wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2021 – 04:16 PM GMT

PDB ID	:	6YBU
Title	:	Crystal structure of a native BcsE (349-523) RQ complex with c-di-GMP and ATP bound
Authors	:	Abidi, W.; Zouhir, S.; Roche, S.; Krasteva, P.V.
Deposited on	:	2020-03-17
Resolution	:	2.49 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

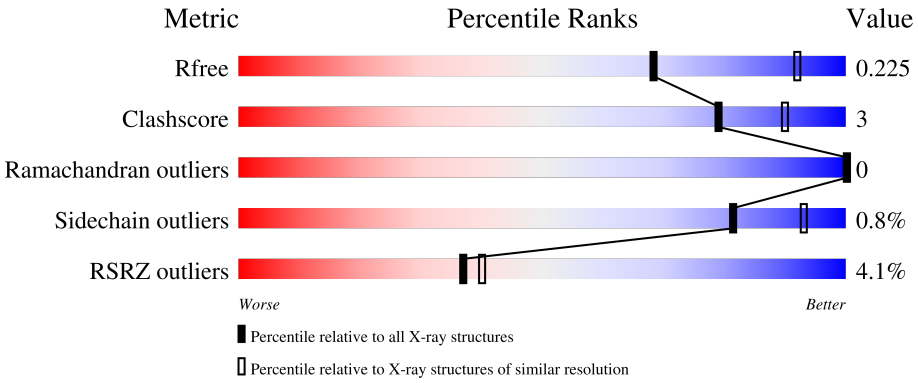
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	250	2% 88% 8% ·
1	B	250	2% 90% 6% ·
1	G	250	90% 6% ·
1	H	250	92% · ·
2	C	67	18% 33% 10% 57%

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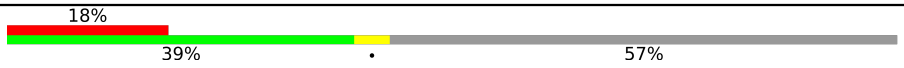
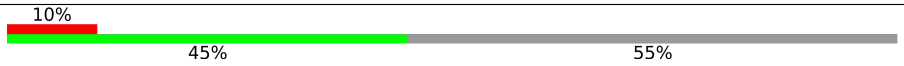
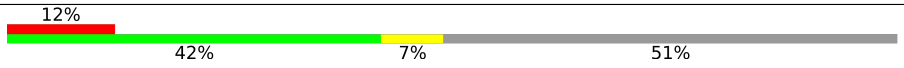
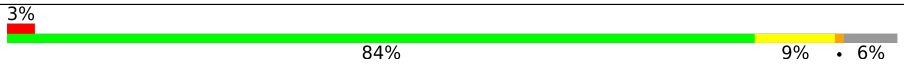
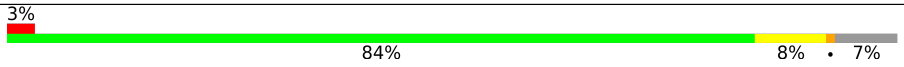
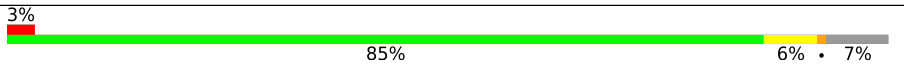
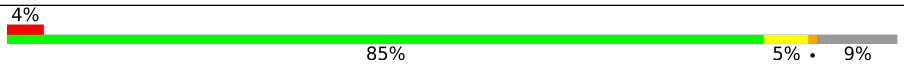
Mol	Chain	Length	Quality of chain
2	D	67	
2	I	67	
2	J	67	
3	E	179	
3	F	179	
3	K	179	
3	L	179	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14546 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 Bacterial cellulose secretion regulator BcsQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1891	1187	342	352	10			
1	B	240	Total	C	N	O	S	0	0	0
			1891	1187	342	352	10			
1	G	240	Total	C	N	O	S	0	1	0
			1899	1191	343	355	10			
1	H	239	Total	C	N	O	S	0	0	0
			1887	1185	341	351	10			

- Molecule 2 is a protein called Bacterial cellulose secretion regulator BcsR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	29	Total	C	N	O	0	0	0
			235	151	40	44			
2	D	29	Total	C	N	O	0	0	0
			237	151	41	45			
2	I	30	Total	C	N	O	0	0	0
			243	157	41	45			
2	J	33	Total	C	N	O	0	0	0
			265	172	44	49			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	expression tag	UNP J7QAC9
C	-3	PRO	-	expression tag	UNP J7QAC9
C	-2	MET	-	expression tag	UNP J7QAC9
C	-1	GLY	-	expression tag	UNP J7QAC9
C	0	SER	-	expression tag	UNP J7QAC9
D	-4	GLY	-	expression tag	UNP J7QAC9
D	-3	PRO	-	expression tag	UNP J7QAC9
D	-2	MET	-	expression tag	UNP J7QAC9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP J7QAC9
D	0	SER	-	expression tag	UNP J7QAC9
I	-4	GLY	-	expression tag	UNP J7QAC9
I	-3	PRO	-	expression tag	UNP J7QAC9
I	-2	MET	-	expression tag	UNP J7QAC9
I	-1	GLY	-	expression tag	UNP J7QAC9
I	0	SER	-	expression tag	UNP J7QAC9
J	-4	GLY	-	expression tag	UNP J7QAC9
J	-3	PRO	-	expression tag	UNP J7QAC9
J	-2	MET	-	expression tag	UNP J7QAC9
J	-1	GLY	-	expression tag	UNP J7QAC9
J	0	SER	-	expression tag	UNP J7QAC9

- Molecule 3 is a protein called Bacterial cellulose secretion regulator BcsE, residues 349-523.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	168	Total	C	N	O	S	0	0	0
			1339	853	241	233	12			
3	F	166	Total	C	N	O	S	0	0	0
			1322	841	239	231	11			
3	K	166	Total	C	N	O	S	0	0	0
			1322	841	239	231	11			
3	L	162	Total	C	N	O	S	0	0	0
			1292	825	235	221	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	345	MET	-	initiating methionine	UNP P37657
E	346	GLY	-	expression tag	UNP P37657
E	347	SER	-	expression tag	UNP P37657
E	348	MET	-	expression tag	UNP P37657
F	345	MET	-	initiating methionine	UNP P37657
F	346	GLY	-	expression tag	UNP P37657
F	347	SER	-	expression tag	UNP P37657
F	348	MET	-	expression tag	UNP P37657
K	345	MET	-	initiating methionine	UNP P37657
K	346	GLY	-	expression tag	UNP P37657
K	347	SER	-	expression tag	UNP P37657
K	348	MET	-	expression tag	UNP P37657
L	345	MET	-	initiating methionine	UNP P37657
L	346	GLY	-	expression tag	UNP P37657

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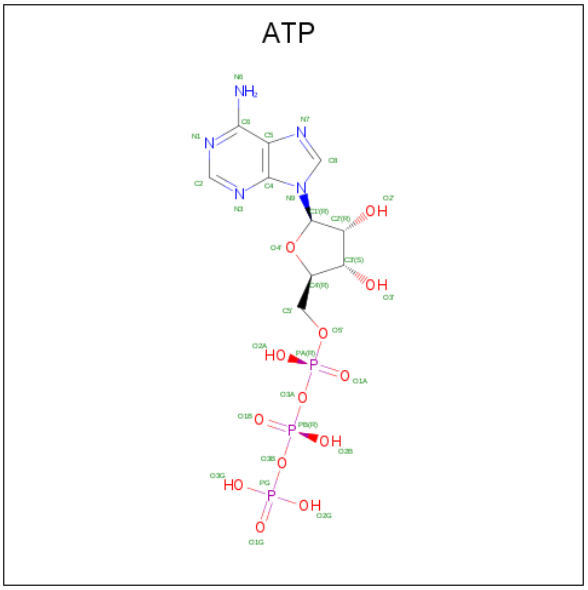
Chain	Residue	Modelled	Actual	Comment	Reference
L	347	SER	-	expression tag	UNP P37657
L	348	MET	-	expression tag	UNP P37657

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		

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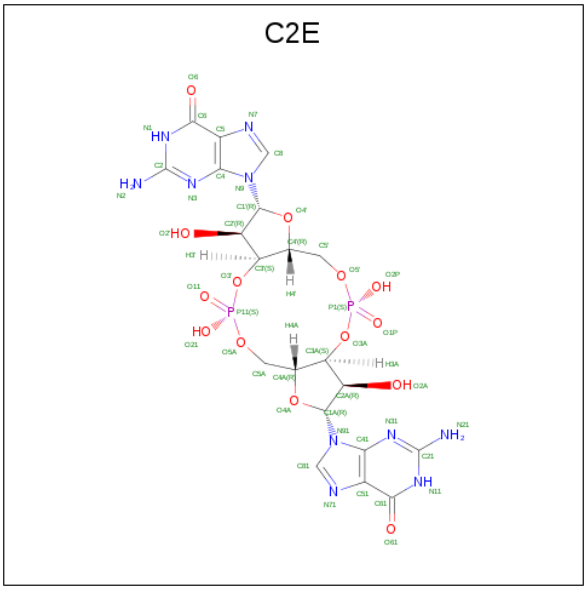
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Mg 1 1	0	0

- Molecule 6 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O P 46 20 10 14 2	0	0
6	E	1	Total C N O P 46 20 10 14 2	0	0
6	F	1	Total C N O P 46 20 10 14 2	0	0
6	F	1	Total C N O P 46 20 10 14 2	0	0
6	K	1	Total C N O P 46 20 10 14 2	0	0
6	K	1	Total C N O P 46 20 10 14 2	0	0
6	L	1	Total C N O P 46 20 10 14 2	0	0
6	L	1	Total C N O P 46 20 10 14 2	0	0

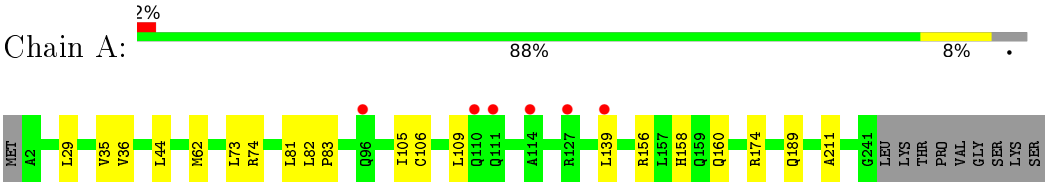
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	36	Total O 36 36	0	0
7	B	35	Total O 35 35	0	0
7	D	3	Total O 3 3	0	0
7	E	18	Total O 18 18	0	0
7	F	18	Total O 18 18	0	0
7	G	35	Total O 35 35	0	0
7	H	36	Total O 36 36	0	0
7	I	3	Total O 3 3	0	0
7	J	1	Total O 1 1	0	0
7	K	20	Total O 20 20	0	0
7	L	22	Total O 22 22	0	0

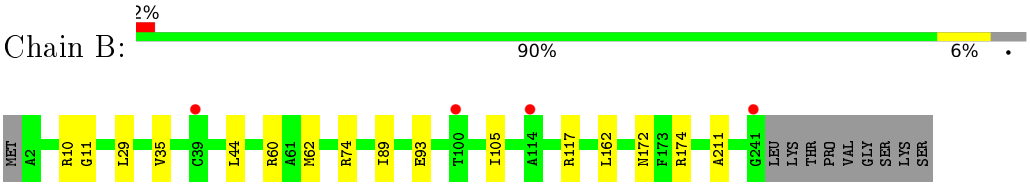
3 Residue-property plots (i)

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

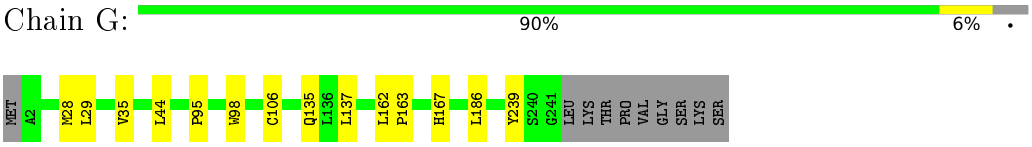
- Molecule 1: Bacterial cellulose secretion regulator BcsQ



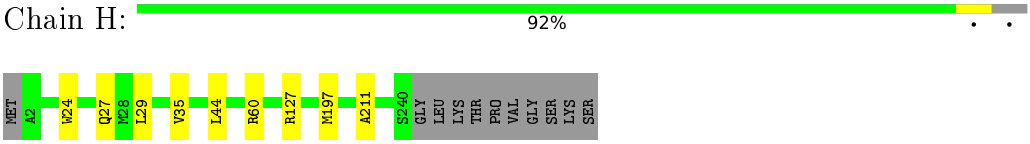
- Molecule 1: Bacterial cellulose secretion regulator BcsQ



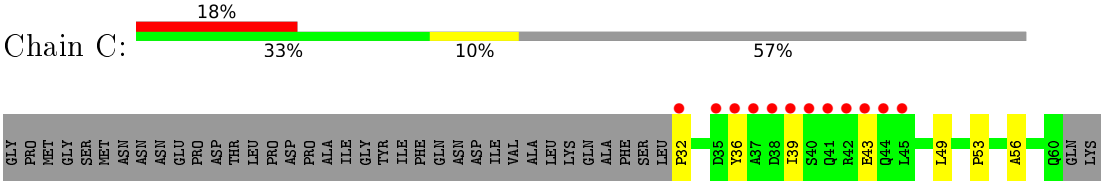
- Molecule 1: Bacterial cellulose secretion regulator BcsQ



- Molecule 1: Bacterial cellulose secretion regulator BcsQ

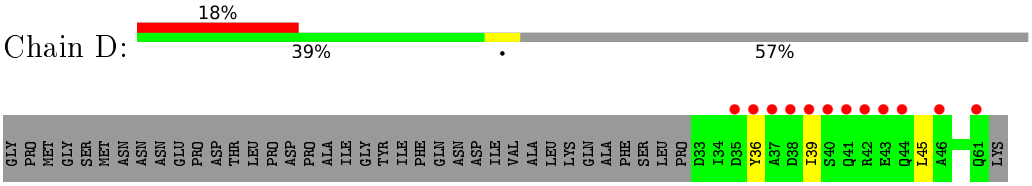


- Molecule 2: Bacterial cellulose secretion regulator BcsR



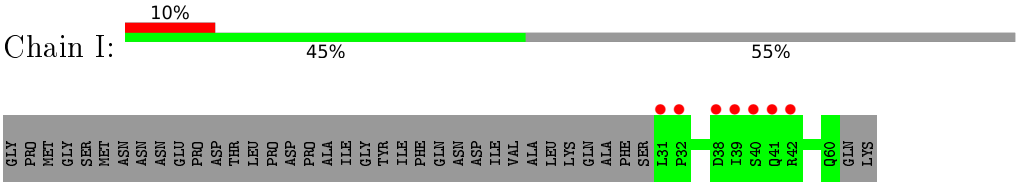
- Molecule 2: Bacterial cellulose secretion regulator BcsR

Chain D:



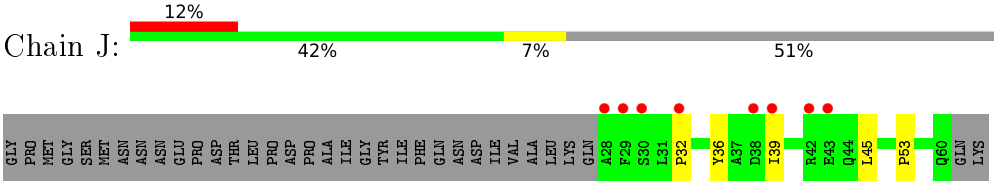
• Molecule 2: Bacterial cellulose secretion regulator BcsR

Chain I:



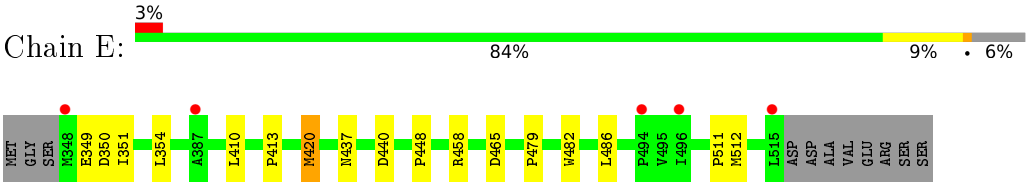
• Molecule 2: Bacterial cellulose secretion regulator BcsR

Chain J:



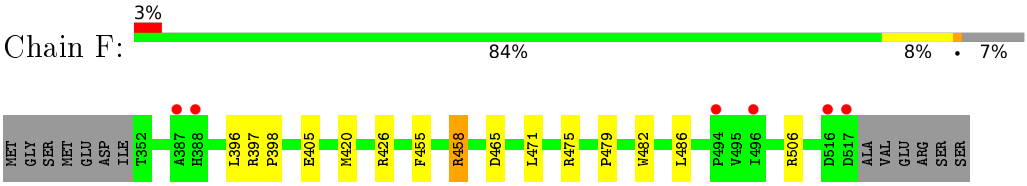
• Molecule 3: Bacterial cellulose secretion regulator BcsE, residues 349-523

Chain E:



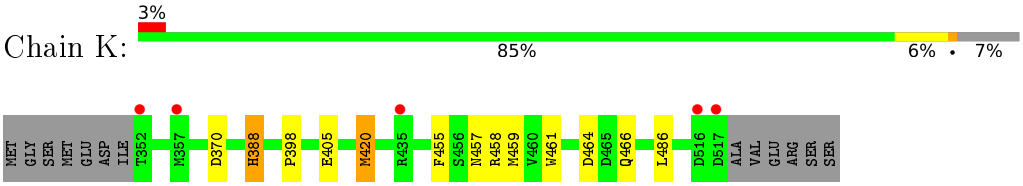
• Molecule 3: Bacterial cellulose secretion regulator BcsE, residues 349-523

Chain F:



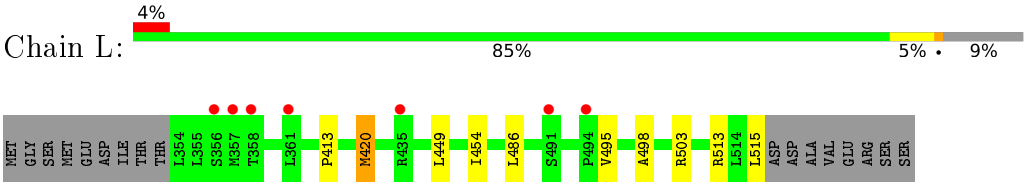
• Molecule 3: Bacterial cellulose secretion regulator BcsE, residues 349-523

Chain K:



• Molecule 3: Bacterial cellulose secretion regulator BcsE, residues 349-523

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.99Å 72.57Å 161.25Å 90.00° 98.37° 90.00°	Depositor
Resolution (Å)	47.71 – 2.49 47.71 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.71-2.49) 98.8 (47.71-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.17rc2_3619	Depositor
R, R_{free}	0.181 , 0.225 0.181 , 0.225	Depositor DCC
R_{free} test set	4331 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14546	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, C2E

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	0.23	0/1928	0.41	0/2623
1	B	0.23	0/1928	0.41	0/2623
1	G	0.23	0/1936	0.41	0/2634
1	H	0.23	0/1924	0.41	0/2618
2	C	0.24	0/240	0.34	0/325
2	D	0.23	0/241	0.33	0/326
2	I	0.24	0/248	0.37	0/337
2	J	0.25	0/271	0.35	0/368
3	E	0.24	0/1371	0.42	0/1864
3	F	0.24	0/1354	0.42	0/1842
3	K	0.24	0/1354	0.42	0/1842
3	L	0.24	0/1324	0.43	0/1800
All	All	0.24	0/14119	0.41	0/19202

There are no bond length outliers.

There are no bond angle outliers.

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	1891	0	1861	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1891	0	1861	12	0
1	G	1899	0	1864	9	0
1	H	1887	0	1858	5	0
2	C	235	0	230	4	0
2	D	237	0	230	4	0
2	I	243	0	240	0	0
2	J	265	0	259	4	0
3	E	1339	0	1361	15	0
3	F	1322	0	1339	10	0
3	K	1322	0	1339	9	0
3	L	1292	0	1317	7	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	G	31	0	12	0	0
4	H	31	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	E	92	0	44	0	0
6	F	92	0	44	0	0
6	K	92	0	44	1	0
6	L	92	0	44	0	0
7	A	36	0	0	0	0
7	B	35	0	0	2	0
7	D	3	0	0	0	0
7	E	18	0	0	0	0
7	F	18	0	0	0	0
7	G	35	0	0	0	0
7	H	36	0	0	1	0
7	I	3	0	0	0	0
7	J	1	0	0	0	0
7	K	20	0	0	0	0
7	L	22	0	0	0	0
All	All	14546	0	13983	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 79 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)
2:J:39:ILE:HG23	2:J:45:LEU:HD23	1.77	0.66
1:B:172:ASN:ND2	7:B:401:HOH:O	2.31	0.64
1:A:174:ARG:HH22	1:B:174:ARG:HE	1.48	0.61
1:A:189:GLN:HG3	2:D:45:LEU:HD11	1.82	0.60
3:E:349:GLU:HG3	3:E:354:LEU:HD21	1.83	0.60

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/250 (95%)	237 (100%)	1 (0%)	0	100	100
1	B	238/250 (95%)	237 (100%)	1 (0%)	0	100	100
1	G	239/250 (96%)	234 (98%)	5 (2%)	0	100	100
1	H	237/250 (95%)	233 (98%)	4 (2%)	0	100	100
2	C	27/67 (40%)	24 (89%)	3 (11%)	0	100	100
2	D	27/67 (40%)	27 (100%)	0	0	100	100
2	I	28/67 (42%)	27 (96%)	1 (4%)	0	100	100
2	J	31/67 (46%)	28 (90%)	3 (10%)	0	100	100
3	E	166/179 (93%)	165 (99%)	1 (1%)	0	100	100
3	F	164/179 (92%)	162 (99%)	2 (1%)	0	100	100
3	K	164/179 (92%)	160 (98%)	4 (2%)	0	100	100
3	L	160/179 (89%)	158 (99%)	2 (1%)	0	100	100
All	All	1719/1984 (87%)	1692 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	202/211 (96%)	202 (100%)	0	100	100
1	B	202/211 (96%)	201 (100%)	1 (0%)	88	96
1	G	203/211 (96%)	202 (100%)	1 (0%)	88	96
1	H	202/211 (96%)	200 (99%)	2 (1%)	76	90
2	C	23/55 (42%)	22 (96%)	1 (4%)	29	53
2	D	23/55 (42%)	23 (100%)	0	100	100
2	I	24/55 (44%)	24 (100%)	0	100	100
2	J	26/55 (47%)	26 (100%)	0	100	100
3	E	150/159 (94%)	149 (99%)	1 (1%)	84	94
3	F	148/159 (93%)	146 (99%)	2 (1%)	67	86
3	K	148/159 (93%)	146 (99%)	2 (1%)	67	86
3	L	144/159 (91%)	142 (99%)	2 (1%)	67	86
All	All	1495/1700 (88%)	1483 (99%)	12 (1%)	81	93

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	197	MET
3	K	388	HIS
3	L	503	ARG
3	K	420	MET
3	F	420	MET

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

Mol	Chain	Res	Type
1	H	97	HIS

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
6	C2E	F	601	-	44,52,52	0.93	2 (4%)	54,82,82	2.23	12 (22%)
6	C2E	L	602	-	44,52,52	0.94	2 (4%)	54,82,82	2.23	12 (22%)
4	ATP	H	301	5	26,33,33	0.61	0	31,52,52	0.61	1 (3%)
6	C2E	E	601	-	44,52,52	0.93	2 (4%)	54,82,82	2.24	12 (22%)
6	C2E	L	601	-	44,52,52	0.93	2 (4%)	54,82,82	2.25	12 (22%)
6	C2E	K	601	3	44,52,52	0.93	2 (4%)	54,82,82	2.24	12 (22%)
4	ATP	B	301	5	26,33,33	0.59	0	31,52,52	0.63	1 (3%)
4	ATP	G	301	5	26,33,33	0.62	0	31,52,52	0.62	1 (3%)
4	ATP	A	301	5	26,33,33	0.61	0	31,52,52	0.60	1 (3%)
6	C2E	K	602	-	44,52,52	0.93	2 (4%)	54,82,82	2.23	12 (22%)
6	C2E	E	602	-	44,52,52	0.93	2 (4%)	54,82,82	2.24	12 (22%)
6	C2E	F	602	3	44,52,52	0.94	2 (4%)	54,82,82	2.23	12 (22%)

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
6	C2E	F	601	-	-	0/22/62/62	0/6/7/7
6	C2E	L	602	-	-	0/22/62/62	0/6/7/7
4	ATP	H	301	5	-	3/18/38/38	0/3/3/3
6	C2E	E	601	-	-	0/22/62/62	0/6/7/7
6	C2E	L	601	-	-	0/22/62/62	0/6/7/7
6	C2E	K	601	3	-	0/22/62/62	0/6/7/7
4	ATP	B	301	5	-	3/18/38/38	0/3/3/3
4	ATP	G	301	5	-	0/18/38/38	0/3/3/3
4	ATP	A	301	5	-	0/18/38/38	0/3/3/3
6	C2E	K	602	-	-	0/22/62/62	0/6/7/7
6	C2E	E	602	-	-	0/22/62/62	0/6/7/7
6	C2E	F	602	3	-	0/22/62/62	0/6/7/7

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	601	C2E	C6-N1	3.23	1.38	1.33
6	E	602	C2E	C6-N1	3.22	1.38	1.33
6	L	602	C2E	C6-N1	3.21	1.38	1.33
6	K	601	C2E	C6-N1	3.20	1.38	1.33
6	F	602	C2E	C6-N1	3.20	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	601	C2E	C51-C61-N11	-8.31	112.06	123.43
6	E	601	C2E	C5-C6-N1	-8.31	112.07	123.43
6	F	602	C2E	C51-C61-N11	-8.30	112.08	123.43
6	L	602	C2E	C51-C61-N11	-8.29	112.09	123.43
6	E	601	C2E	C51-C61-N11	-8.28	112.11	123.43

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

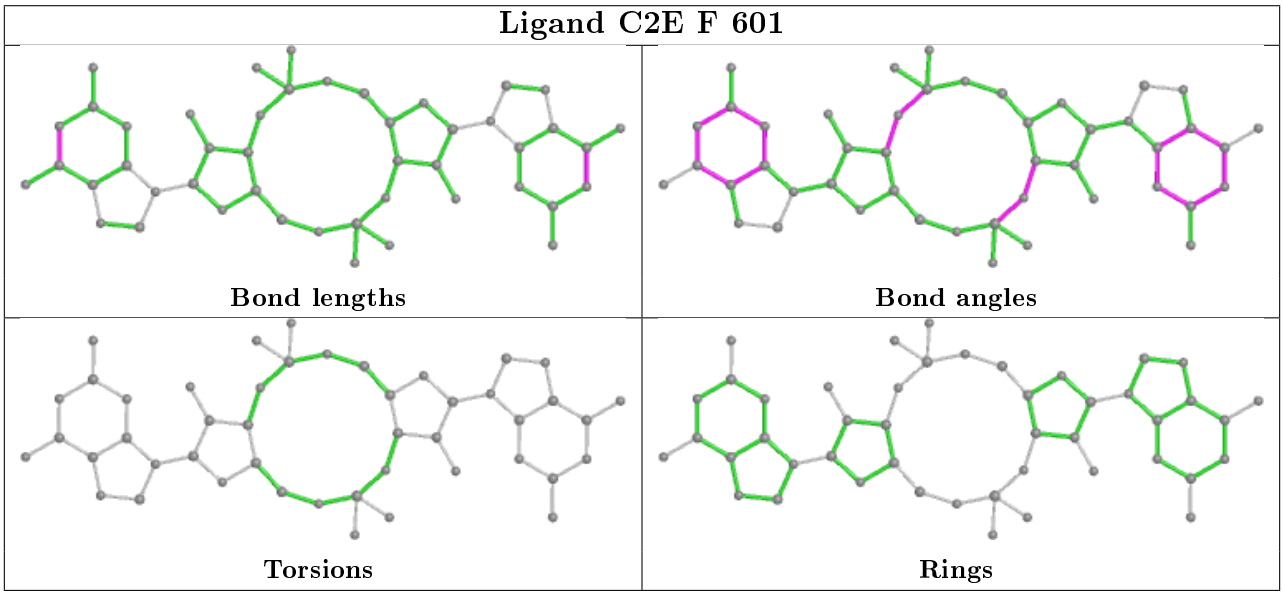
Mol	Chain	Res	Type	Atoms
4	B	301	ATP	PB-O3B-PG-O3G
4	H	301	ATP	PB-O3B-PG-O3G
4	B	301	ATP	PB-O3B-PG-O1G
4	H	301	ATP	PB-O3B-PG-O1G
4	B	301	ATP	PB-O3B-PG-O2G

There are no ring outliers.

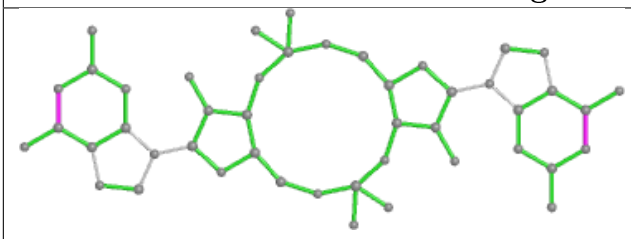
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	601	C2E	1	0

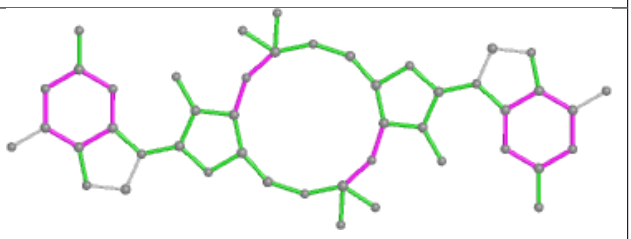
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



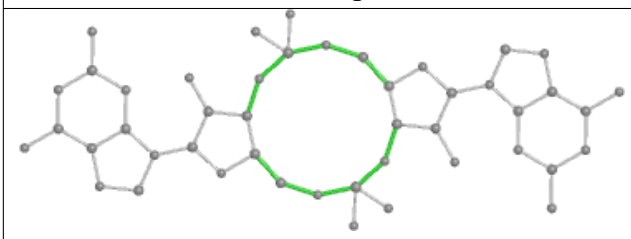
Ligand C2E L 602



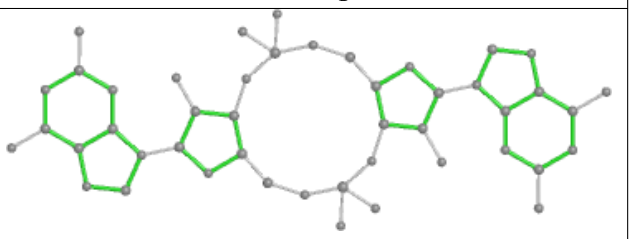
Bond lengths



Bond angles

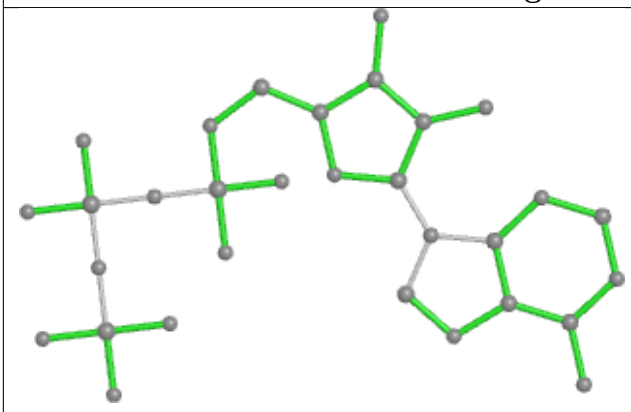


Torsions



Rings

Ligand ATP H 301



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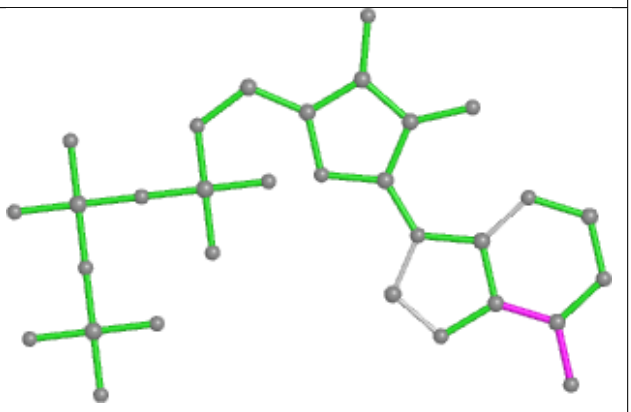

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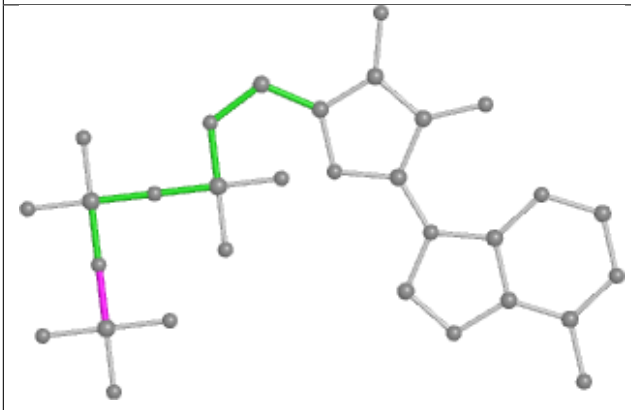

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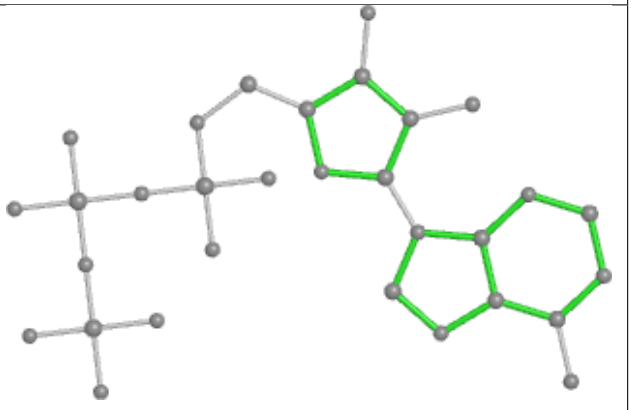
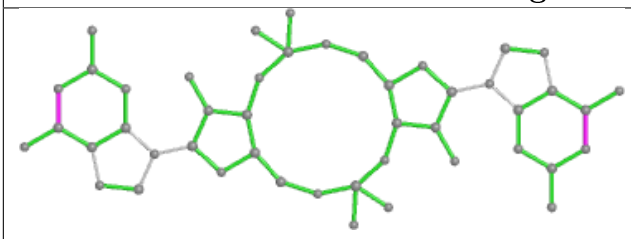


Rings

Ligand C2E E 601



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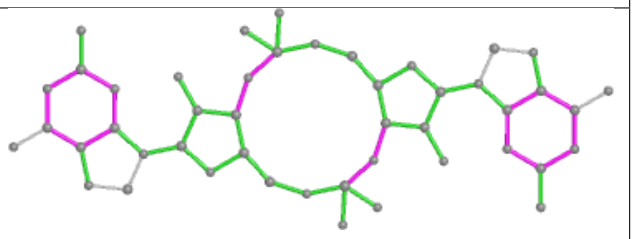

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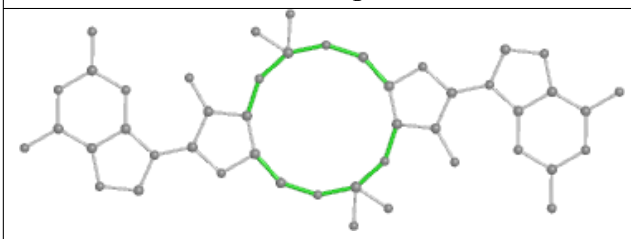

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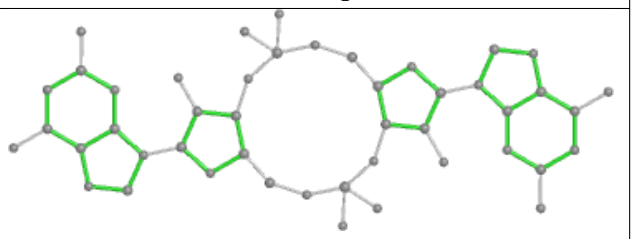
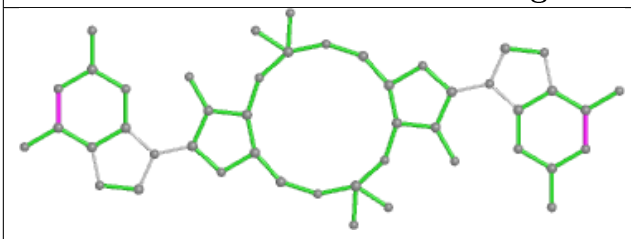


Rings

Ligand C2E L 601



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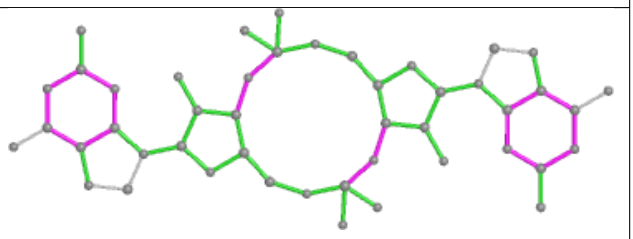

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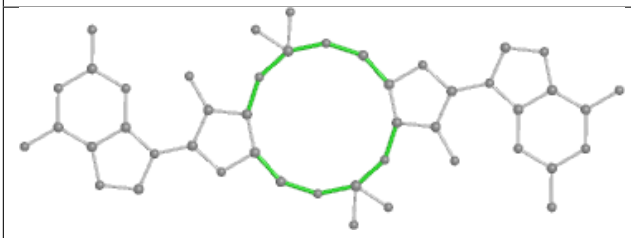

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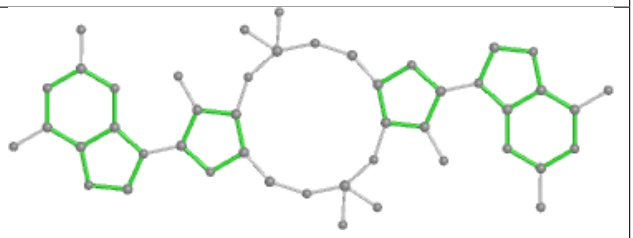
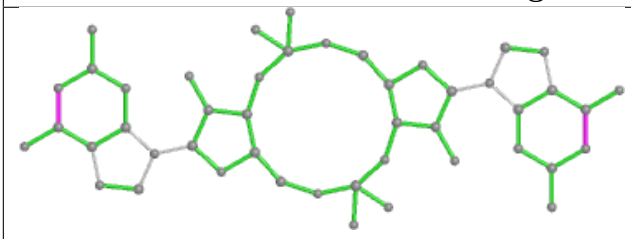


Rings

Ligand C2E K 601



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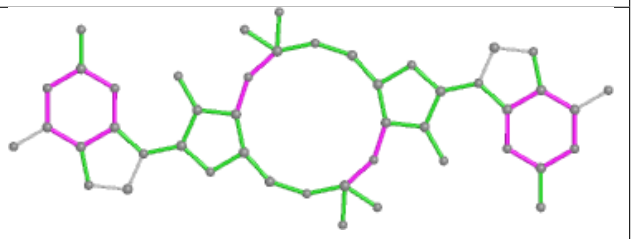

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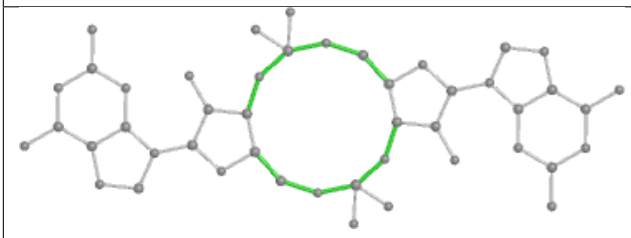

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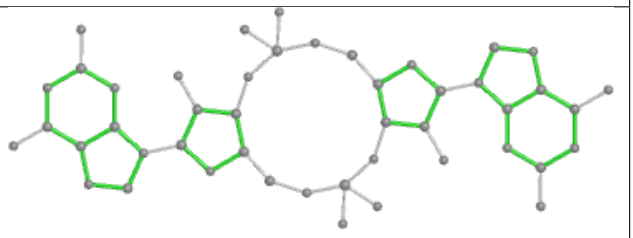
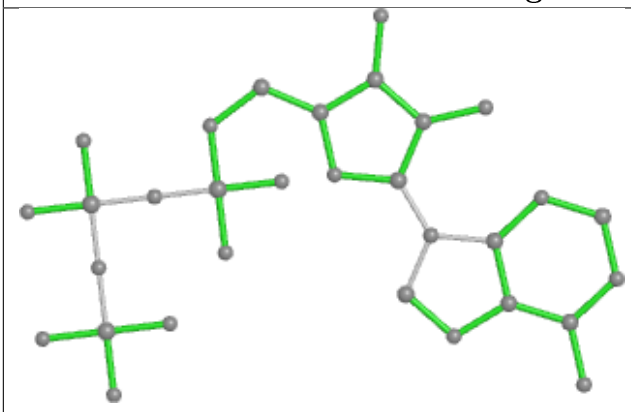


Rings

Ligand ATP B 301



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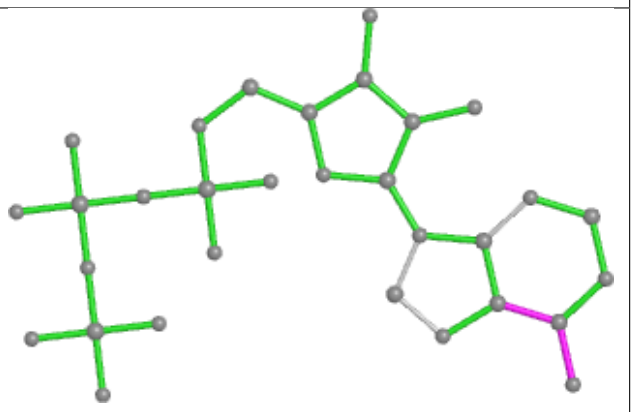
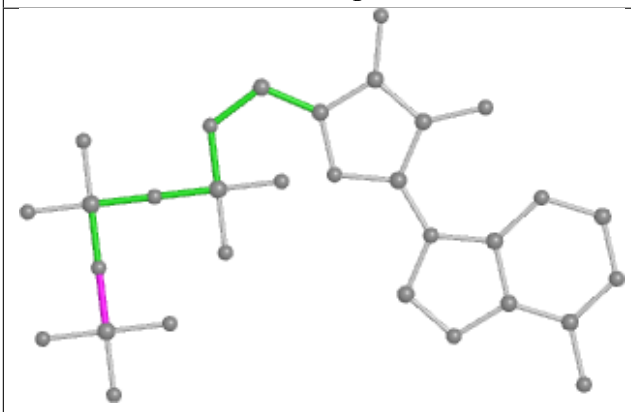


Bond angles



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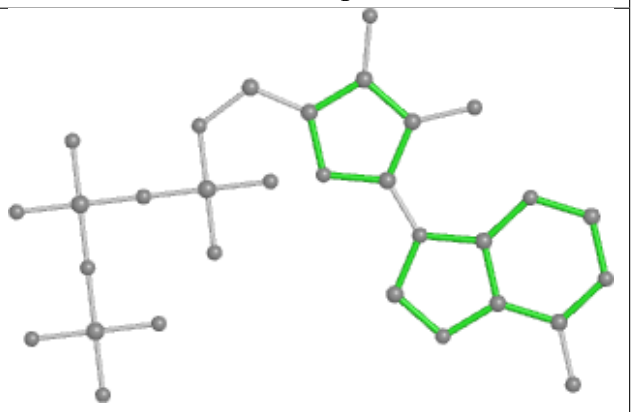
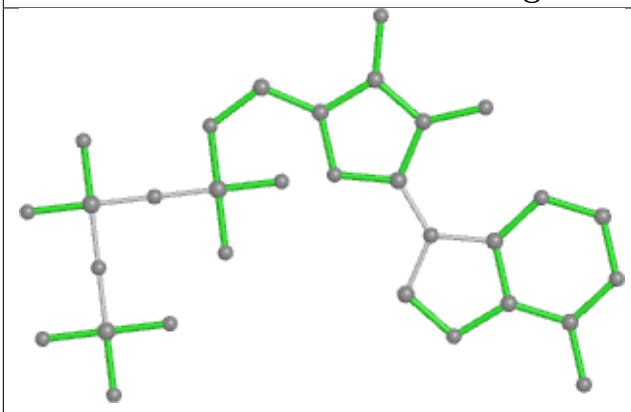
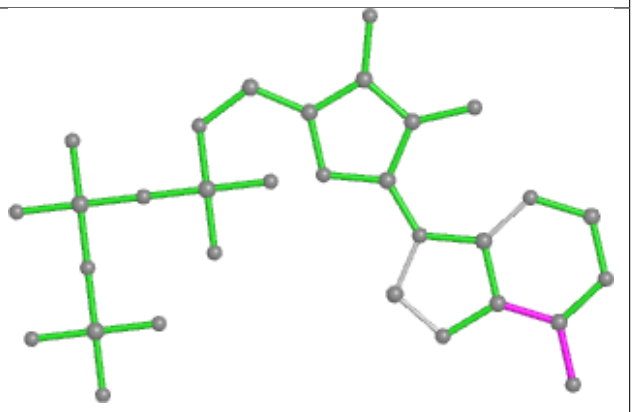


Rings

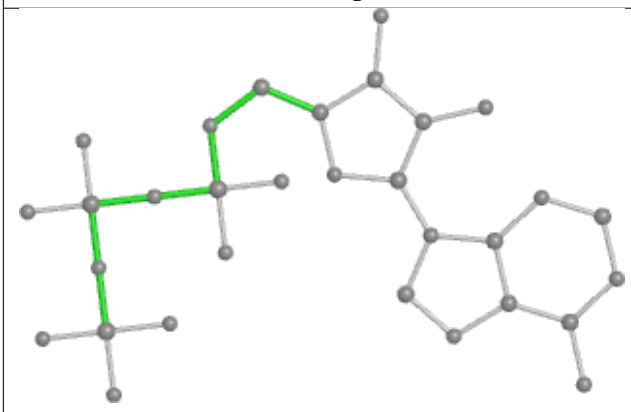
Ligand ATP G 301



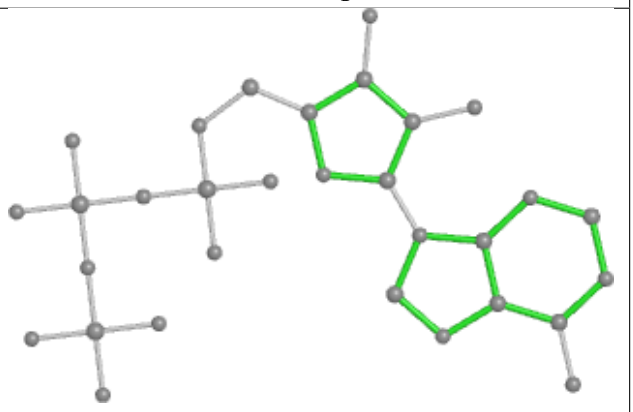
Bond lengths



Bond angles

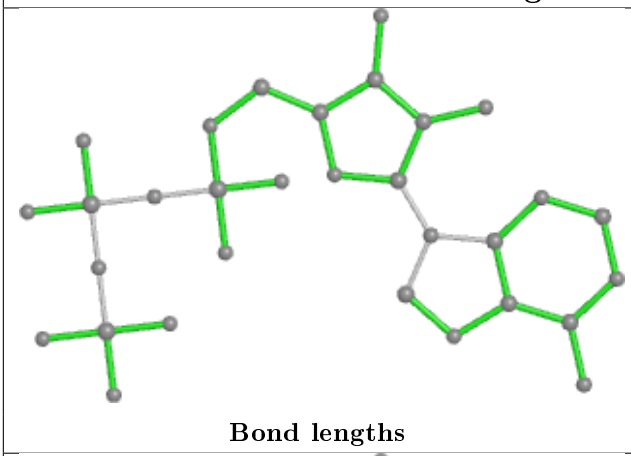


Torsions

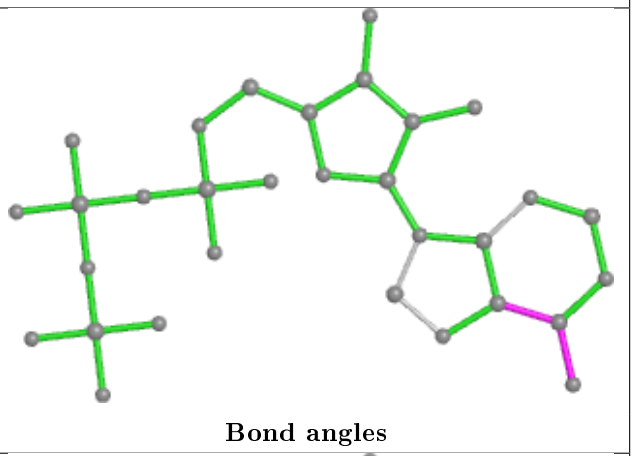


Rings

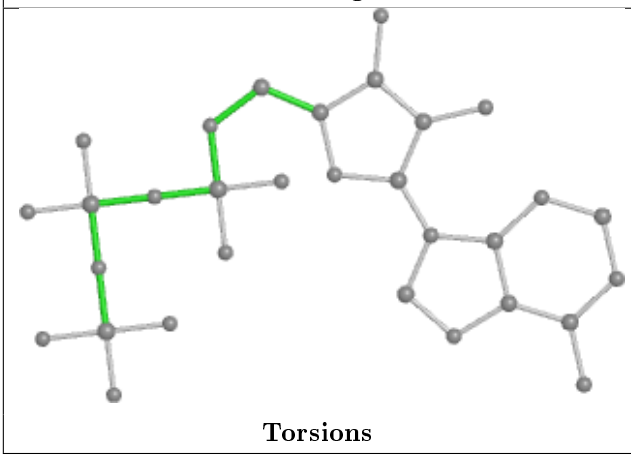
Ligand ATP A 301



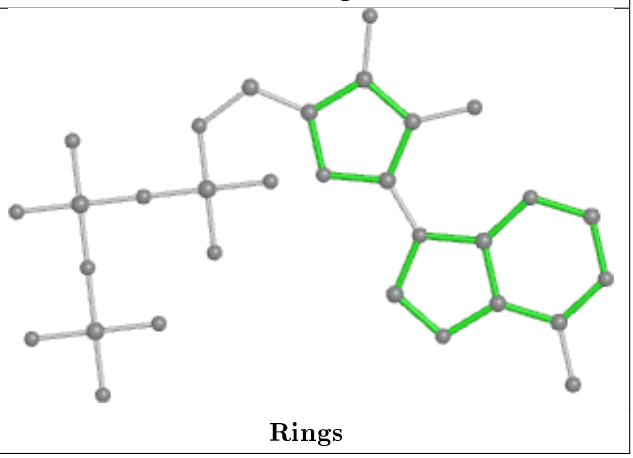
Bond lengths



Bond angles

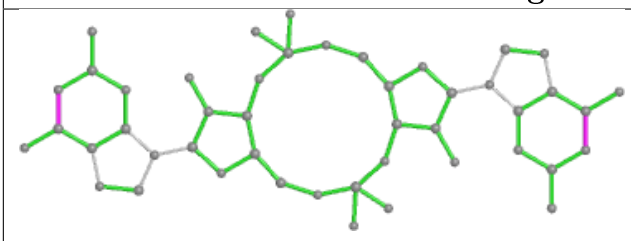


Torsions

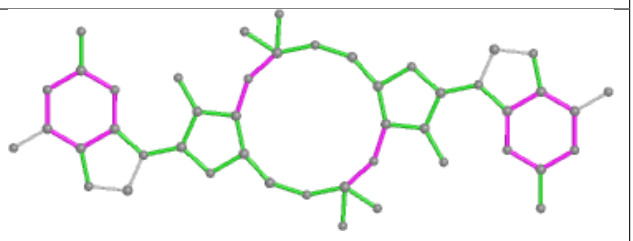


Rings

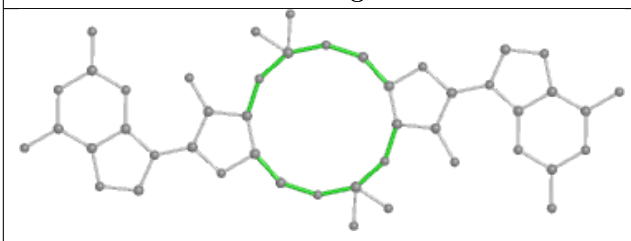
Ligand C2E K 602



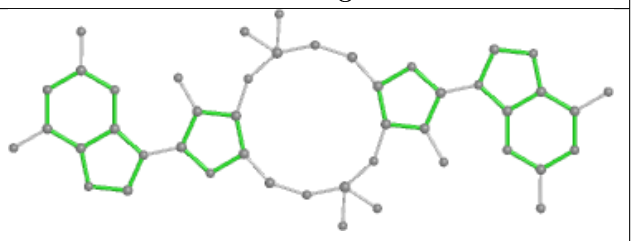
Bond lengths



Bond angles

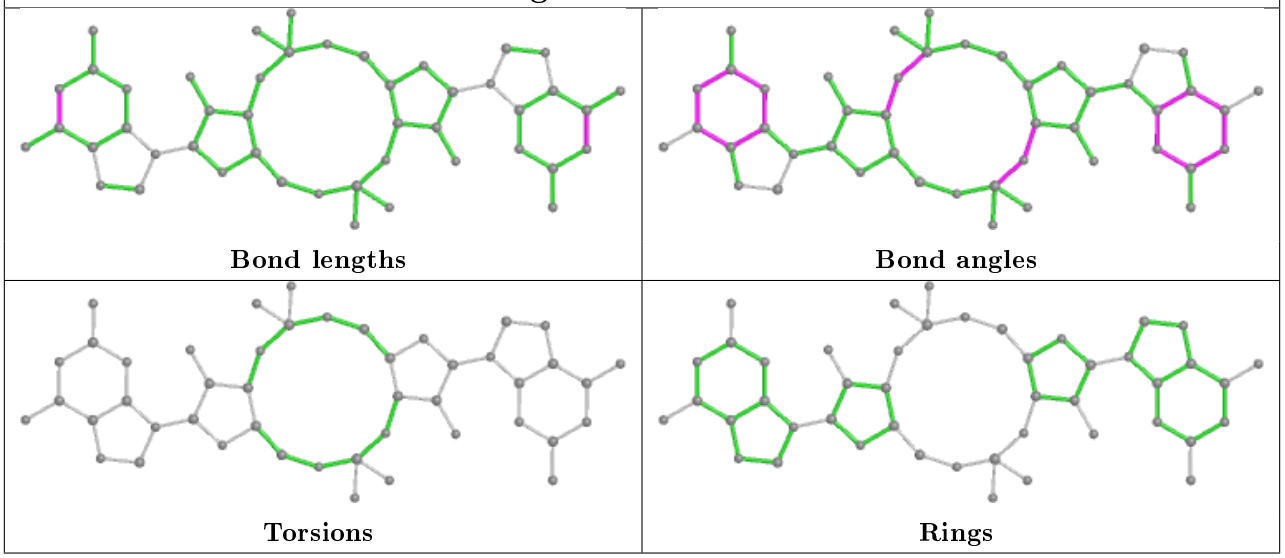


Torsions

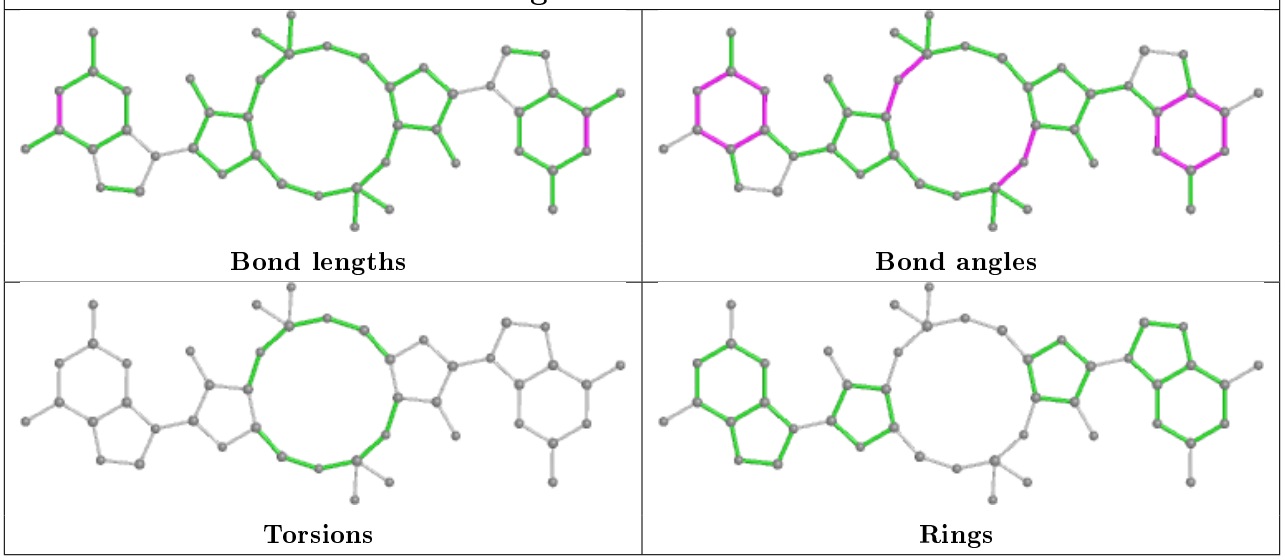


Rings

Ligand C2E E 602



Ligand C2E F 602



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	240/250 (96%)	0.04	6 (2%) 57 61	41, 56, 101, 135	0
1	B	240/250 (96%)	-0.06	4 (1%) 70 72	40, 56, 89, 102	0
1	G	240/250 (96%)	-0.20	0 100 100	38, 52, 83, 93	0
1	H	239/250 (95%)	-0.14	0 100 100	37, 52, 87, 110	0
2	C	29/67 (43%)	1.67	12 (41%) 0 0	52, 86, 137, 153	0
2	D	29/67 (43%)	1.82	12 (41%) 0 0	48, 79, 140, 153	0
2	I	30/67 (44%)	1.06	7 (23%) 0 0	44, 73, 142, 153	0
2	J	33/67 (49%)	1.15	8 (24%) 0 0	49, 74, 127, 139	0
3	E	168/179 (93%)	-0.06	5 (2%) 50 53	40, 59, 99, 141	0
3	F	166/179 (92%)	-0.08	6 (3%) 42 46	41, 60, 90, 126	0
3	K	166/179 (92%)	-0.01	5 (3%) 50 53	35, 54, 103, 131	0
3	L	162/179 (90%)	-0.04	7 (4%) 35 38	37, 56, 103, 120	0
All	All	1742/1984 (87%)	0.03	72 (4%) 37 40	35, 56, 102, 153	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	39	ILE	6.4
2	I	41	GLN	6.2
2	D	40	SER	6.1
2	J	32	PRO	5.9
2	I	31	LEU	5.7

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

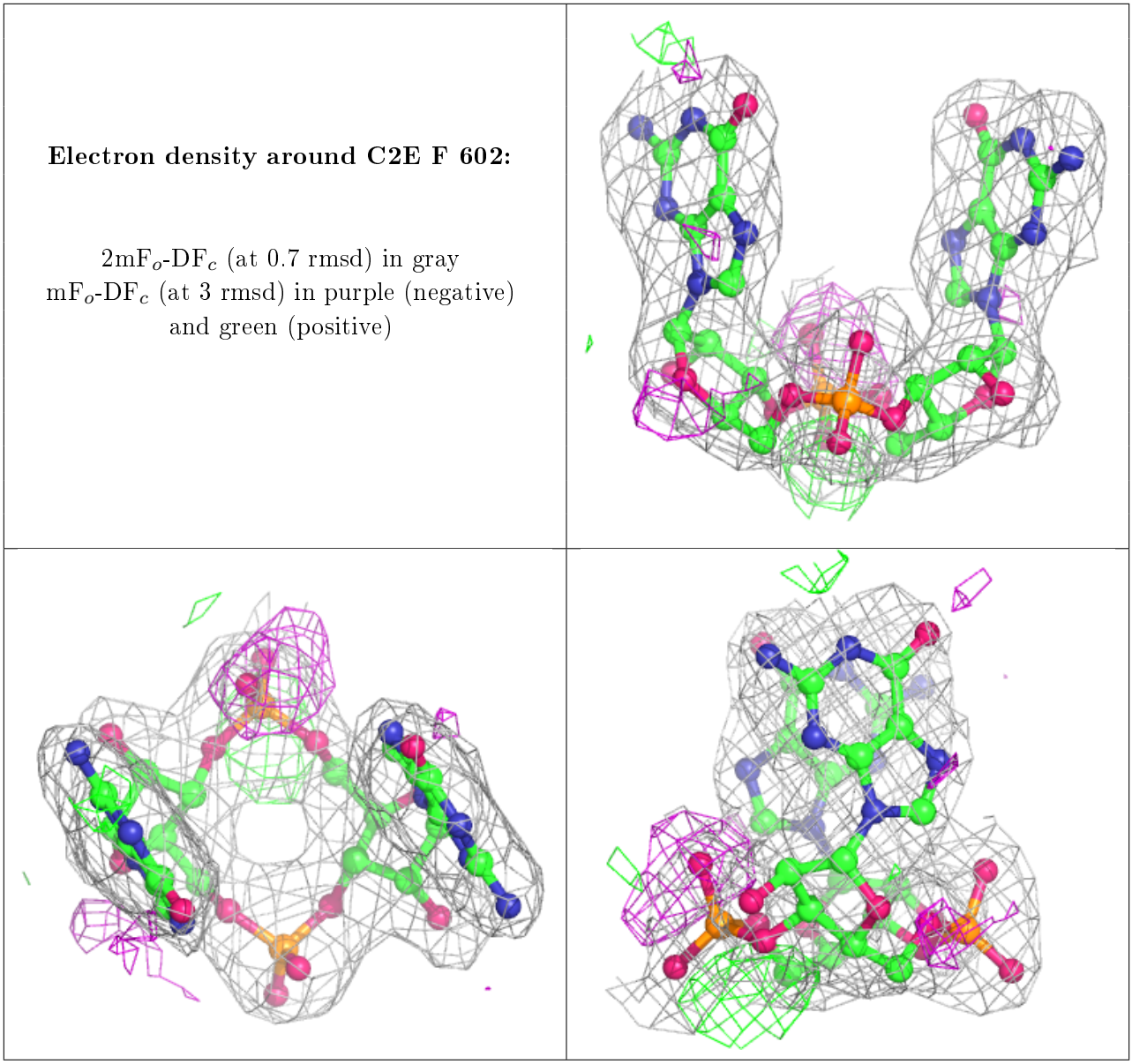
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	C2E	F	602	46/46	0.94	0.14	47,56,64,74	0
6	C2E	K	601	46/46	0.94	0.14	45,58,68,72	0
6	C2E	L	601	46/46	0.95	0.12	43,53,61,69	0
6	C2E	E	601	46/46	0.96	0.14	46,54,67,71	0
5	MG	G	302	1/1	0.96	0.16	43,43,43,43	0
5	MG	H	302	1/1	0.97	0.14	46,46,46,46	0
6	C2E	E	602	46/46	0.97	0.12	44,52,61,67	0
6	C2E	K	602	46/46	0.97	0.13	44,53,63,68	0
6	C2E	F	601	46/46	0.97	0.12	50,60,64,67	0
6	C2E	L	602	46/46	0.97	0.14	36,51,58,71	0
5	MG	A	302	1/1	0.98	0.14	41,41,41,41	0
5	MG	B	302	1/1	0.98	0.17	45,45,45,45	0
4	ATP	B	301	31/31	0.98	0.15	37,46,55,56	0
4	ATP	A	301	31/31	0.99	0.15	37,47,55,63	0
4	ATP	G	301	31/31	0.99	0.17	31,43,51,61	0
4	ATP	H	301	31/31	0.99	0.17	35,46,51,53	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.

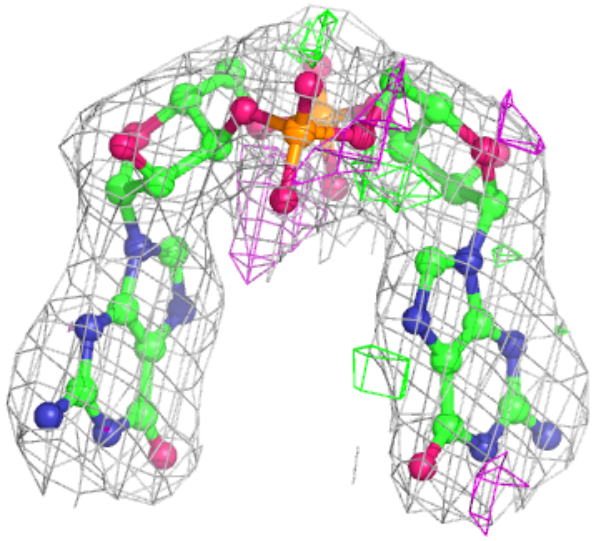
Electron density around C2E F 602:

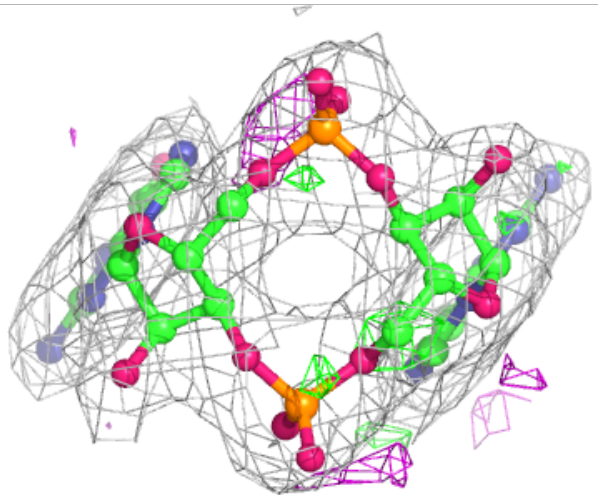
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

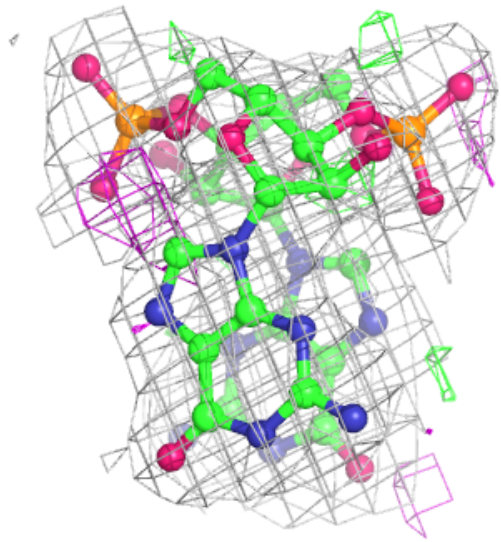


Electron density around C2E K 601:

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

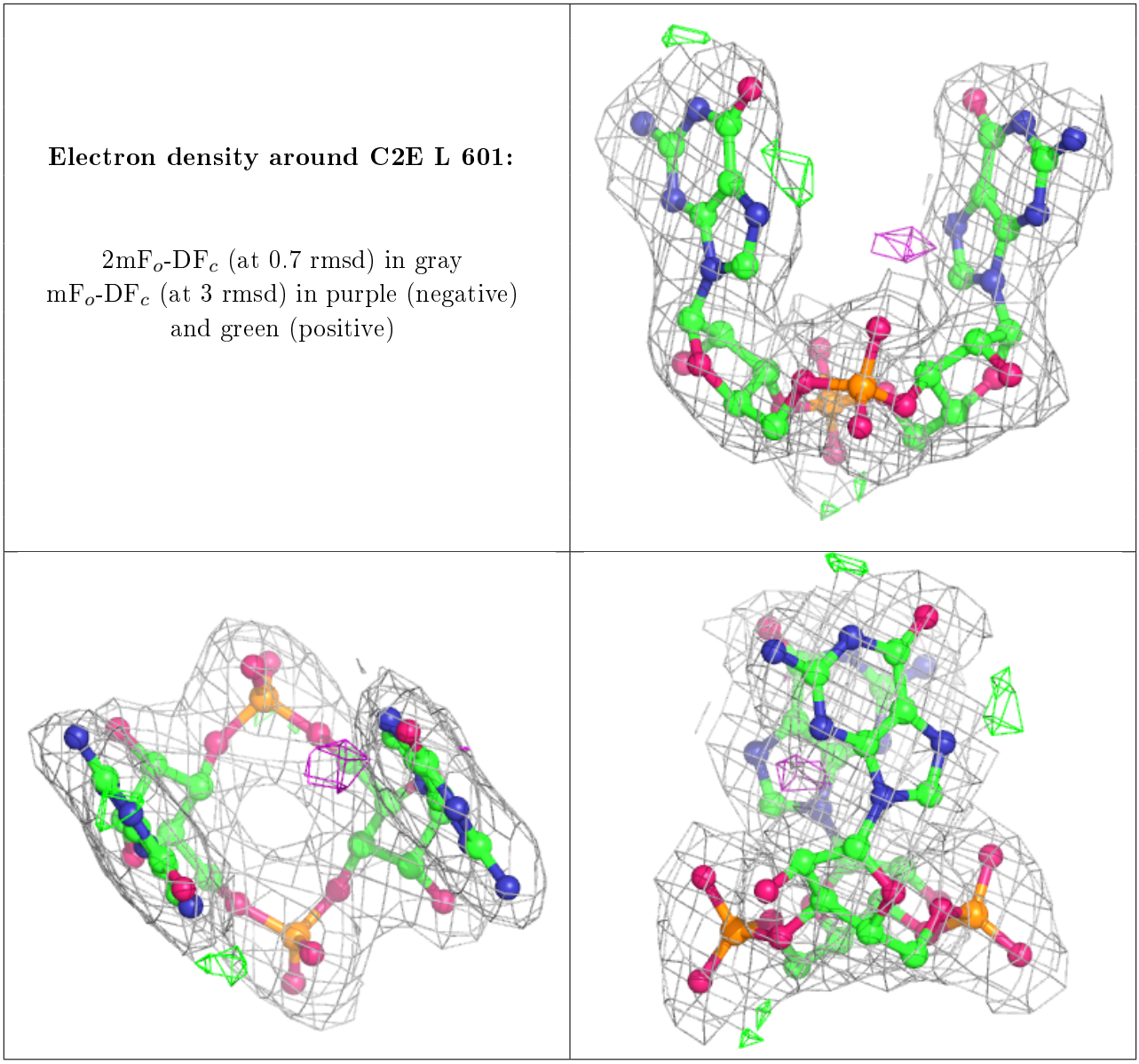






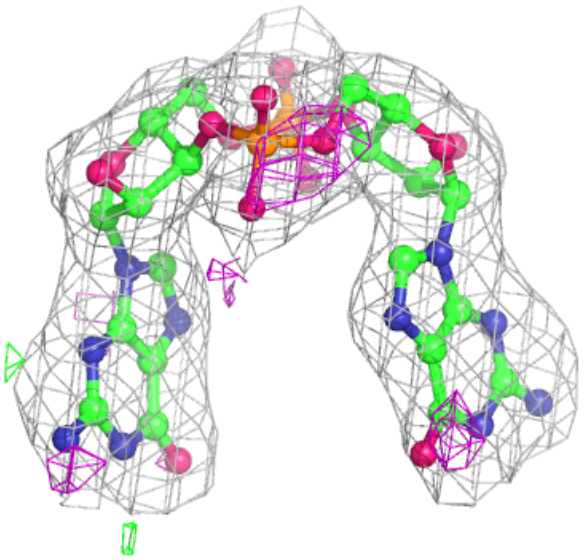
Electron density around C2E L 601:

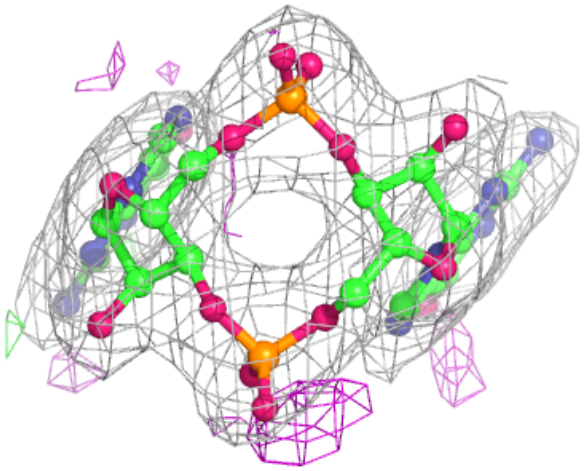
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

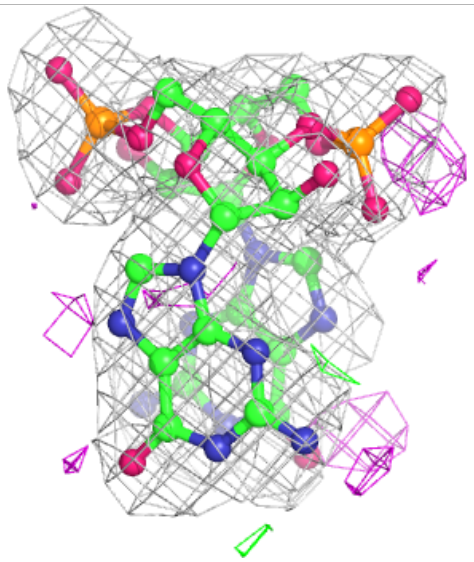


Electron density around C2E E 601:

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

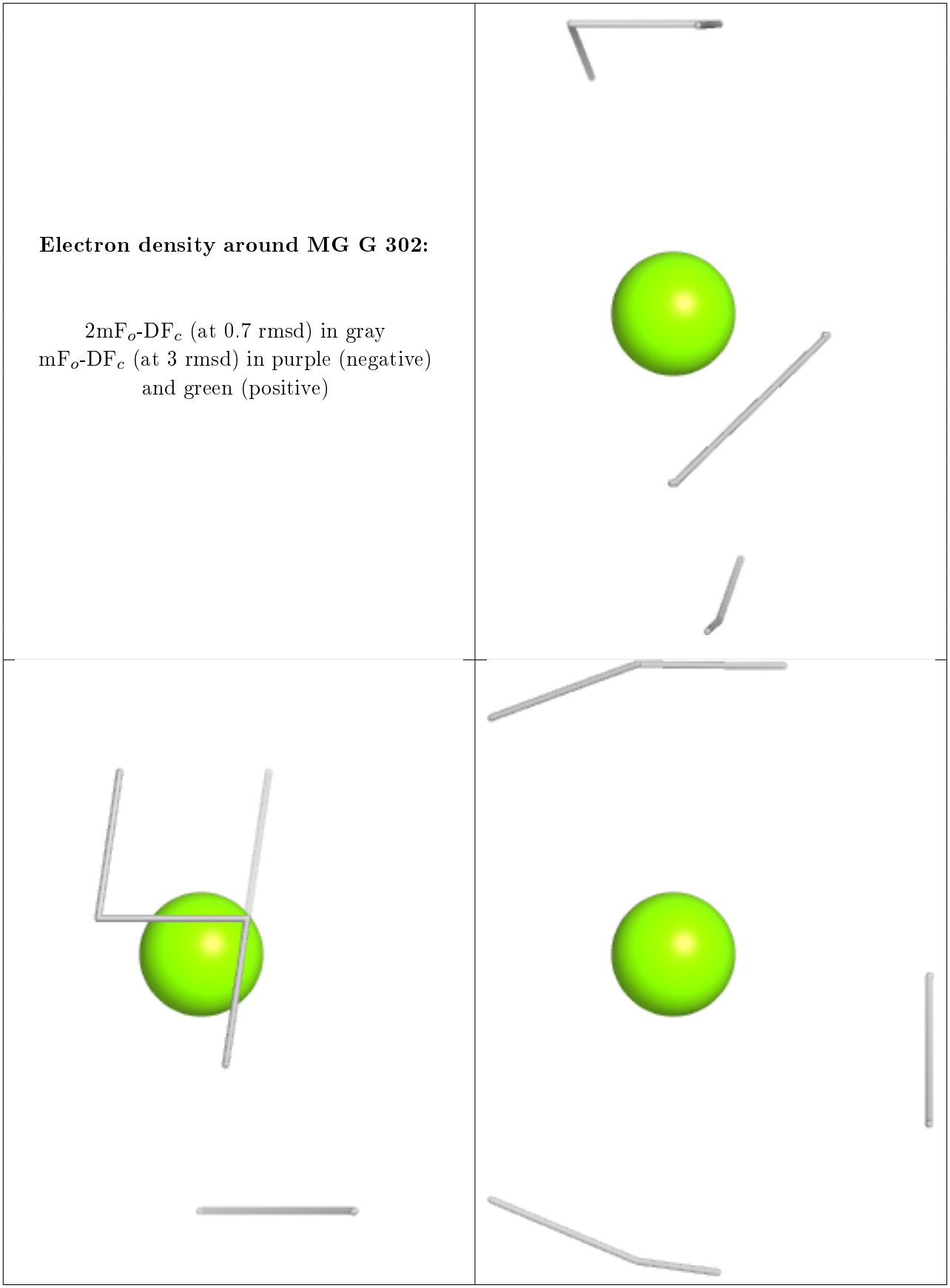






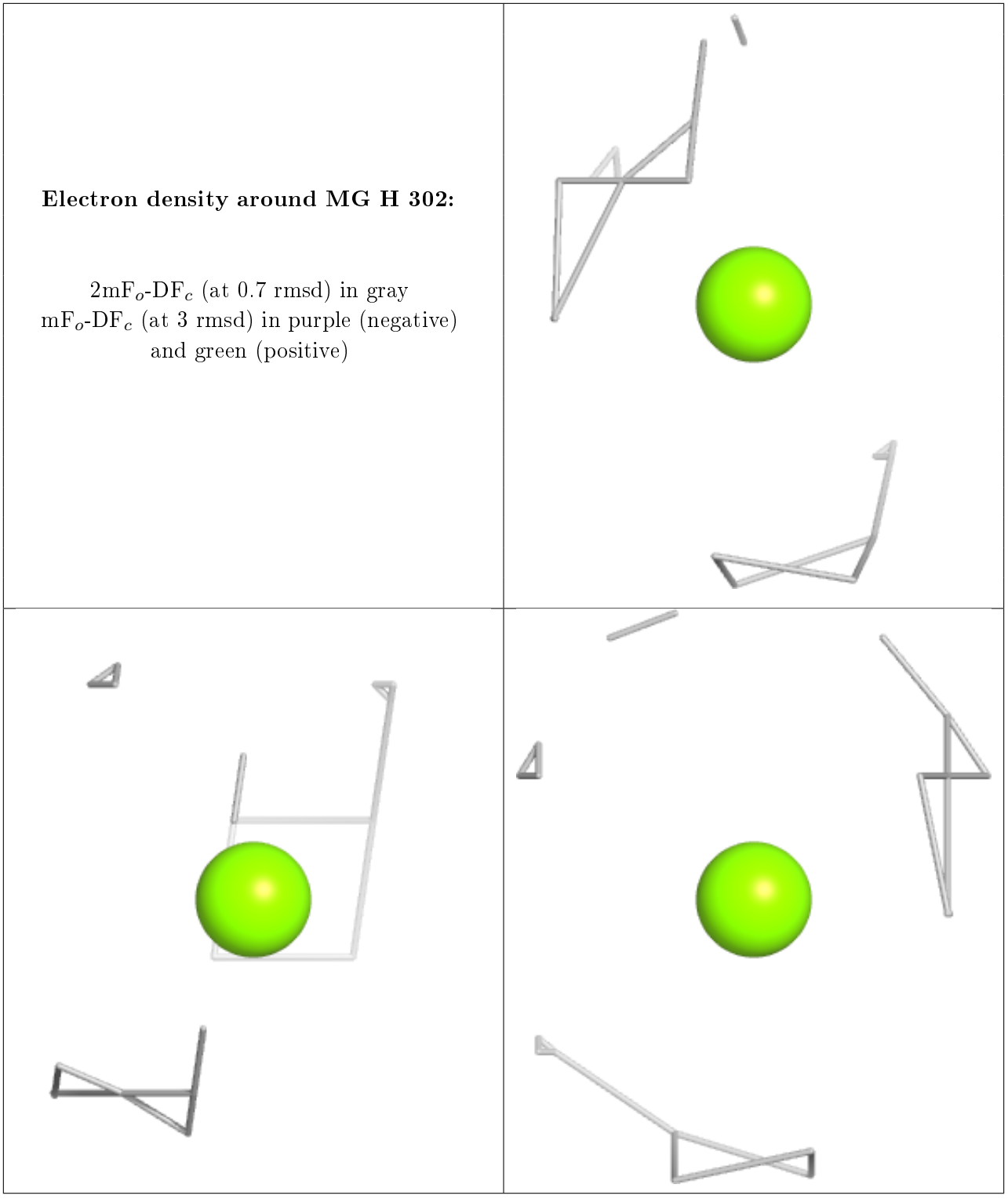
Electron density around MG G 302:

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



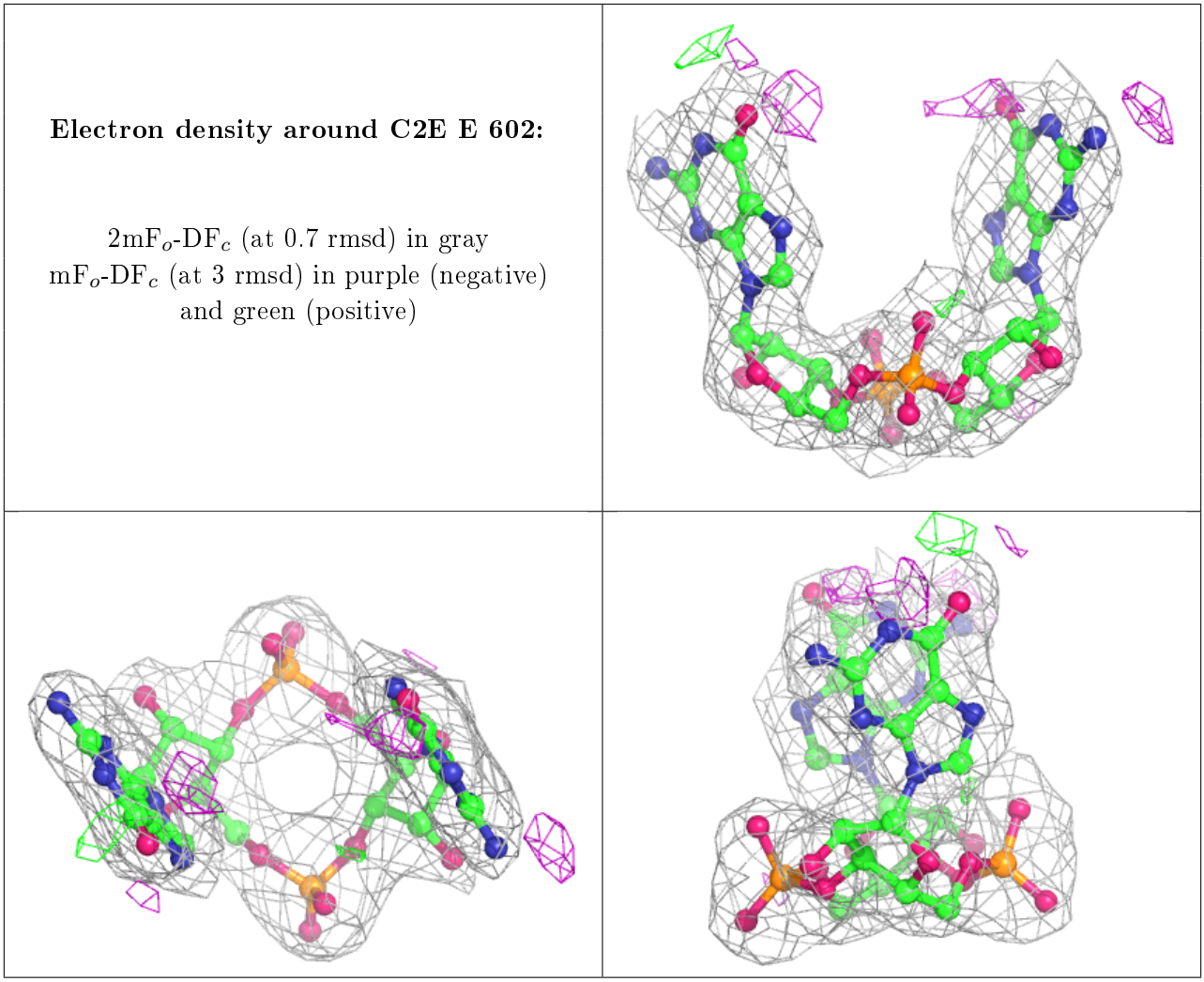
Electron density around MG H 302:

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



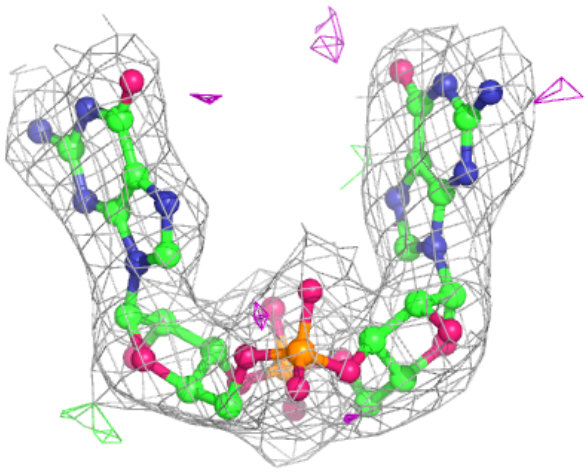
Electron density around C2E E 602:

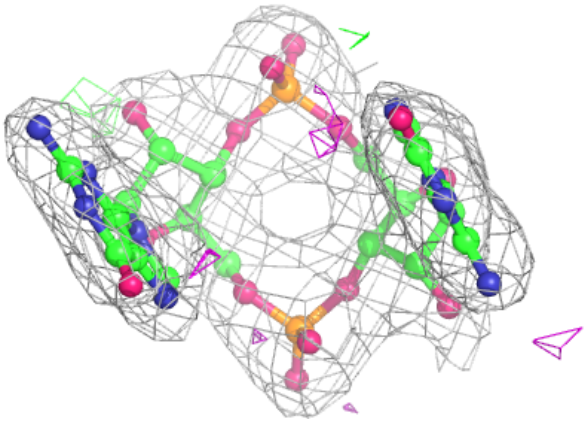
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

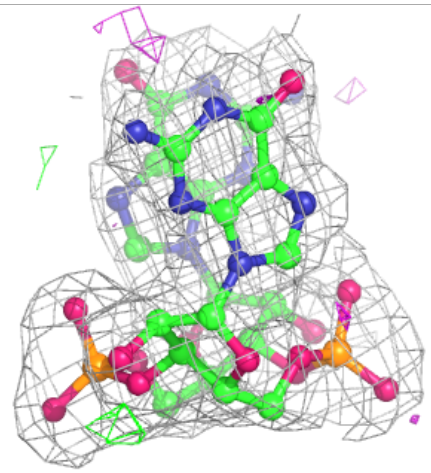


Electron density around C2E K 602:

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

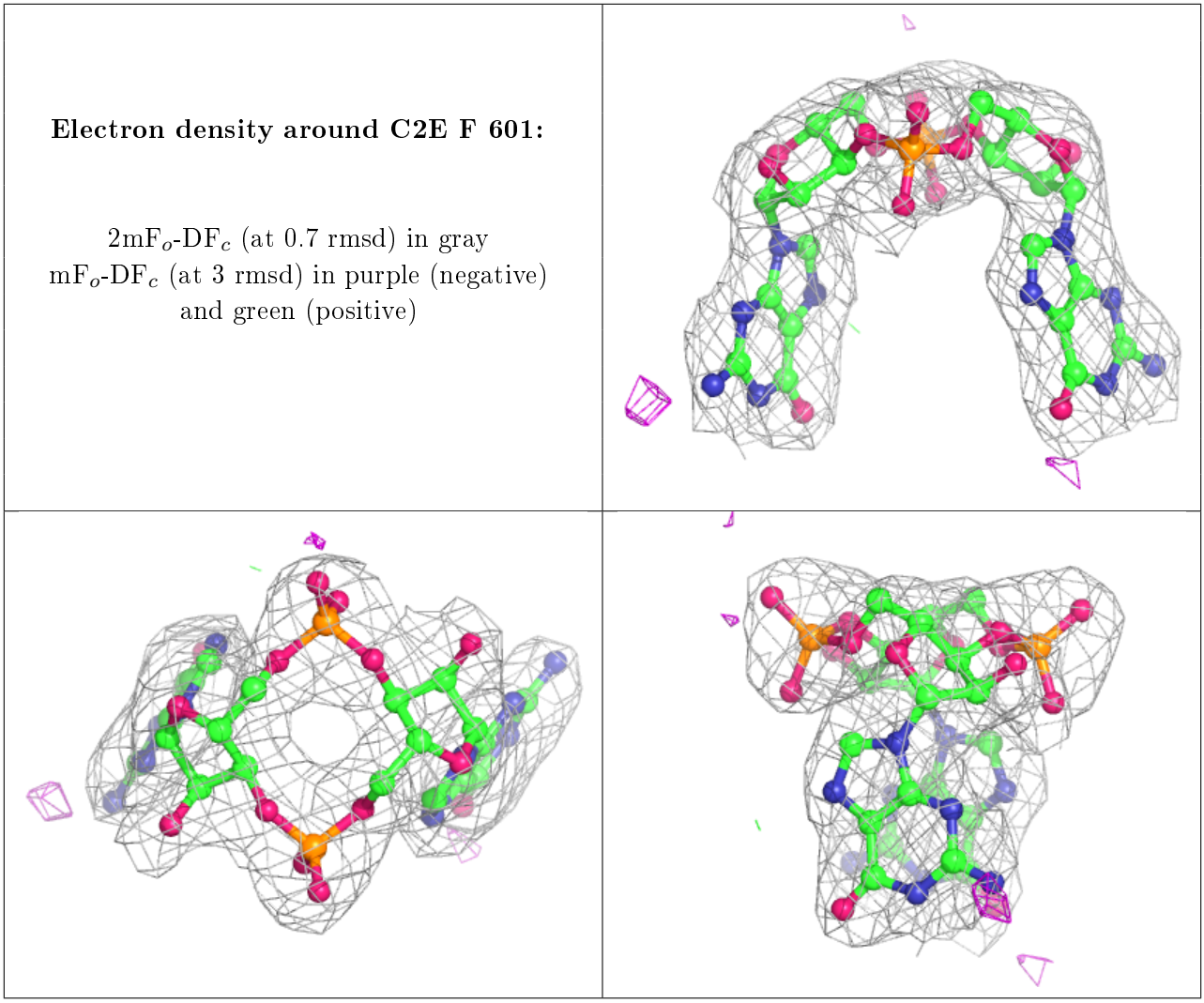






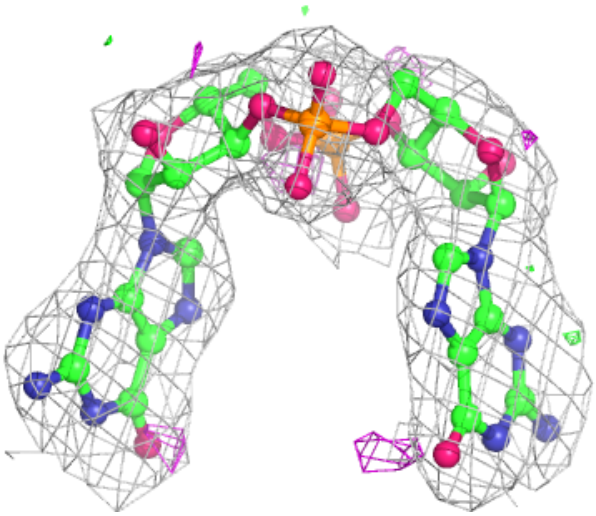
Electron density around C2E F 601:

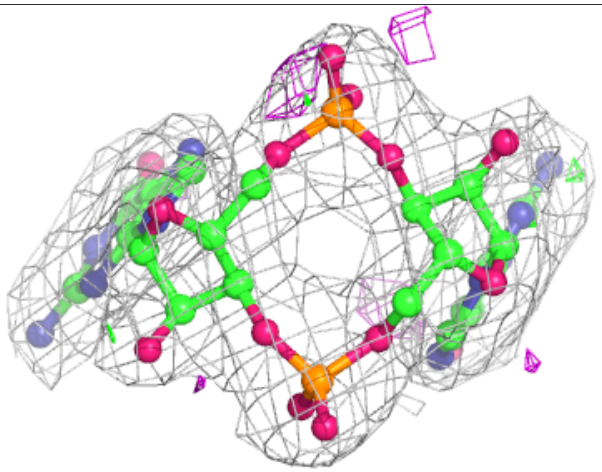
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

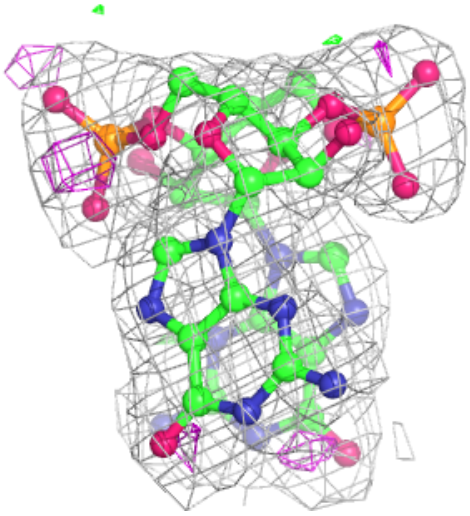


Electron density around C2E L 602:

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

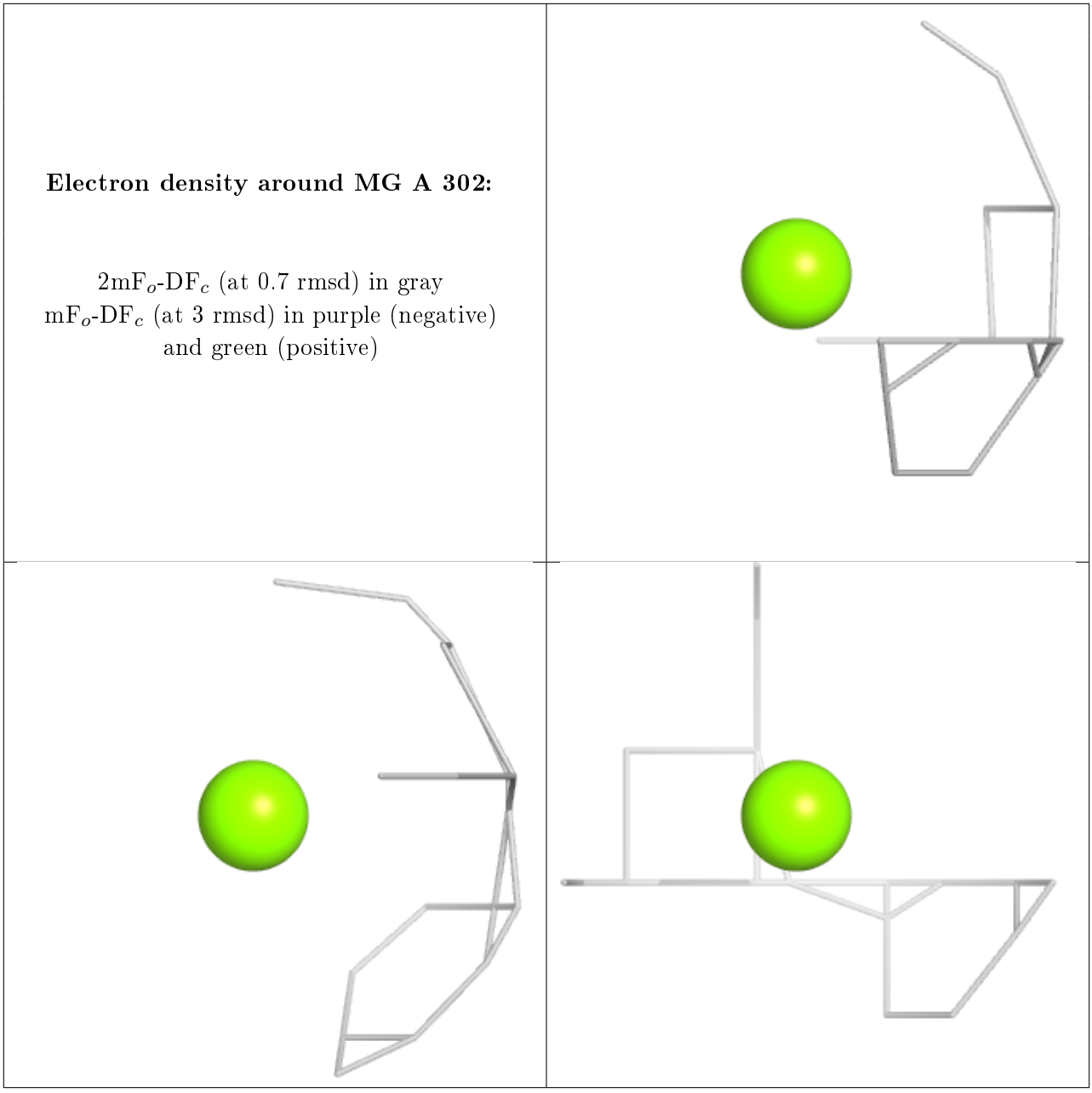






Electron density around MG A 302:

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

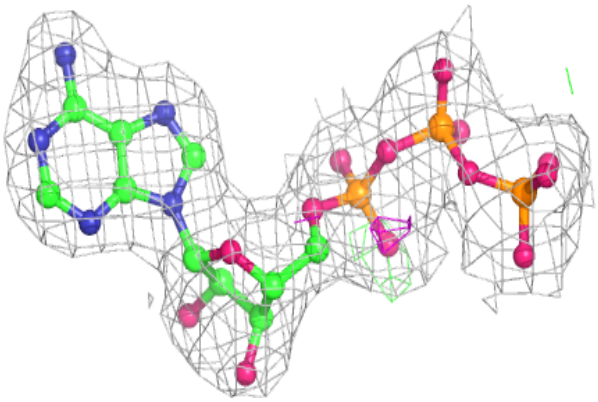


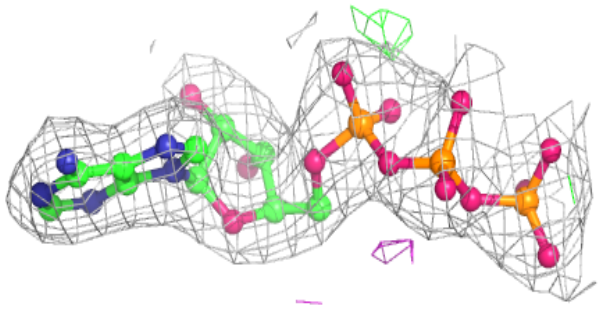
Electron density around MG B 302:

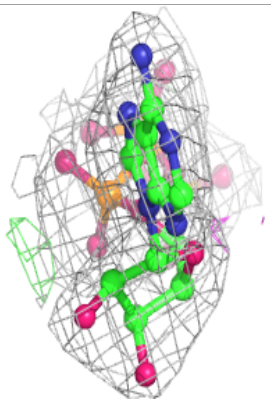
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

Electron density around ATP B 301:

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

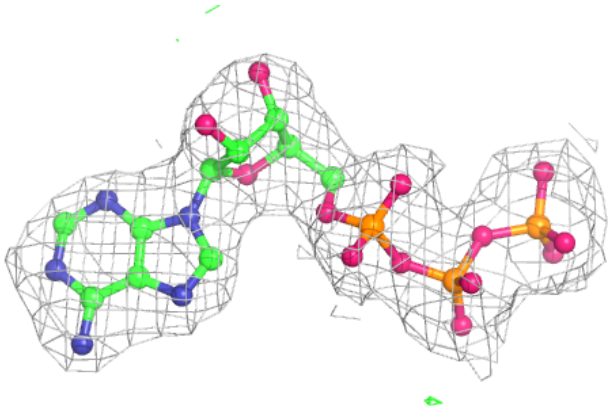


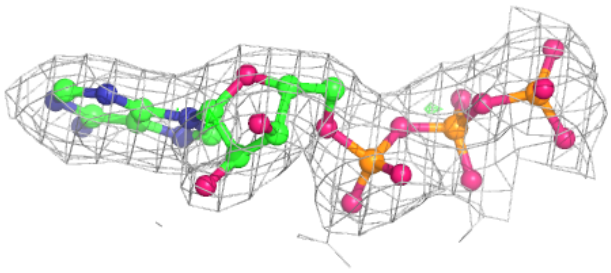


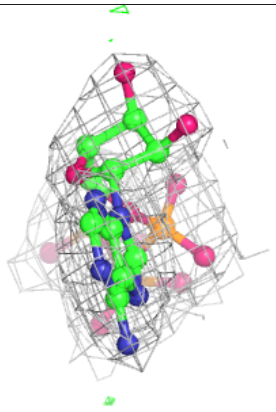


Electron density around ATP A 301:

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

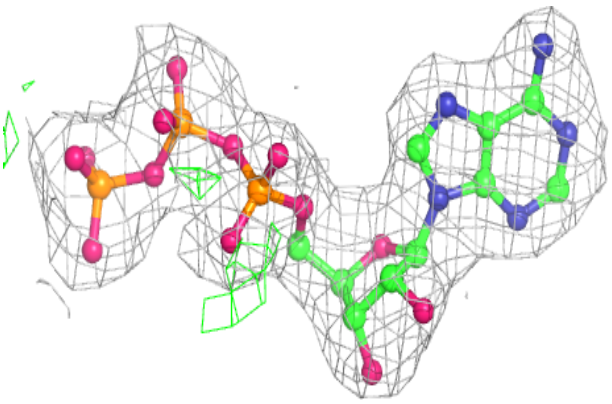


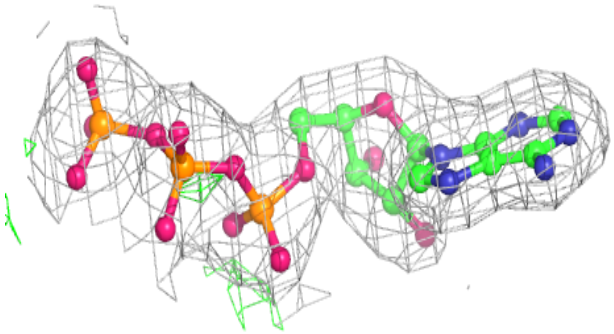


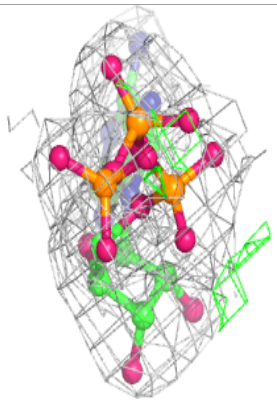


Electron density around ATP G 301:

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

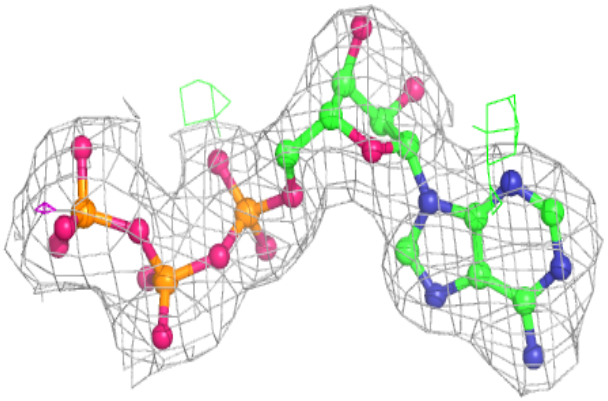


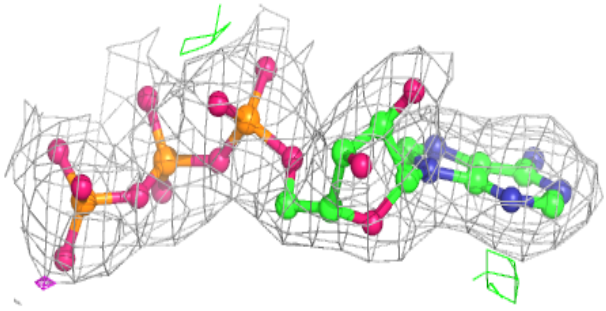


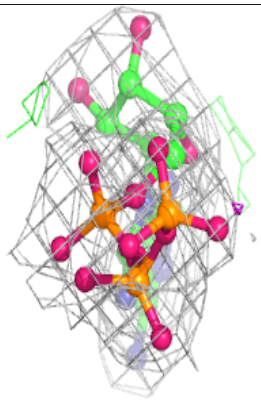


Electron density around ATP H 301:

$2mF_o$-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.