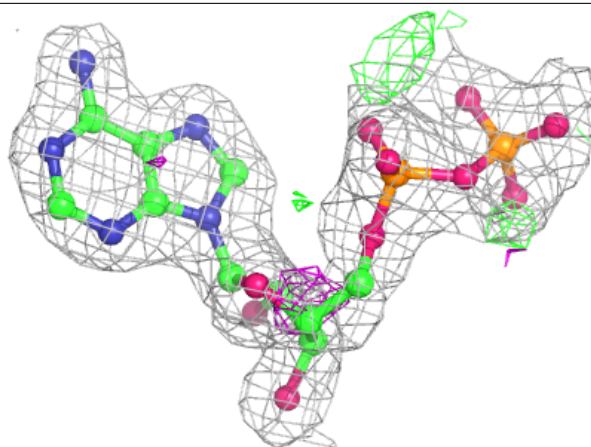
**Electron density around ADP F 506 (B):**

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

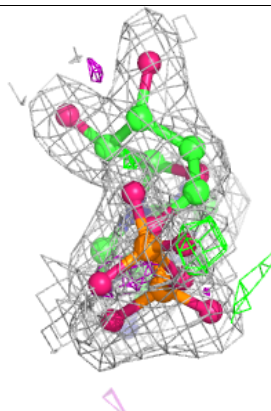
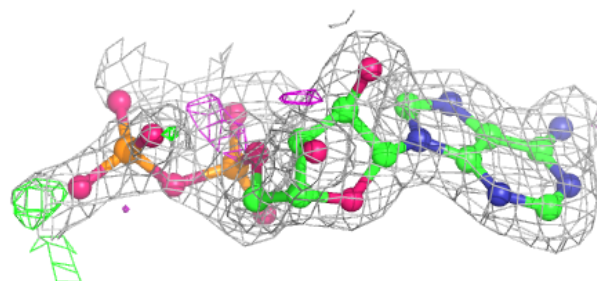
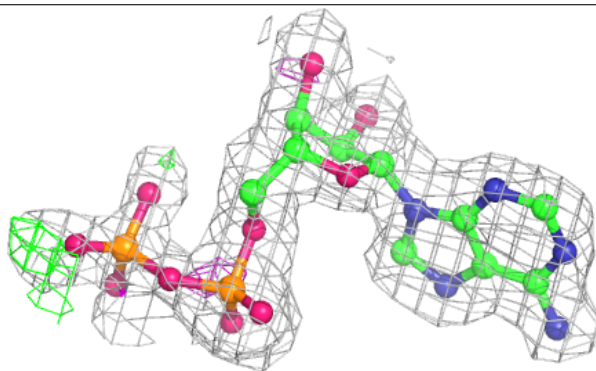


Electron density around ADP F 506 (A):

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

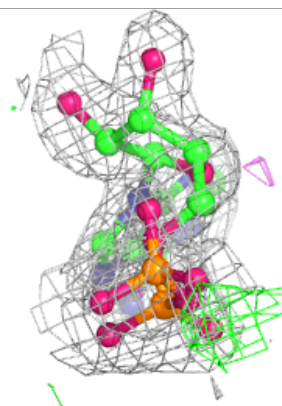
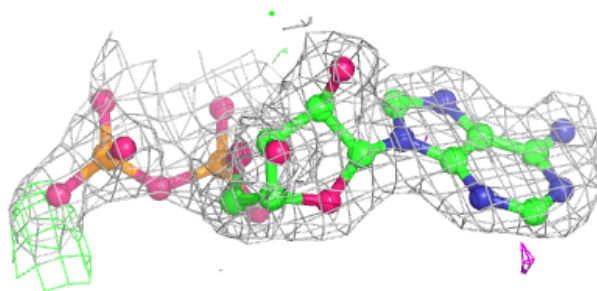
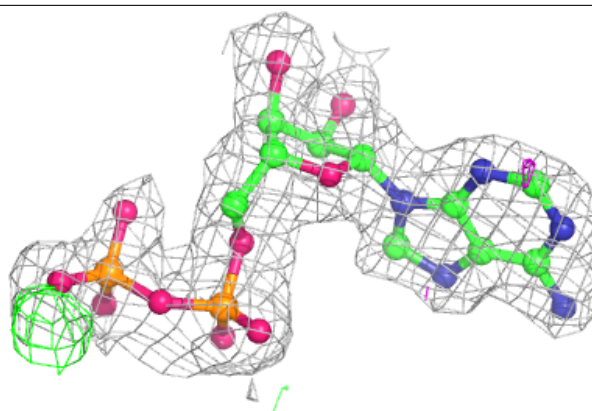
**Electron density around ADP H 508 (B):**

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

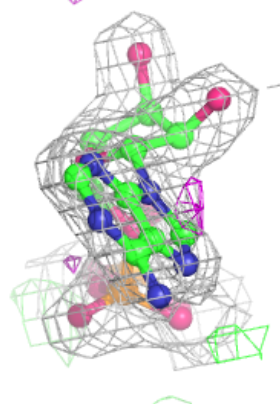
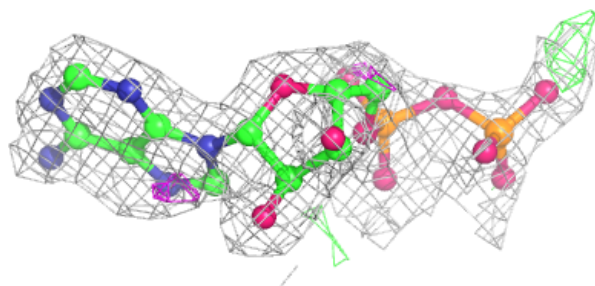
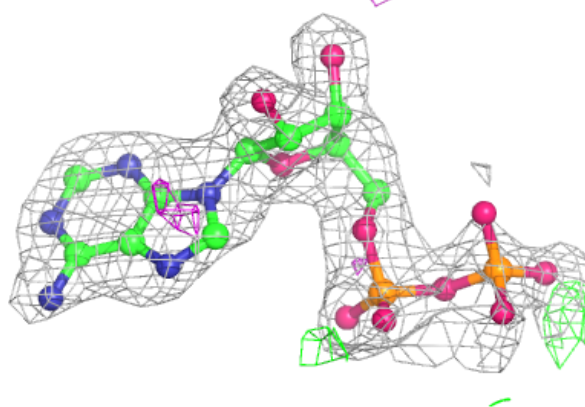


Electron density around ADP G 507 (B):

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

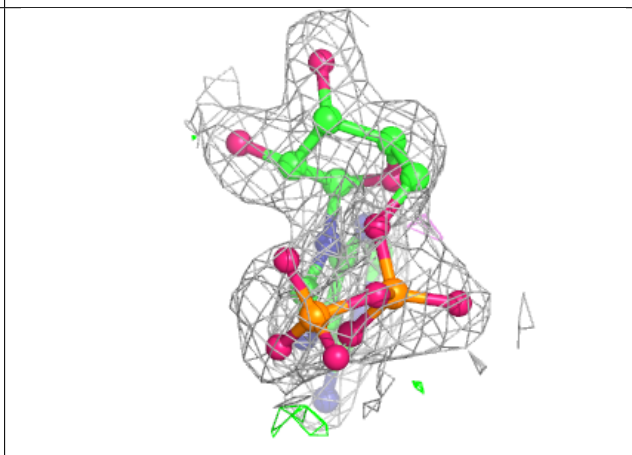
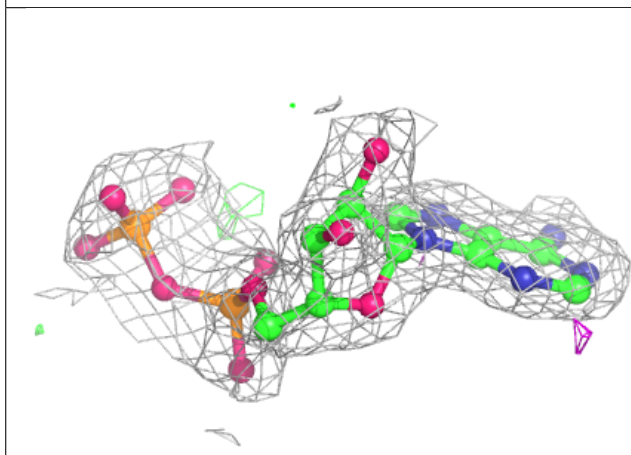
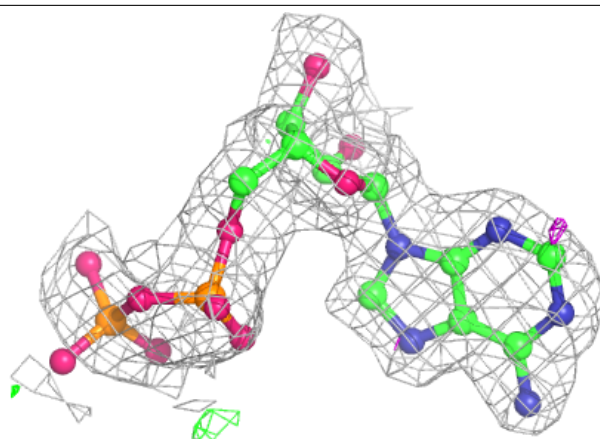
**Electron density around ADP D 504 (B):**

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



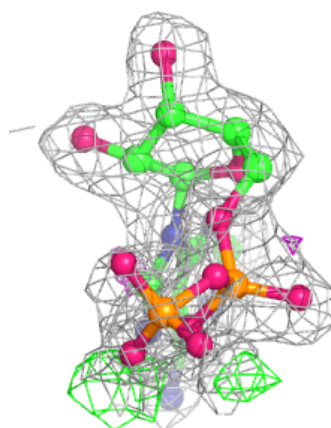
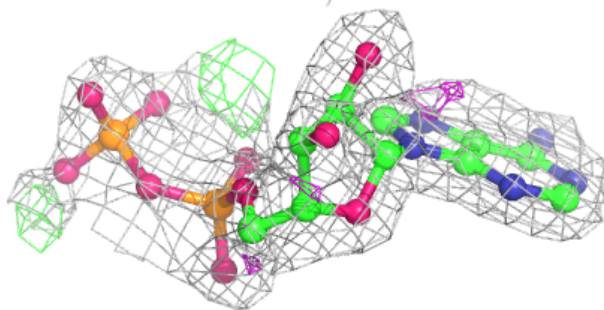
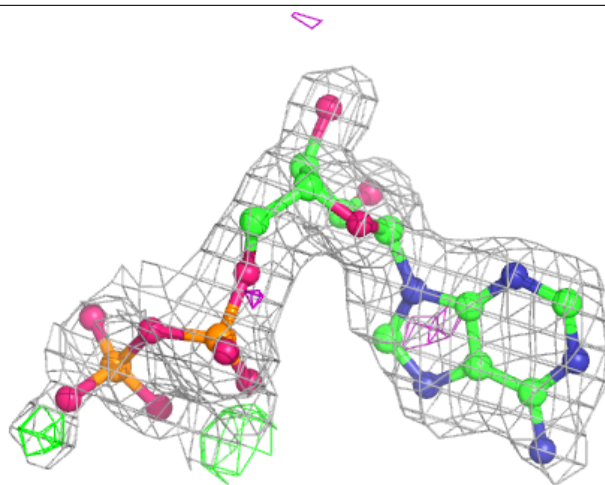
Electron density around ADP G 507 (A):

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



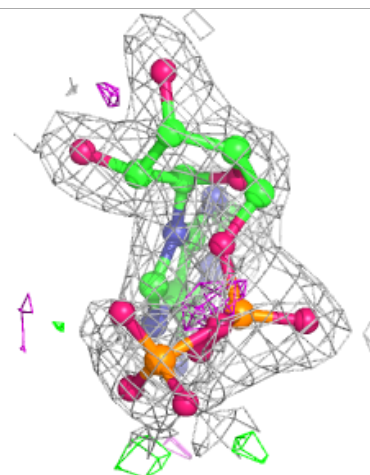
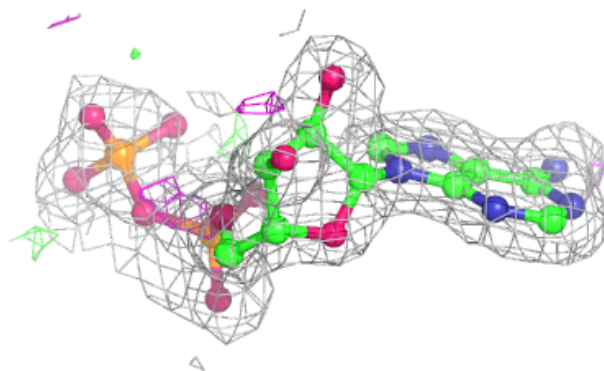
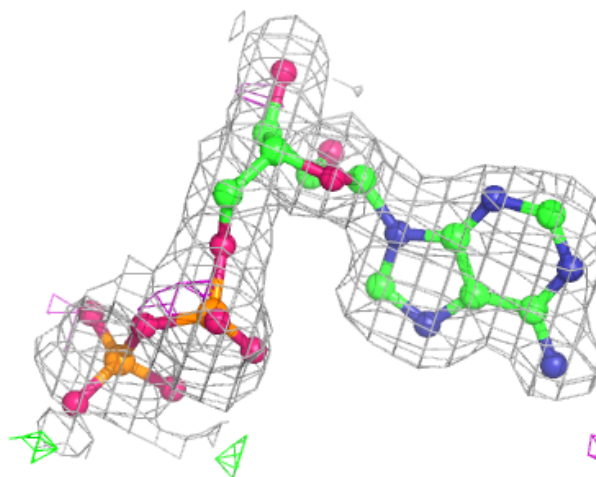
Electron density around ADP D 504 (A):

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



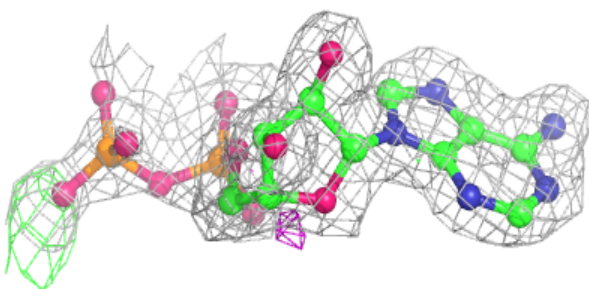
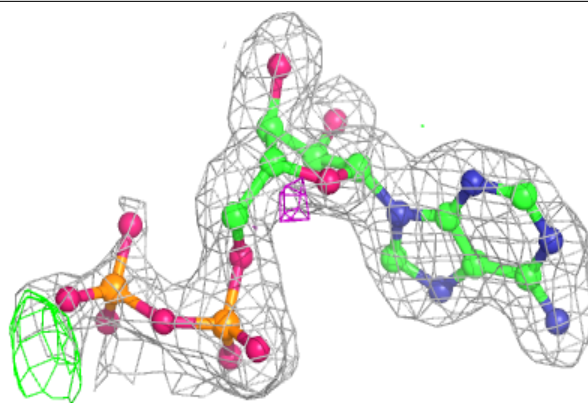
Electron density around ADP H 508 (A):

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



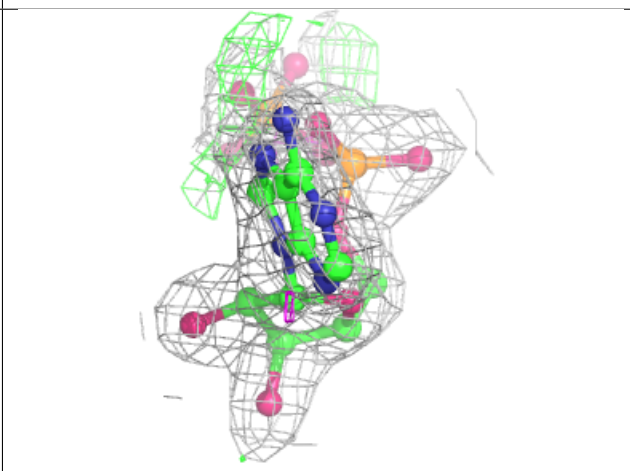
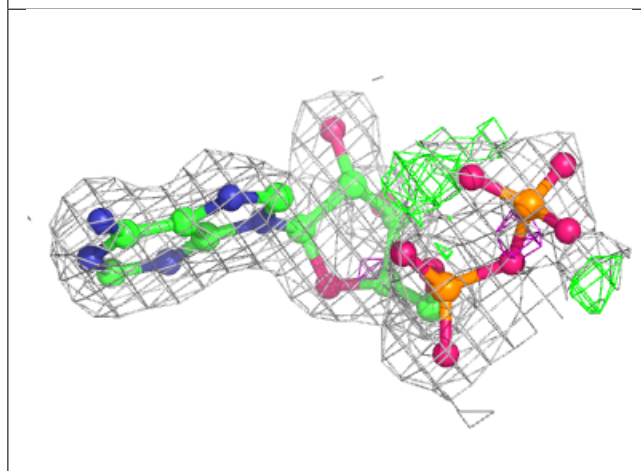
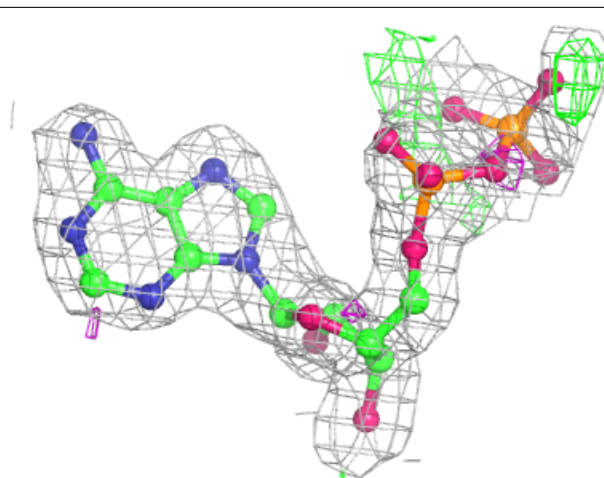
Electron density around ADP C 503 (B):

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



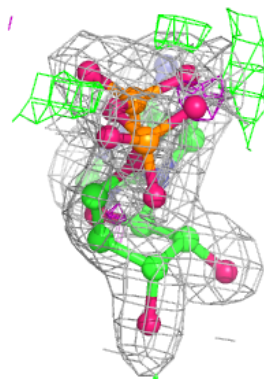
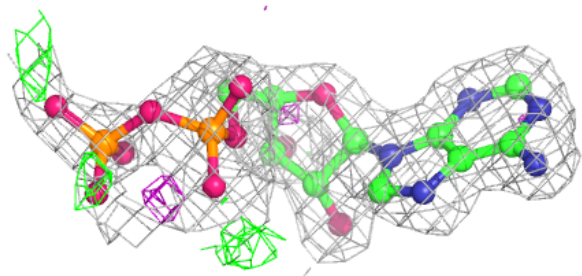
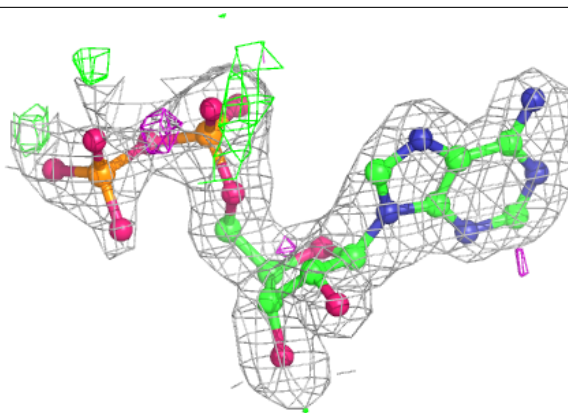
Electron density around ADP E 505 (A):

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

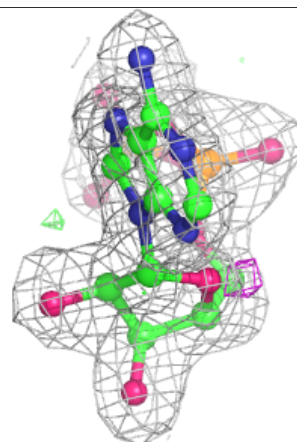
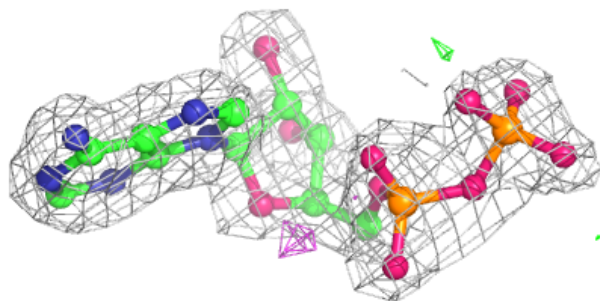
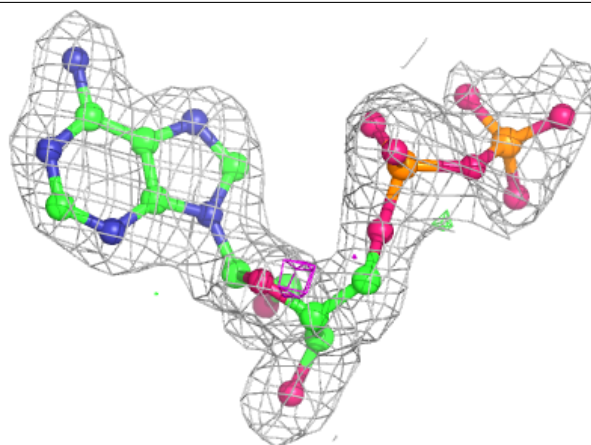


Electron density around ADP E 505 (B):

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

**Electron density around ADP C 503 (A):**

$2mF_o - DF_c$ (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.