



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 03:06 AM EST

PDB ID : 2D3C
Title : Crystal Structure of the Maize Glutamine Synthetase complexed with ADP and Phosphinothricin Phosphate
Authors : Unno, H.; Uchida, T.; Sugawara, H.; Kurisu, G.; Sugiyama, T.; Yamaya, T.; Sakakibara, H.; Hase, T.; Kusunoki, M.
Deposited on : 2005-09-26
Resolution : 3.81 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 types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

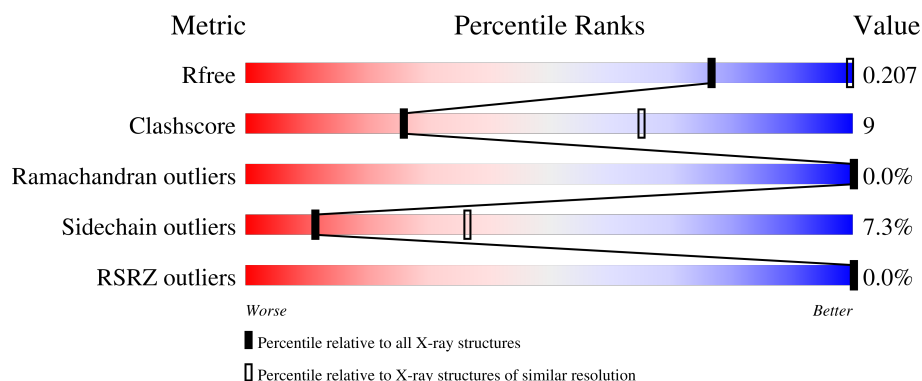
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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}	164625	1155 (4.00-3.64)
Clashscore	180529	1222 (4.00-3.64)
Ramachandran outliers	177936	1182 (4.00-3.64)
Sidechain outliers	177891	1174 (4.00-3.64)
RSRZ outliers	164620	1156 (4.00-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	356	<div> <div>79%</div> <div>17%</div> <div>..</div> </div>
1	B	356	<div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	C	356	<div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	D	356	<div> <div>77%</div> <div>19%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	356	 78% 19% ..
1	F	356	 78% 19% ..
1	G	356	 78% 18% ..
1	H	356	 79% 17% ..
1	I	356	 76% 19% ..
1	J	356	 78% 19% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28138 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 glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	B	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	C	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	D	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	E	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	F	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	G	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	H	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	I	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			
1	J	353	Total	C	N	O	S	0	0	0
			2745	1739	470	525	11			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

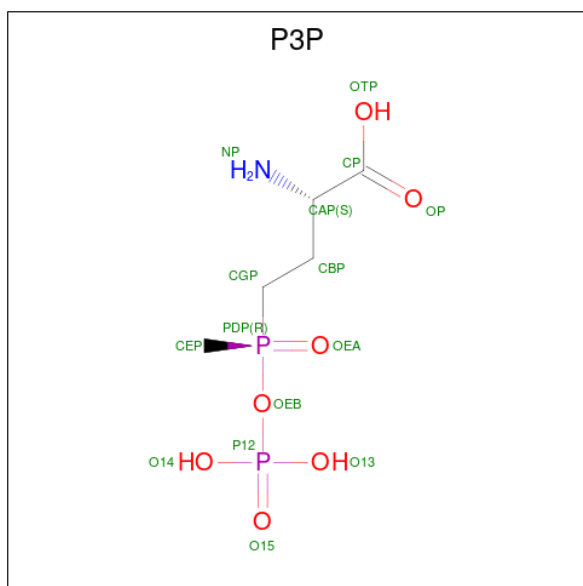
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		
2	C	3	Total	Mn	0	0
			3	3		
2	D	3	Total	Mn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	3	Total	Mn	0	0
			3	3		
2	F	3	Total	Mn	0	0
			3	3		
2	G	3	Total	Mn	0	0
			3	3		
2	H	3	Total	Mn	0	0
			3	3		
2	I	3	Total	Mn	0	0
			3	3		
2	J	3	Total	Mn	0	0
			3	3		

- Molecule 3 is (2S)-2-AMINO-4-[METHYL(PHOSPHONOOXY)PHOSPHORYL]BUTANOIC ACID (three-letter code: P3P) (formula: C₅H₁₃NO₇P₂).



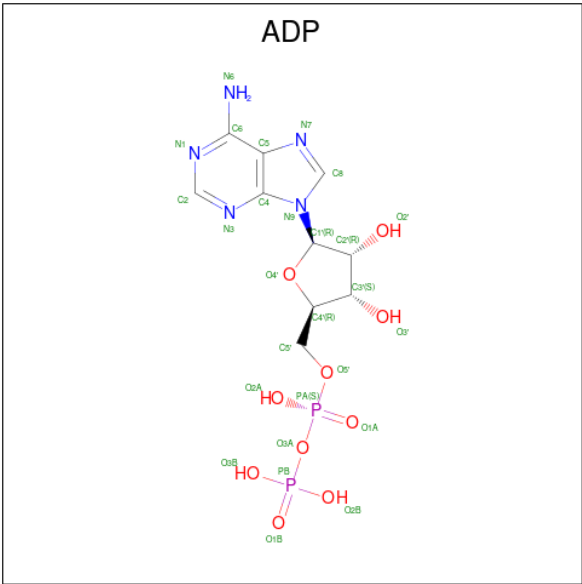
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	B	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	C	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	D	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	E	1	Total	C	N	O	P	0	0
			15	5	1	7	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	G	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	H	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	I	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
3	J	1	Total	C	N	O	P	0	0
			15	5	1	7	2		

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



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

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

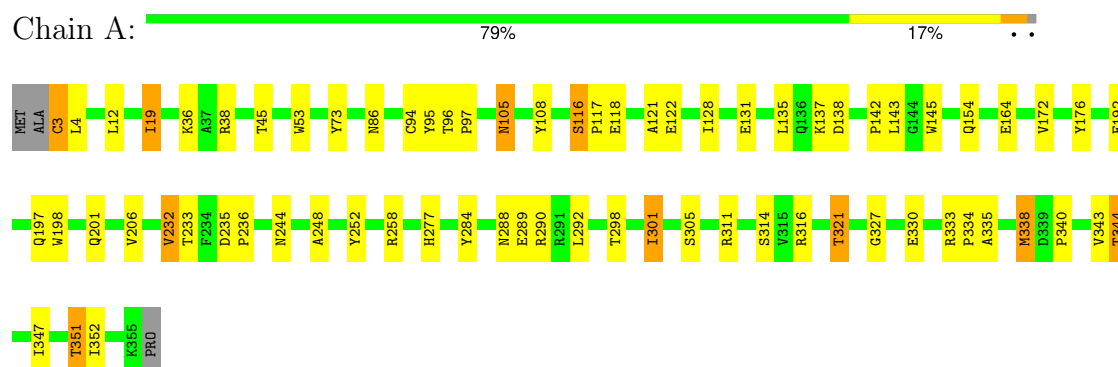
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total	O	0	0
			25	25		
5	B	26	Total	O	0	0
			26	26		
5	C	11	Total	O	0	0
			11	11		
5	D	30	Total	O	0	0
			30	30		
5	E	30	Total	O	0	0
			30	30		
5	F	31	Total	O	0	0
			31	31		
5	G	22	Total	O	0	0
			22	22		
5	H	21	Total	O	0	0
			21	21		
5	I	27	Total	O	0	0
			27	27		
5	J	15	Total	O	0	0
			15	15		

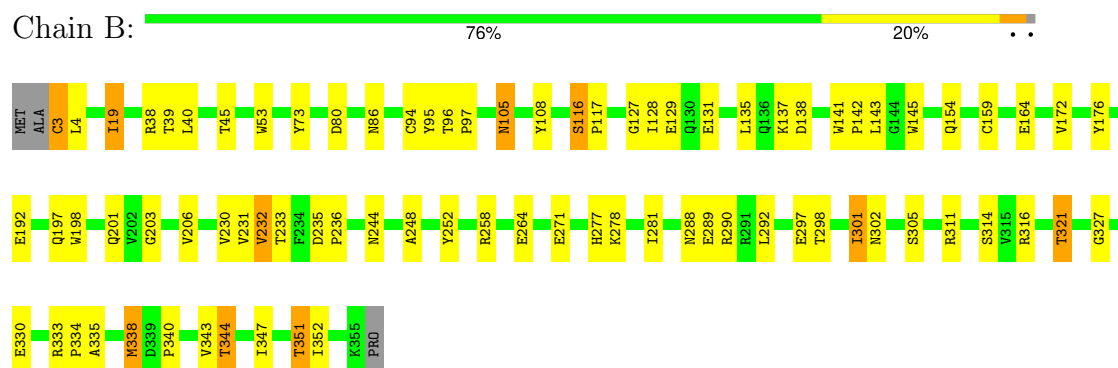
3 Residue-property plots [i](#)

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

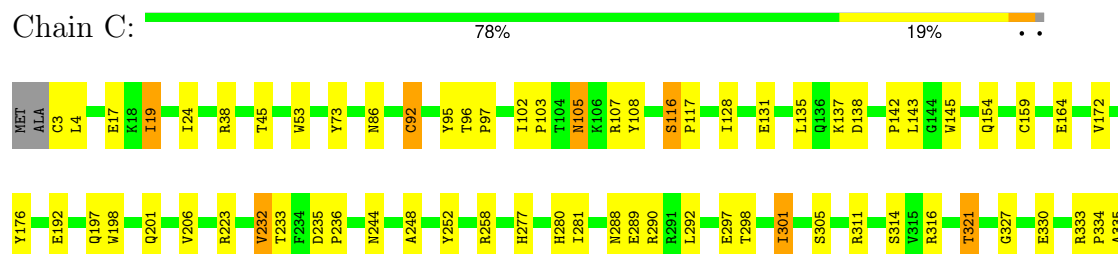
- Molecule 1: glutamine synthetase



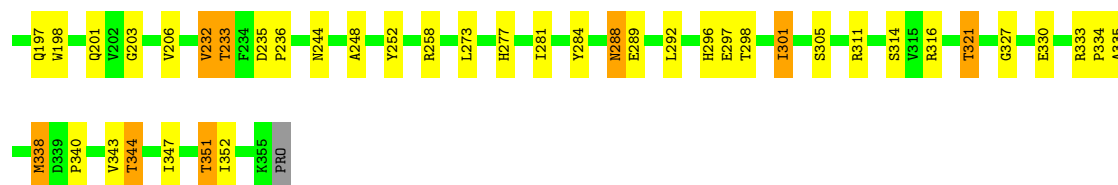
- Molecule 1: glutamine synthetase



- Molecule 1: glutamine synthetase

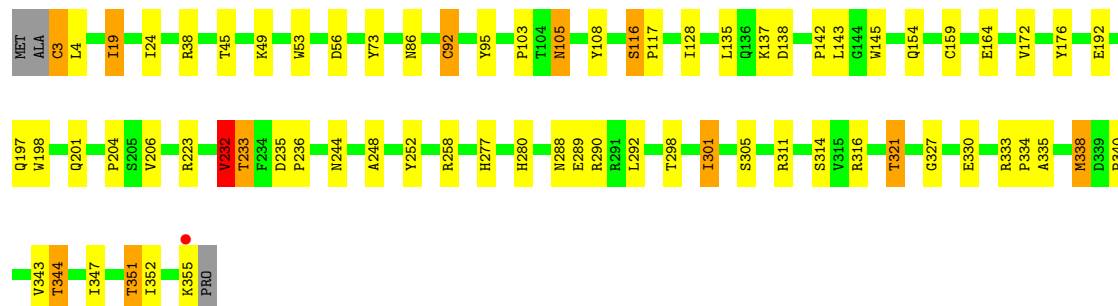






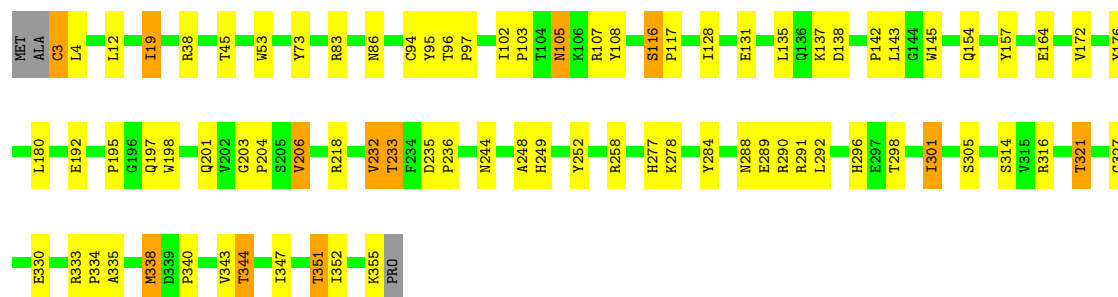
- Molecule 1: glutamine synthetase

Chain H: 79% 17%



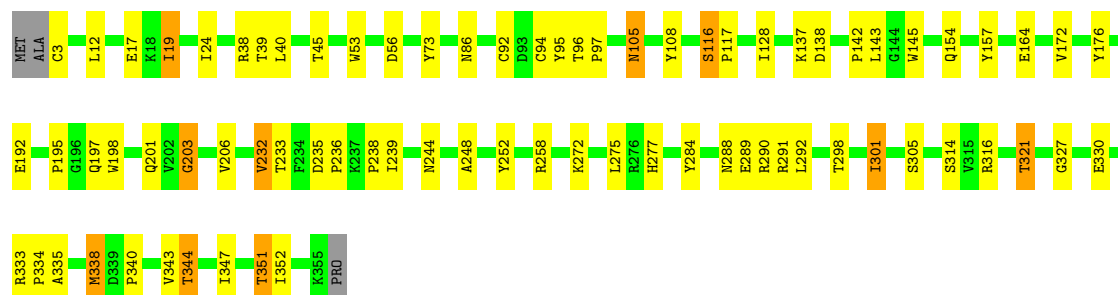
- Molecule 1: glutamine synthetase

Chain I: 76% 19%



- Molecule 1: glutamine synthetase

Chain J: 78% 19%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.96Å 191.01Å 118.12Å 90.00° 101.23° 90.00°	Depositor
Resolution (Å)	27.36 – 3.81 27.36 – 3.81	Depositor EDS
% Data completeness (in resolution range)	83.0 (27.36-3.81) 82.9 (27.36-3.81)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.185 , 0.229 0.170 , 0.207	Depositor DCC
R_{free} test set	1718 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	86.9	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28138	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MN, P3P

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	0.96	1/2819 (0.0%)	0.81	1/3834 (0.0%)
1	B	0.98	2/2819 (0.1%)	0.82	1/3834 (0.0%)
1	C	0.99	3/2819 (0.1%)	0.81	1/3834 (0.0%)
1	D	0.98	1/2819 (0.0%)	0.84	1/3834 (0.0%)
1	E	0.99	3/2819 (0.1%)	0.84	3/3834 (0.1%)
1	F	1.01	2/2819 (0.1%)	0.83	1/3834 (0.0%)
1	G	0.98	1/2819 (0.0%)	0.83	1/3834 (0.0%)
1	H	0.95	2/2819 (0.1%)	0.81	1/3834 (0.0%)
1	I	0.98	1/2819 (0.0%)	0.81	1/3834 (0.0%)
1	J	0.99	2/2819 (0.1%)	0.83	2/3834 (0.1%)
All	All	0.98	18/28190 (0.1%)	0.82	13/38340 (0.0%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	94	CYS	CB-SG	-9.28	1.66	1.82
1	B	159	CYS	CB-SG	-8.08	1.68	1.82
1	A	94	CYS	CB-SG	-7.07	1.70	1.82
1	C	92	CYS	CB-SG	-6.33	1.71	1.82
1	J	94	CYS	CB-SG	-6.04	1.72	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	290	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	D	232	VAL	CB-CA-C	-5.50	100.95	111.40
1	F	232	VAL	CB-CA-C	-5.44	101.06	111.40
1	G	232	VAL	CB-CA-C	-5.39	101.15	111.40
1	E	232	VAL	CB-CA-C	-5.39	101.16	111.40

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	2745	0	2653	47	0
1	B	2745	0	2653	51	1
1	C	2745	0	2653	46	0
1	D	2745	0	2653	55	0
1	E	2745	0	2653	48	0
1	F	2745	0	2653	52	0
1	G	2745	0	2653	53	0
1	H	2745	0	2653	47	1
1	I	2745	0	2653	56	0
1	J	2745	0	2653	44	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
3	A	15	0	10	5	0
3	B	15	0	10	3	0
3	C	15	0	10	4	0
3	D	15	0	10	3	0
3	E	15	0	10	4	0
3	F	15	0	10	4	0
3	G	15	0	10	2	0
3	H	15	0	10	2	0
3	I	15	0	10	4	0
3	J	15	0	10	0	0
4	A	27	0	12	0	0
4	B	27	0	12	2	0
4	C	27	0	12	0	0
4	D	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	27	0	12	0	0
4	F	27	0	12	2	0
4	G	27	0	12	3	0
4	H	27	0	12	0	0
4	I	27	0	12	2	0
4	J	27	0	12	1	0
5	A	25	0	0	7	0
5	B	26	0	0	5	0
5	C	11	0	0	1	0
5	D	30	0	0	11	0
5	E	30	0	0	10	0
5	F	31	0	0	8	0
5	G	22	0	0	7	0
5	H	21	0	0	7	0
5	I	27	0	0	8	0
5	J	15	0	0	3	0
All	All	28138	0	26750	507	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 9.

The worst 5 of 507 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:B:278:LYS:HA	5:B:6021:HOH:O	1.22	1.29
1:B:344:THR:HG21	5:B:6024:HOH:O	1.44	1.18
1:B:271:GLU:OE1	5:B:6016:HOH:O	1.63	1.14
1:D:123:GLU:HA	5:D:6013:HOH:O	1.54	1.05
1:J:117:PRO:HD2	5:J:6022:HOH:O	1.57	1.03

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:B:302:ASN:O	1:H:355:LYS:CB[2_655]	2.16	0.04

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	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	B	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	C	351/356 (99%)	332 (95%)	19 (5%)	0	100	100
1	D	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	E	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	F	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	G	351/356 (99%)	334 (95%)	17 (5%)	0	100	100
1	H	351/356 (99%)	332 (95%)	19 (5%)	0	100	100
1	I	351/356 (99%)	333 (95%)	18 (5%)	0	100	100
1	J	351/356 (99%)	336 (96%)	14 (4%)	1 (0%)	37	70
All	All	3510/3560 (99%)	3334 (95%)	175 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	203	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	288/290 (99%)	267 (93%)	21 (7%)	11	36
1	B	288/290 (99%)	267 (93%)	21 (7%)	11	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	288/290 (99%)	267 (93%)	21 (7%)	11	36
1	D	288/290 (99%)	268 (93%)	20 (7%)	13	38
1	E	288/290 (99%)	267 (93%)	21 (7%)	11	36
1	F	288/290 (99%)	267 (93%)	21 (7%)	11	36
1	G	288/290 (99%)	267 (93%)	21 (7%)	11	36
1	H	288/290 (99%)	266 (92%)	22 (8%)	11	35
1	I	288/290 (99%)	267 (93%)	21 (7%)	11	36
1	J	288/290 (99%)	267 (93%)	21 (7%)	11	36
All	All	2880/2900 (99%)	2670 (93%)	210 (7%)	11	36

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	232	VAL
1	G	338	MET
1	J	206	VAL
1	F	289	GLU
1	G	128	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	190	ASN
1	H	288	ASN
1	G	201	GLN
1	H	154	GLN
1	I	154	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 30 are monoatomic - leaving 20 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$
3	P3P	A	5001	2	9,14,14	4.00	2 (22%)	11,21,21	1.36	2 (18%)
3	P3P	C	5003	2	9,14,14	3.33	1 (11%)	11,21,21	2.64	8 (72%)
3	P3P	F	5007	2	9,14,14	2.49	1 (11%)	11,21,21	2.50	5 (45%)
3	P3P	H	5010	2	9,14,14	4.67	3 (33%)	11,21,21	1.56	2 (18%)
3	P3P	I	5008	2	9,14,14	3.63	2 (22%)	11,21,21	2.18	3 (27%)
4	ADP	E	6004	2	24,29,29	1.53	3 (12%)	29,45,45	2.11	10 (34%)
4	ADP	I	6008	2	24,29,29	1.35	2 (8%)	29,45,45	2.13	9 (31%)
4	ADP	H	6010	2	24,29,29	1.29	3 (12%)	29,45,45	2.12	8 (27%)
4	ADP	A	6001	2	24,29,29	1.45	5 (20%)	29,45,45	2.88	13 (44%)
4	ADP	G	6006	2	24,29,29	1.16	2 (8%)	29,45,45	1.61	6 (20%)
4	ADP	F	6007	2	24,29,29	1.37	2 (8%)	29,45,45	2.35	5 (17%)
4	ADP	B	6002	2	24,29,29	1.53	4 (16%)	29,45,45	2.69	7 (24%)
3	P3P	G	5006	2	9,14,14	3.52	2 (22%)	11,21,21	2.03	4 (36%)
3	P3P	B	5002	2	9,14,14	2.94	3 (33%)	11,21,21	2.22	5 (45%)
3	P3P	J	5009	2	9,14,14	2.97	1 (11%)	11,21,21	2.02	5 (45%)
3	P3P	E	5005	2	9,14,14	1.89	3 (33%)	11,21,21	1.83	3 (27%)
4	ADP	J	6009	2	24,29,29	1.21	2 (8%)	29,45,45	2.25	6 (20%)
4	ADP	C	6003	2	24,29,29	1.46	3 (12%)	29,45,45	2.44	10 (34%)
3	P3P	D	5004	2	9,14,14	3.55	3 (33%)	11,21,21	1.72	3 (27%)
4	ADP	D	6005	2	24,29,29	1.46	4 (16%)	29,45,45	2.33	9 (31%)

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
3	P3P	A	5001	2	-	6/12/16/16	-
3	P3P	C	5003	2	-	10/12/16/16	-
3	P3P	F	5007	2	-	7/12/16/16	-
3	P3P	H	5010	2	-	9/12/16/16	-
3	P3P	I	5008	2	-	7/12/16/16	-
4	ADP	E	6004	2	-	4/12/32/32	0/3/3/3
4	ADP	I	6008	2	-	3/12/32/32	0/3/3/3
4	ADP	H	6010	2	-	1/12/32/32	0/3/3/3
4	ADP	A	6001	2	-	2/12/32/32	0/3/3/3
4	ADP	G	6006	2	-	7/12/32/32	0/3/3/3
4	ADP	F	6007	2	-	6/12/32/32	0/3/3/3
4	ADP	B	6002	2	-	4/12/32/32	0/3/3/3
3	P3P	G	5006	2	-	4/12/16/16	-
3	P3P	B	5002	2	-	9/12/16/16	-
3	P3P	J	5009	2	-	8/12/16/16	-
3	P3P	E	5005	2	-	9/12/16/16	-
4	ADP	J	6009	2	-	4/12/32/32	0/3/3/3
4	ADP	C	6003	2	-	3/12/32/32	0/3/3/3
3	P3P	D	5004	2	-	7/12/16/16	-
4	ADP	D	6005	2	-	5/12/32/32	0/3/3/3

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	5010	P3P	PDP-CGP	-13.18	1.67	1.79
3	A	5001	P3P	PDP-CGP	-11.38	1.69	1.79
3	I	5008	P3P	PDP-CGP	-10.02	1.70	1.79
3	G	5006	P3P	PDP-CGP	-9.84	1.70	1.79
3	D	5004	P3P	PDP-CGP	-9.67	1.70	1.79

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	6002	ADP	N3-C2-N1	-9.13	116.28	128.67
4	J	6009	ADP	O4'-C1'-N9	8.74	120.33	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	6001	ADP	O4'-C1'-N9	7.71	118.97	108.75
4	A	6001	ADP	N3-C2-N1	-7.42	118.60	128.67
4	F	6007	ADP	O4'-C1'-N9	7.41	118.57	108.75

There are no chirality outliers.

5 of 115 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5001	P3P	PDP-OEB-P12-O13
3	B	5002	P3P	NP-CAP-CP-OP
3	B	5002	P3P	CP-CAP-CBP-CGP
3	B	5002	P3P	NP-CAP-CBP-CGP
3	B	5002	P3P	CAP-CBP-CGP-PDP

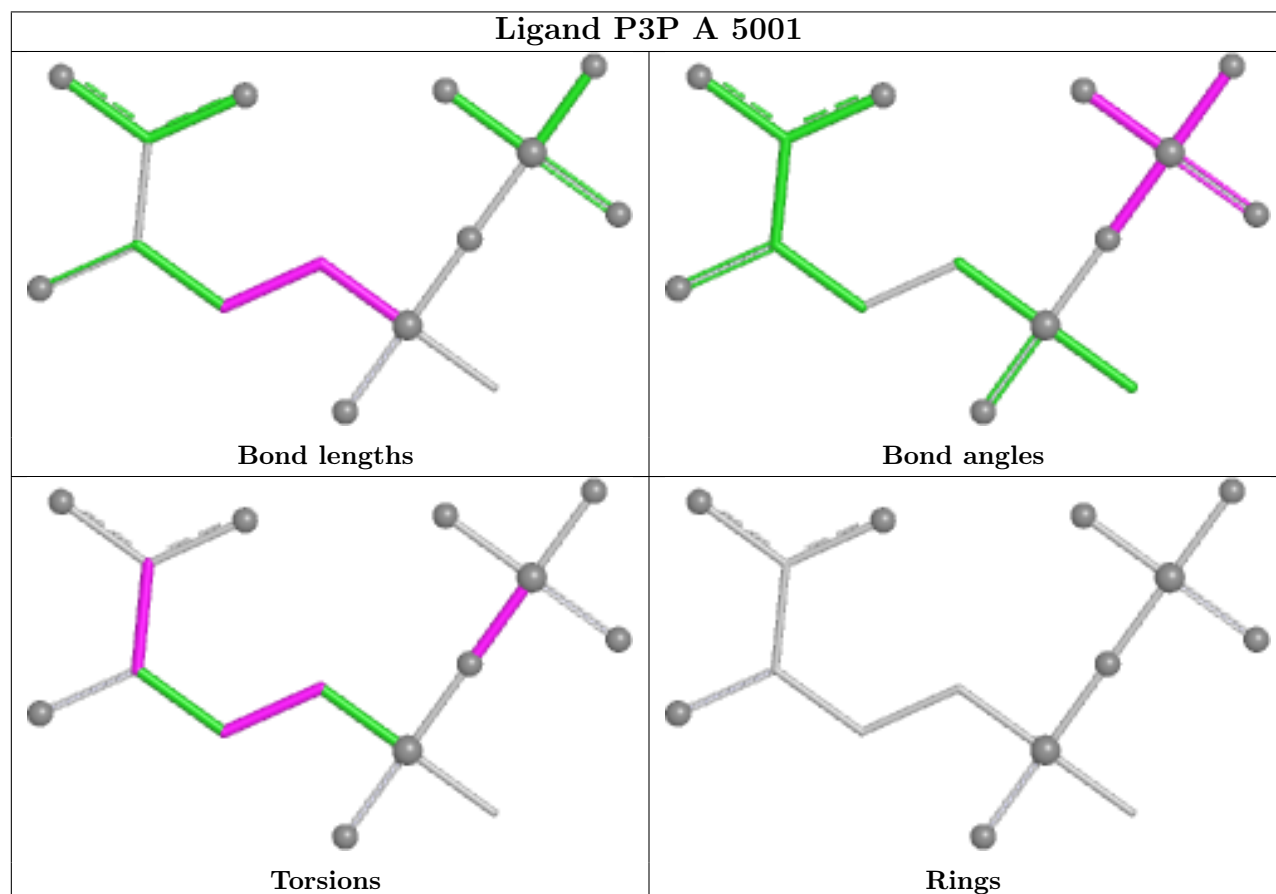
There are no ring outliers.

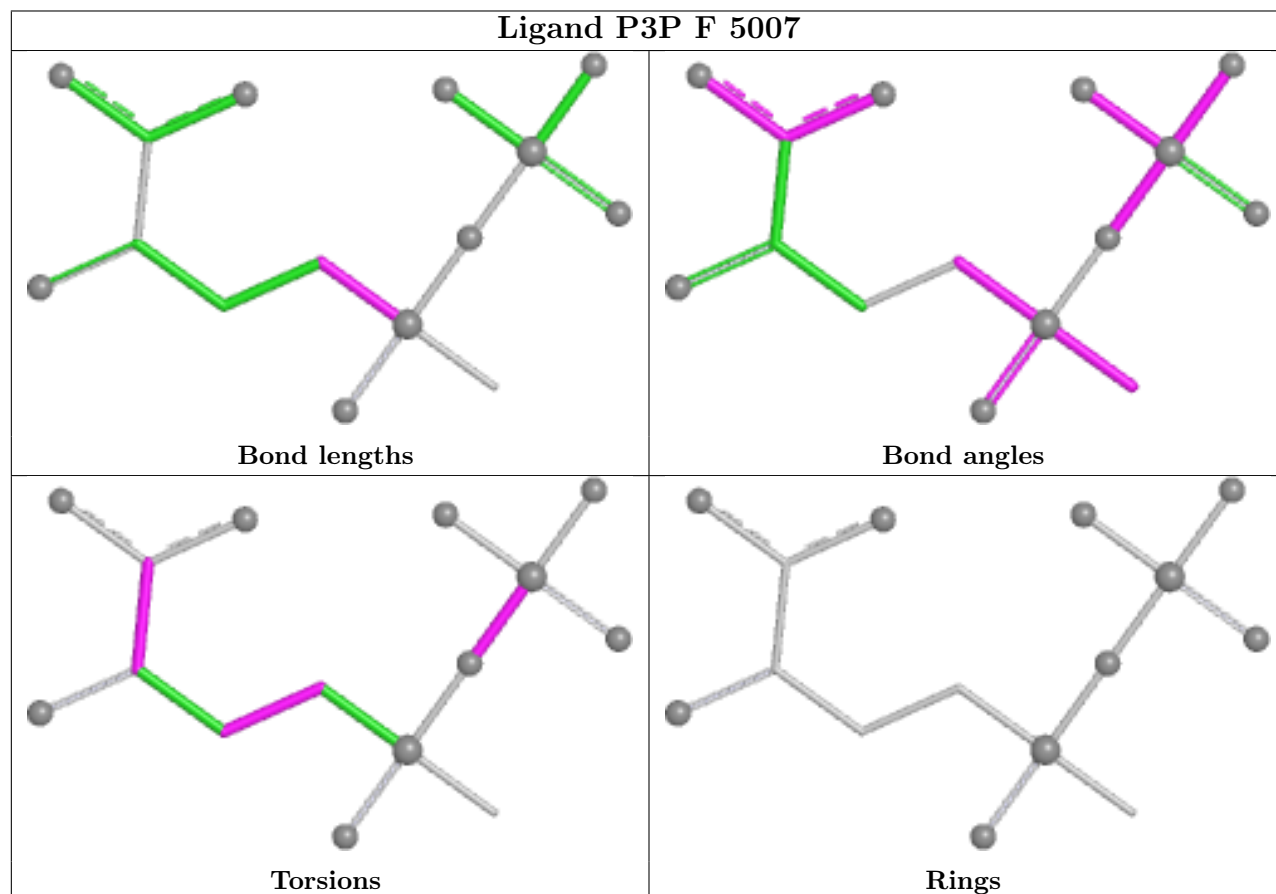
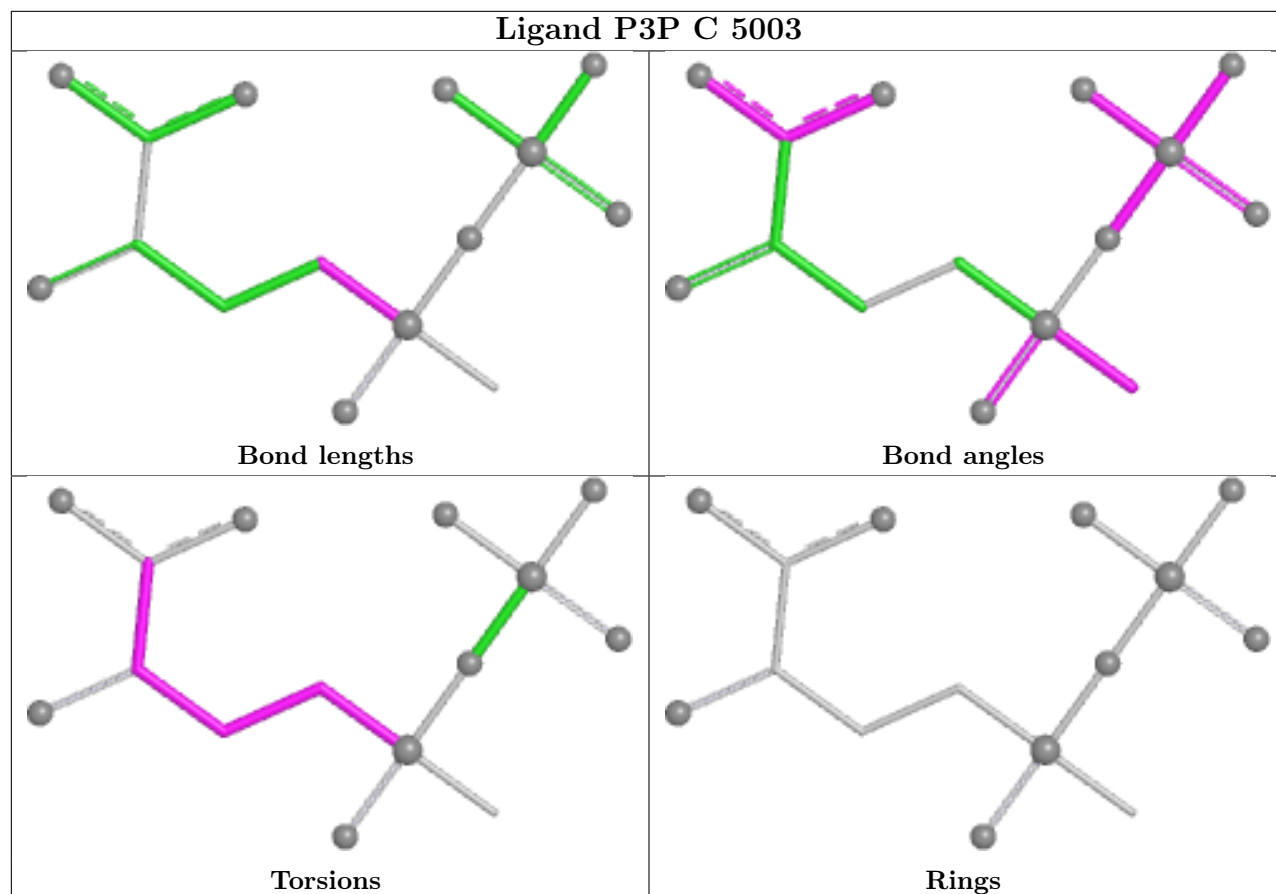
15 monomers are involved in 41 short contacts:

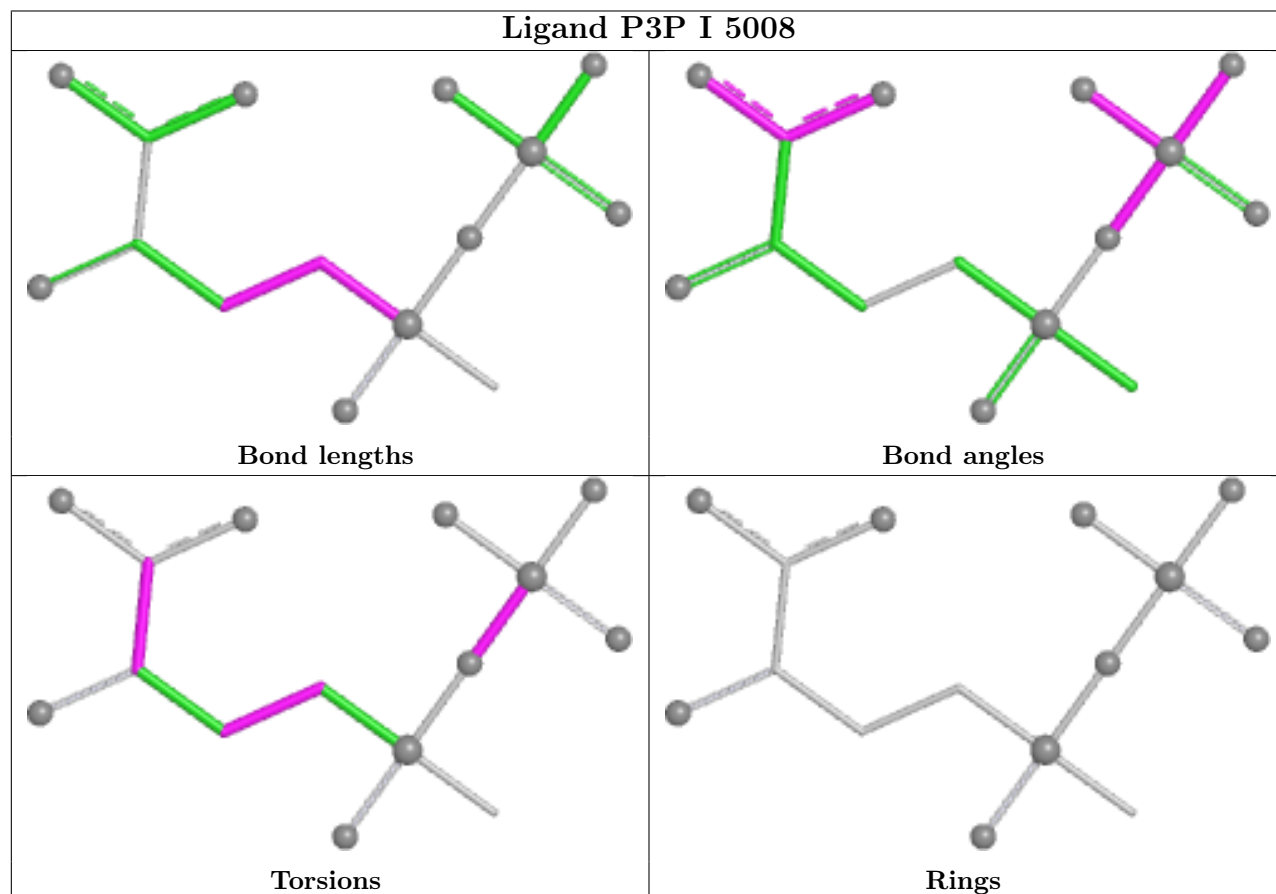
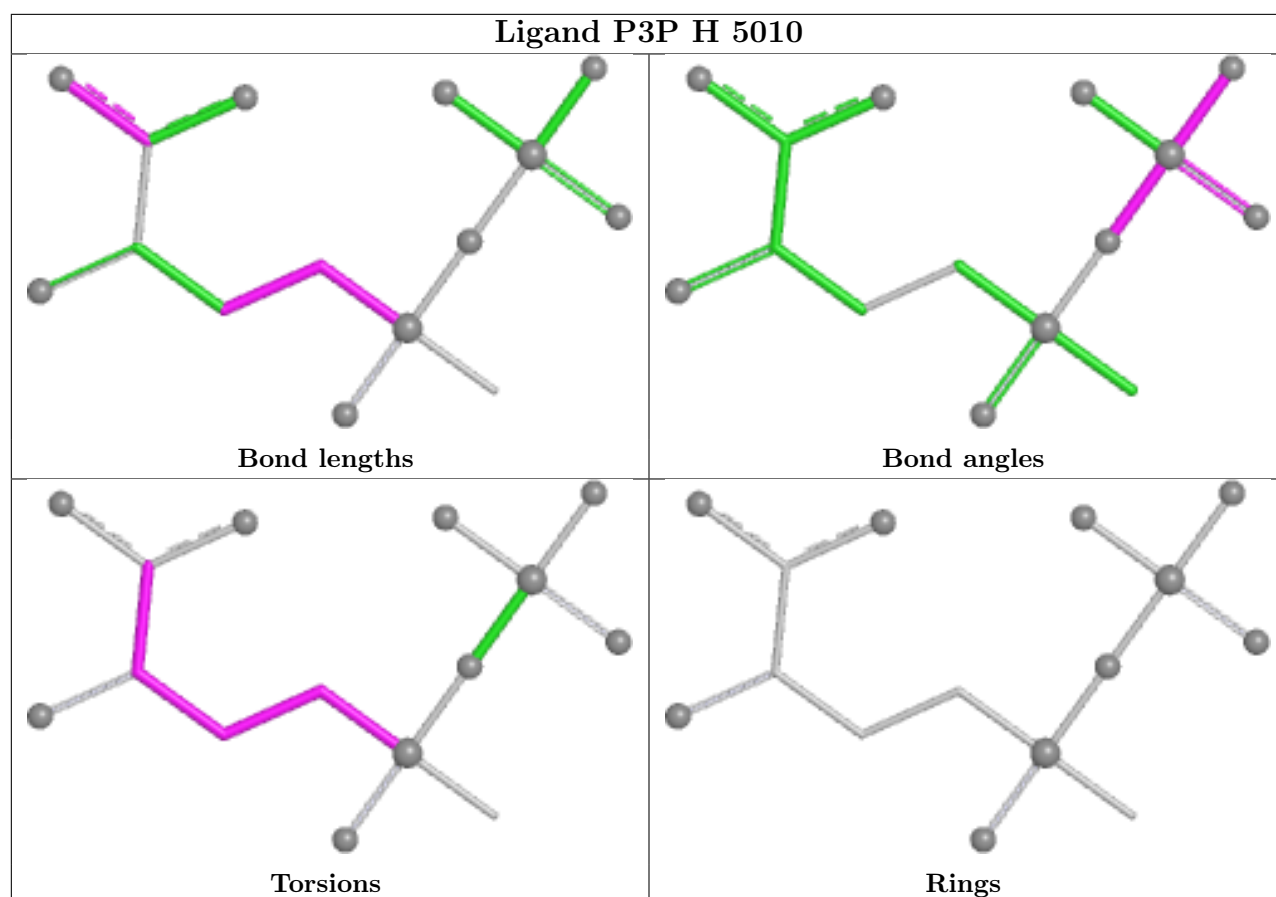
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5001	P3P	5	0
3	C	5003	P3P	4	0
3	F	5007	P3P	4	0
3	H	5010	P3P	2	0
3	I	5008	P3P	4	0
4	I	6008	ADP	2	0
4	G	6006	ADP	3	0
4	F	6007	ADP	2	0
4	B	6002	ADP	2	0
3	G	5006	P3P	2	0
3	B	5002	P3P	3	0
3	E	5005	P3P	4	0
4	J	6009	ADP	1	0
3	D	5004	P3P	3	0
4	D	6005	ADP	1	0

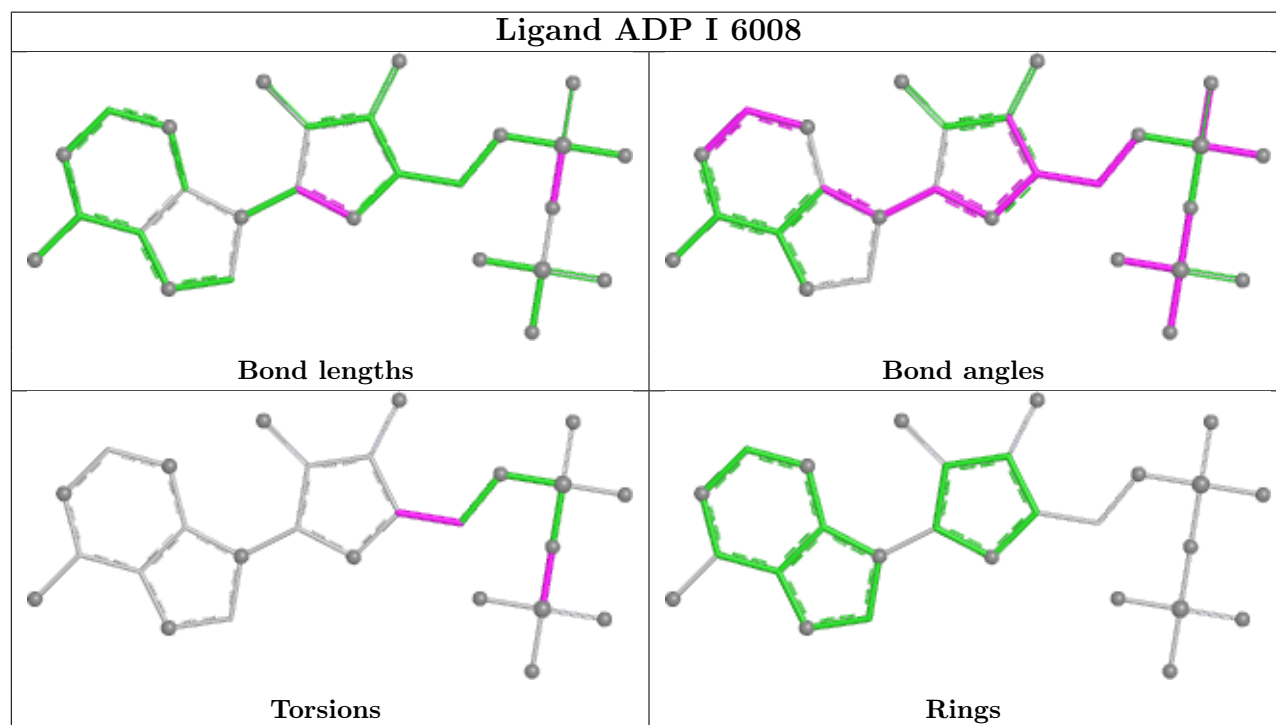
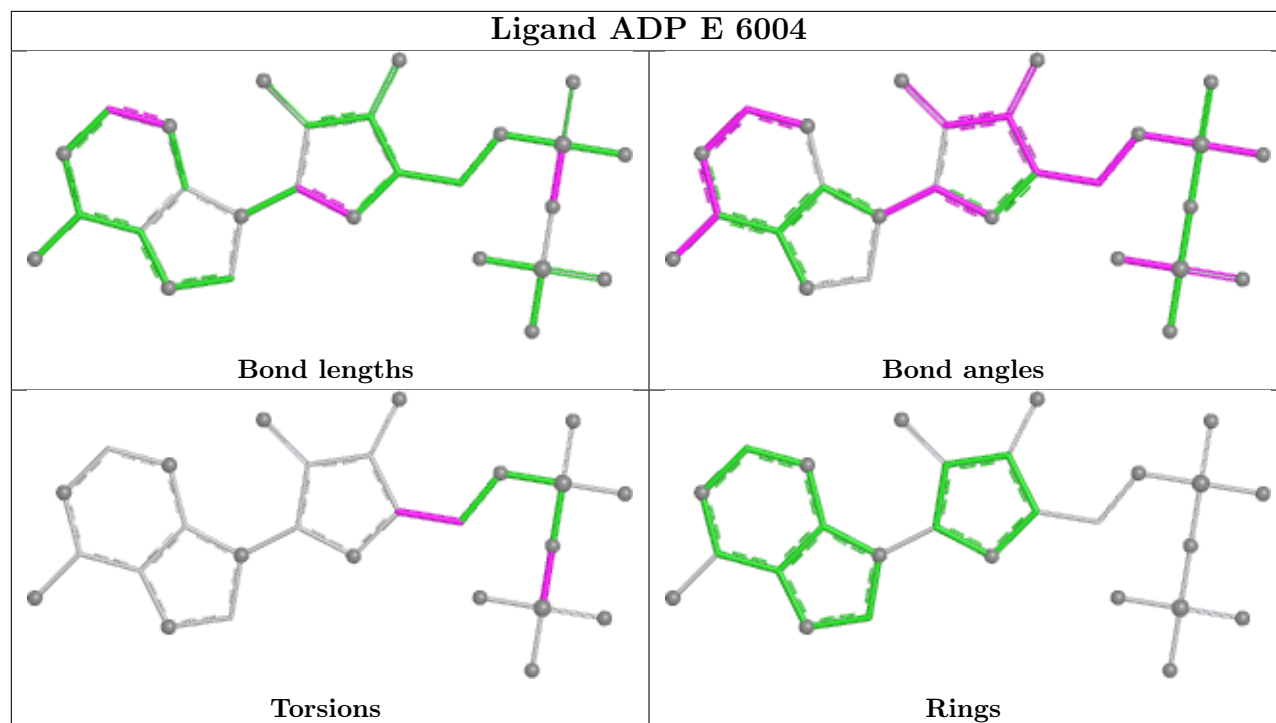
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

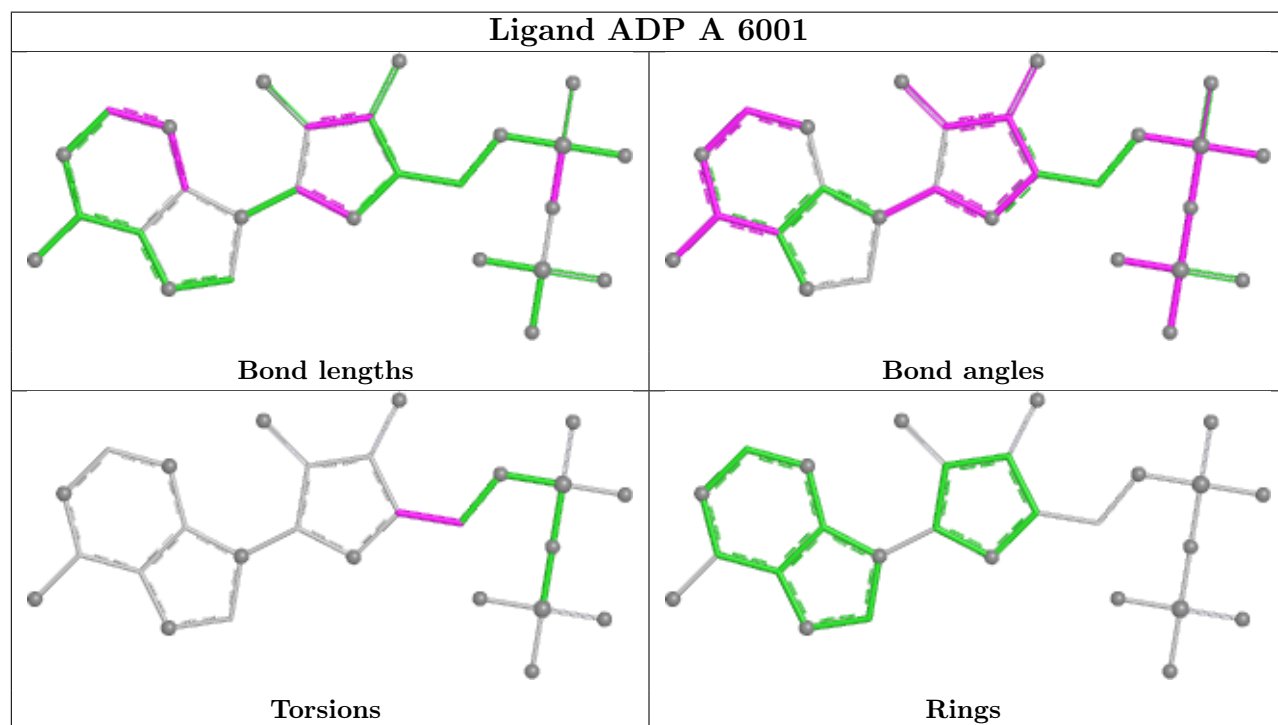
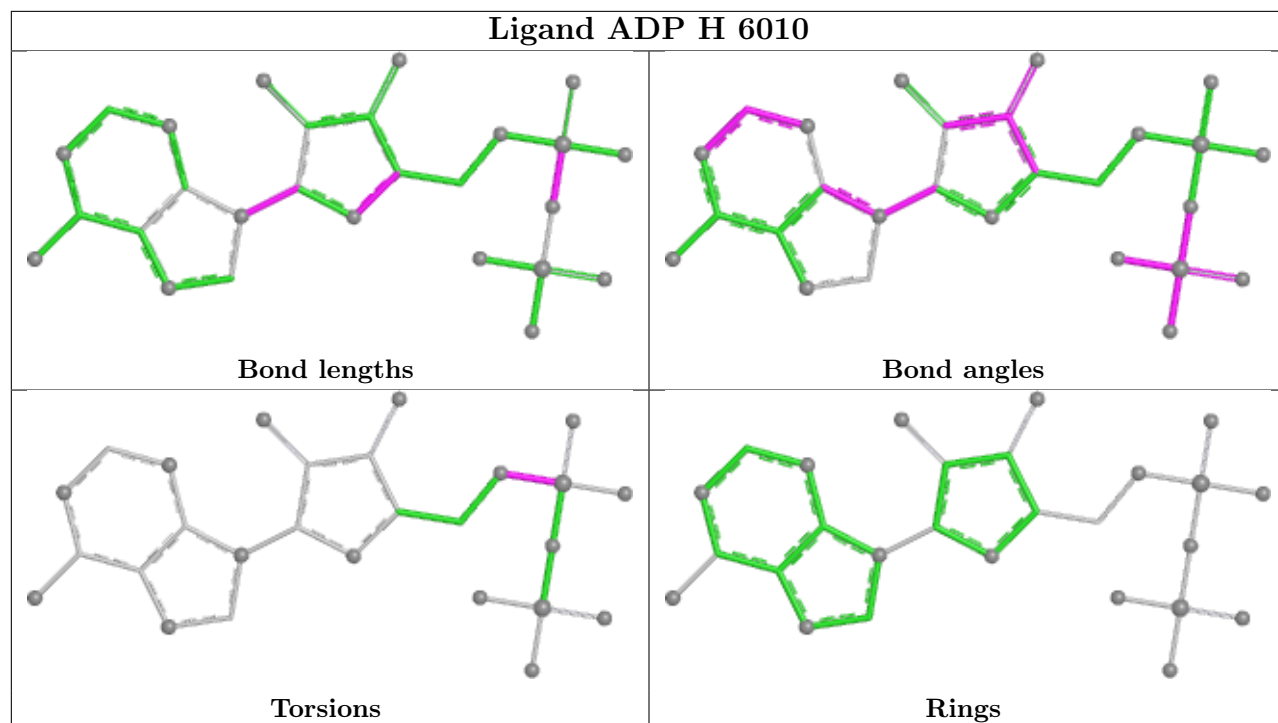
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

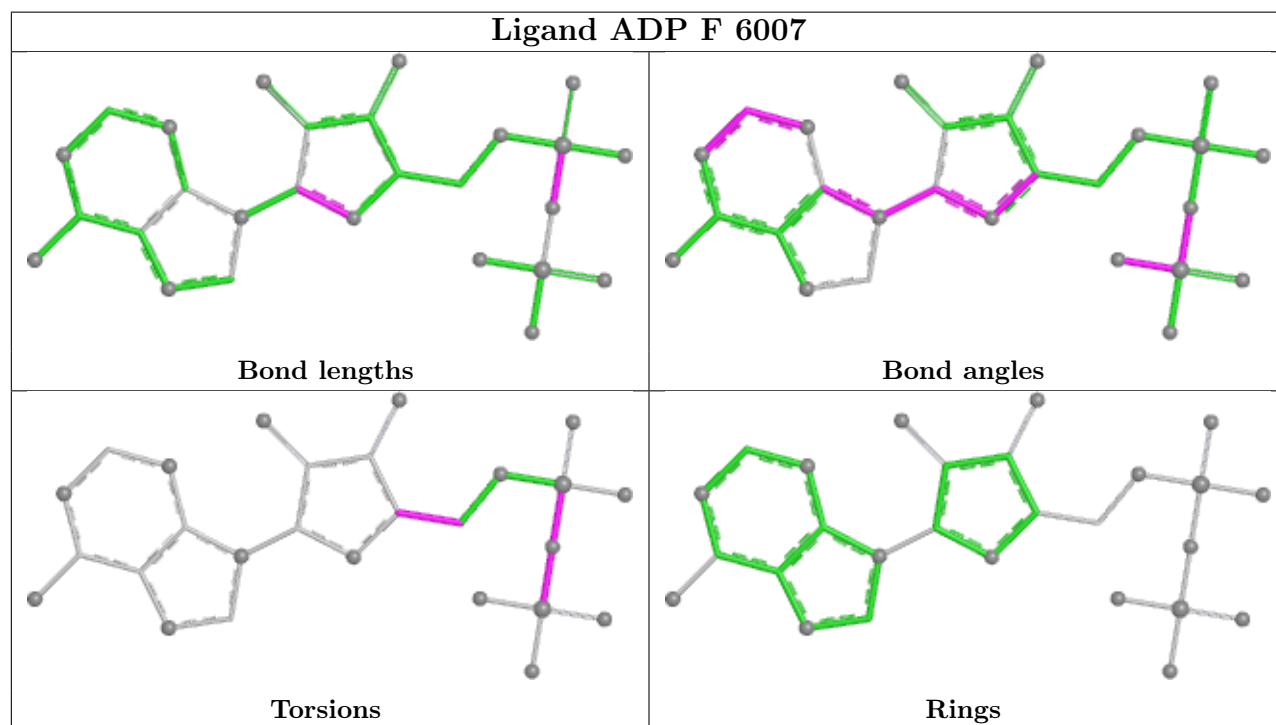
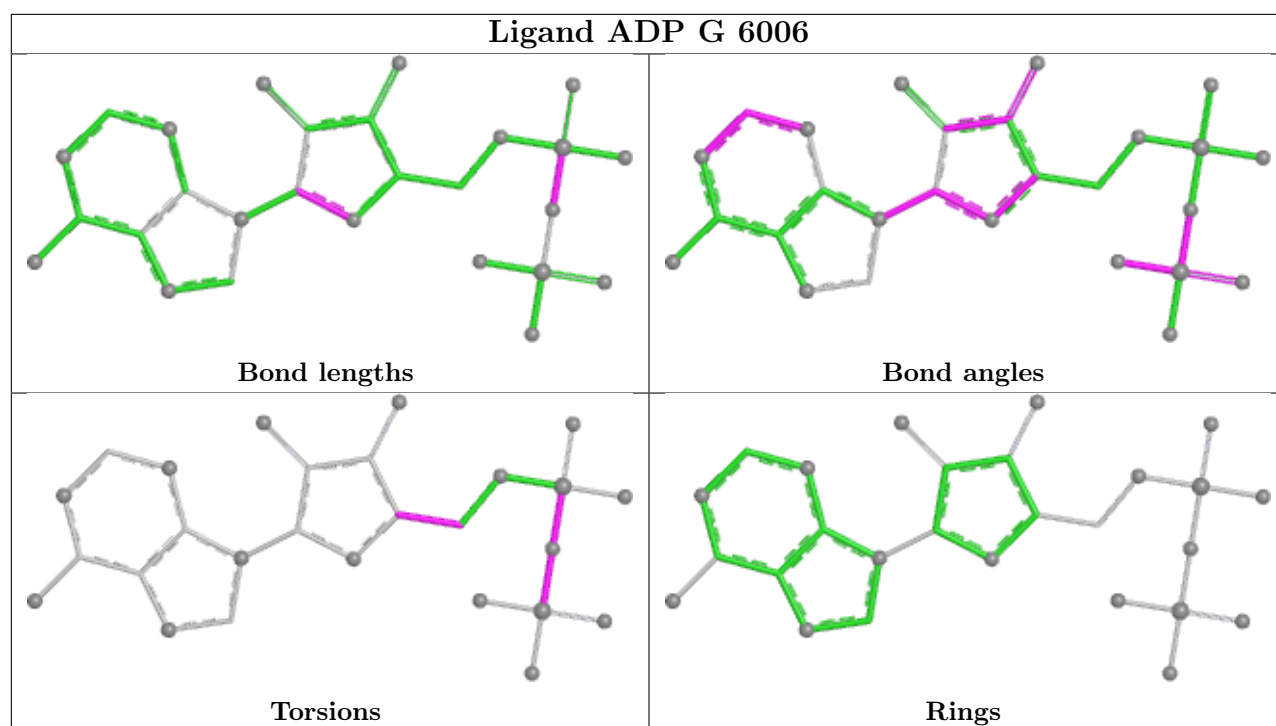




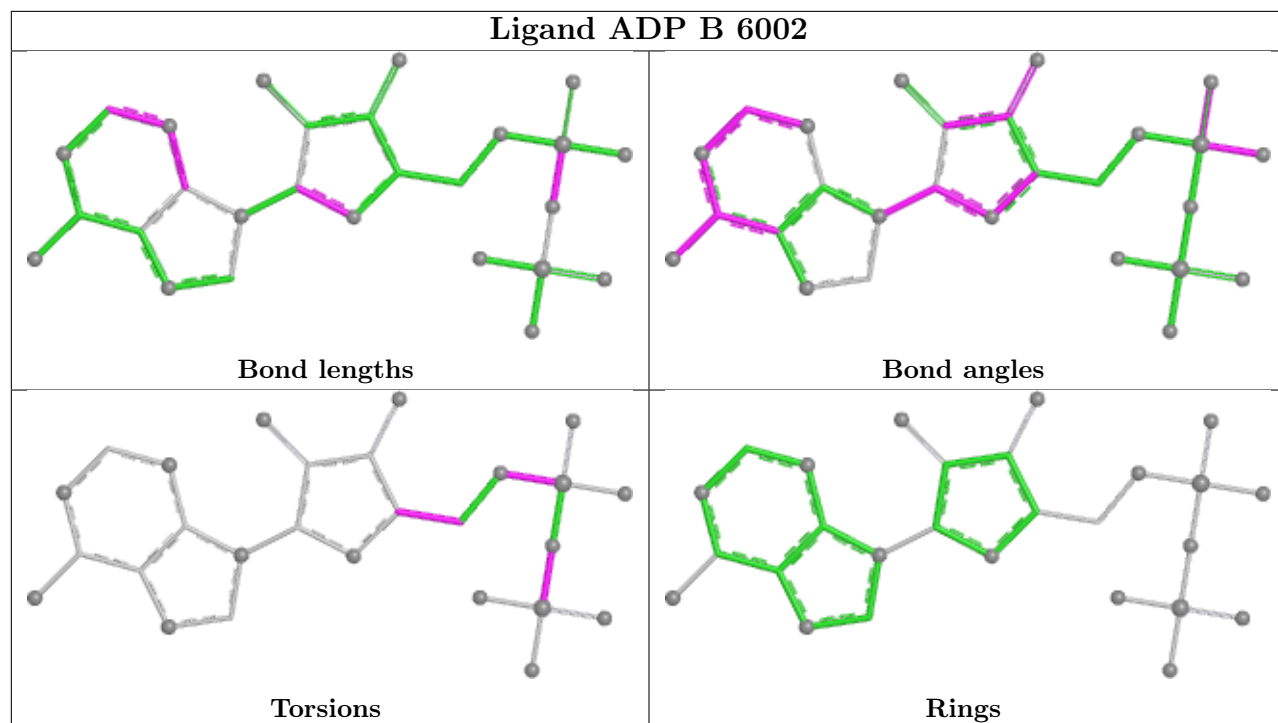




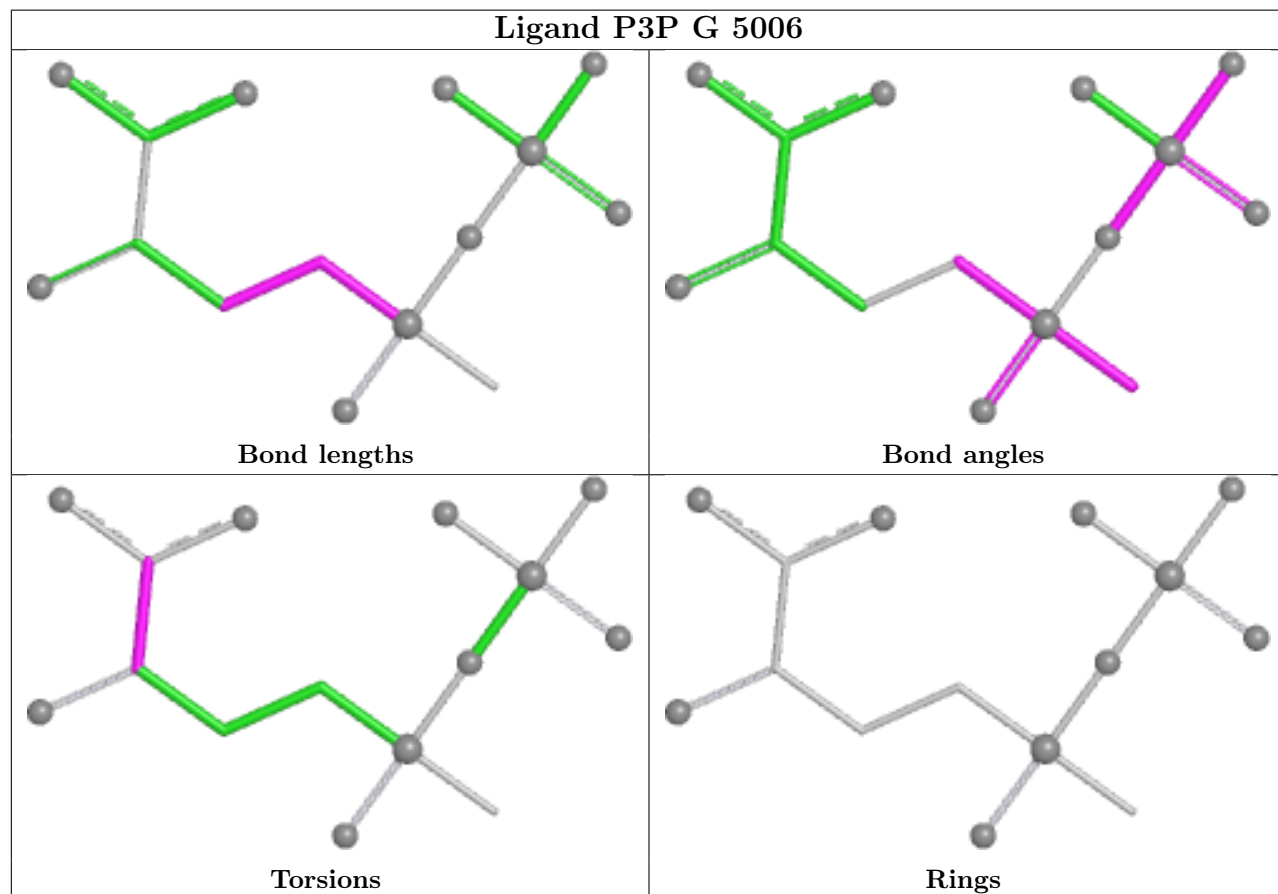


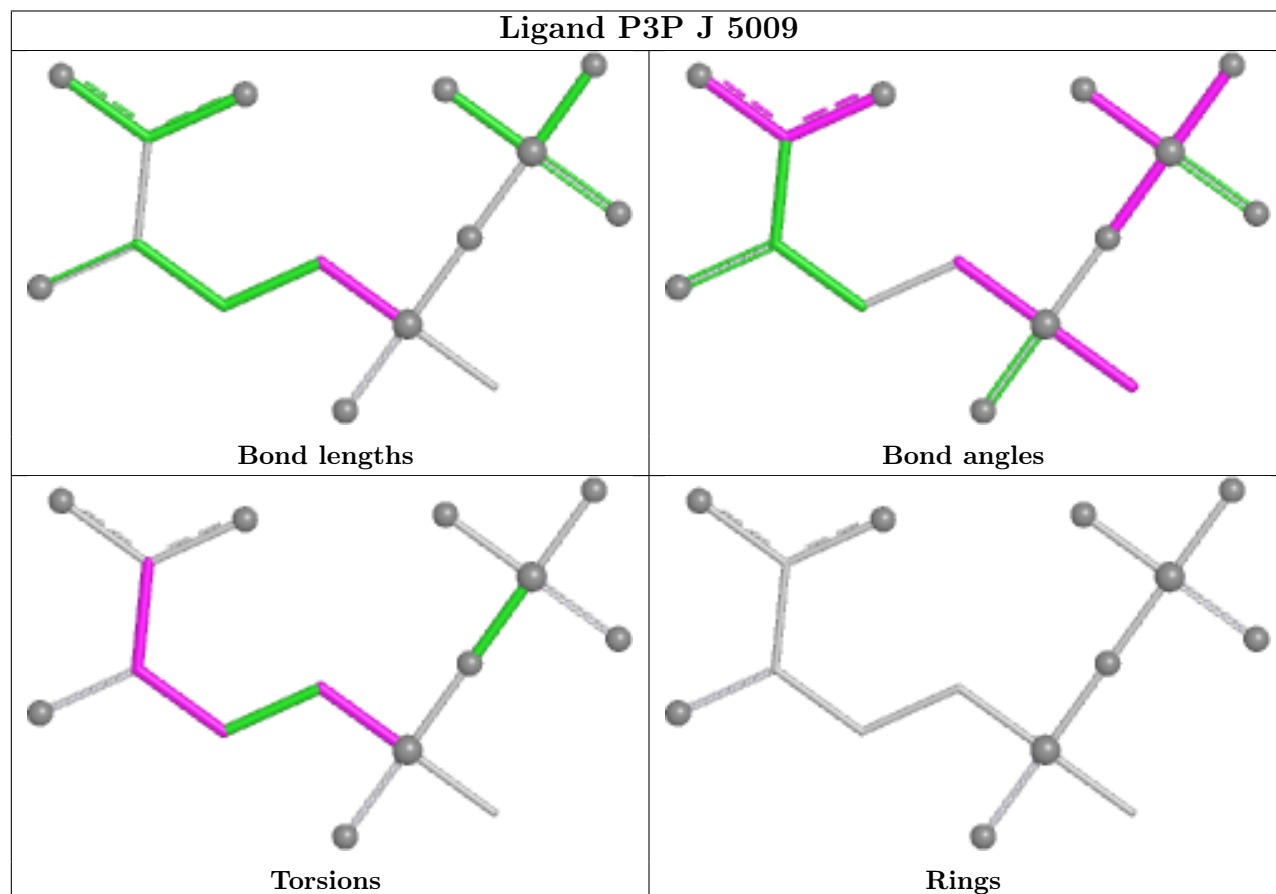
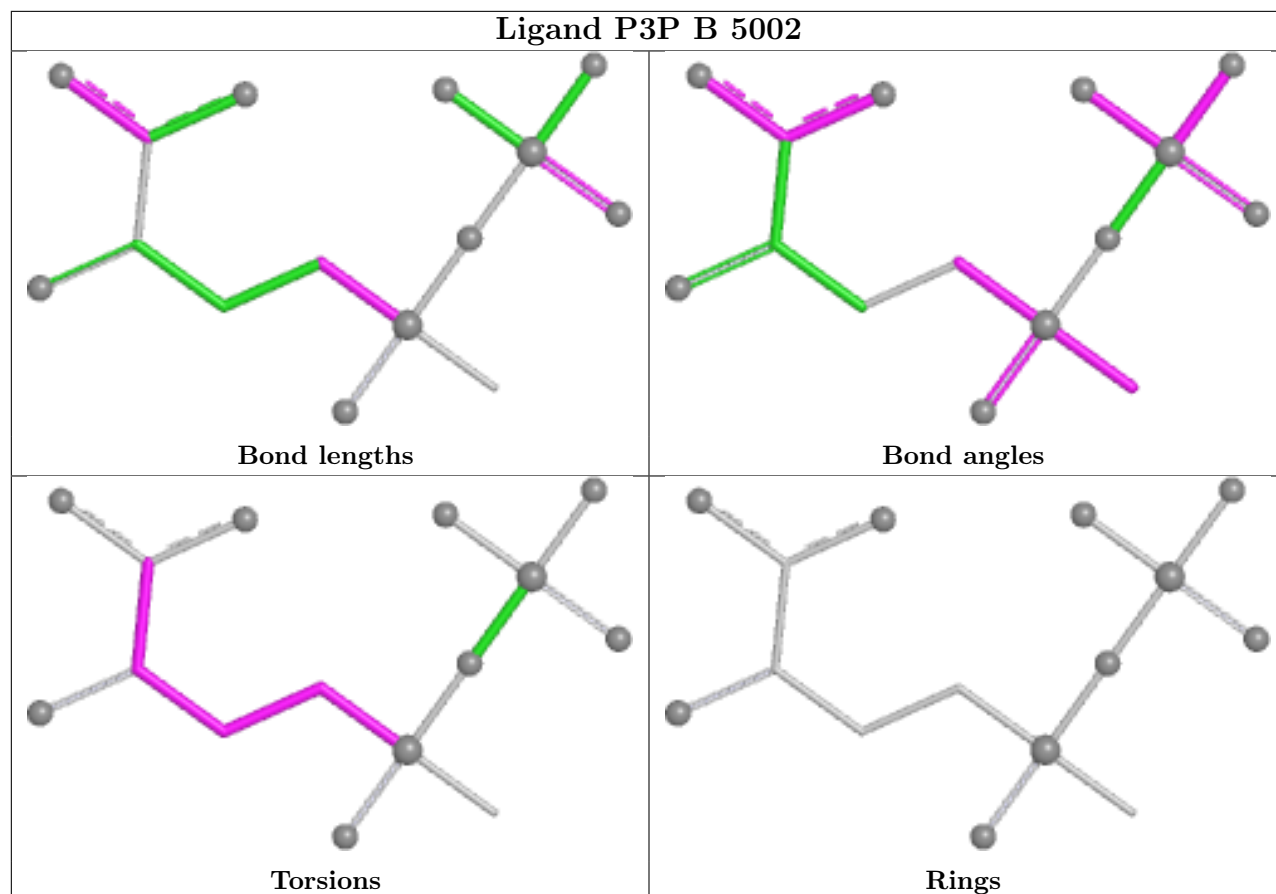


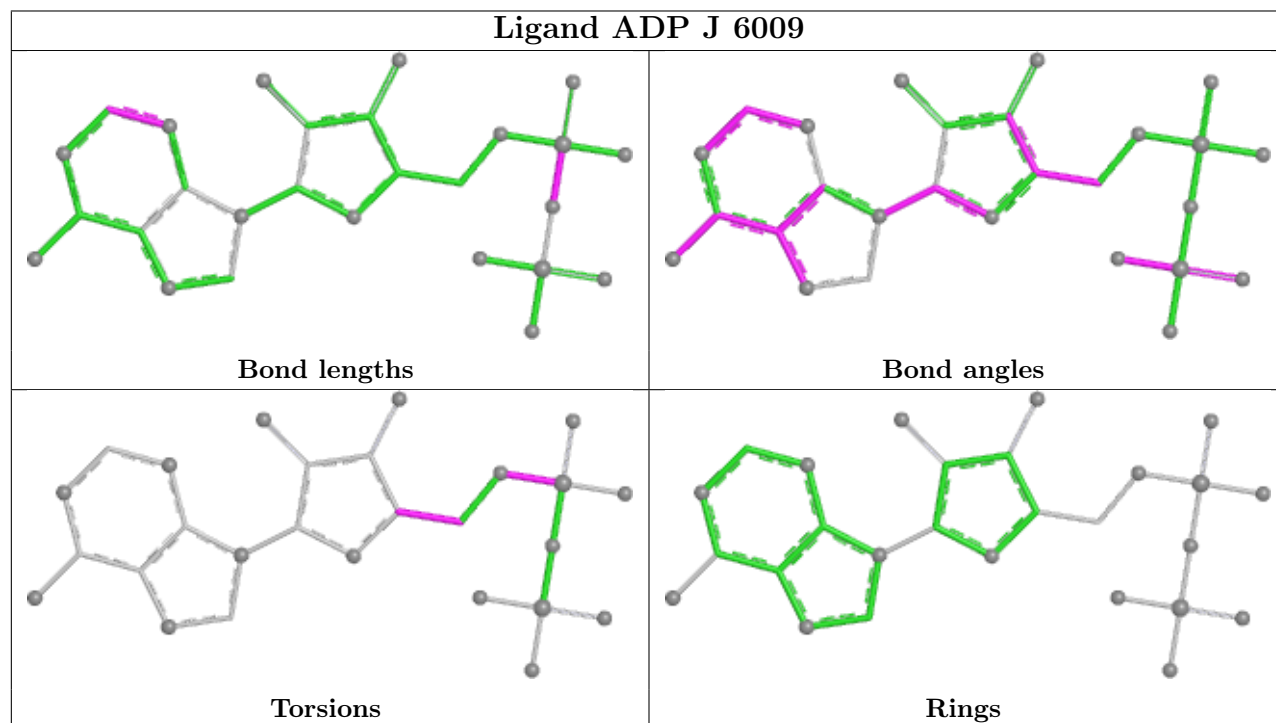
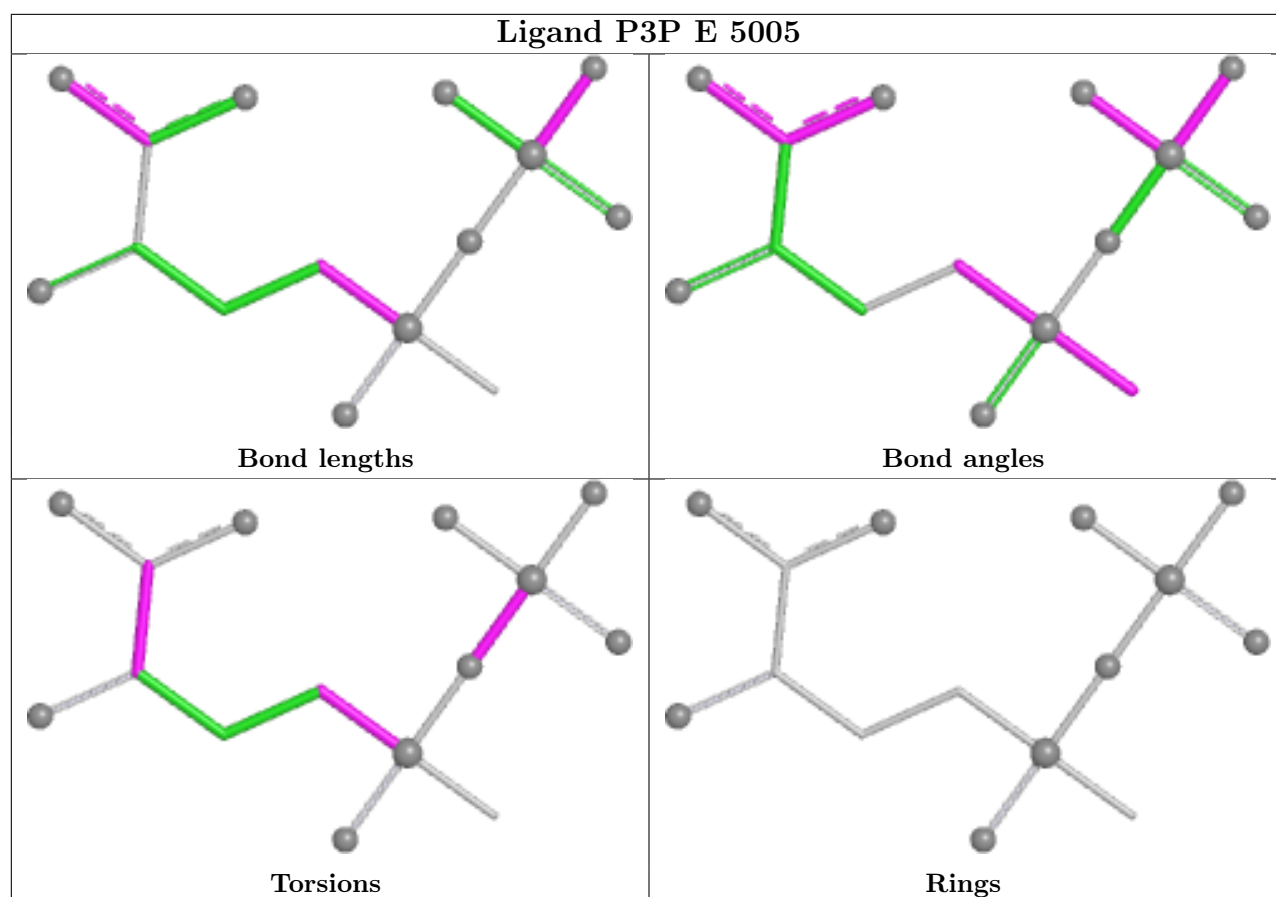
Ligand ADP B 6002



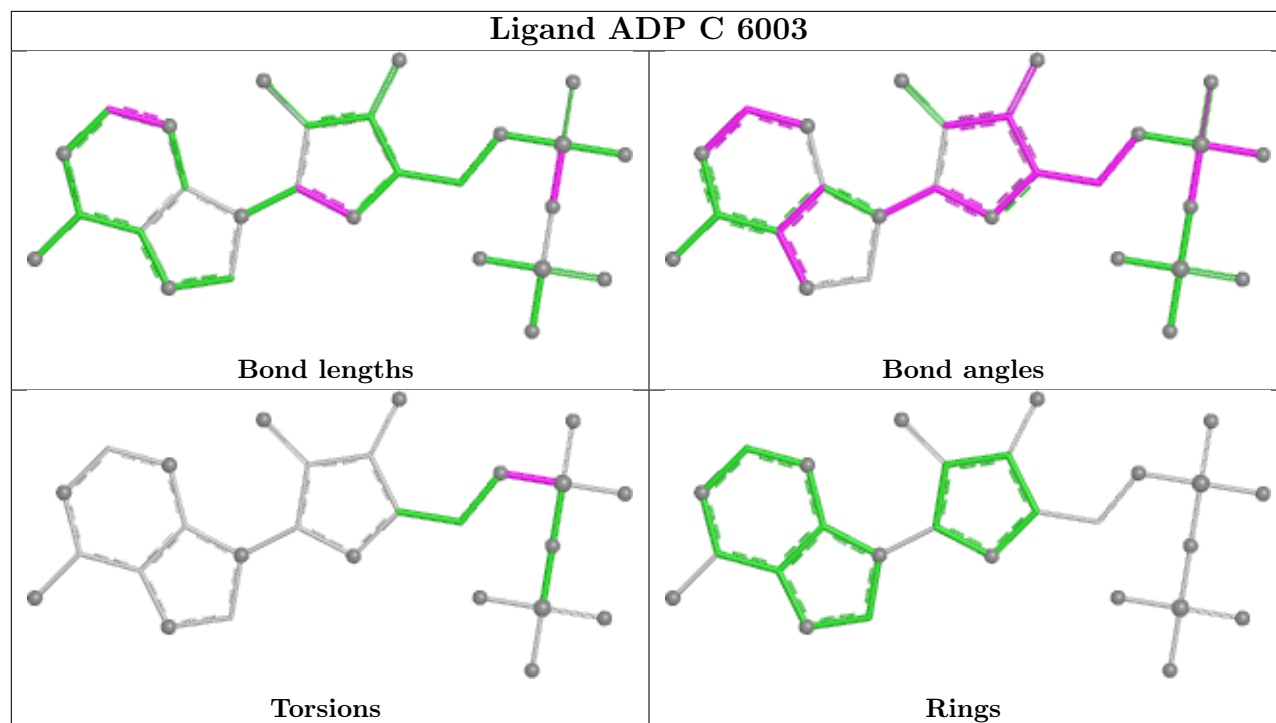
Ligand P3P G 5006



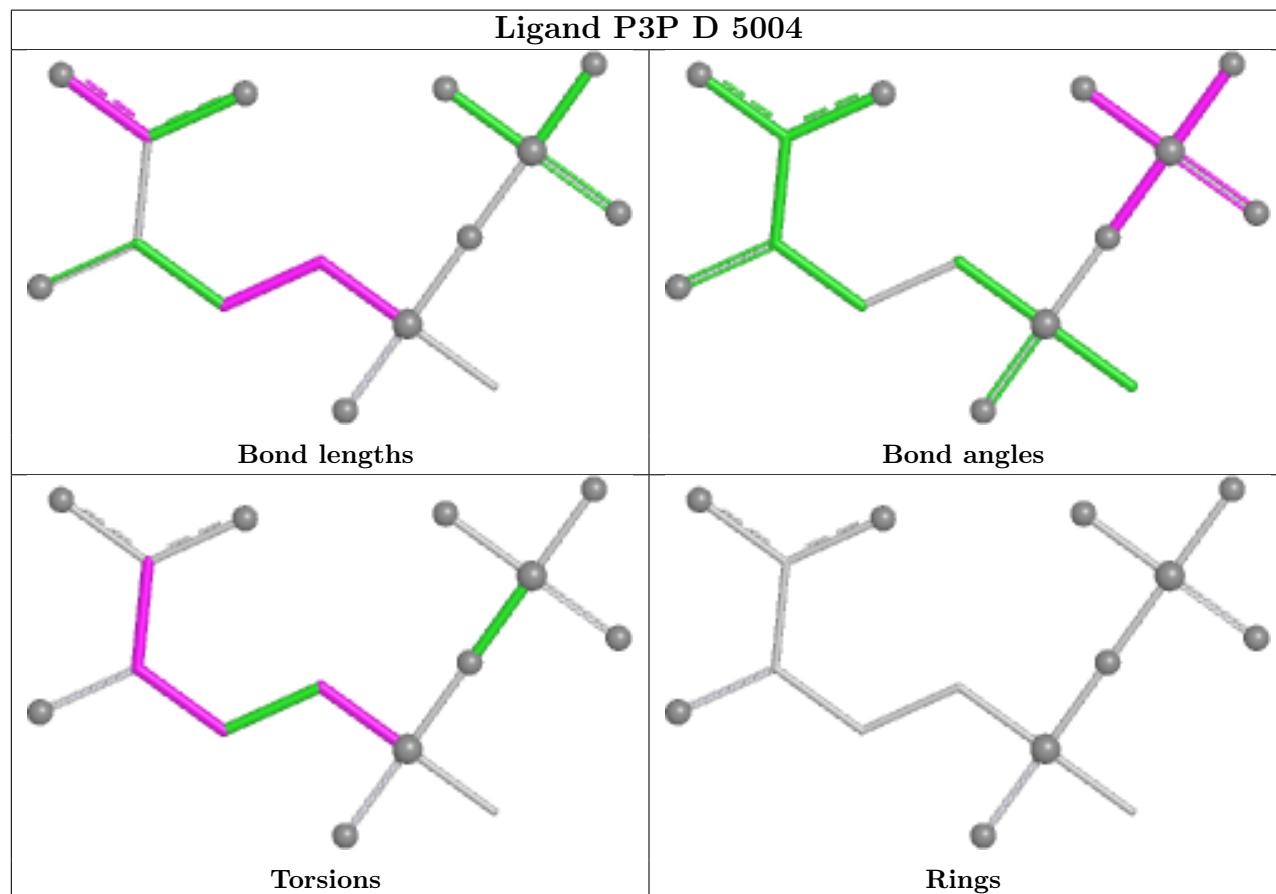


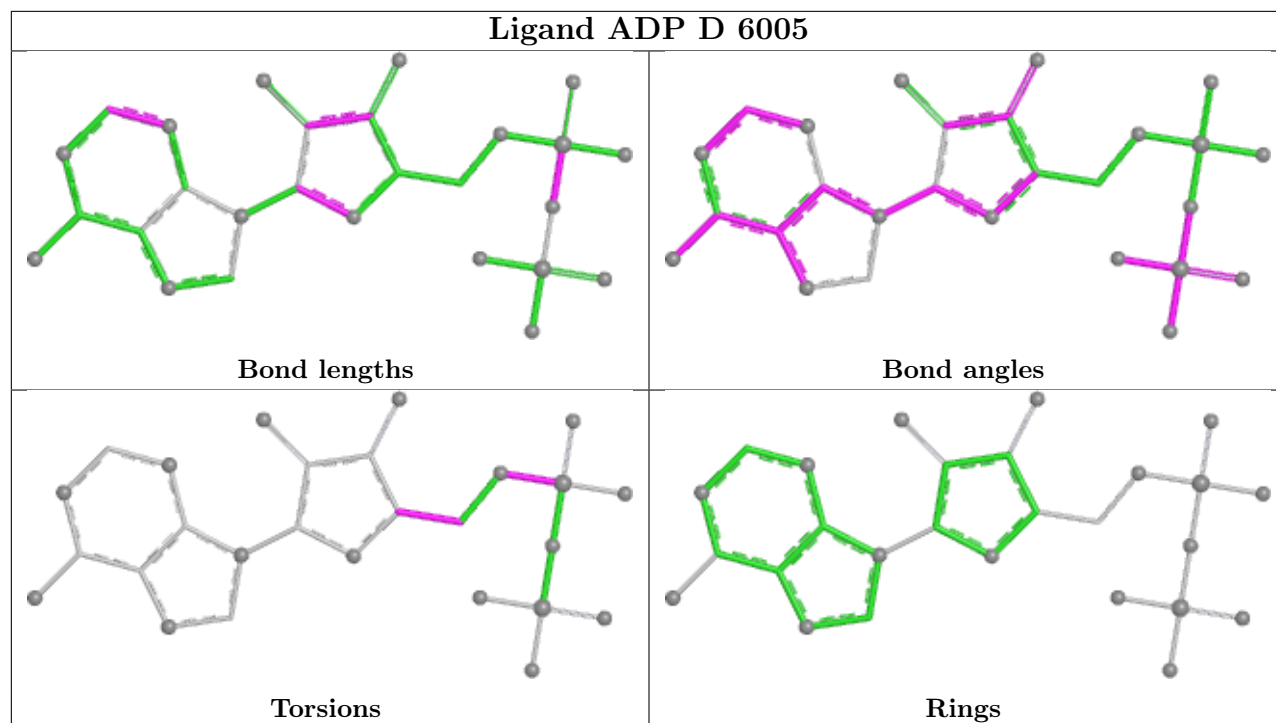


Ligand ADP C 6003



Ligand P3P D 5004





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	353/356 (99%)	-0.88	0 100 100	49, 66, 89, 100	0
1	B	353/356 (99%)	-0.78	0 100 100	49, 66, 89, 100	0
1	C	353/356 (99%)	-0.87	0 100 100	49, 66, 89, 100	0
1	D	353/356 (99%)	-0.82	0 100 100	49, 67, 89, 100	0
1	E	353/356 (99%)	-0.83	0 100 100	49, 66, 89, 100	0
1	F	353/356 (99%)	-0.79	0 100 100	49, 67, 89, 100	0
1	G	353/356 (99%)	-0.88	0 100 100	49, 67, 89, 100	0
1	H	353/356 (99%)	-0.77	1 (0%) 90 81	49, 66, 89, 100	0
1	I	353/356 (99%)	-0.89	0 100 100	49, 66, 89, 100	0
1	J	353/356 (99%)	-0.82	0 100 100	49, 66, 89, 100	0
All	All	3530/3560 (99%)	-0.83	1 (0%) 100 100	49, 67, 89, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	355	LYS	2.4

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	MN	C	1021	1/1	0.88	0.08	88,88,88,88	0
2	MN	E	1041	1/1	0.91	0.07	68,68,68,68	0
2	MN	A	1001	1/1	0.94	0.06	52,52,52,52	0
2	MN	B	1011	1/1	0.94	0.07	61,61,61,61	0
2	MN	H	1071	1/1	0.94	0.05	52,52,52,52	0
2	MN	E	1043	1/1	0.96	0.05	71,71,71,71	0
4	ADP	E	6004	27/27	0.96	0.07	81,87,94,95	0
2	MN	B	1013	1/1	0.97	0.04	54,54,54,54	0
2	MN	G	1061	1/1	0.97	0.03	58,58,58,58	0
2	MN	A	1003	1/1	0.97	0.04	40,40,40,40	0
3	P3P	C	5003	15/15	0.97	0.06	48,53,58,59	0
3	P3P	D	5004	15/15	0.97	0.06	64,67,75,76	0
3	P3P	I	5008	15/15	0.97	0.07	41,49,59,59	0
4	ADP	A	6001	27/27	0.97	0.06	55,76,90,90	0
4	ADP	C	6003	27/27	0.97	0.07	45,68,81,83	0
4	ADP	D	6005	27/27	0.97	0.06	67,73,90,90	0
2	MN	A	1002	1/1	0.97	0.04	62,62,62,62	0
4	ADP	F	6007	27/27	0.97	0.05	76,85,92,92	0
4	ADP	I	6008	27/27	0.97	0.05	62,71,74,75	0
3	P3P	F	5007	15/15	0.98	0.06	66,68,73,77	0
2	MN	D	1032	1/1	0.98	0.03	83,83,83,83	0
3	P3P	J	5009	15/15	0.98	0.05	46,48,56,58	0
2	MN	I	1083	1/1	0.98	0.03	64,64,64,64	0
3	P3P	A	5001	15/15	0.98	0.06	50,54,64,65	0
3	P3P	B	5002	15/15	0.98	0.05	30,32,40,41	0
2	MN	F	1051	1/1	0.98	0.04	86,86,86,86	0
2	MN	D	1031	1/1	0.98	0.04	57,57,57,57	0
4	ADP	G	6006	27/27	0.98	0.05	55,68,76,79	0
3	P3P	E	5005	15/15	0.98	0.07	65,73,78,81	0
2	MN	G	1062	1/1	0.99	0.02	69,69,69,69	0
2	MN	G	1063	1/1	0.99	0.02	51,51,51,51	0
3	P3P	G	5006	15/15	0.99	0.05	61,67,80,80	0
3	P3P	H	5010	15/15	0.99	0.06	30,35,41,41	0
2	MN	E	1042	1/1	0.99	0.02	73,73,73,73	0
2	MN	I	1081	1/1	0.99	0.02	53,53,53,53	0
2	MN	C	1023	1/1	0.99	0.02	56,56,56,56	0
4	ADP	B	6002	27/27	0.99	0.04	37,46,53,54	0

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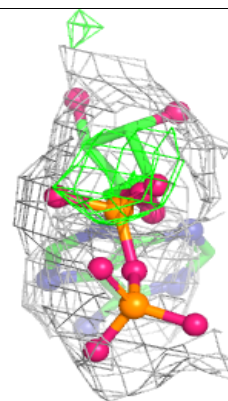
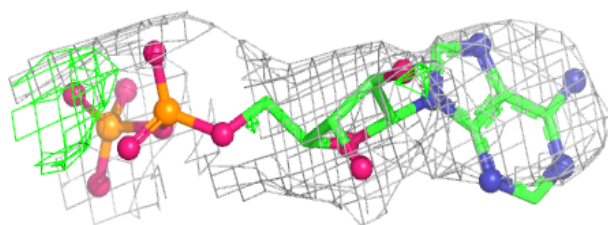
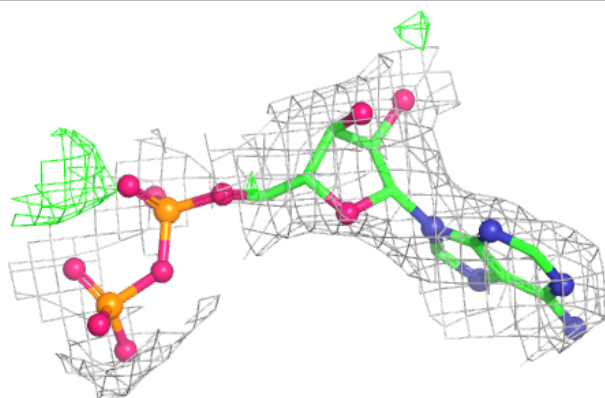
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MN	J	1091	1/1	0.99	0.02	52,52,52,52	0
2	MN	J	1093	1/1	0.99	0.03	41,41,41,41	0
2	MN	D	1033	1/1	0.99	0.03	51,51,51,51	0
2	MN	F	1052	1/1	0.99	0.03	54,54,54,54	0
2	MN	F	1053	1/1	0.99	0.02	63,63,63,63	0
4	ADP	H	6010	27/27	0.99	0.04	29,31,40,43	0
2	MN	B	1012	1/1	0.99	0.02	32,32,32,32	0
4	ADP	J	6009	27/27	0.99	0.04	44,54,60,62	0
2	MN	I	1082	1/1	1.00	0.01	67,67,67,67	0
2	MN	H	1072	1/1	1.00	0.02	49,49,49,49	0
2	MN	H	1073	1/1	1.00	0.02	28,28,28,28	0
2	MN	J	1092	1/1	1.00	0.02	61,61,61,61	0
2	MN	C	1022	1/1	1.00	0.02	51,51,51,51	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.

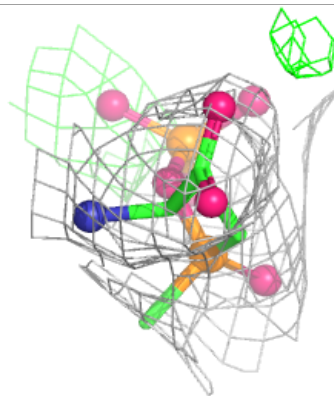
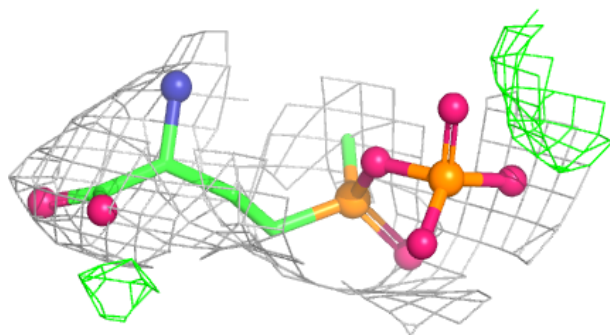
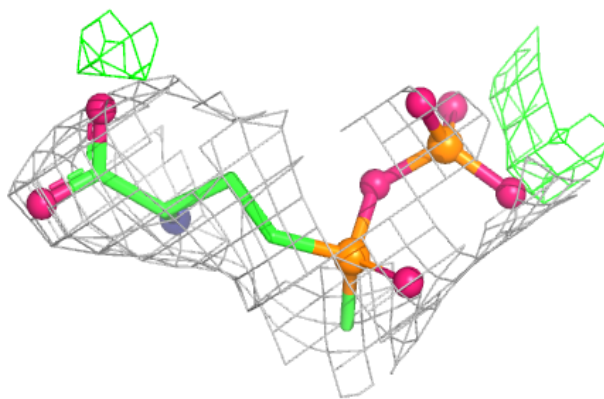
Electron density around ADP E 6004:

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

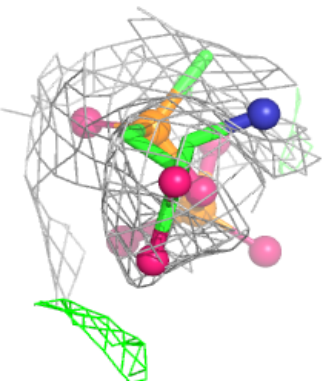
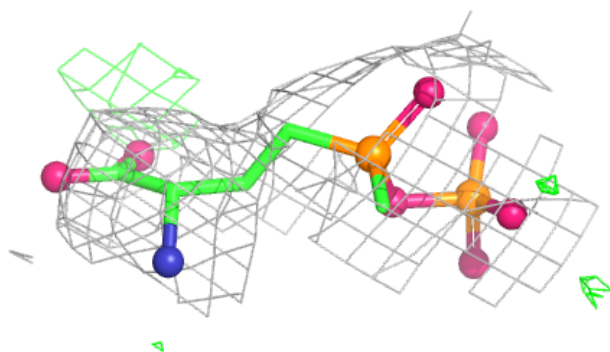
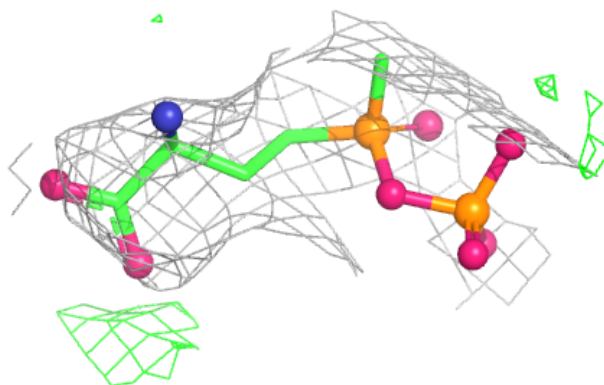


Electron density around P3P C 5003:

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

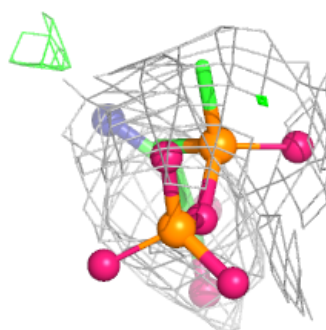
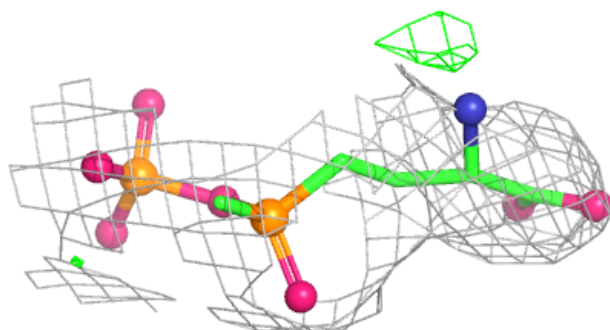
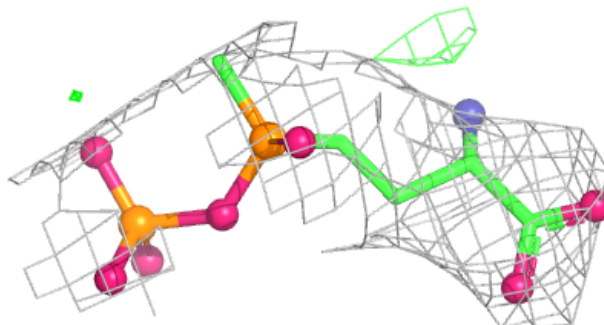
**Electron density around P3P D 5004:**

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

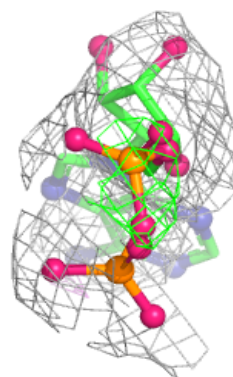
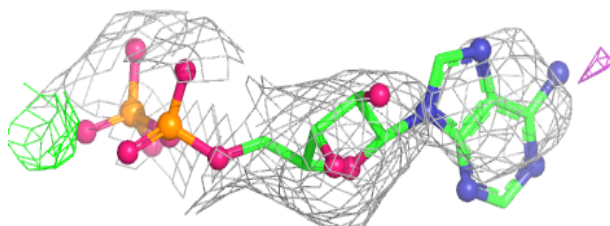
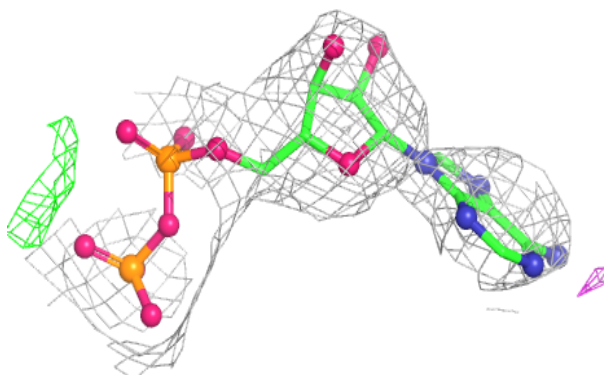


Electron density around P3P I 5008:

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

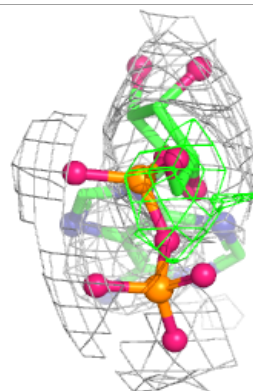
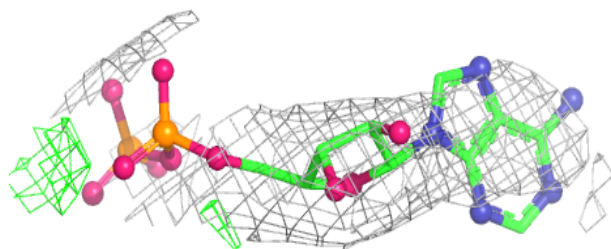
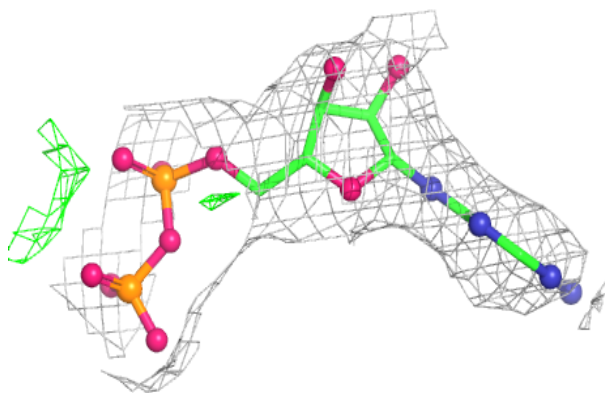
**Electron density around ADP A 6001:**

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

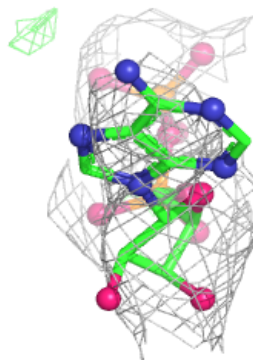
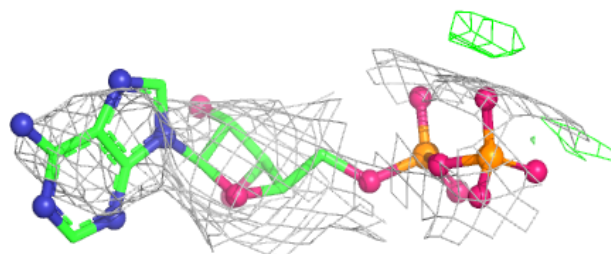
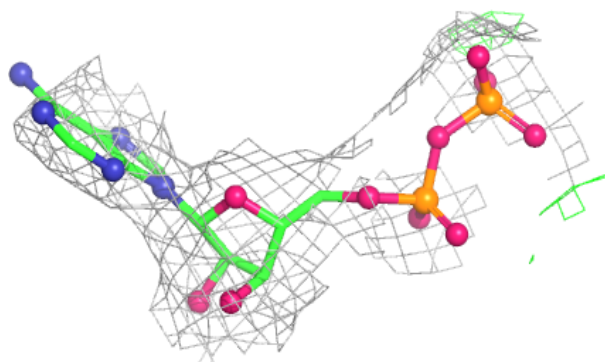


Electron density around ADP C 6003:

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

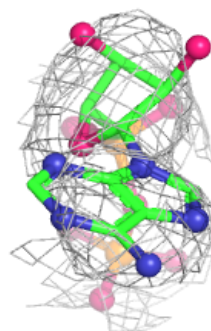
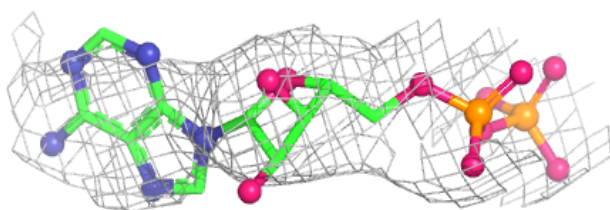
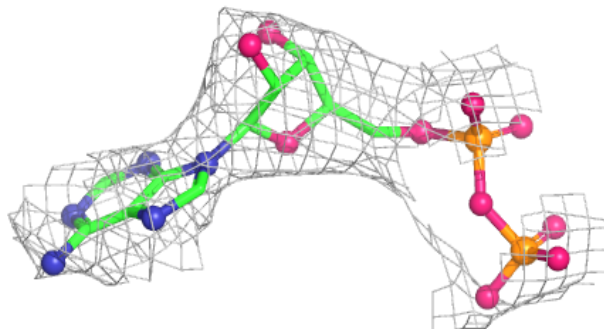
**Electron density around ADP D 6005:**

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

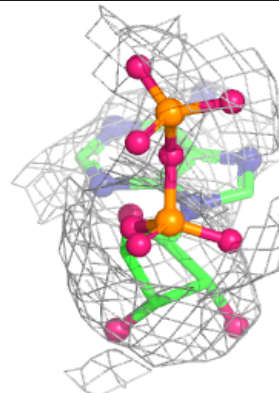
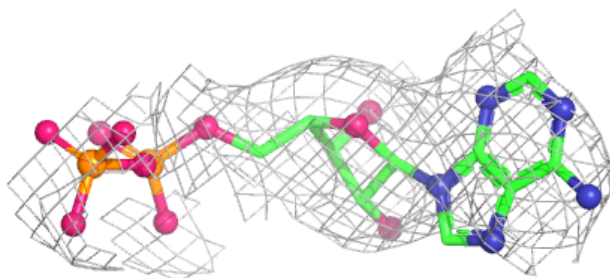
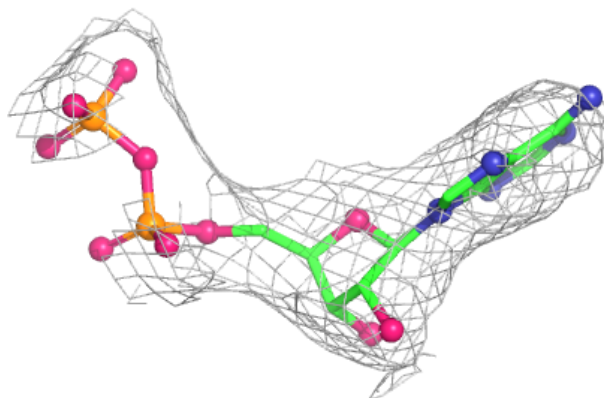


Electron density around ADP F 6007:

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

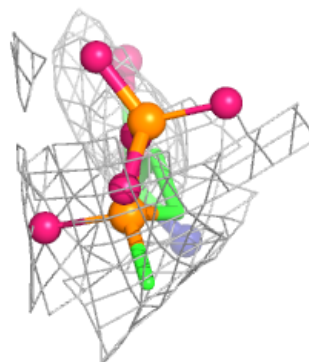
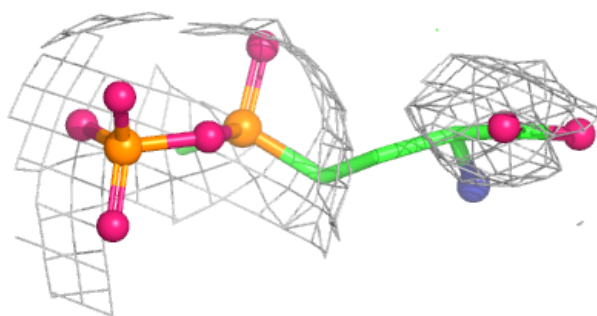
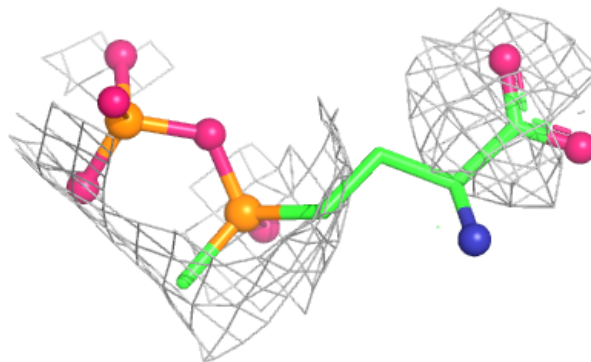
**Electron density around ADP I 6008:**

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

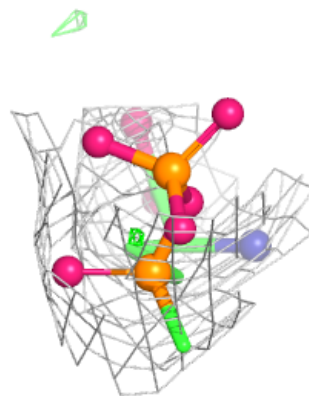
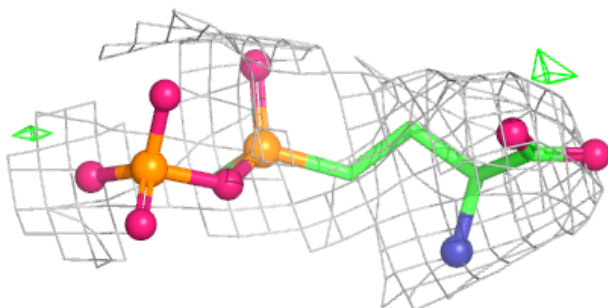
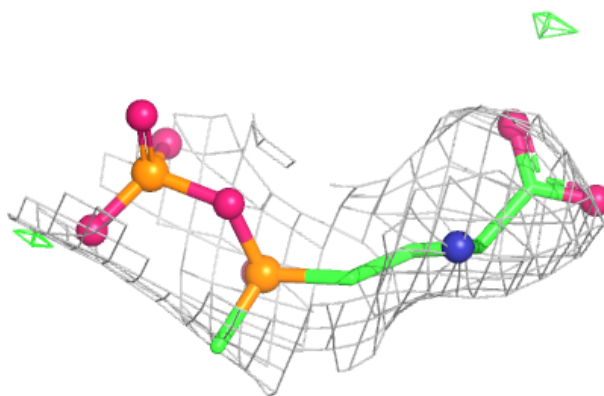


Electron density around P3P F 5007:

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

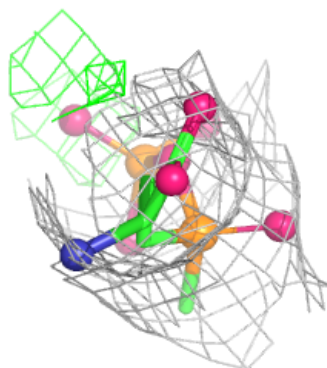
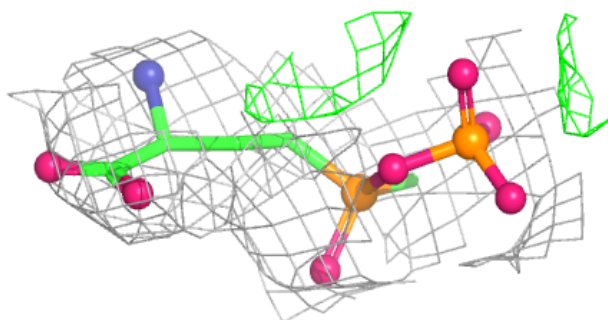
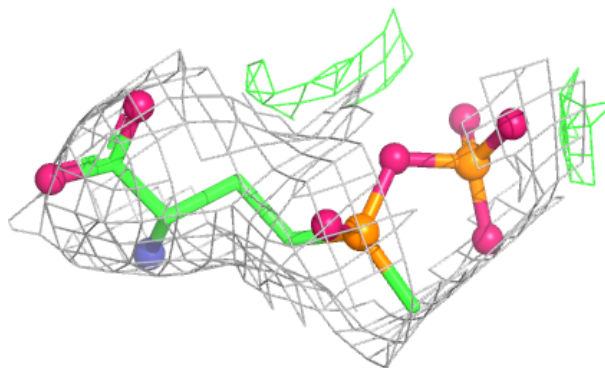
**Electron density around P3P J 5009:**

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

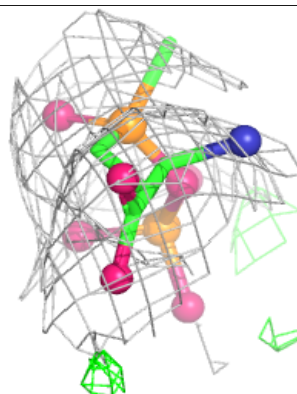
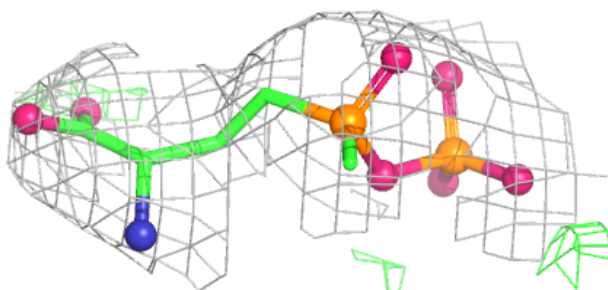
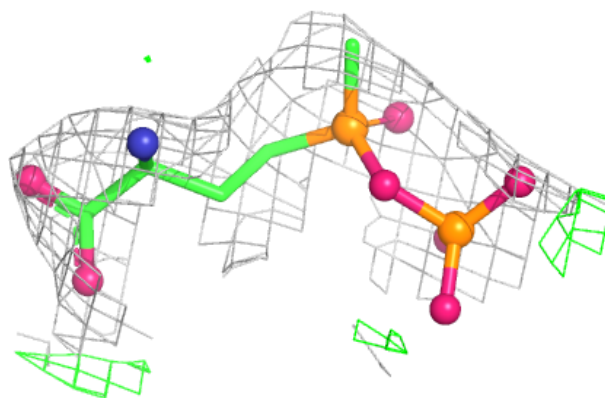


Electron density around P3P A 5001:

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

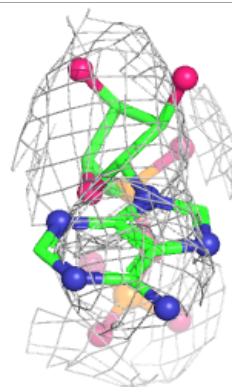
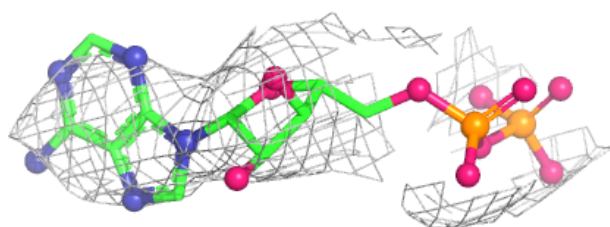
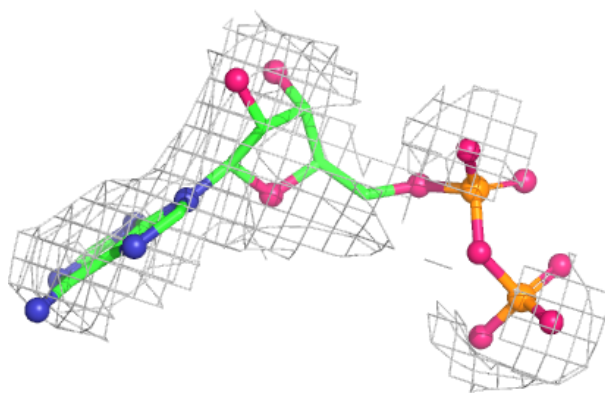
**Electron density around P3P B 5002:**

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

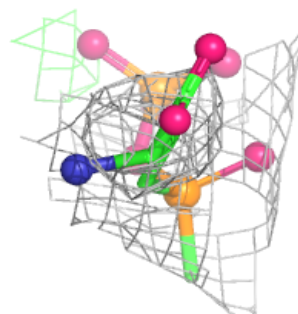
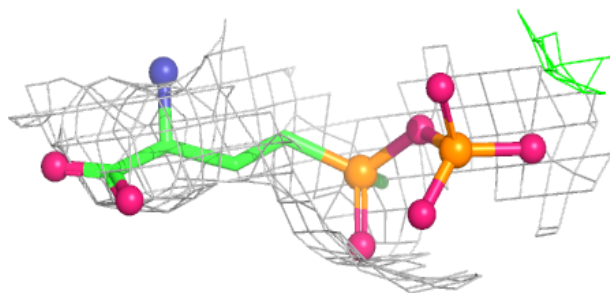
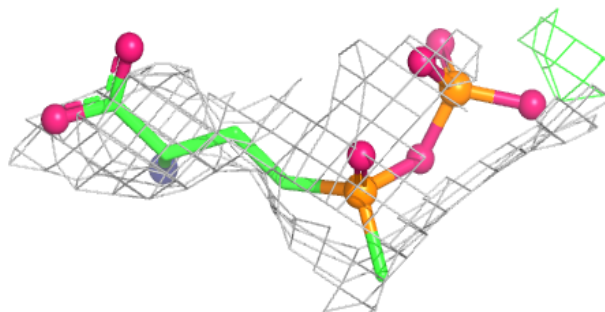


Electron density around ADP G 6006:

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

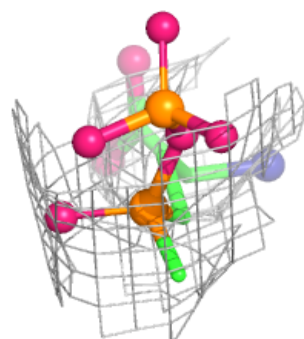
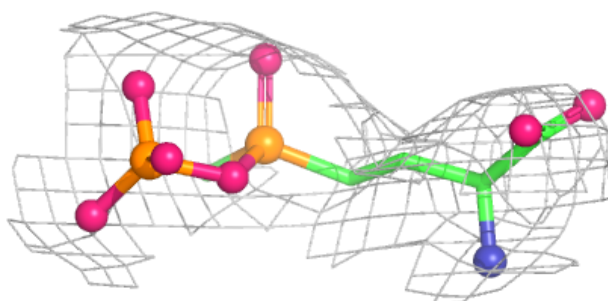
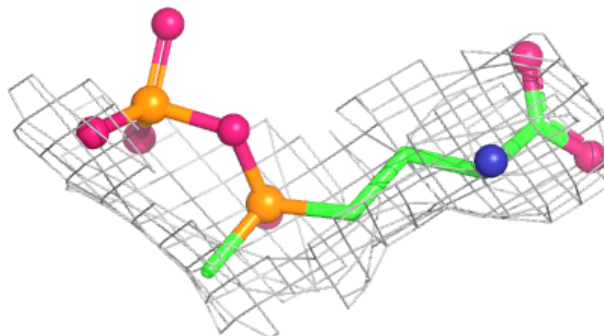
**Electron density around P3P E 5005:**

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

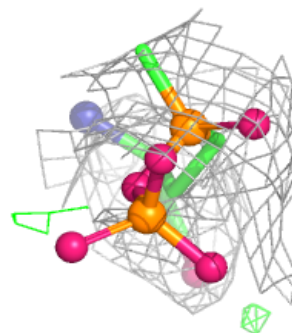
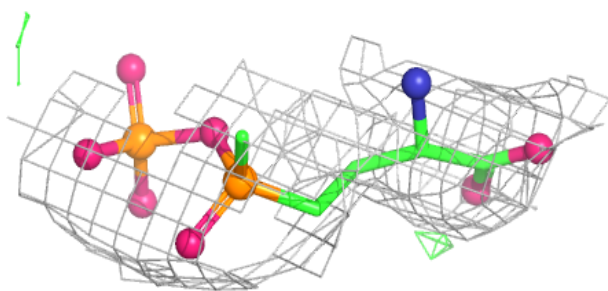
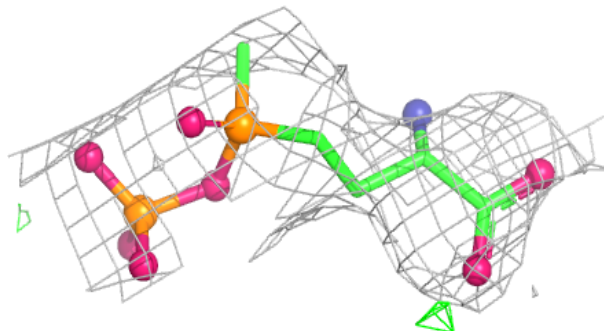


Electron density around P3P G 5006:

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

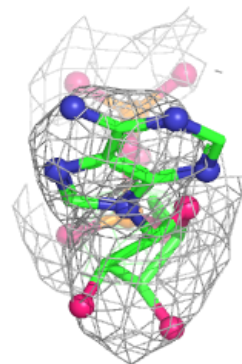
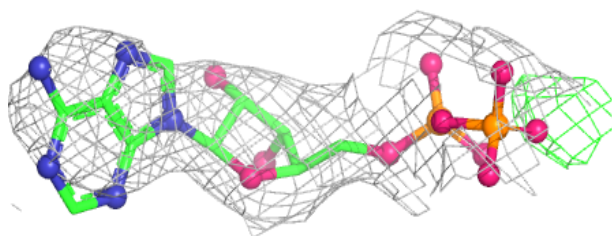
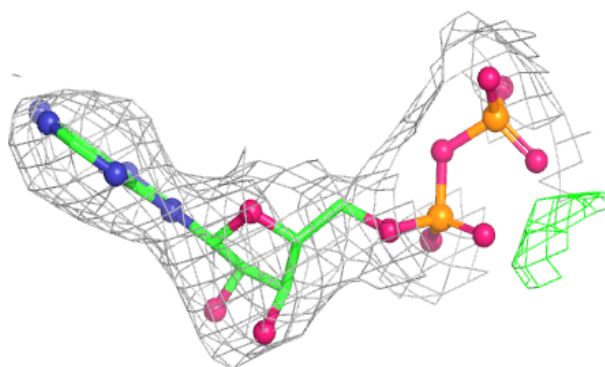
**Electron density around P3P H 5010:**

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

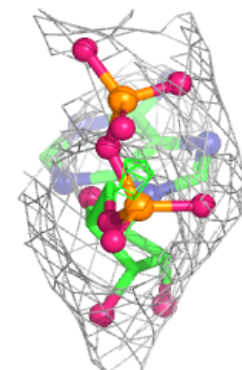
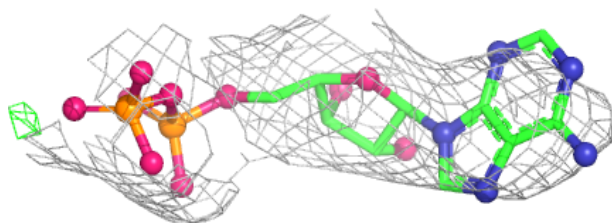
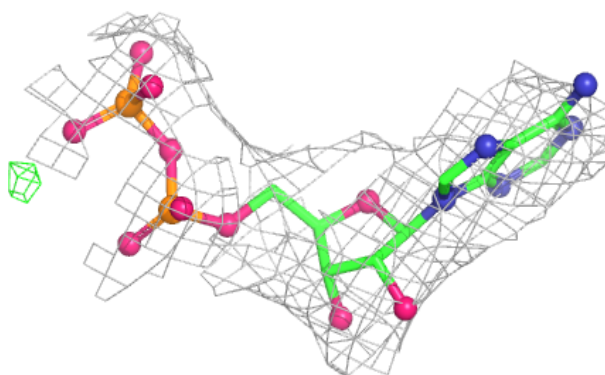


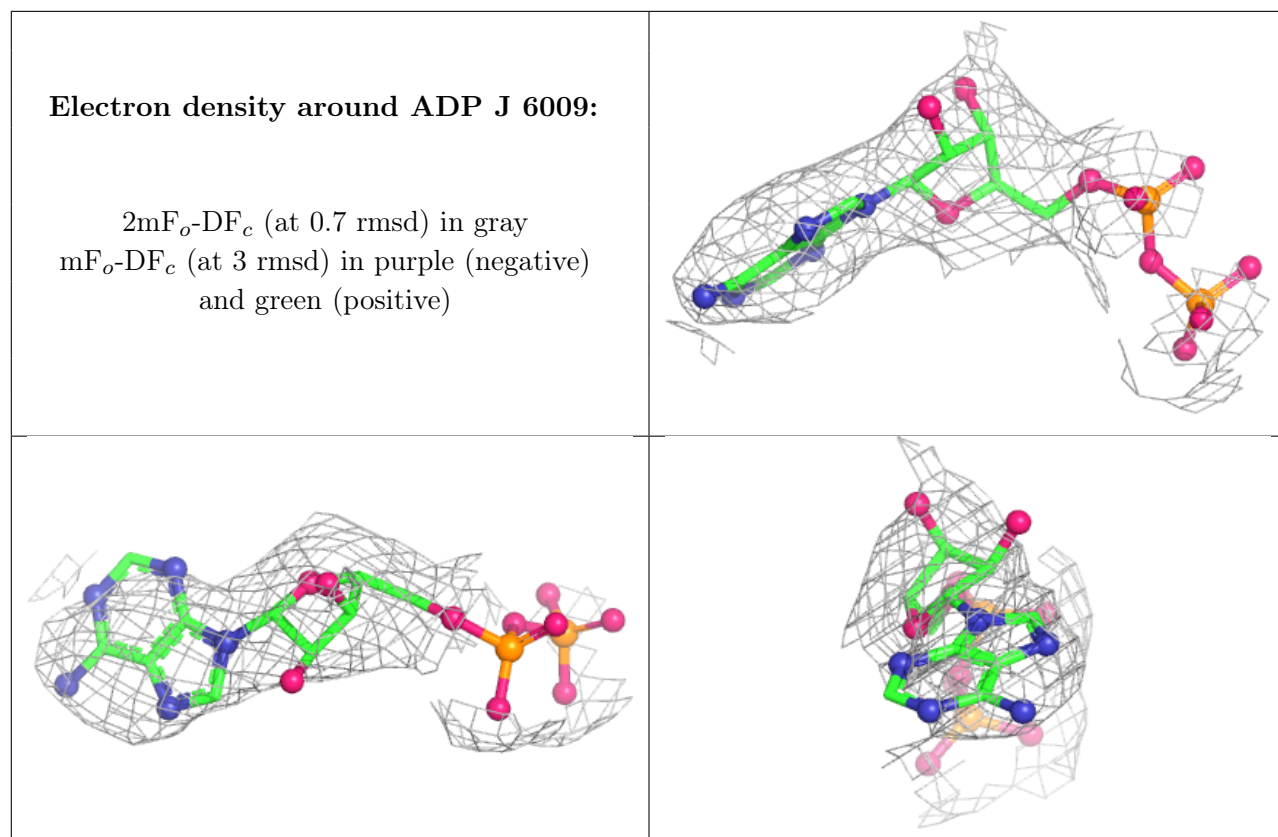
Electron density around ADP B 6002:

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

**Electron density around ADP H 6010:**

$2mF_o-DF_c$ (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.