



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 12:57 PM BST

PDB ID : 2DCN
Title : Crystal structure of 2-keto-3-deoxygluconate kinase from *Sulfolobus tokodaii* complexed with 2-keto-6-phosphogluconate (alpha-furanose form)
Authors : Okazaki, S.; Onda, H.; Suzuki, A.; Kuramitsu, S.; Masui, R.; Yamane, T.
Deposited on : 2006-01-10
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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	:	2.13.1
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)	:	2.13.1

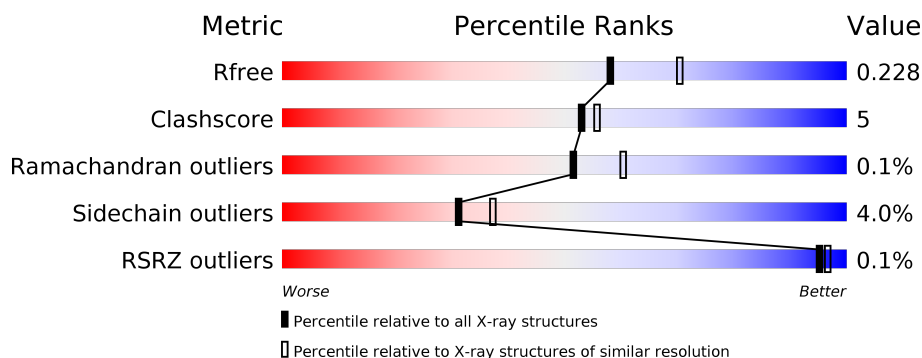
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	311	
1	B	311	
1	C	311	
1	D	311	
1	E	311	
1	F	311	

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Mol	Chain	Length	Quality of chain
1	G	311	<div> <div>%</div> <div> <div>84%13%..</div> </div> </div>
1	H	311	<div> <div>85%13%..</div> </div>
1	I	311	<div> <div>86%11%..</div> </div>
1	J	311	<div> <div>86%11%..</div> </div>
1	K	311	<div> <div>85%13%..</div> </div>
1	L	311	<div> <div>85%13%..</div> </div>

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
2	MG	G	4025	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31709 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 hypothetical fructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	3	0
			2432	1561	392	472	7			
1	B	308	Total	C	N	O	S	0	2	0
			2423	1555	390	471	7			
1	C	308	Total	C	N	O	S	0	3	0
			2432	1560	391	474	7			
1	D	308	Total	C	N	O	S	0	2	0
			2423	1555	390	471	7			
1	E	308	Total	C	N	O	S	0	2	0
			2423	1555	390	471	7			
1	F	308	Total	C	N	O	S	0	5	0
			2450	1571	394	478	7			
1	G	308	Total	C	N	O	S	0	0	0
			2405	1545	388	465	7			
1	H	308	Total	C	N	O	S	0	1	0
			2414	1550	389	468	7			
1	I	308	Total	C	N	O	S	0	4	0
			2441	1566	393	475	7			
1	J	308	Total	C	N	O	S	0	4	0
			2443	1567	396	473	7			
1	K	308	Total	C	N	O	S	0	5	0
			2452	1571	396	478	7			
1	L	308	Total	C	N	O	S	0	6	0
			2456	1574	395	479	8			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	6	Total	Mg	0	0
			6	6		
2	J	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	4	Total 4	Mg 4	0	0
2	K	3	Total 3	Mg 3	0	0
2	E	3	Total 3	Mg 3	0	0
2	H	3	Total 3	Mg 3	0	0
2	B	4	Total 5	Mg 5	0	1
2	I	3	Total 3	Mg 3	0	0
2	C	3	Total 3	Mg 3	0	0
2	A	5	Total 5	Mg 5	0	0
2	L	4	Total 4	Mg 4	0	0
2	F	2	Total 2	Mg 2	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

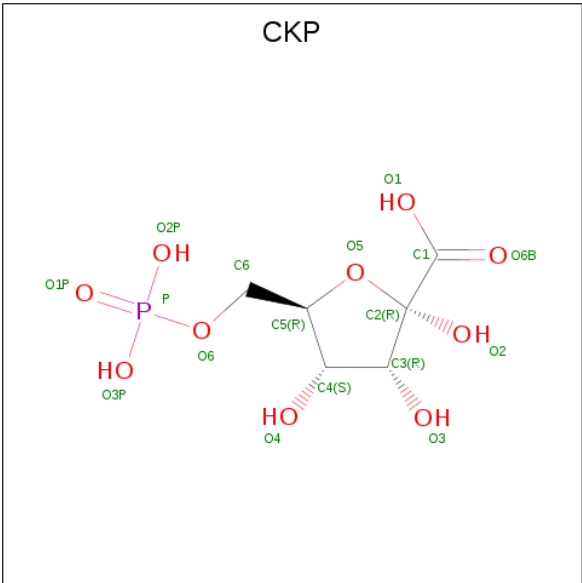
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	K 1	0	0
3	J	1	Total 1	K 1	0	0
3	D	1	Total 1	K 1	0	0
3	K	1	Total 1	K 1	0	0
3	E	1	Total 1	K 1	0	0
3	H	1	Total 1	K 1	0	0
3	B	1	Total 1	K 1	0	0
3	I	1	Total 1	K 1	0	0
3	C	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	L	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		

- Molecule 4 is 6-O-phosphono-beta-D-psicofuranosonic acid (three-letter code: CKP) (formula: C₆H₁₁O₁₀P).



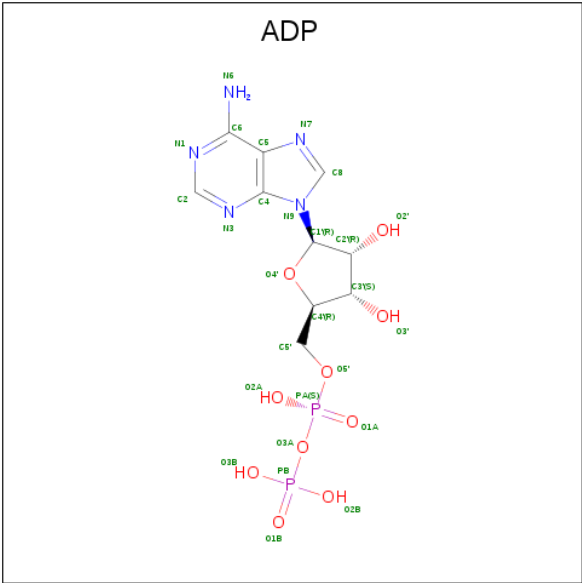
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			17	6	10	1		
4	B	1	Total	C	O	P	0	0
			17	6	10	1		
4	C	1	Total	C	O	P	0	0
			17	6	10	1		
4	D	1	Total	C	O	P	0	0
			17	6	10	1		
4	E	1	Total	C	O	P	0	0
			17	6	10	1		
4	F	1	Total	C	O	P	0	0
			17	6	10	1		
4	G	1	Total	C	O	P	0	0
			17	6	10	1		
4	H	1	Total	C	O	P	0	0
			17	6	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	I	1	Total	C	O	P	0	0
			17	6	10	1		
4	J	1	Total	C	O	P	0	0
			17	6	10	1		
4	K	1	Total	C	O	P	0	0
			17	6	10	1		
4	L	1	Total	C	O	P	0	0
			17	6	10	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

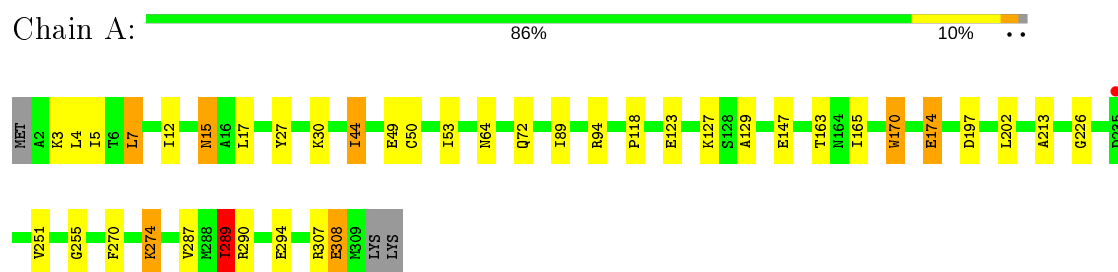
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	141	Total	O	0	0
			141	141		
6	B	158	Total	O	0	0
			158	158		
6	C	189	Total	O	0	0
			189	189		
6	D	177	Total	O	0	0
			177	177		
6	E	156	Total	O	0	0
			156	156		
6	F	163	Total	O	0	0
			163	163		
6	G	135	Total	O	0	0
			135	135		
6	H	179	Total	O	0	0
			179	179		
6	I	176	Total	O	0	0
			176	176		
6	J	169	Total	O	0	0
			169	169		
6	K	124	Total	O	0	0
			124	124		
6	L	163	Total	O	0	0
			163	163		

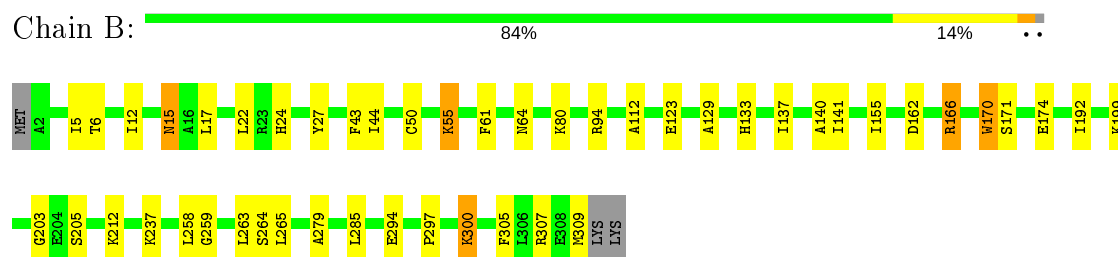
3 Residue-property plots

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.

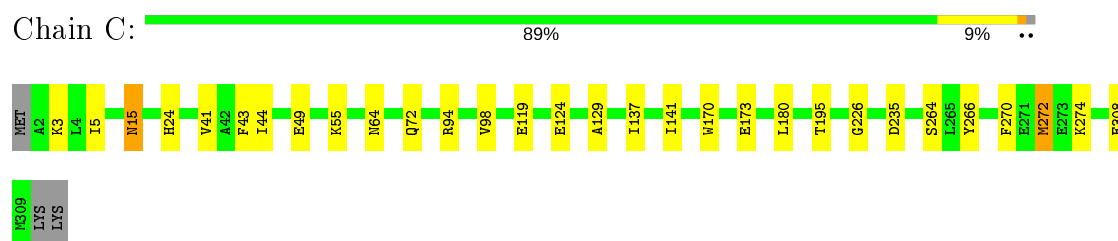
- Molecule 1: hypothetical fructokinase



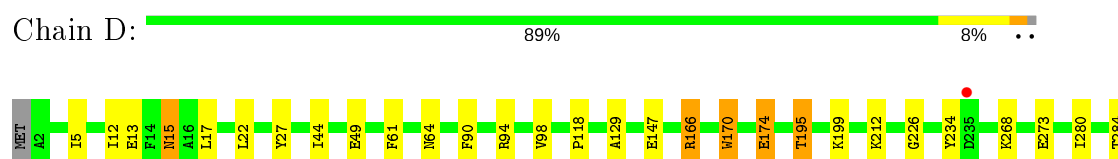
- Molecule 1: hypothetical fructokinase

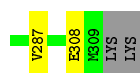


- Molecule 1: hypothetical fructokinase



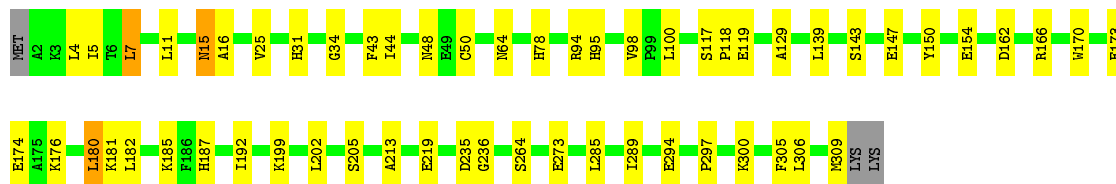
- Molecule 1: hypothetical fructokinase





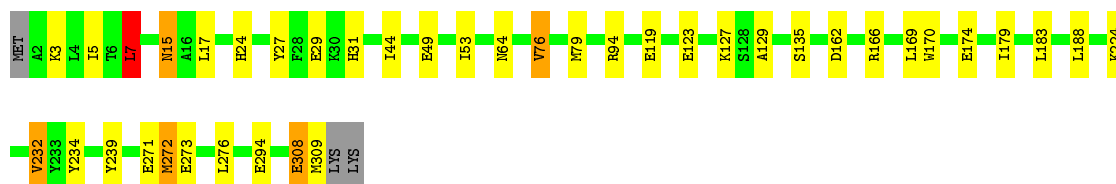
- Molecule 1: hypothetical fructokinase

Chain E: 81% 17% ..



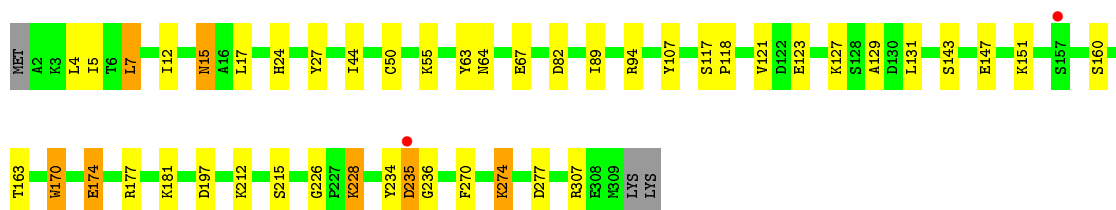
- Molecule 1: hypothetical fructokinase

Chain F: 86% 11% ..



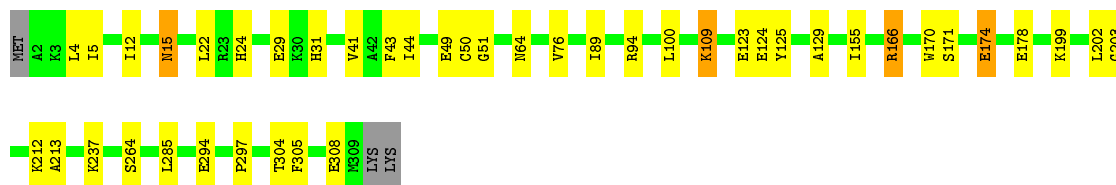
- Molecule 1: hypothetical fructokinase

Chain G: 84% 13% ..



- Molecule 1: hypothetical fructokinase

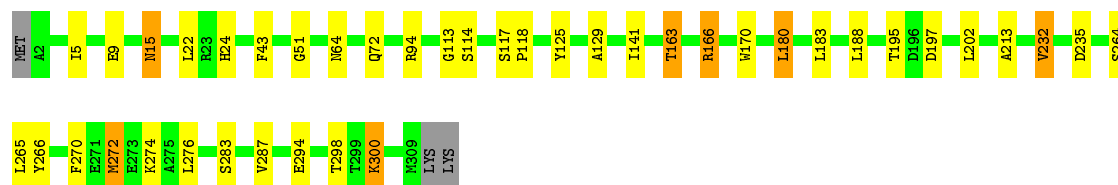
Chain H: 85% 13% ..



- Molecule 1: hypothetical fructokinase

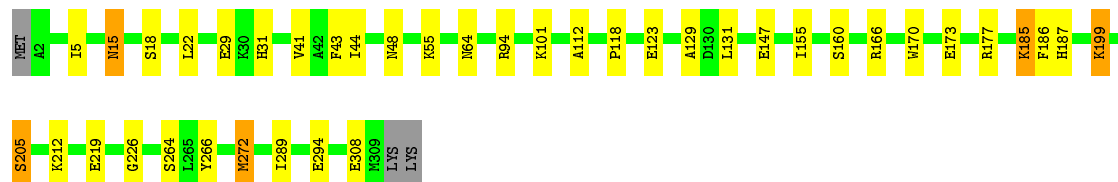
Chain I: 86% 11% ..





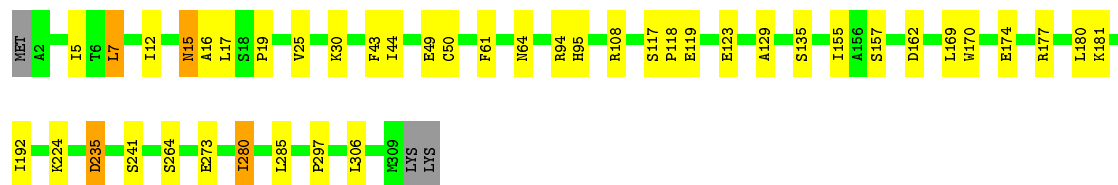
- Molecule 1: hypothetical fructokinase

Chain J: 86% 11% ..



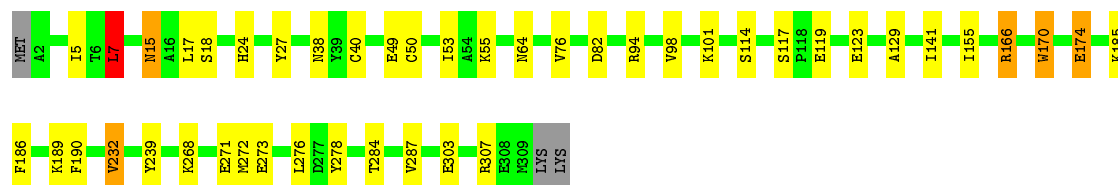
- Molecule 1: hypothetical fructokinase

Chain K: 85% 13% ..



- Molecule 1: hypothetical fructokinase

Chain L: 85% 13% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.64Å 150.23Å 154.76Å 90.00° 93.73° 90.00°	Depositor
Resolution (Å)	46.37 – 2.25 46.36 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.1 (46.37-2.25) 98.0 (46.36-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.175 , 0.228 0.175 , 0.228	Depositor DCC
R_{free} test set	9064 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31709	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 49.84 % 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 7.0435e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.55	0/2483	0.63	2/3352 (0.1%)
1	B	0.60	0/2474	0.65	2/3341 (0.1%)
1	C	0.57	0/2483	0.61	0/3353
1	D	0.59	0/2474	0.65	1/3341 (0.0%)
1	E	0.55	0/2474	0.65	1/3341 (0.0%)
1	F	0.57	0/2501	0.65	1/3376 (0.0%)
1	G	0.55	0/2456	0.64	1/3317 (0.0%)
1	H	0.58	0/2465	0.66	2/3329 (0.1%)
1	I	0.59	0/2492	0.65	1/3364 (0.0%)
1	J	0.58	0/2494	0.62	0/3366
1	K	0.56	0/2503	0.64	1/3379 (0.0%)
1	L	0.57	0/2507	0.66	1/3384 (0.0%)
All	All	0.57	0/29806	0.64	13/40243 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	7	LEU	CA-CB-CG	8.54	134.95	115.30
1	E	7	LEU	CA-CB-CG	8.28	134.33	115.30
1	L	7	LEU	CA-CB-CG	8.26	134.29	115.30
1	F	7	LEU	CA-CB-CG	7.77	133.18	115.30
1	K	7	LEU	CA-CB-CG	7.64	132.87	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2432	0	2412	25	0
1	B	2423	0	2400	33	0
1	C	2432	0	2405	20	1
1	D	2423	0	2400	21	0
1	E	2423	0	2400	39	0
1	F	2450	0	2422	26	0
1	G	2405	0	2390	27	0
1	H	2414	0	2395	25	0
1	I	2441	0	2417	30	0
1	J	2443	0	2424	25	0
1	K	2452	0	2422	24	0
1	L	2456	0	2426	23	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
2	E	3	0	0	0	0
2	F	2	0	0	0	0
2	G	6	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	4	0	0	0	0
2	K	3	0	0	0	0
2	L	4	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	17	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	17	0	5	2	0
4	C	17	0	5	0	0
4	D	17	0	5	1	0
4	E	17	0	5	1	0
4	F	17	0	5	1	0
4	G	17	0	5	0	0
4	H	17	0	5	2	0
4	I	17	0	5	1	0
4	J	17	0	5	1	0
4	K	17	0	5	0	0
4	L	17	0	5	2	0
5	A	27	0	12	2	0
5	B	27	0	12	0	0
5	C	27	0	12	1	0
5	D	27	0	12	1	0
5	E	27	0	12	0	0
5	F	27	0	12	1	0
5	G	27	0	12	1	0
5	H	27	0	12	0	0
5	I	27	0	12	0	0
5	J	27	0	12	1	0
5	K	27	0	12	1	0
5	L	27	0	12	0	0
6	A	141	0	0	5	0
6	B	158	0	0	5	0
6	C	189	0	0	2	0
6	D	177	0	0	5	0
6	E	156	0	0	10	1
6	F	163	0	0	1	0
6	G	135	0	0	3	0
6	H	179	0	0	7	0
6	I	176	0	0	1	0
6	J	169	0	0	4	0
6	K	124	0	0	4	0
6	L	163	0	0	3	0
All	All	31709	0	29117	317	1

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 5.

The worst 5 of 317 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:E:150:TYR:O	1:E:154:GLU:HG3	1.61	1.00
1:D:5:ILE:HD12	1:D:129:ALA:HB2	1.51	0.92
1:A:44:ILE:HG21	6:A:5129:HOH:O	1.74	0.87
1:I:15:ASN:HD21	1:I:94:ARG:HD3	1.41	0.84
1:A:307:ARG:NH2	6:A:5125:HOH:O	2.11	0.83

All (1) 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:C:173[A]:GLU:OE2	6:E:5094:HOH:O[2_645]	2.17	0.03

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	309/311 (99%)	301 (97%)	8 (3%)	0	100	100
1	B	308/311 (99%)	305 (99%)	3 (1%)	0	100	100
1	C	309/311 (99%)	304 (98%)	5 (2%)	0	100	100
1	D	308/311 (99%)	302 (98%)	6 (2%)	0	100	100
1	E	308/311 (99%)	301 (98%)	7 (2%)	0	100	100
1	F	311/311 (100%)	307 (99%)	4 (1%)	0	100	100
1	G	306/311 (98%)	296 (97%)	8 (3%)	2 (1%)	22	21
1	H	307/311 (99%)	303 (99%)	4 (1%)	0	100	100
1	I	310/311 (100%)	306 (99%)	4 (1%)	0	100	100
1	J	310/311 (100%)	303 (98%)	7 (2%)	0	100	100
1	K	311/311 (100%)	307 (99%)	4 (1%)	0	100	100
1	L	312/311 (100%)	309 (99%)	3 (1%)	0	100	100
All	All	3709/3732 (99%)	3644 (98%)	63 (2%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	235	ASP
1	G	236	GLY

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	260/260 (100%)	251 (96%)	9 (4%)	36	43
1	B	259/260 (100%)	251 (97%)	8 (3%)	40	49
1	C	260/260 (100%)	253 (97%)	7 (3%)	44	54
1	D	259/260 (100%)	247 (95%)	12 (5%)	27	30
1	E	259/260 (100%)	251 (97%)	8 (3%)	40	49
1	F	262/260 (101%)	249 (95%)	13 (5%)	24	26
1	G	257/260 (99%)	249 (97%)	8 (3%)	40	49
1	H	258/260 (99%)	247 (96%)	11 (4%)	29	33
1	I	261/260 (100%)	249 (95%)	12 (5%)	27	30
1	J	261/260 (100%)	249 (95%)	12 (5%)	27	30
1	K	262/260 (101%)	251 (96%)	11 (4%)	30	34
1	L	263/260 (101%)	250 (95%)	13 (5%)	25	27
All	All	3121/3120 (100%)	2997 (96%)	124 (4%)	31	37

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	309	MET
1	H	109	LYS
1	L	49	GLU
1	G	7	LEU
1	G	174	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such

sidechains are listed below:

Mol	Chain	Res	Type
1	F	24	HIS
1	G	72	GLN
1	K	95	HIS
1	F	31	HIS
1	F	245	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 81 ligands modelled in this entry, 57 are monoatomic - leaving 24 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	CKP	L	2012	2	14,17,17	0.92	1 (7%)	20,27,27	1.79	6 (30%)
4	CKP	H	2008	2	14,17,17	0.84	1 (7%)	20,27,27	2.21	5 (25%)
4	CKP	J	2010	2	14,17,17	0.82	1 (7%)	20,27,27	1.98	5 (25%)
5	ADP	G	3007	2	24,29,29	0.95	1 (4%)	29,45,45	1.37	4 (13%)
5	ADP	J	3010	2	24,29,29	0.98	3 (12%)	29,45,45	1.39	3 (10%)
5	ADP	H	3008	2	24,29,29	1.00	2 (8%)	29,45,45	1.39	2 (6%)
4	CKP	I	2009	2	14,17,17	0.81	1 (7%)	20,27,27	1.90	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	A	3001	2	24,29,29	1.05	1 (4%)	29,45,45	1.28	4 (13%)
4	CKP	D	2004	2	14,17,17	0.90	1 (7%)	20,27,27	1.84	5 (25%)
4	CKP	K	2011	2	14,17,17	0.83	1 (7%)	20,27,27	1.50	3 (15%)
5	ADP	B	3002	2	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
5	ADP	I	3009	2	24,29,29	1.02	1 (4%)	29,45,45	1.33	4 (13%)
4	CKP	G	2007	2	14,17,17	0.86	1 (7%)	20,27,27	1.72	5 (25%)
5	ADP	E	3005	2	24,29,29	1.05	3 (12%)	29,45,45	1.25	3 (10%)
5	ADP	F	3006	2	24,29,29	1.02	1 (4%)	29,45,45	1.29	3 (10%)
5	ADP	K	3011	2	24,29,29	0.96	1 (4%)	29,45,45	1.29	4 (13%)
4	CKP	E	2005	2	14,17,17	0.92	1 (7%)	20,27,27	1.64	3 (15%)
4	CKP	F	2006	2	14,17,17	0.88	1 (7%)	20,27,27	2.03	6 (30%)
5	ADP	L	3012	2	24,29,29	0.98	1 (4%)	29,45,45	1.31	4 (13%)
4	CKP	C	2003	2	14,17,17	0.80	1 (7%)	20,27,27	1.86	8 (40%)
4	CKP	A	2001	2	14,17,17	0.78	1 (7%)	20,27,27	1.72	4 (20%)
5	ADP	C	3003	2	24,29,29	1.01	1 (4%)	29,45,45	1.23	3 (10%)
4	CKP	B	2002	2	14,17,17	0.88	1 (7%)	20,27,27	1.77	3 (15%)
5	ADP	D	3004	2	24,29,29	0.98	3 (12%)	29,45,45	1.41	3 (10%)

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	CKP	L	2012	2	-	2/6/31/31	0/1/1/1
4	CKP	H	2008	2	-	3/6/31/31	0/1/1/1
4	CKP	J	2010	2	-	2/6/31/31	0/1/1/1
5	ADP	G	3007	2	-	0/12/32/32	0/3/3/3
5	ADP	J	3010	2	-	0/12/32/32	0/3/3/3
5	ADP	H	3008	2	-	0/12/32/32	0/3/3/3
4	CKP	I	2009	2	-	1/6/31/31	0/1/1/1
5	ADP	A	3001	2	-	0/12/32/32	0/3/3/3
4	CKP	D	2004	2	-	1/6/31/31	0/1/1/1
4	CKP	K	2011	2	-	4/6/31/31	0/1/1/1
5	ADP	B	3002	2	-	0/12/32/32	0/3/3/3
5	ADP	I	3009	2	-	0/12/32/32	0/3/3/3
4	CKP	G	2007	2	-	1/6/31/31	0/1/1/1
5	ADP	E	3005	2	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	F	3006	2	-	0/12/32/32	0/3/3/3
5	ADP	K	3011	2	-	0/12/32/32	0/3/3/3
4	CKP	E	2005	2	-	3/6/31/31	0/1/1/1
4	CKP	F	2006	2	-	2/6/31/31	0/1/1/1
5	ADP	L	3012	2	-	0/12/32/32	0/3/3/3
4	CKP	C	2003	2	-	3/6/31/31	0/1/1/1
4	CKP	A	2001	2	-	3/6/31/31	0/1/1/1
5	ADP	C	3003	2	-	0/12/32/32	0/3/3/3
4	CKP	B	2002	2	-	1/6/31/31	0/1/1/1
5	ADP	D	3004	2	-	0/12/32/32	0/3/3/3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3006	ADP	C5-C4	2.99	1.48	1.40
5	G	3007	ADP	C5-C4	2.89	1.48	1.40
5	L	3012	ADP	C5-C4	2.84	1.48	1.40
4	F	2006	CKP	O2-C2	2.83	1.45	1.40
4	L	2012	CKP	O2-C2	2.73	1.45	1.40

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2008	CKP	O5-C2-C3	-7.54	94.67	105.77
4	F	2006	CKP	O5-C2-C3	-6.08	96.82	105.77
4	I	2009	CKP	O5-C2-C3	-5.71	97.36	105.77
4	J	2010	CKP	O5-C2-C3	-5.53	97.63	105.77
4	B	2002	CKP	O5-C2-C3	-5.48	97.70	105.77

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

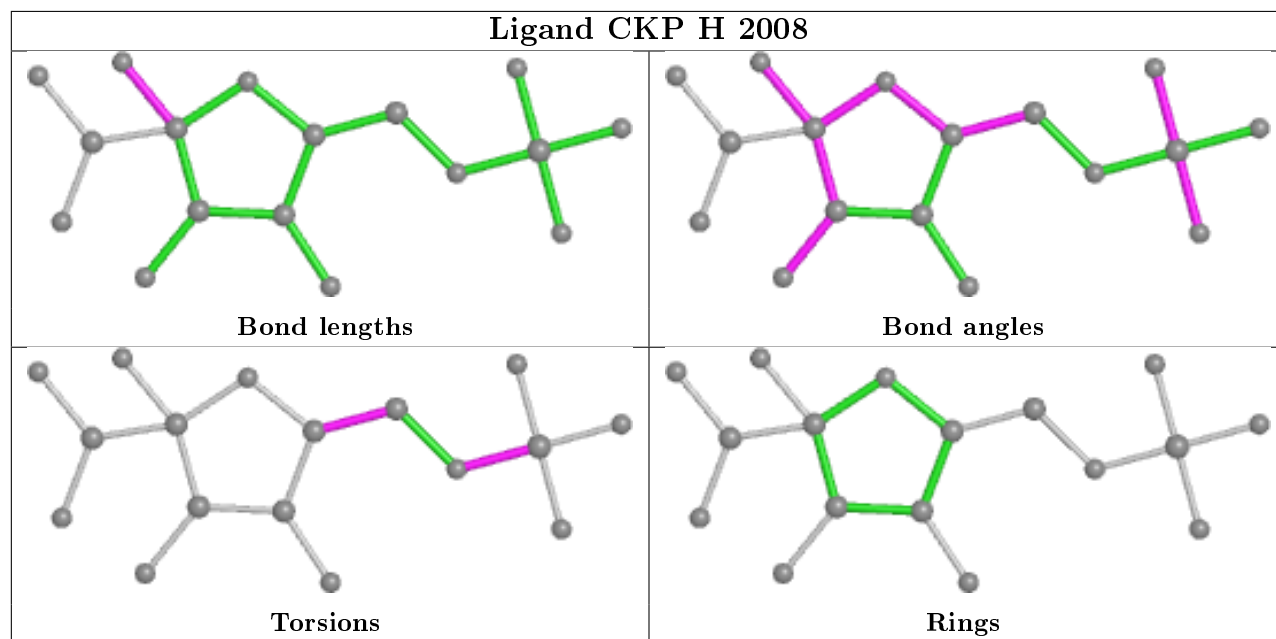
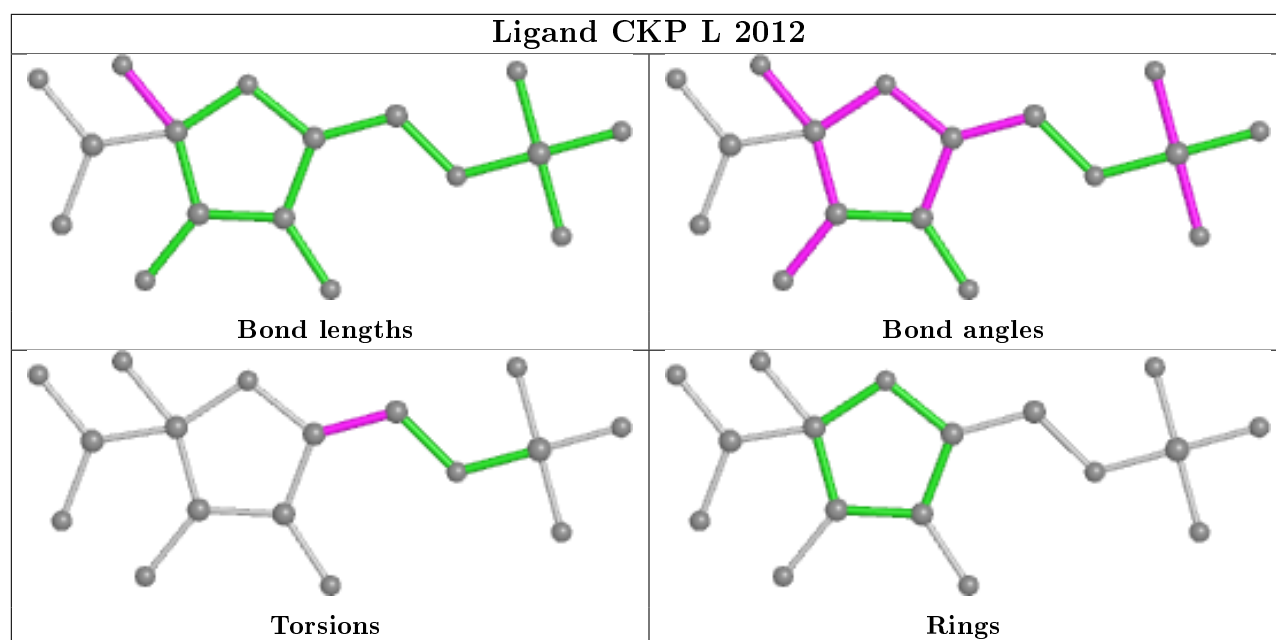
Mol	Chain	Res	Type	Atoms
4	E	2005	CKP	C6-O6-P-O3P
4	E	2005	CKP	C6-O6-P-O1P
4	E	2005	CKP	C6-O6-P-O2P
4	C	2003	CKP	C6-O6-P-O1P
4	K	2011	CKP	C6-O6-P-O3P

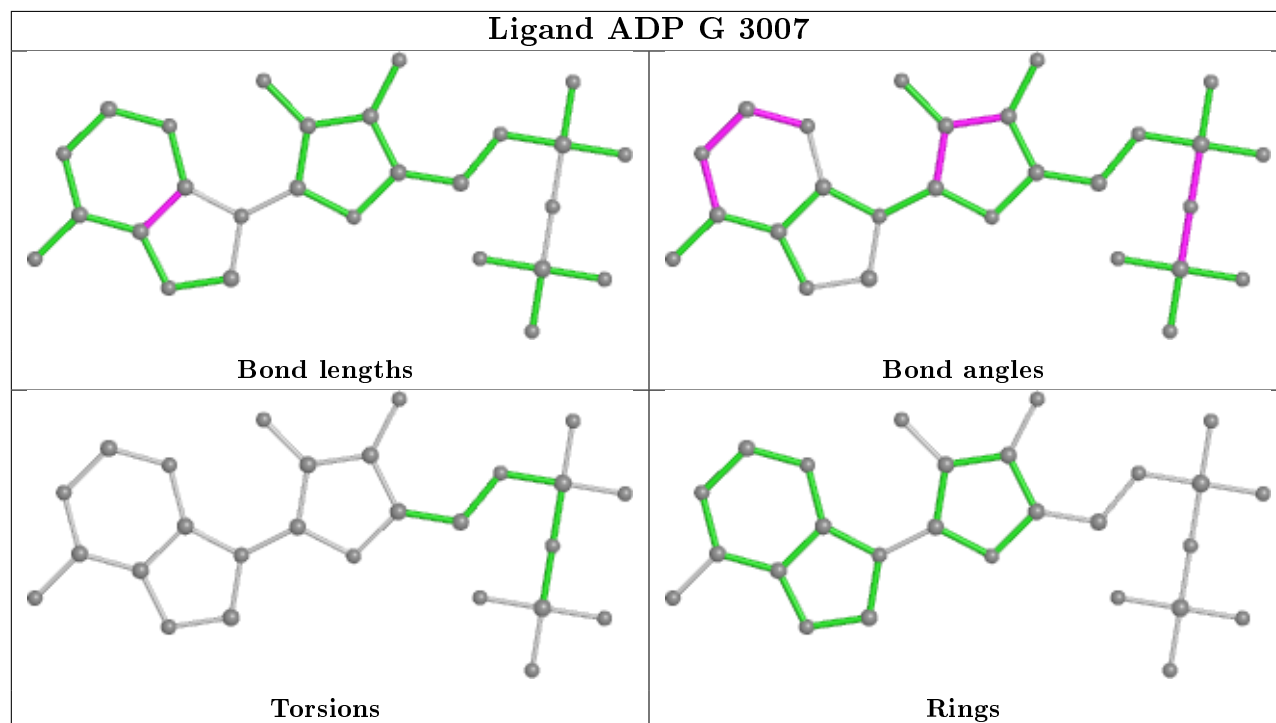
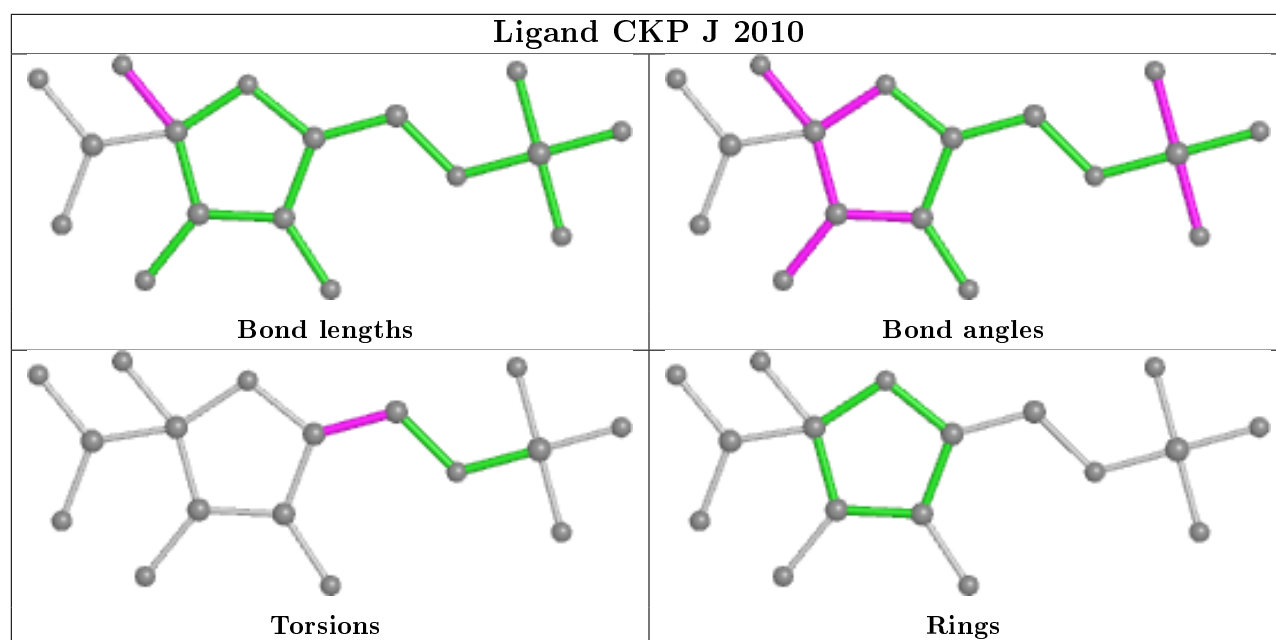
There are no ring outliers.

16 monomers are involved in 20 short contacts:

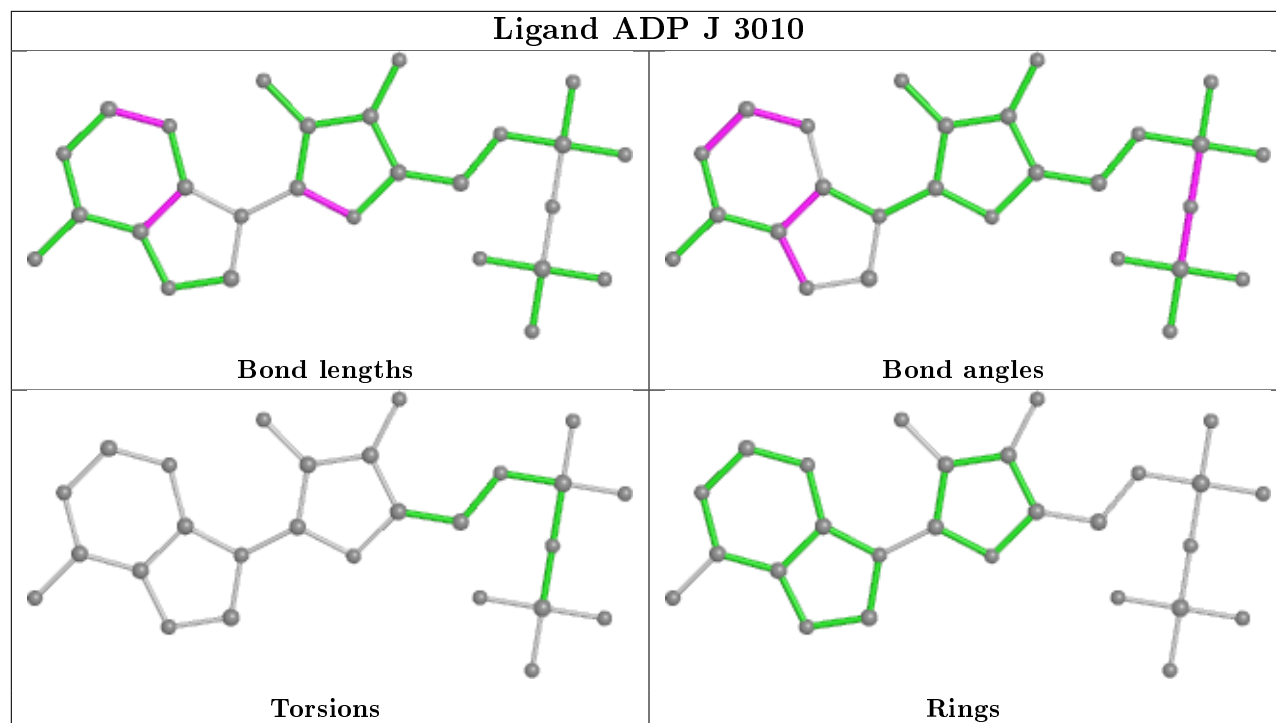
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	2012	CKP	2	0
4	H	2008	CKP	2	0
4	J	2010	CKP	1	0
5	G	3007	ADP	1	0
5	J	3010	ADP	1	0
4	I	2009	CKP	1	0
5	A	3001	ADP	2	0
4	D	2004	CKP	1	0
5	F	3006	ADP	1	0
5	K	3011	ADP	1	0
4	E	2005	CKP	1	0
4	F	2006	CKP	1	0
4	A	2001	CKP	1	0
5	C	3003	ADP	1	0
4	B	2002	CKP	2	0
5	D	3004	ADP	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.

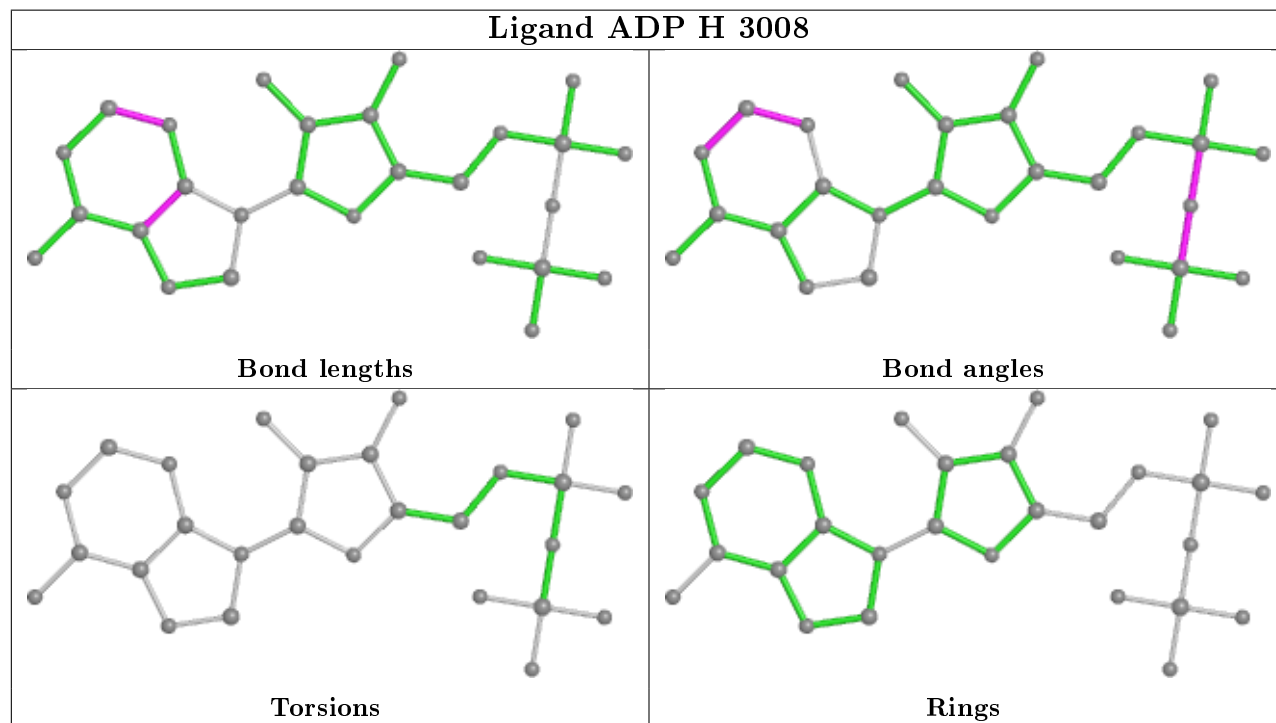


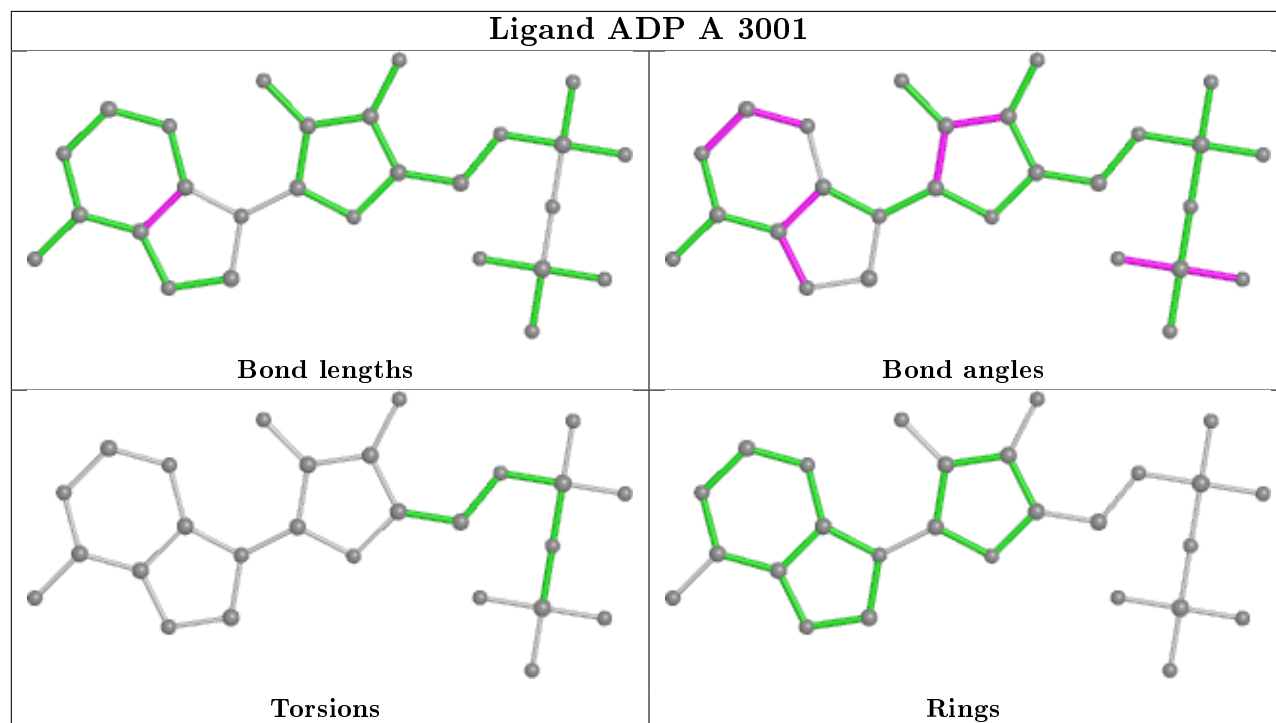
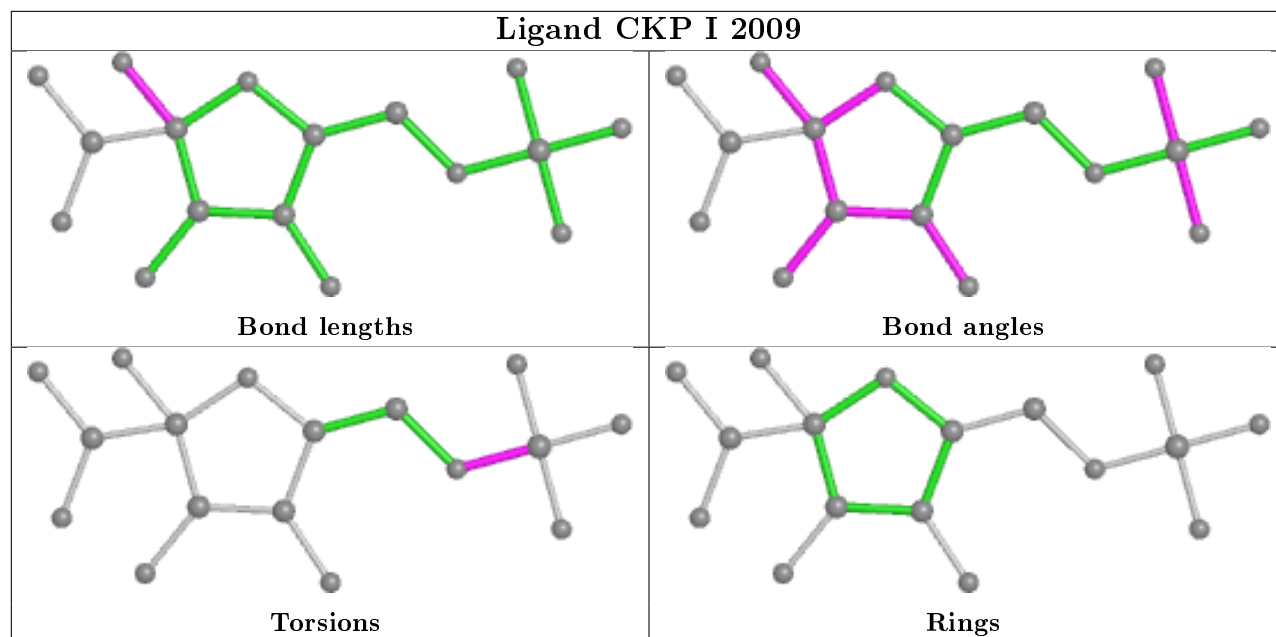


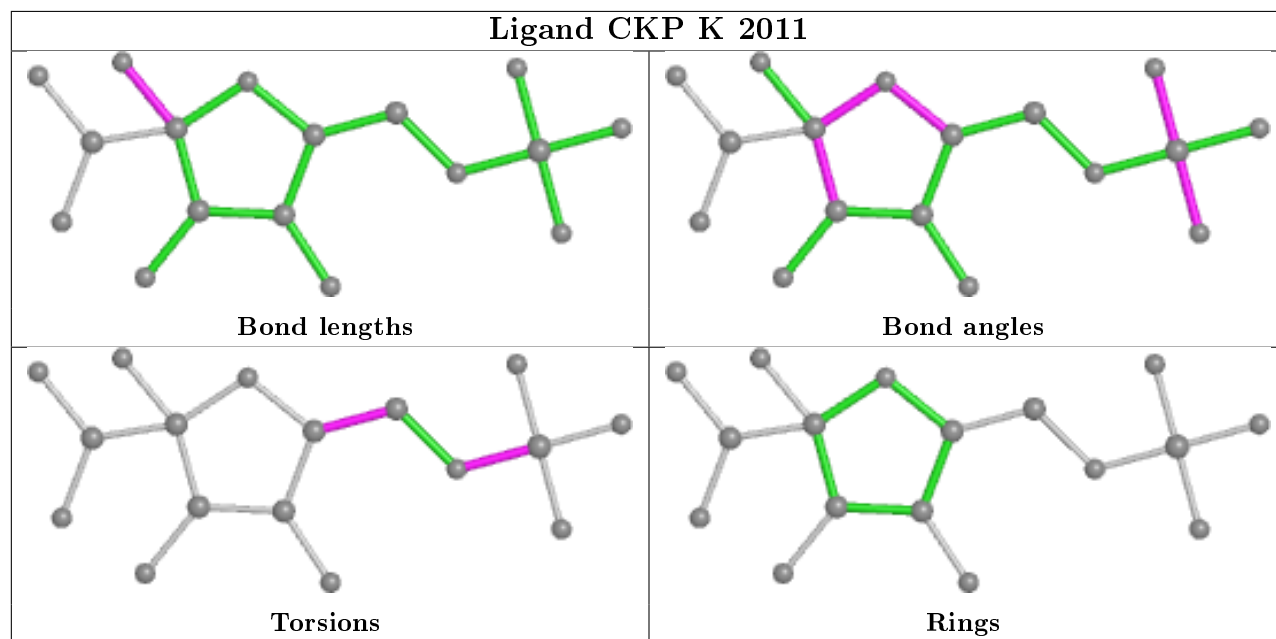
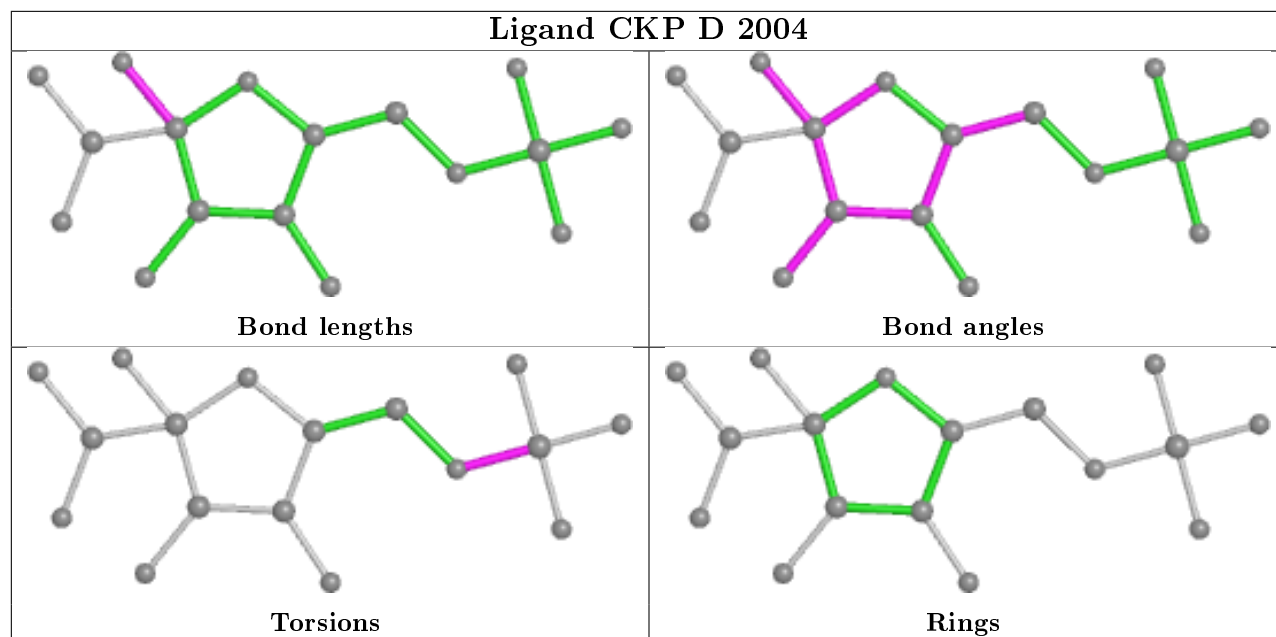
Ligand ADP J 3010



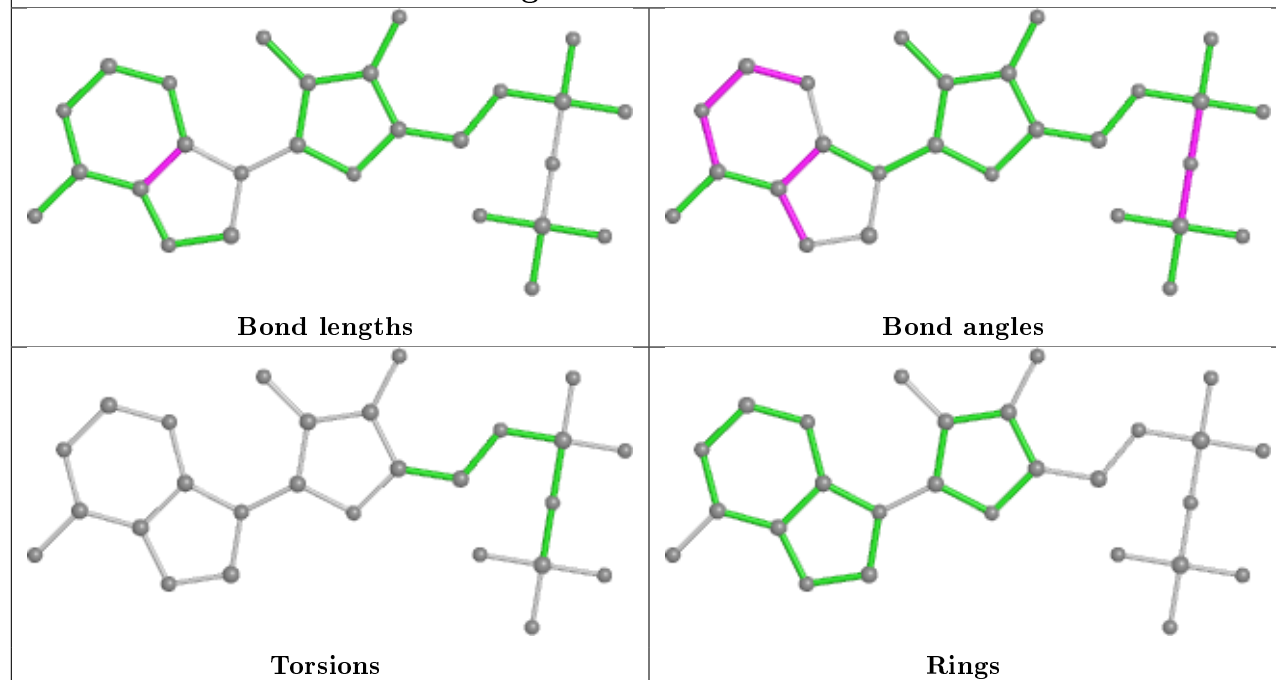
Ligand ADP H 3008



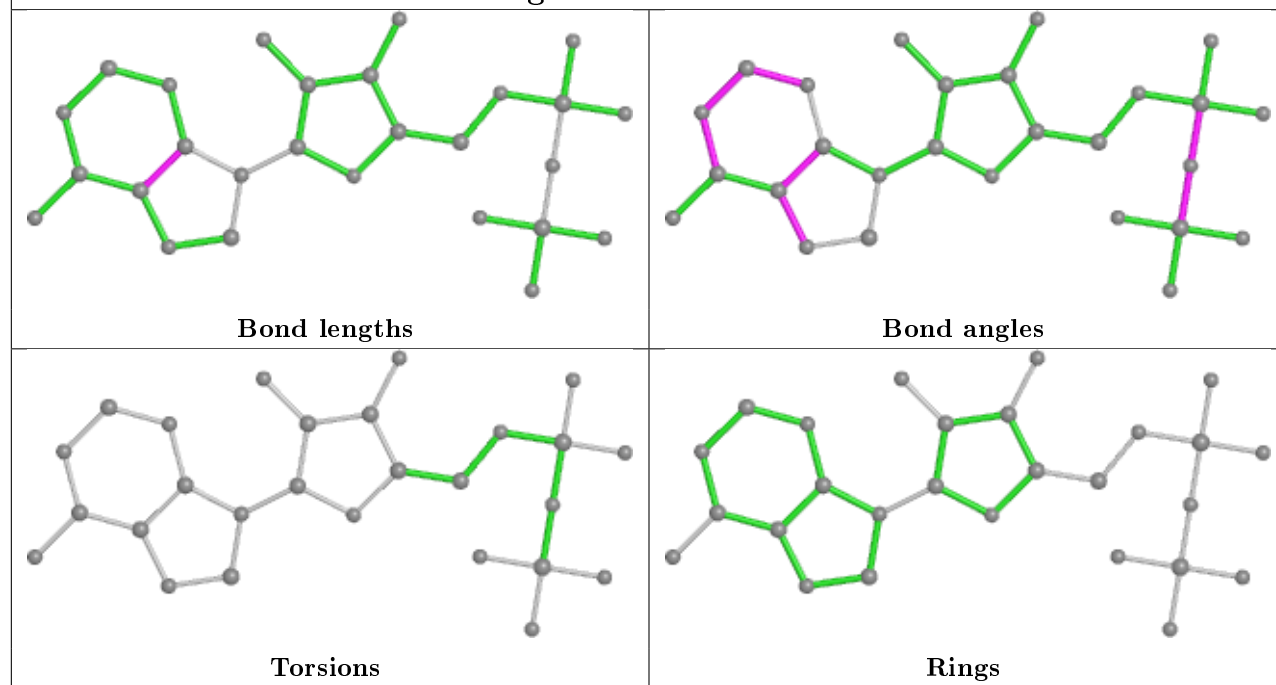


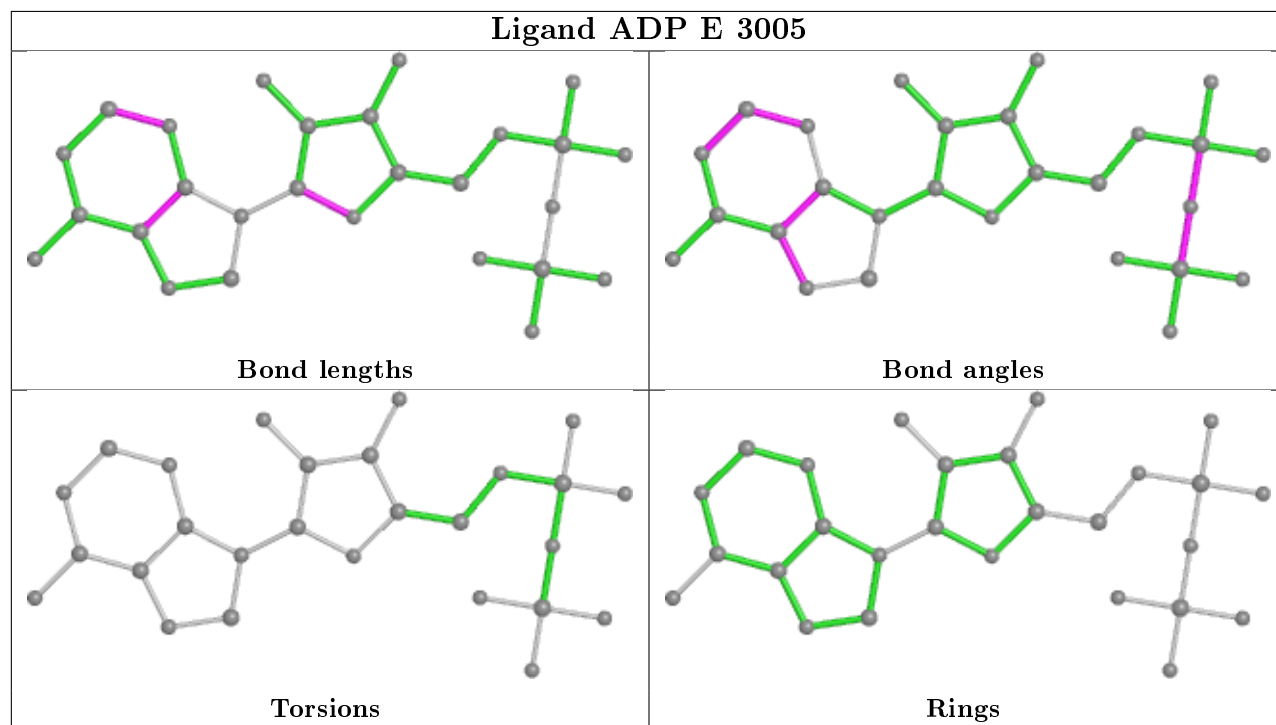
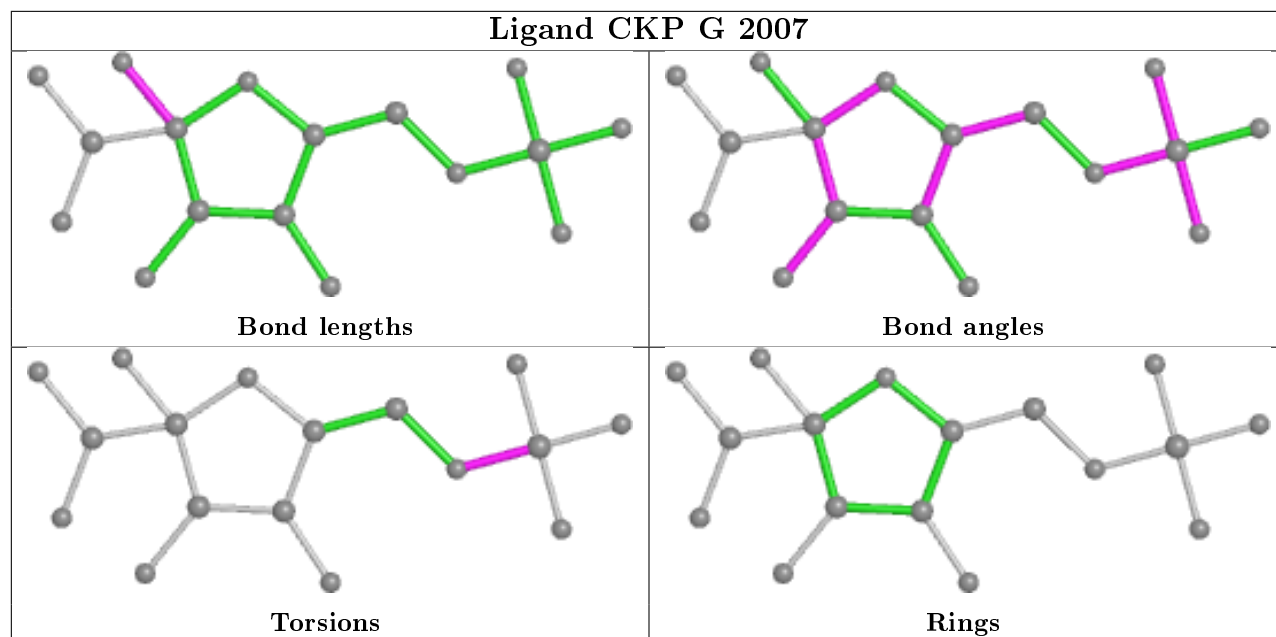


Ligand ADP B 3002

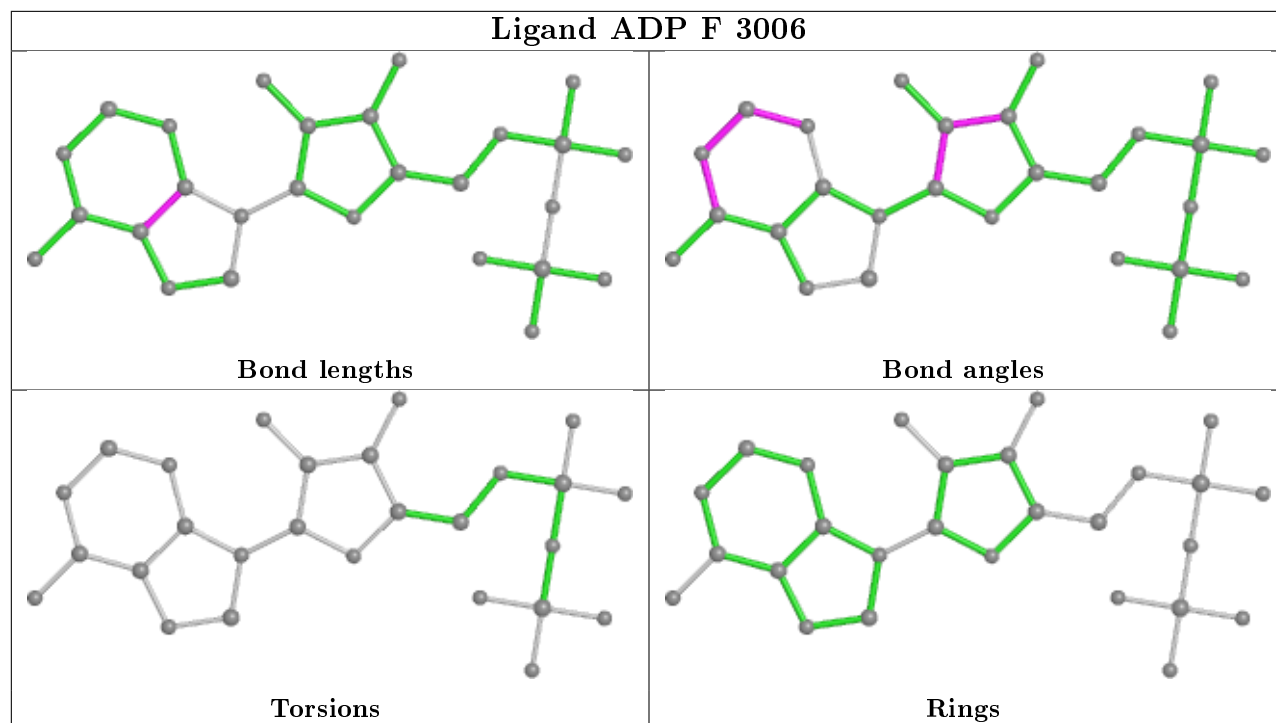


Ligand ADP I 3009

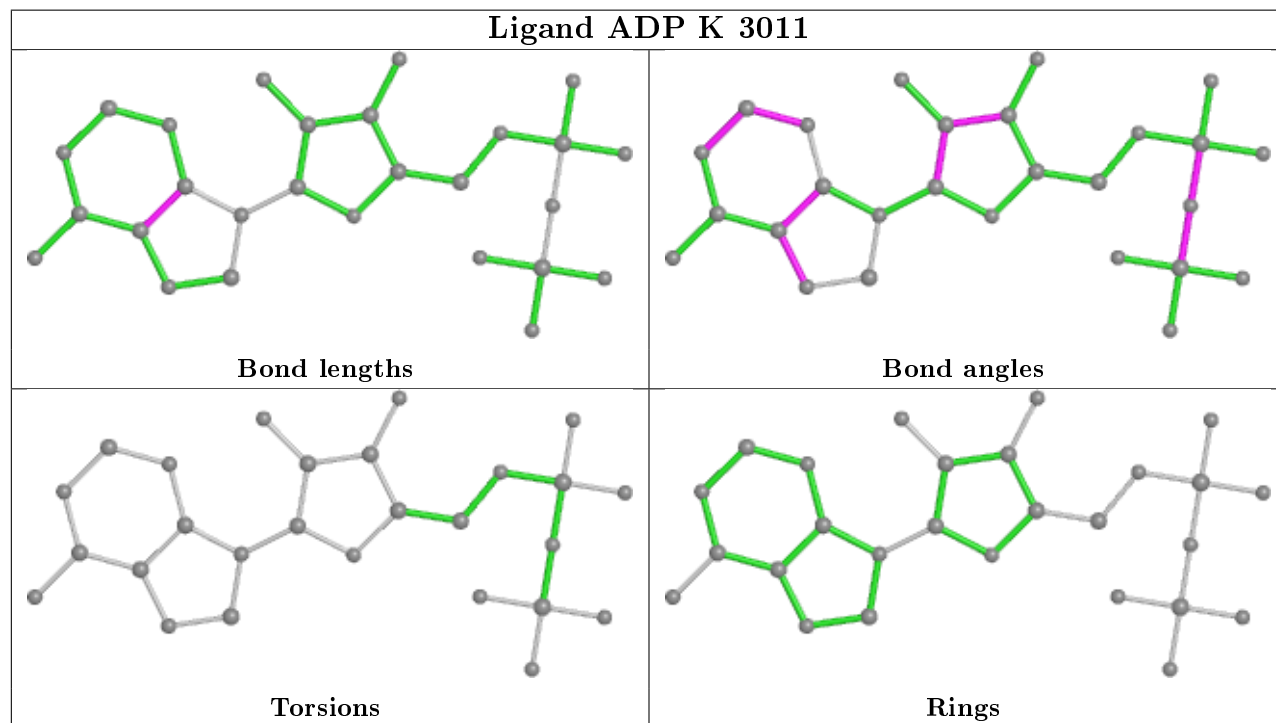


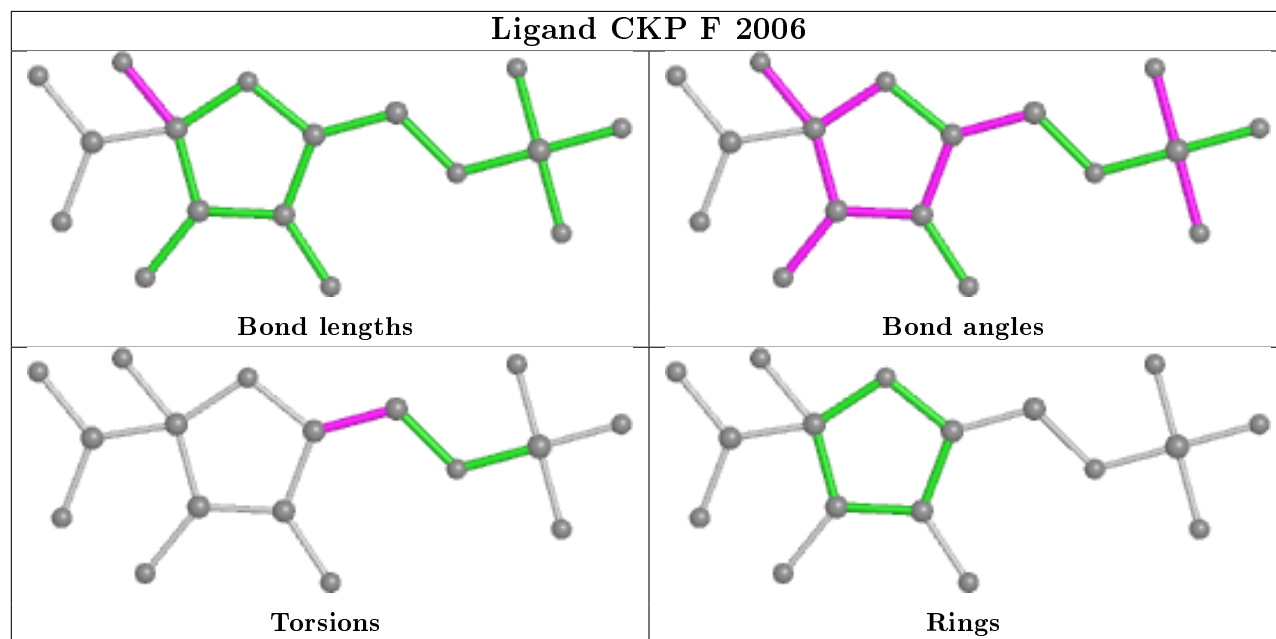
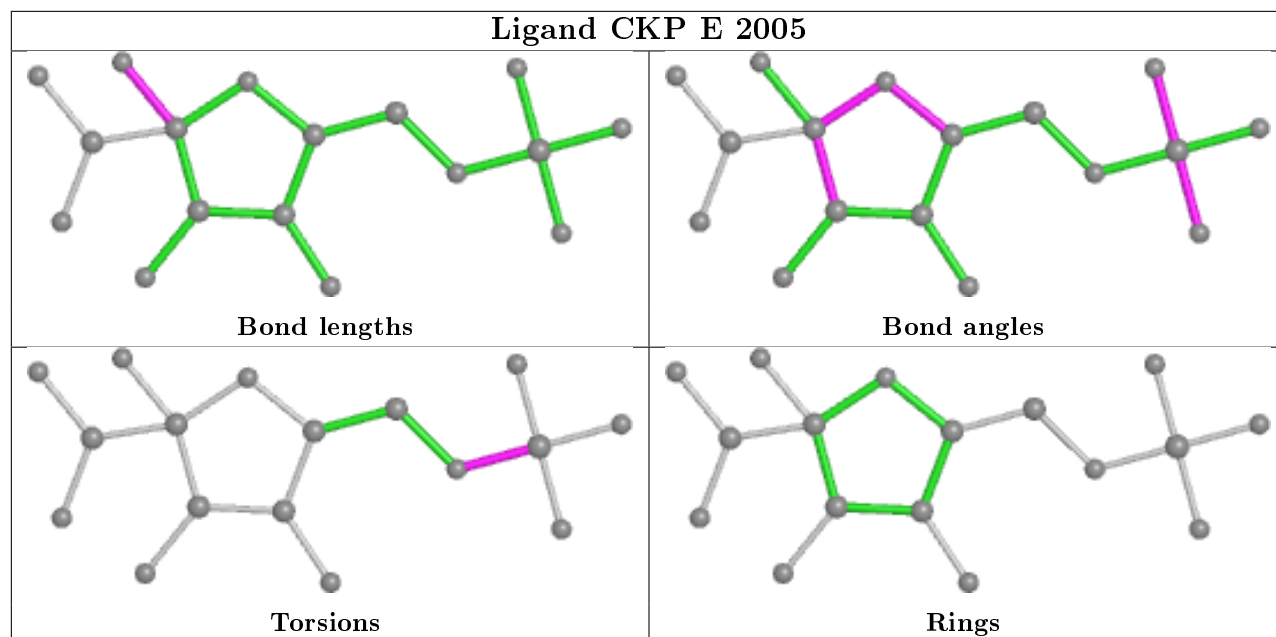


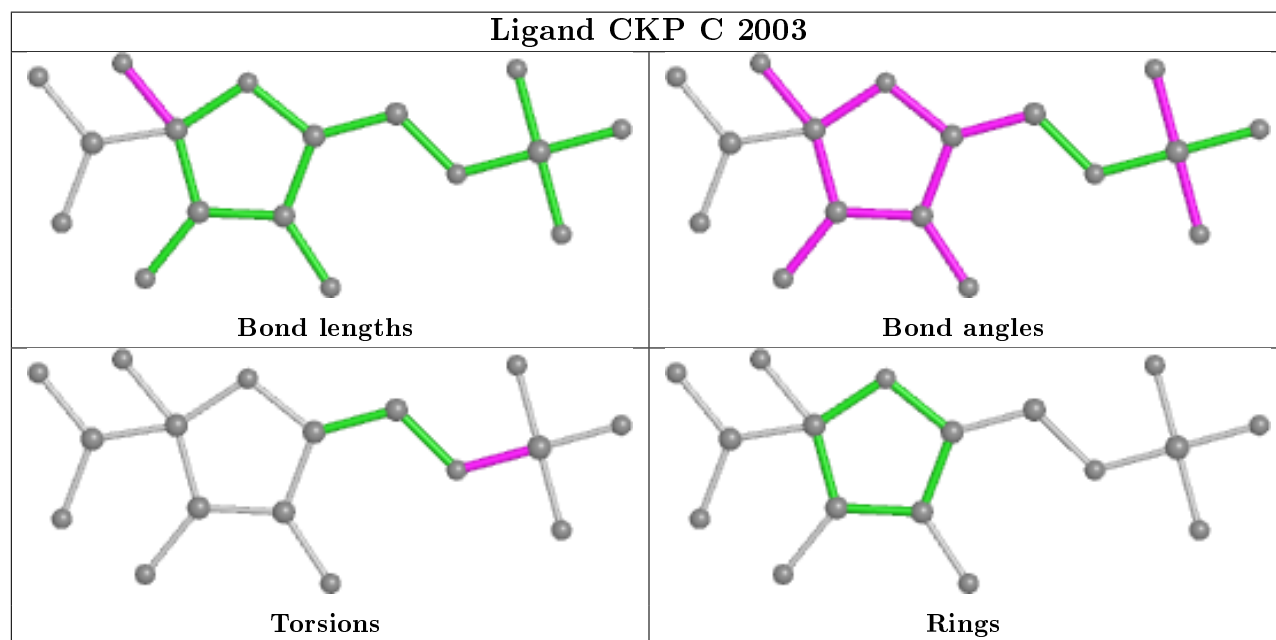
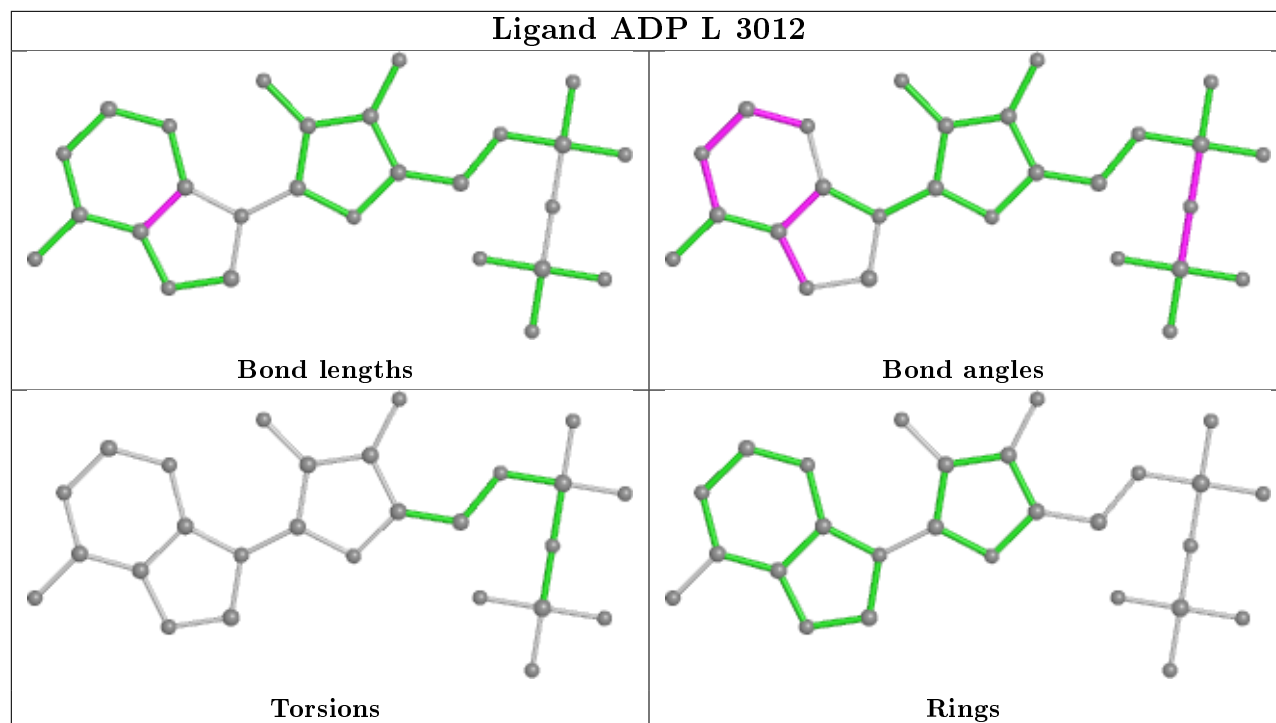
Ligand ADP F 3006

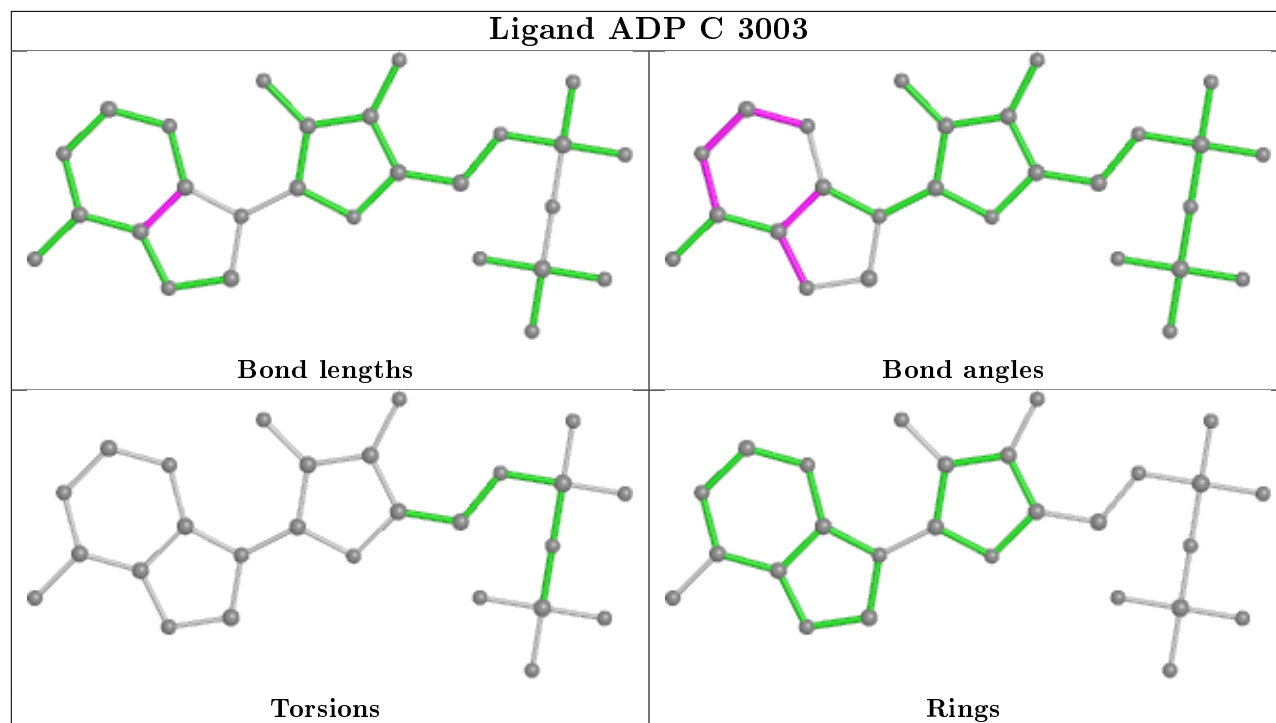
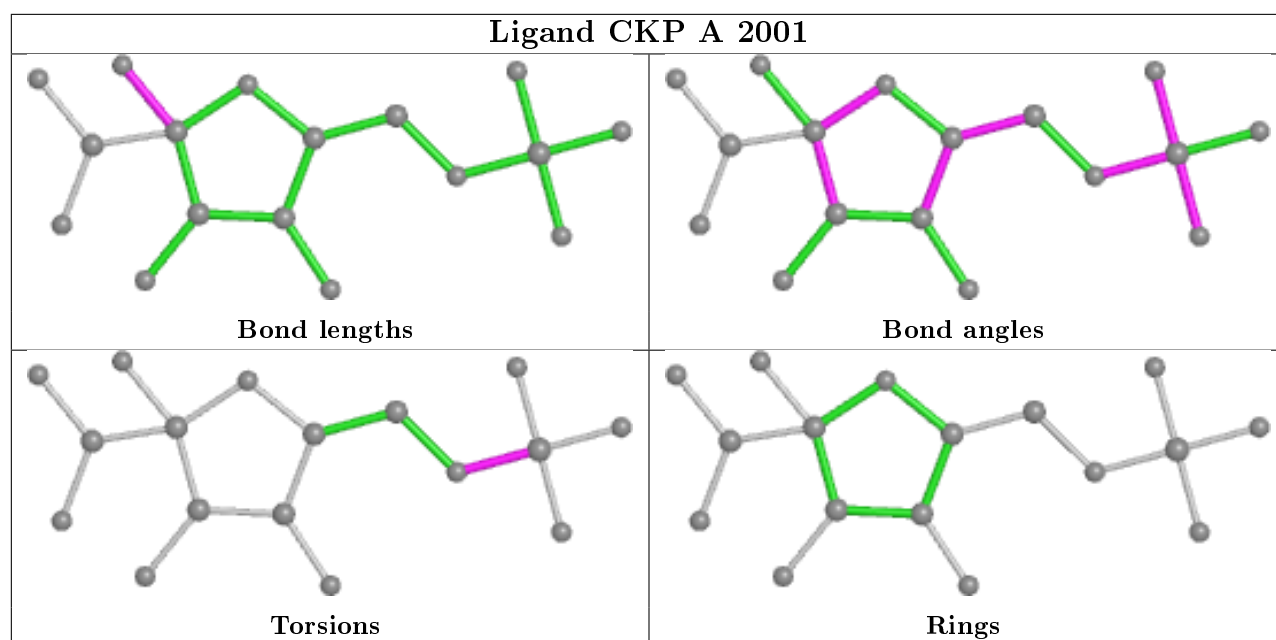


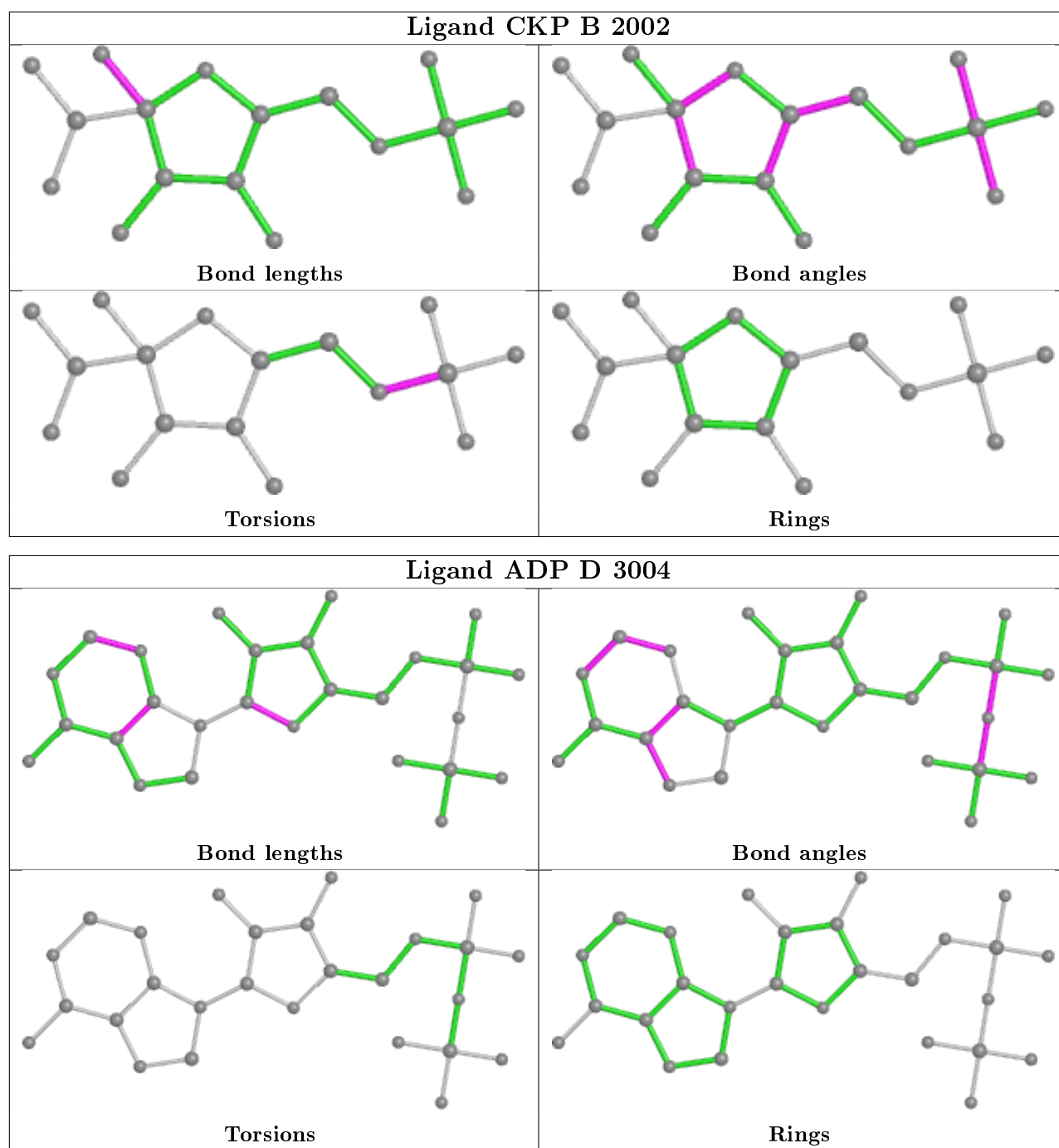
Ligand ADP K 3011











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	308/311 (99%)	-0.40	1 (0%) 94 94	17, 25, 47, 53	0
1	B	308/311 (99%)	-0.69	0 100 100	15, 22, 36, 43	0
1	C	308/311 (99%)	-0.69	0 100 100	14, 22, 32, 49	0
1	D	308/311 (99%)	-0.60	1 (0%) 94 94	15, 22, 35, 46	0
1	E	308/311 (99%)	-0.56	0 100 100	15, 25, 45, 52	0
1	F	308/311 (99%)	-0.53	0 100 100	16, 24, 36, 48	0
1	G	308/311 (99%)	-0.49	2 (0%) 89 89	16, 26, 44, 49	0
1	H	308/311 (99%)	-0.69	0 100 100	15, 23, 35, 42	0
1	I	308/311 (99%)	-0.63	0 100 100	14, 22, 33, 49	0
1	J	308/311 (99%)	-0.55	0 100 100	14, 22, 39, 46	0
1	K	308/311 (99%)	-0.58	0 100 100	16, 25, 44, 54	0
1	L	308/311 (99%)	-0.47	0 100 100	15, 24, 36, 45	0
All	All	3696/3732 (99%)	-0.57	4 (0%) 95 96	14, 23, 39, 54	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	157	SER	3.3
1	A	235	ASP	2.2
1	G	235	ASP	2.1
1	D	235	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	MG	A	4004	1/1	0.66	0.24	40,40,40,40	1
2	MG	G	4025	1/1	0.72	0.46	41,41,41,41	1
2	MG	G	4026	1/1	0.72	0.28	34,34,34,34	1
2	MG	J	4037	1/1	0.76	0.34	31,31,31,31	1
2	MG	B	4009[A]	1/1	0.83	0.47	30,30,30,30	1
2	MG	B	4009[B]	1/1	0.83	0.47	18,18,18,18	1
2	MG	B	4007	1/1	0.85	0.11	33,33,33,33	0
2	MG	L	4044	1/1	0.85	0.42	45,45,45,45	1
2	MG	L	4041	1/1	0.85	0.83	34,34,34,34	1
2	MG	A	4003	1/1	0.86	0.42	37,37,37,37	1
2	MG	D	4015	1/1	0.87	0.43	47,47,47,47	1
2	MG	H	4030	1/1	0.87	0.13	38,38,38,38	0
2	MG	C	4012	1/1	0.87	0.28	42,42,42,42	0
2	MG	G	4023	1/1	0.88	0.21	30,30,30,30	0
2	MG	K	4040	1/1	0.88	0.55	37,37,37,37	1
2	MG	A	4002	1/1	0.89	0.17	33,33,33,33	0
2	MG	H	4027	1/1	0.89	0.62	39,39,39,39	1
2	MG	J	4036	1/1	0.90	0.63	44,44,44,44	1
2	MG	J	4035	1/1	0.91	0.16	34,34,34,34	0
2	MG	D	4016	1/1	0.91	0.21	40,40,40,40	0
2	MG	L	4043	1/1	0.92	0.21	30,30,30,30	0
4	CKP	B	2002	17/17	0.92	0.11	18,23,36,38	0
2	MG	G	4028	1/1	0.92	0.30	41,41,41,41	1
2	MG	A	4005	1/1	0.93	0.43	29,29,29,29	1
4	CKP	H	2008	17/17	0.94	0.12	22,25,36,38	0
2	MG	E	4018	1/1	0.94	0.17	40,40,40,40	0
2	MG	E	4019	1/1	0.94	0.38	44,44,44,44	1
4	CKP	L	2012	17/17	0.94	0.10	22,25,32,33	0
4	CKP	C	2003	17/17	0.94	0.11	17,19,27,27	0
4	CKP	E	2005	17/17	0.95	0.10	22,25,38,39	0
2	MG	G	4024	1/1	0.95	0.26	36,36,36,36	1
4	CKP	F	2006	17/17	0.95	0.11	17,22,32,34	0

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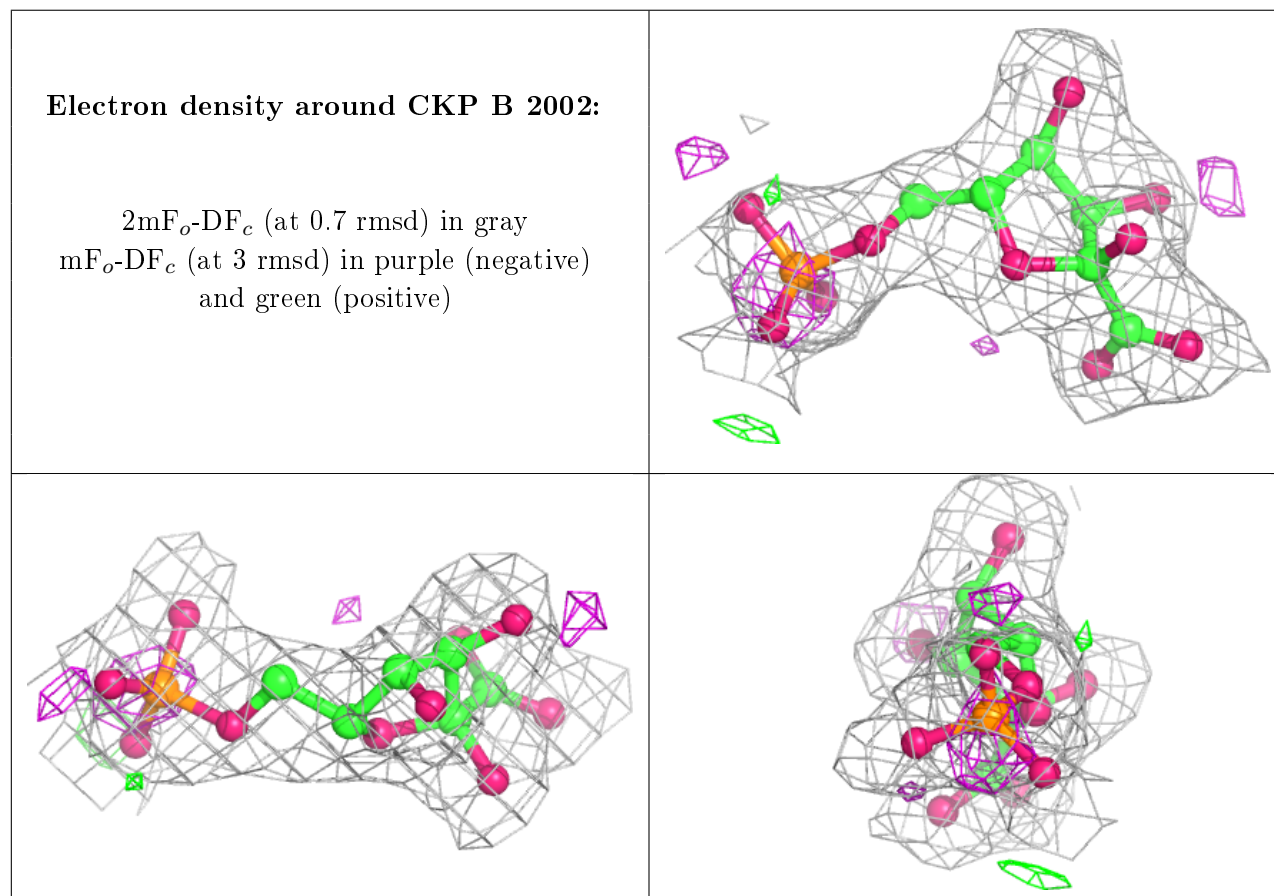
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CKP	J	2010	17/17	0.95	0.10	20,23,35,35	0
4	CKP	K	2011	17/17	0.95	0.10	21,25,38,38	0
4	CKP	D	2004	17/17	0.95	0.10	18,23,33,35	0
4	CKP	G	2007	17/17	0.95	0.10	21,27,33,34	0
2	MG	K	4039	1/1	0.95	0.17	28,28,28,28	0
4	CKP	A	2001	17/17	0.95	0.11	21,23,34,36	0
4	CKP	I	2009	17/17	0.95	0.11	15,19,30,30	0
2	MG	D	4014	1/1	0.95	0.06	26,26,26,26	0
5	ADP	A	3001	27/27	0.96	0.09	20,24,38,40	0
2	MG	F	4021	1/1	0.96	0.17	25,25,25,25	0
5	ADP	E	3005	27/27	0.96	0.09	20,26,35,38	0
5	ADP	J	3010	27/27	0.96	0.09	21,23,34,36	0
2	MG	I	4033	1/1	0.96	0.45	43,43,43,43	1
5	ADP	D	3004	27/27	0.96	0.08	19,22,32,36	0
2	MG	B	4006	1/1	0.96	0.09	13,13,13,13	0
2	MG	B	4008	1/1	0.97	0.51	31,31,31,31	1
5	ADP	K	3011	27/27	0.97	0.09	19,21,30,35	0
5	ADP	G	3007	27/27	0.97	0.08	22,26,35,36	0
2	MG	I	4032	1/1	0.97	0.11	26,26,26,26	0
5	ADP	F	3006	27/27	0.97	0.09	19,21,26,32	0
2	MG	K	4038	1/1	0.98	0.10	13,13,13,13	0
2	MG	C	4011	1/1	0.98	0.07	22,22,22,22	0
5	ADP	C	3003	27/27	0.98	0.07	17,19,27,29	0
5	ADP	B	3002	27/27	0.98	0.08	20,22,30,35	0
5	ADP	H	3008	27/27	0.98	0.08	19,21,30,35	0
5	ADP	L	3012	27/27	0.98	0.08	18,20,29,33	0
3	K	C	5003	1/1	0.98	0.07	22,22,22,22	0
5	ADP	I	3009	27/27	0.98	0.09	18,21,26,30	0
2	MG	G	4022	1/1	0.98	0.11	10,10,10,10	0
3	K	D	5004	1/1	0.99	0.06	20,20,20,20	0
2	MG	C	4010	1/1	0.99	0.07	7,7,7,7	0
3	K	F	5006	1/1	0.99	0.07	24,24,24,24	0
3	K	L	5012	1/1	0.99	0.08	22,22,22,22	0
2	MG	L	4042	1/1	0.99	0.09	8,8,8,8	0
3	K	J	5010	1/1	0.99	0.09	20,20,20,20	0
3	K	B	5002	1/1	0.99	0.04	19,19,19,19	0
2	MG	D	4013	1/1	0.99	0.08	10,10,10,10	0
2	MG	I	4031	1/1	0.99	0.10	10,10,10,10	0
3	K	I	5009	1/1	0.99	0.04	21,21,21,21	0
2	MG	E	4017	1/1	0.99	0.15	13,13,13,13	0
3	K	E	5005	1/1	0.99	0.06	23,23,23,23	0
3	K	G	5007	1/1	0.99	0.07	26,26,26,26	0

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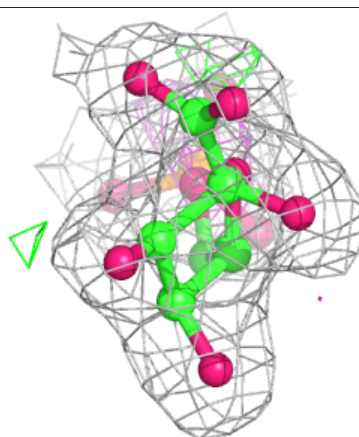
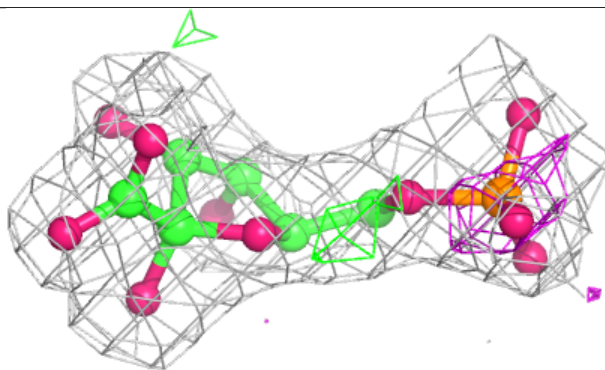
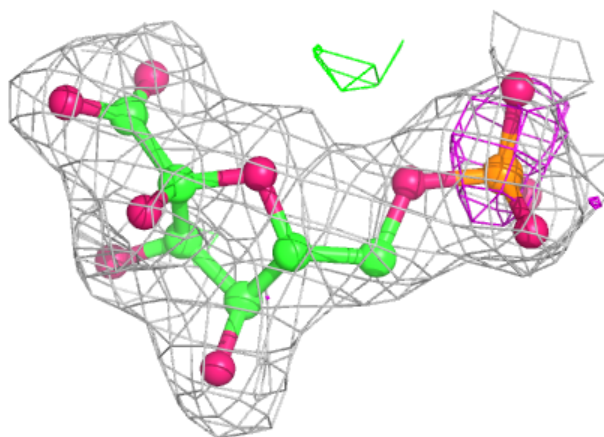
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	F	4020	1/1	0.99	0.11	11,11,11,11	0
2	MG	J	4034	1/1	0.99	0.11	12,12,12,12	0
2	MG	A	4001	1/1	0.99	0.08	11,11,11,11	0
3	K	H	5008	1/1	1.00	0.06	23,23,23,23	0
3	K	K	5011	1/1	1.00	0.06	23,23,23,23	0
3	K	A	5001	1/1	1.00	0.10	21,21,21,21	0
2	MG	H	4029	1/1	1.00	0.09	12,12,12,12	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.



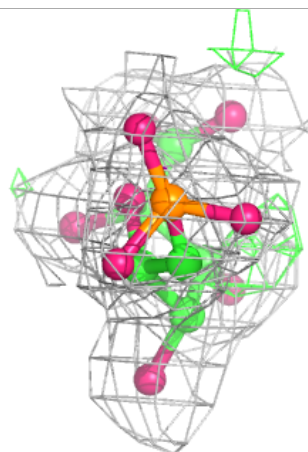
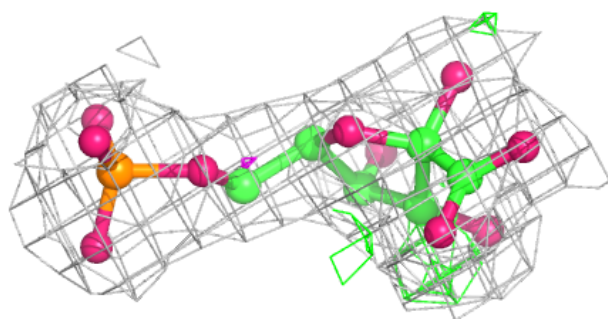
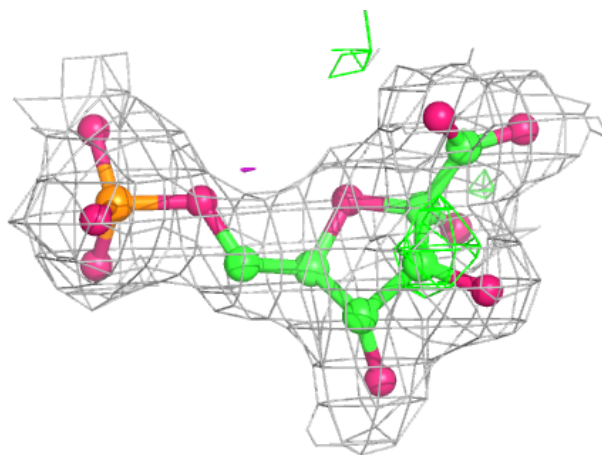
Electron density around CKP H 2008:

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



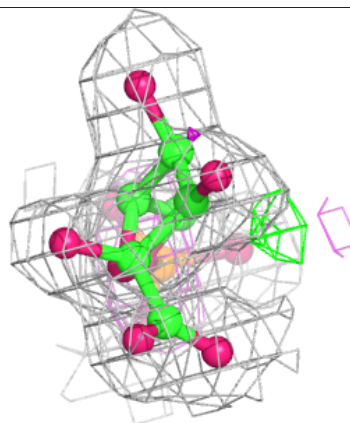
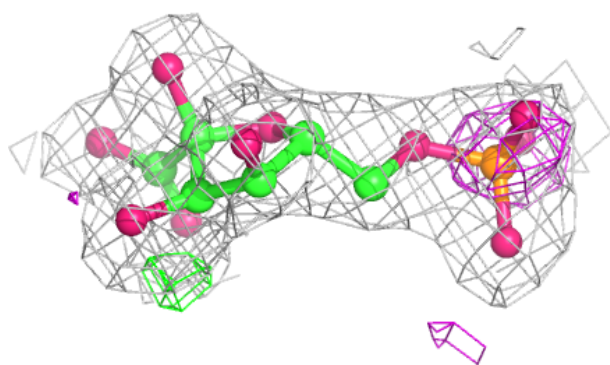
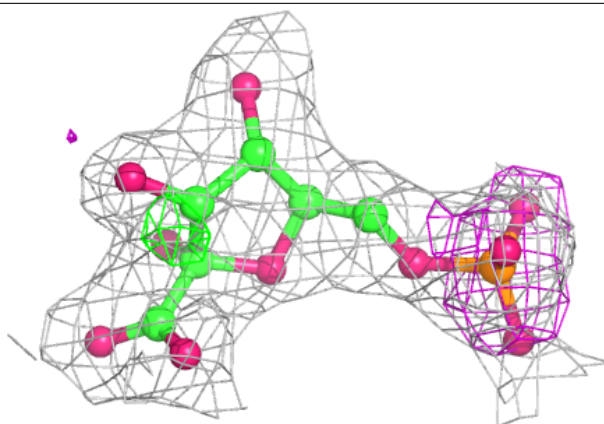
Electron density around CKP L 2012:

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



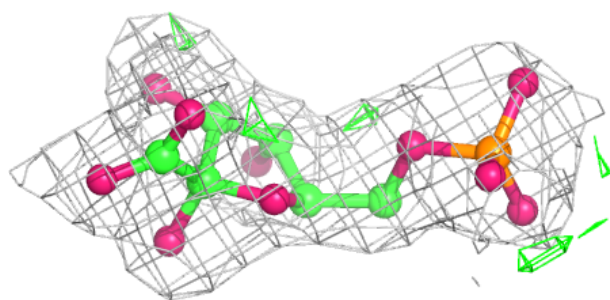
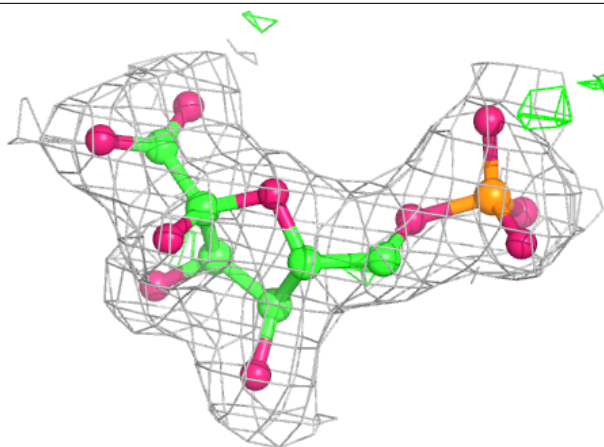
Electron density around CKP C 2003:

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



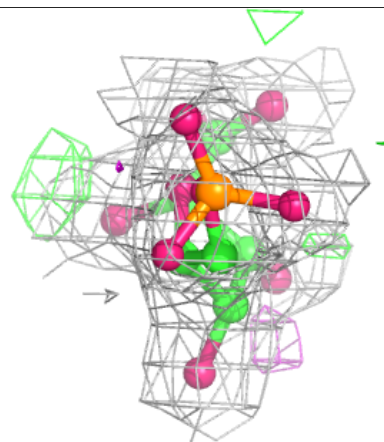
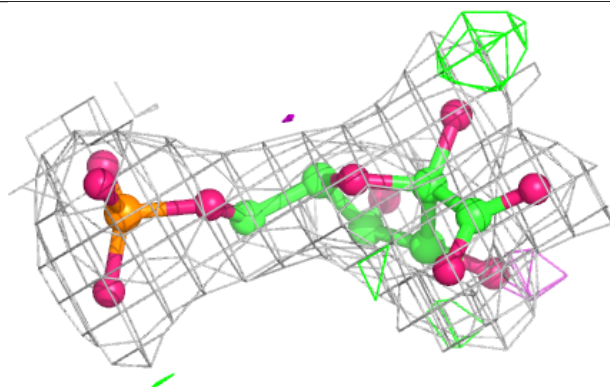
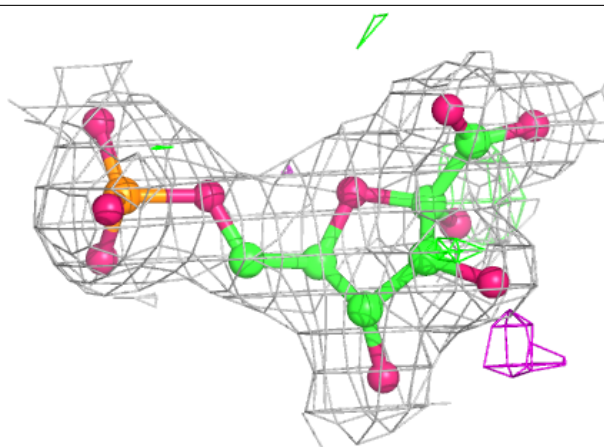
Electron density around CKP E 2005:

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

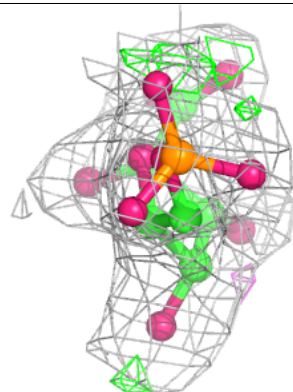
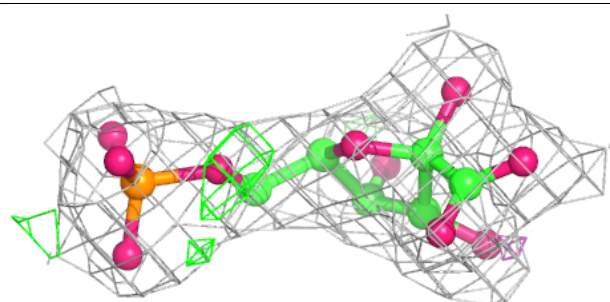
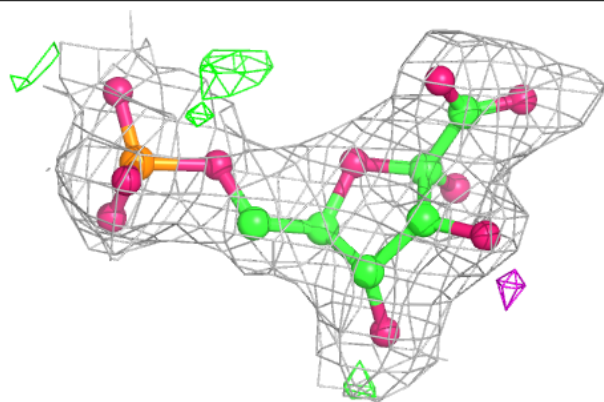


Electron density around CKP F 2006:

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

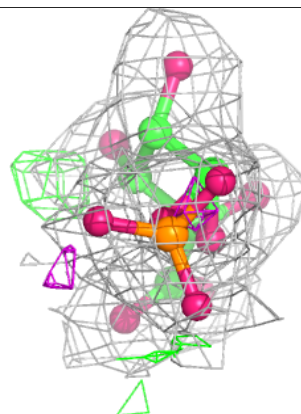
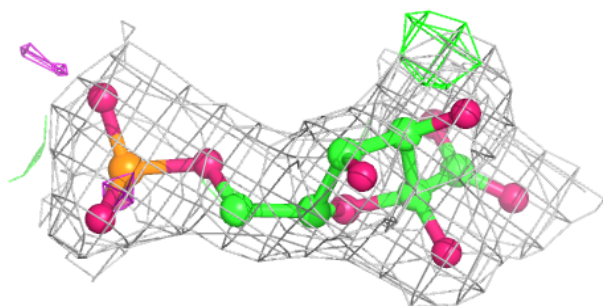
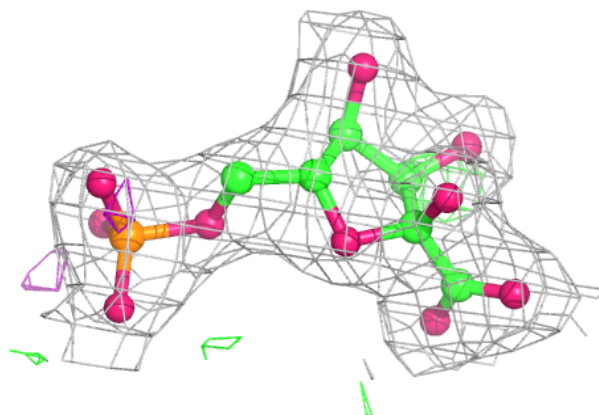
**Electron density around CKP J 2010:**

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

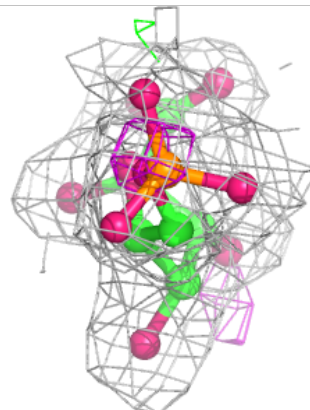
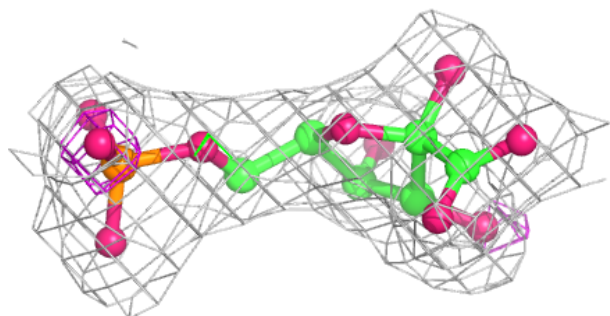
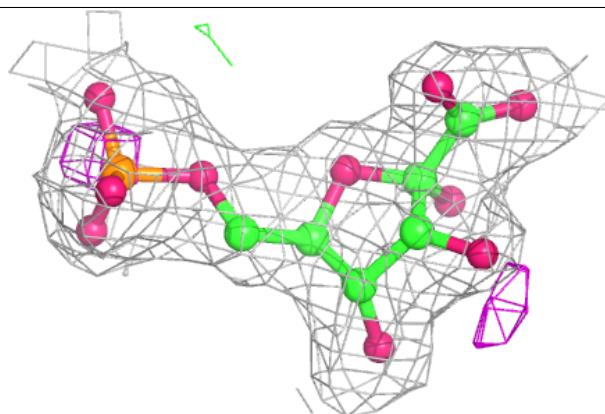


Electron density around CKP K 2011:

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

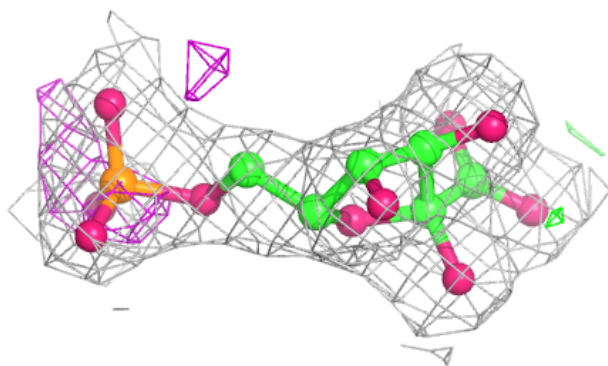
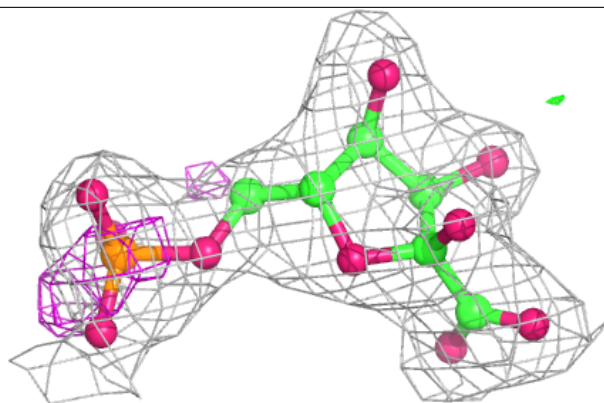
**Electron density around CKP D 2004:**

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

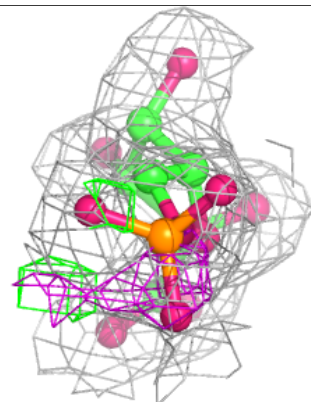
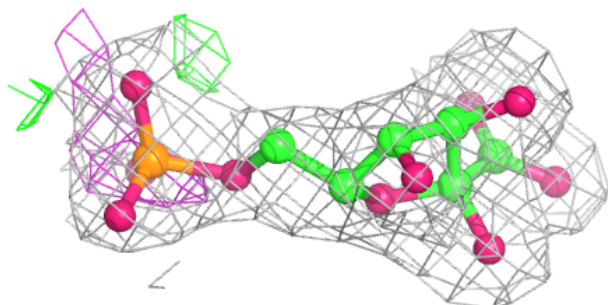
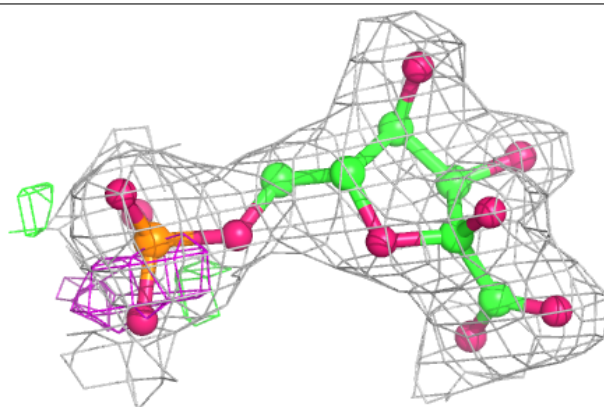


Electron density around CKP G 2007:

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

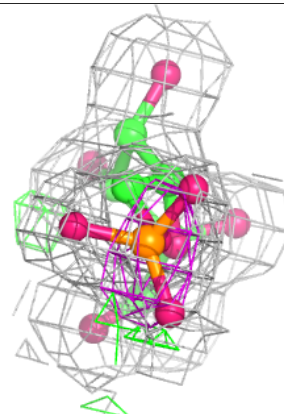
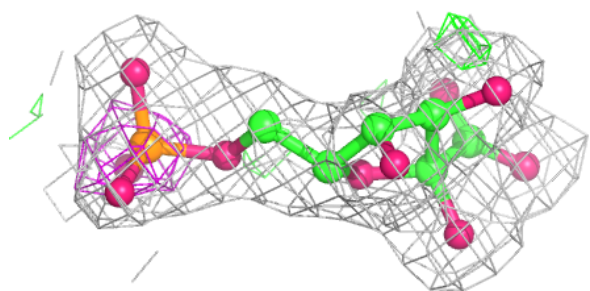
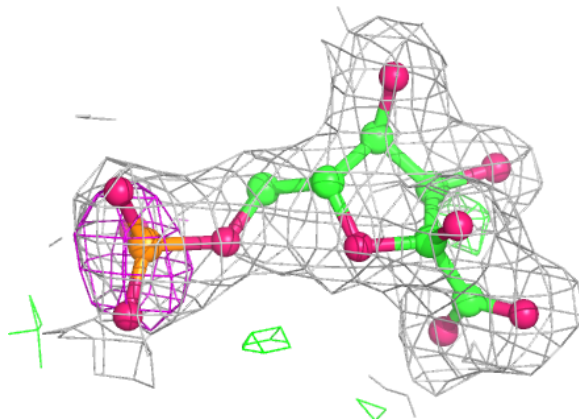
**Electron density around CKP A 2001:**

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

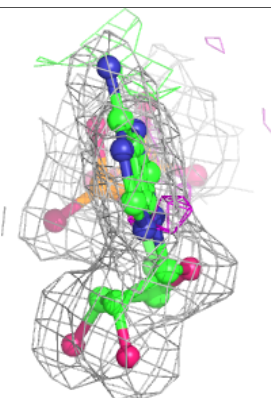
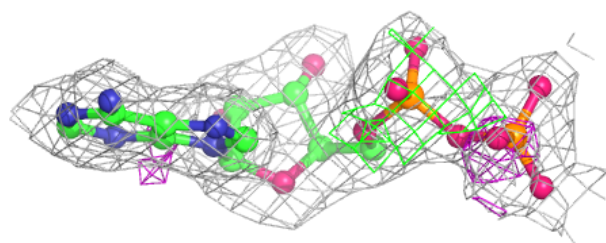
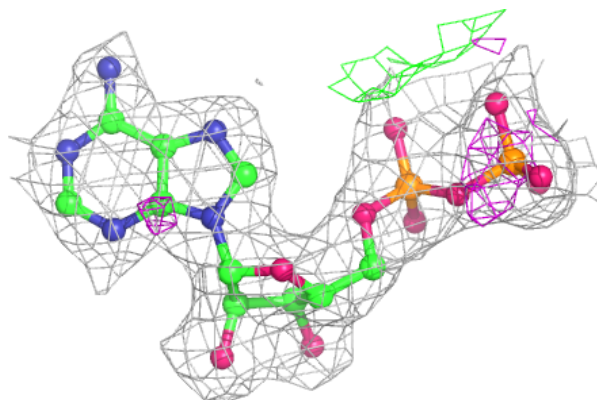


Electron density around CKP I 2009:

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and green (positive)

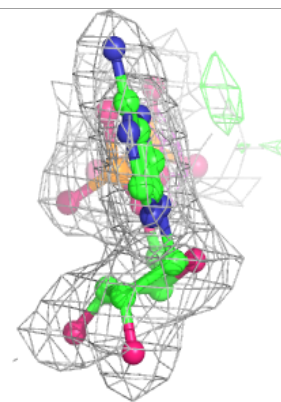
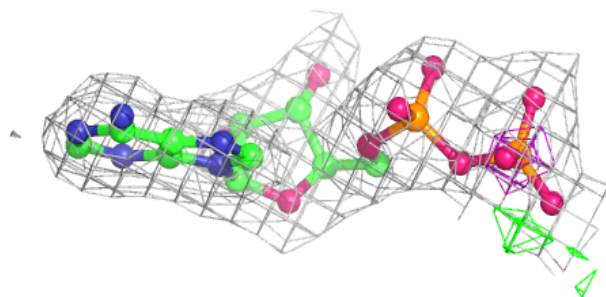
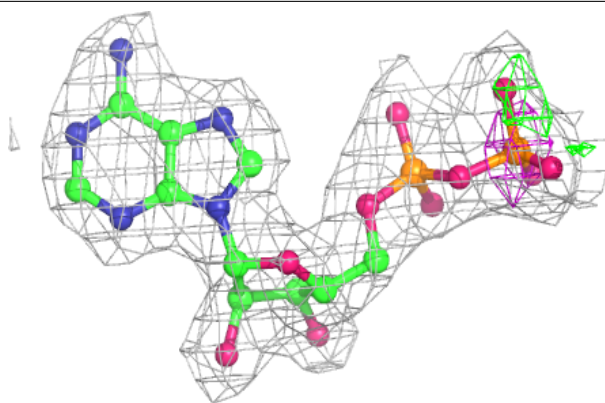
**Electron density around ADP A 3001:**

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and green (positive)

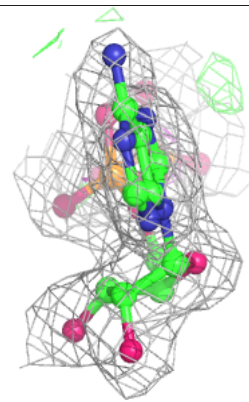
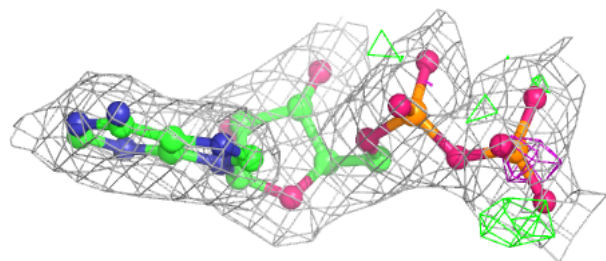
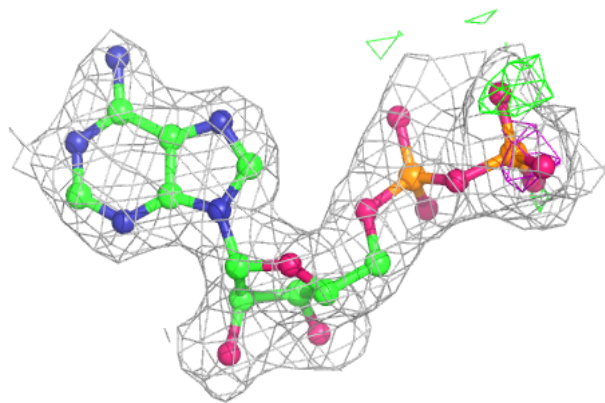


Electron density around ADP E 3005:

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and green (positive)

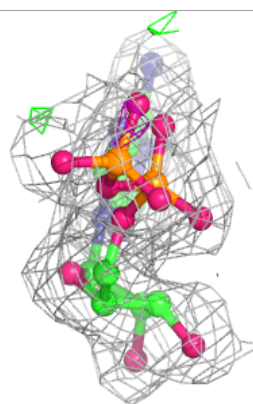
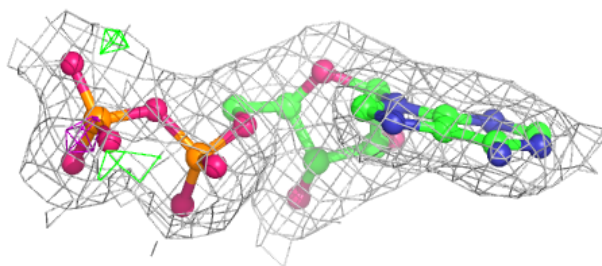
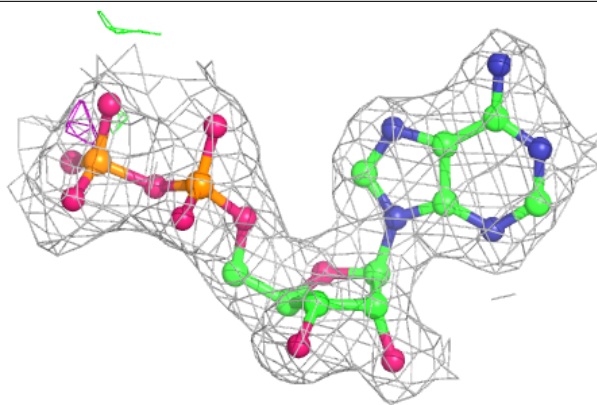
**Electron density around ADP J 3010:**

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

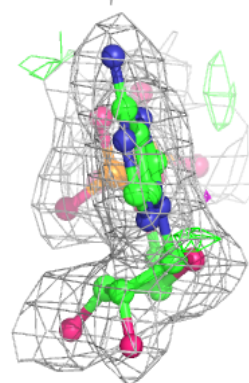
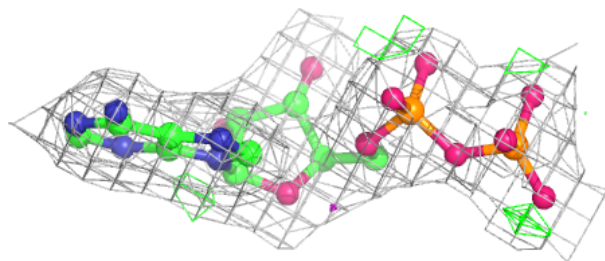
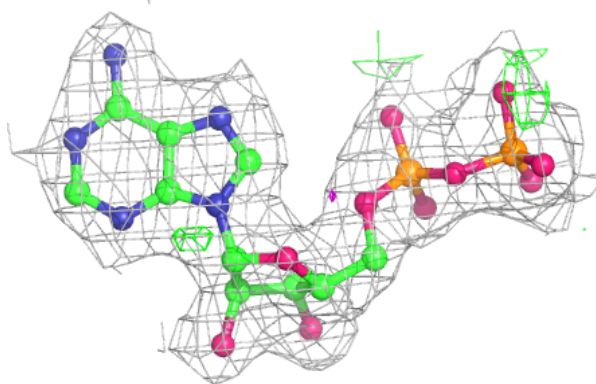


Electron density around ADP D 3004:

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

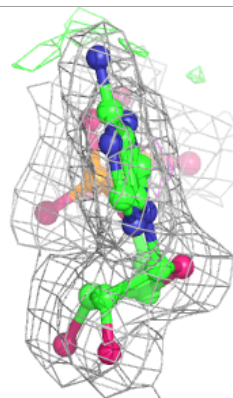
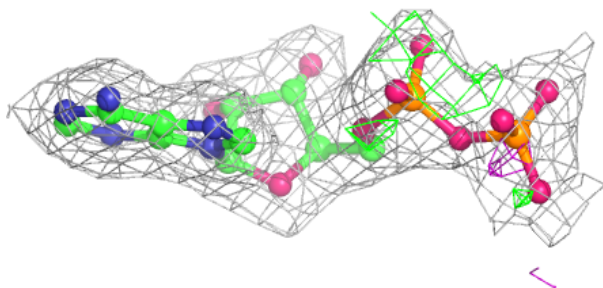
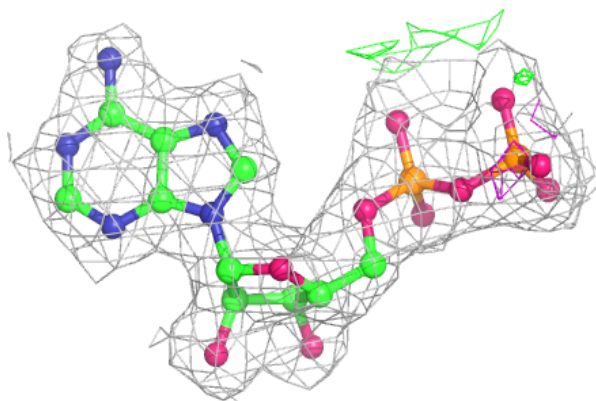
**Electron density around ADP K 3011:**

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

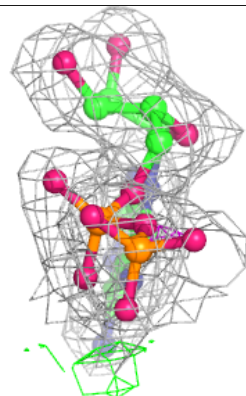
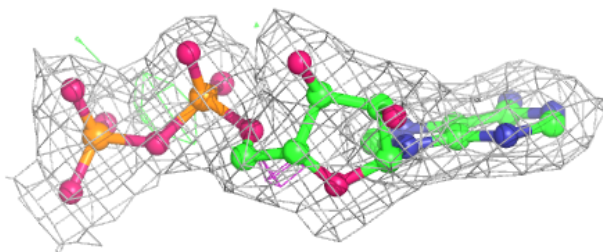
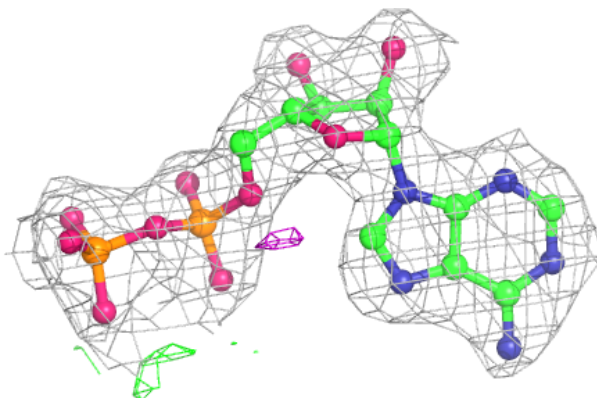


Electron density around ADP G 3007:

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

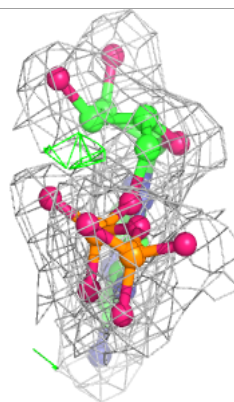
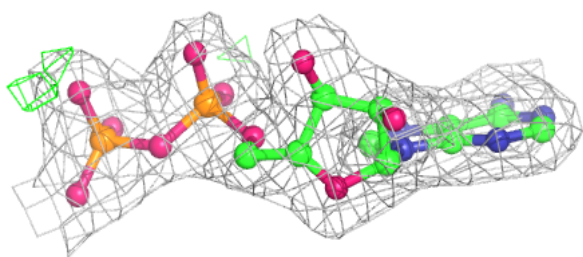
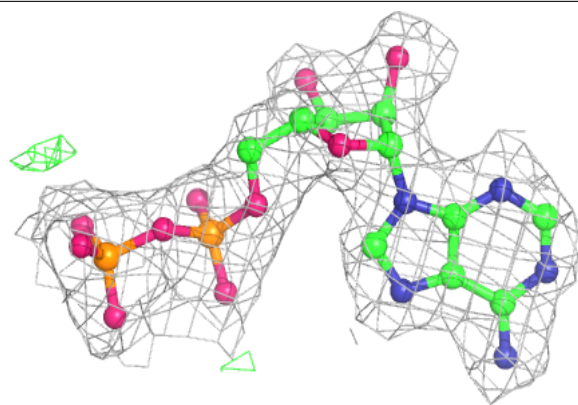
**Electron density around ADP F 3006:**

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

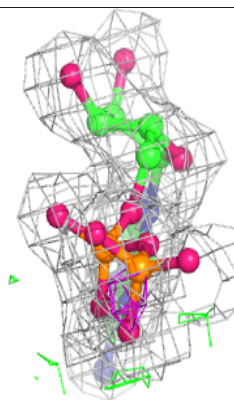
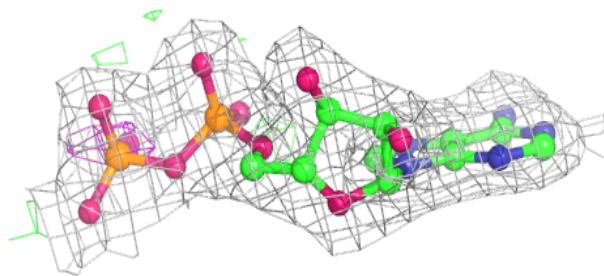
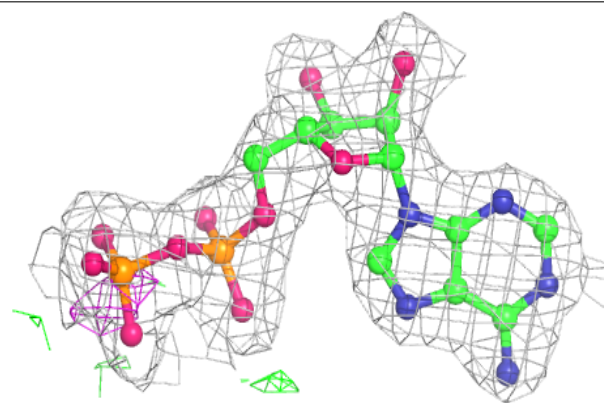


Electron density around ADP C 3003:

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and green (positive)

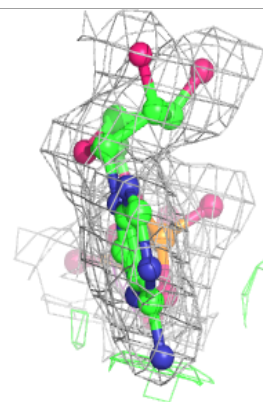
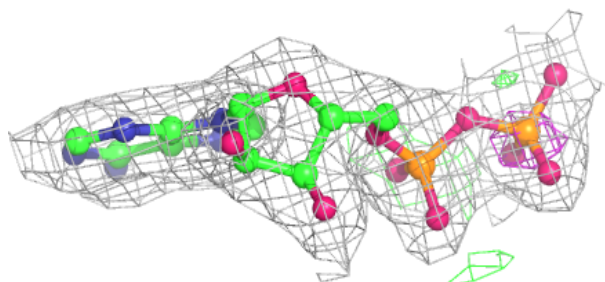
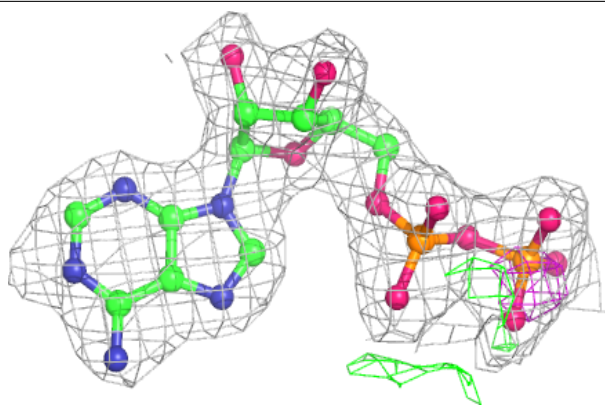
**Electron density around ADP B 3002:**

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

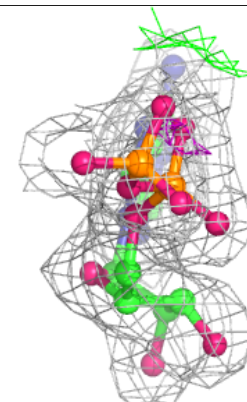
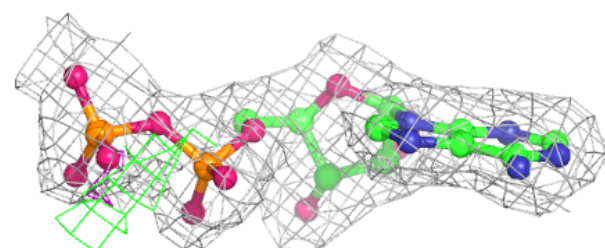
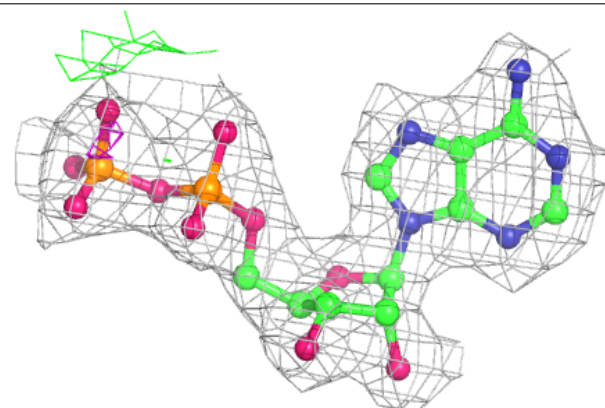


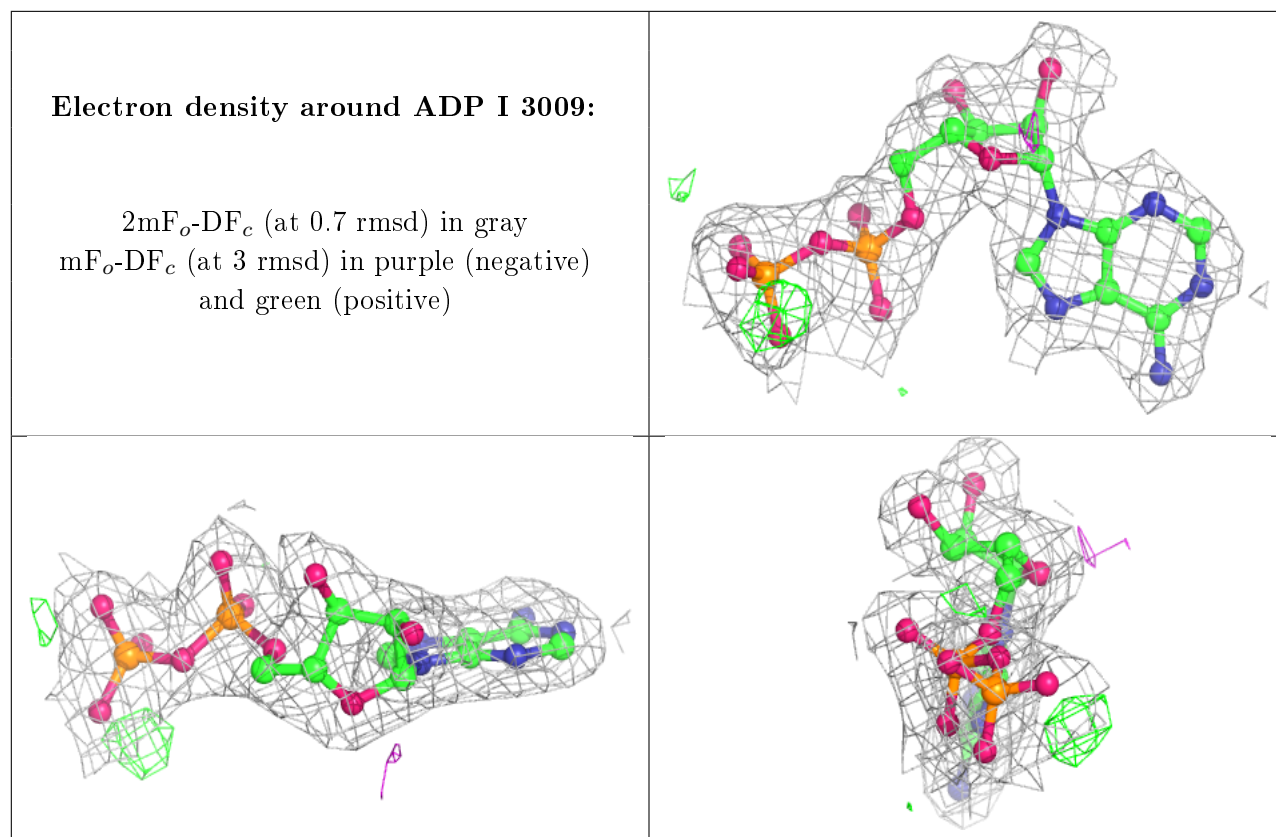
Electron density around ADP H 3008:

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

**Electron density around ADP L 3012:**

$2mF_o-DF_c$ (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.