Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:38 pm BST

PDB ID	:	3WBZ
Title	:	Crystal structure of C. albicans tRNA(His) guanylyltransferase (Thg1) with ATP
Authors	:	Nakamura, A.; Nemoto, T.; Sonoda, T.; Yamashita, K.; Tanaka, I.; Yao, M.
Deposited on	:	2013-05-24
Resolution	:	2.39 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

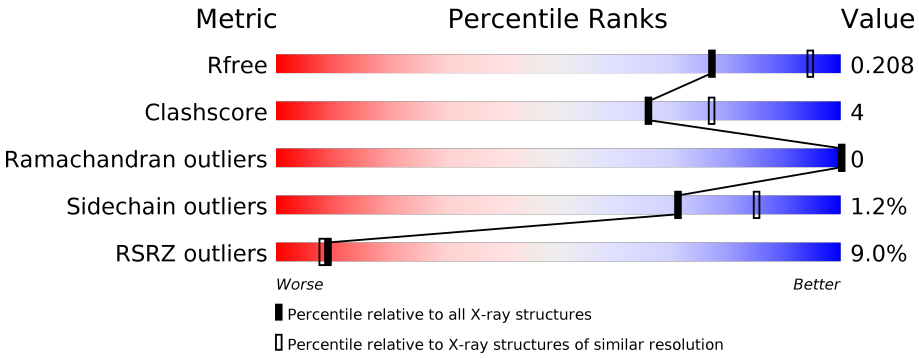
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	271	6% 79% 11% 10%
1	B	271	3% 79% 11% 10%
1	C	271	8% 85% 13%
1	D	271	10% 86% 12%
1	E	271	10% 85% 14%
1	F	271	10% 86% 8% 6%

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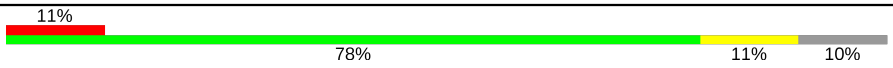
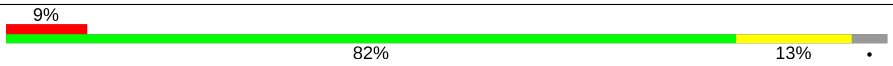
Mol	Chain	Length	Quality of chain
1	G	271	
1	H	271	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18389 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 Likely histidyl tRNA-specific guanylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			2085	1354	339	380	12			
1	B	243	Total	C	N	O	S	0	0	0
			2077	1350	337	378	12			
1	C	265	Total	C	N	O	S	0	1	0
			2277	1470	378	417	12			
1	D	266	Total	C	N	O	S	0	0	0
			2275	1468	377	418	12			
1	E	268	Total	C	N	O	S	0	1	0
			2298	1482	382	421	13			
1	F	255	Total	C	N	O	S	0	0	0
			2186	1417	361	396	12			
1	G	243	Total	C	N	O	S	0	1	0
			2087	1356	340	379	12			
1	H	259	Total	C	N	O	S	0	0	0
			2219	1436	369	402	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
A	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
A	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
B	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
B	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
B	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
C	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
C	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
C	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
D	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
D	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
D	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
E	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5

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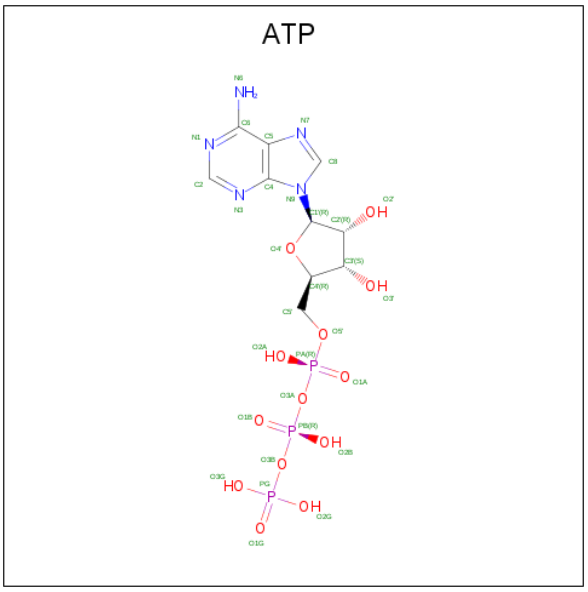
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
E	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
F	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
F	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
F	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
G	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
G	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
G	0	SER	-	EXPRESSION TAG	UNP Q5AFK5
H	-2	GLY	-	EXPRESSION TAG	UNP Q5AFK5
H	-1	GLY	-	EXPRESSION TAG	UNP Q5AFK5
H	0	SER	-	EXPRESSION TAG	UNP Q5AFK5

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	H	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total	Mg	0	0
			3	3		
3	D	3	Total	Mg	0	0
			3	3		
3	E	3	Total	Mg	0	0
			3	3		
3	H	3	Total	Mg	0	0
			3	3		
3	B	3	Total	Mg	0	0
			3	3		
3	C	3	Total	Mg	0	0
			3	3		
3	A	3	Total	Mg	0	0
			3	3		
3	F	3	Total	Mg	0	0
			3	3		

- Molecule 4 is water.

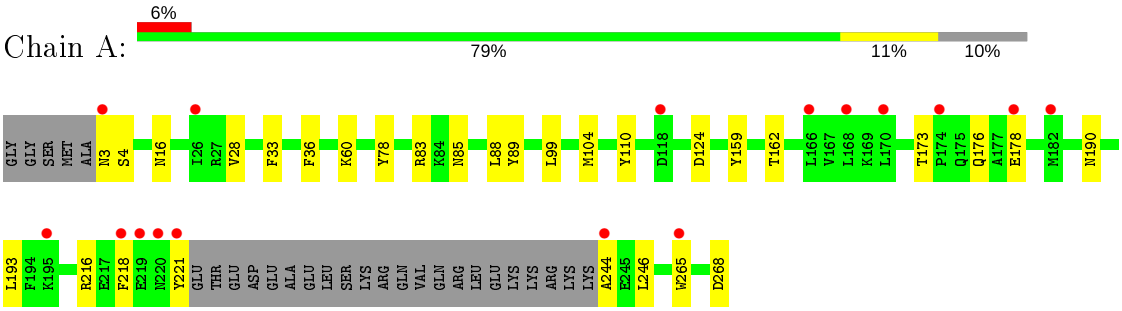
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	59	Total O 59 59	0	0
4	B	65	Total O 65 65	0	0
4	C	52	Total O 52 52	0	0
4	D	47	Total O 47 47	0	0
4	E	51	Total O 51 51	0	0
4	F	39	Total O 39 39	0	0
4	G	23	Total O 23 23	0	0
4	H	29	Total O 29 29	0	0

3 Residue-property plots (i)

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

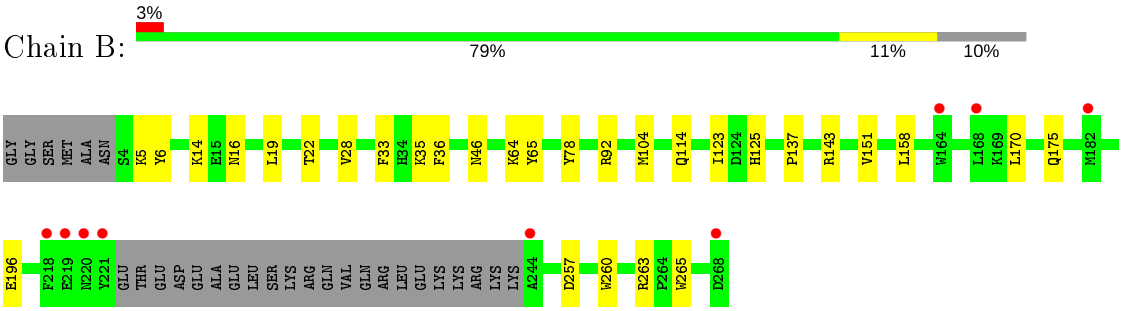
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain A:



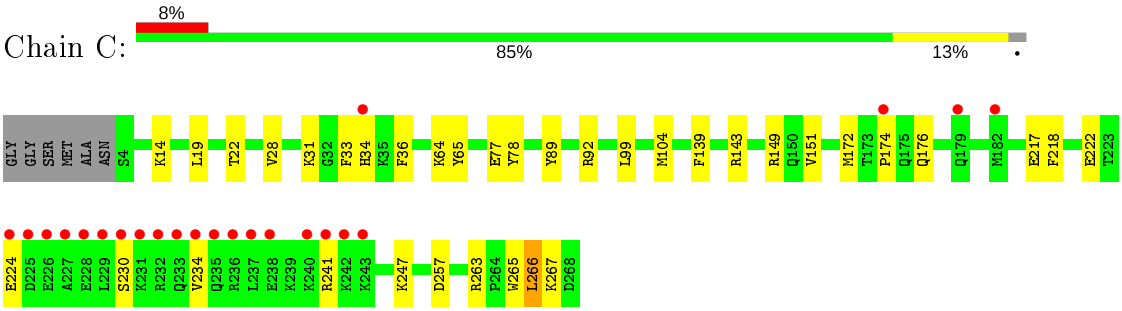
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain B:



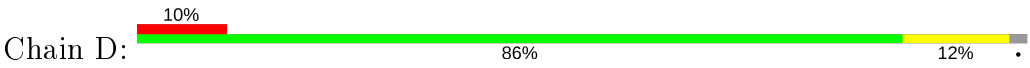
- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

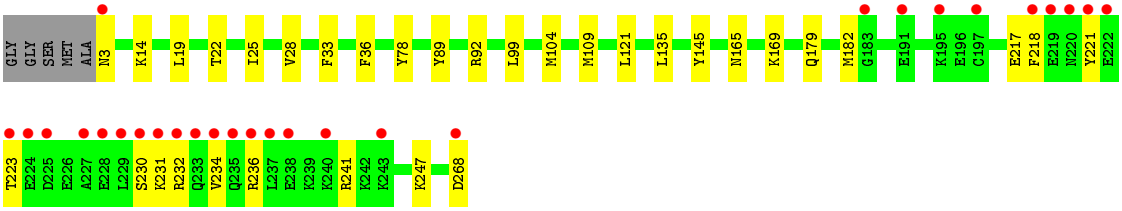
Chain C:



- Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

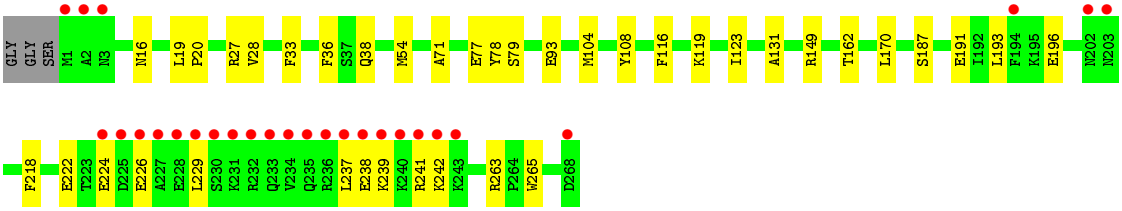
Chain D:





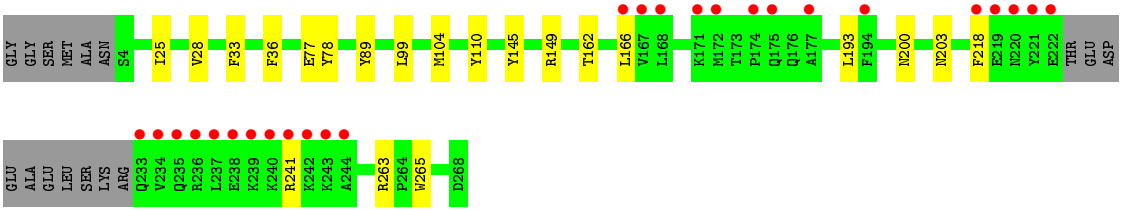
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain E:



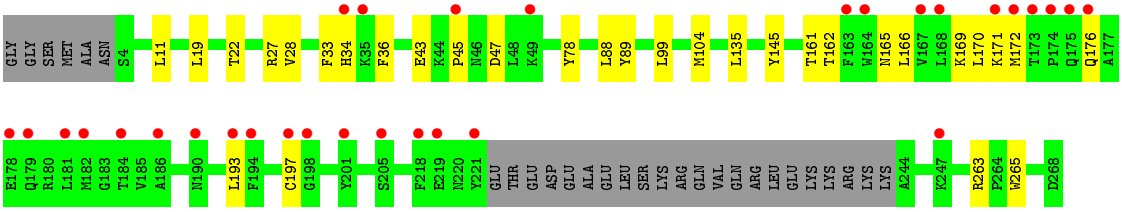
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain F:



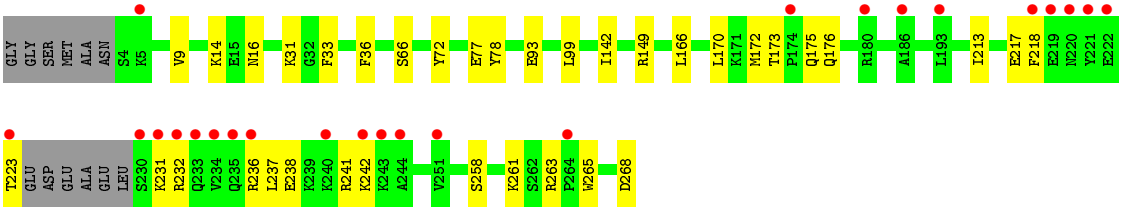
• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain G:



• Molecule 1: Likely histidyl tRNA-specific guanylyltransferase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.83Å 217.87Å 87.24Å 90.00° 113.68° 90.00°	Depositor
Resolution (Å)	42.26 – 2.39 42.64 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.26-2.39) 97.4 (42.64-2.39)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.176 , 0.208 0.176 , 0.208	Depositor DCC
R_{free} test set	3528 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18389	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: MG, ATP

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	0.48	0/2144	0.58	0/2894
1	B	0.52	0/2136	0.60	0/2883
1	C	0.47	0/2338	0.59	0/3150
1	D	0.44	0/2335	0.58	0/3146
1	E	0.47	0/2359	0.57	0/3178
1	F	0.44	0/2245	0.53	0/3024
1	G	0.39	0/2147	0.52	0/2898
1	H	0.41	0/2278	0.54	0/3067
All	All	0.45	0/17982	0.57	0/24240

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	2085	0	2016	17	0
1	B	2077	0	2010	21	0
1	C	2277	0	2219	24	0
1	D	2275	0	2219	24	0
1	E	2298	0	2242	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2186	0	2136	10	0
1	G	2087	0	2016	18	0
1	H	2219	0	2174	20	0
2	A	62	0	24	1	0
2	B	62	0	24	0	0
2	C	62	0	24	3	0
2	D	62	0	24	2	0
2	E	62	0	24	0	0
2	F	62	0	24	0	0
2	G	62	0	24	2	0
2	H	62	0	24	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
4	A	59	0	0	0	0
4	B	65	0	0	1	0
4	C	52	0	0	1	0
4	D	47	0	0	0	0
4	E	51	0	0	1	0
4	F	39	0	0	0	0
4	G	23	0	0	0	0
4	H	29	0	0	0	0
All	All	18389	0	17224	141	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 4.

All (141) 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:H:217:GLU:OE2	1:H:263:ARG:NH2	2.15	0.79
1:H:238:GLU:HG2	1:H:242:LYS:HE3	1.63	0.78
1:C:151:VAL:HG11	1:D:3:ASN:HB2	1.68	0.75
1:G:33:PHE:HA	1:G:36:PHE:HB3	1.71	0.72
1:A:159:TYR:OH	1:A:178:GLU:OE1	2.09	0.69
2:C:402:ATP:O3G	1:D:92:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ARG:NH2	2:D:402:ATP:O3G	2.26	0.68
1:C:19:LEU:HD23	1:C:22:THR:HG21	1.77	0.67
1:D:221:TYR:OH	1:D:268:ASP:OD2	2.15	0.65
1:A:28:VAL:HG21	1:A:104:MET:HG3	1.79	0.64
1:C:77:GLU:OE1	1:C:149:ARG:HD3	1.98	0.64
1:F:89:TYR:HE2	1:F:99:LEU:HD22	1.64	0.62
1:C:31:LYS:NZ	1:D:89:TYR:OH	2.28	0.62
1:H:166:LEU:HD23	1:H:170:LEU:HD22	1.82	0.62
1:C:89:TYR:HE2	1:C:99:LEU:HD22	1.64	0.62
1:D:217:GLU:HG3	1:D:247:LYS:HD2	1.82	0.60
1:B:143:ARG:NH2	1:B:257:ASP:OD1	2.34	0.59
1:E:123:ILE:HD13	1:F:110:TYR:CD2	2.38	0.58
1:A:110:TYR:CD2	1:B:123:ILE:HD13	2.39	0.58
1:A:221:TYR:OH	1:A:268:ASP:OD2	2.22	0.58
1:C:143:ARG:NH1	1:C:257:ASP:OD1	2.30	0.56
1:C:33:PHE:HA	1:C:36:PHE:HB3	1.86	0.56
1:D:19:LEU:HD23	1:D:22:THR:HG21	1.87	0.56
1:G:45:PRO:HG3	1:G:161:THR:HA	1.87	0.56
1:B:46:ASN:ND2	4:B:549:HOH:O	2.37	0.55
1:G:19:LEU:HD23	1:G:22:THR:HG21	1.89	0.55
1:D:33:PHE:HA	1:D:36:PHE:HB3	1.87	0.55
1:B:175:GLN:OE1	1:E:38:GLN:NE2	2.37	0.55
2:C:402:ATP:PG	1:D:92:ARG:HH22	2.31	0.54
1:F:200:ASN:ND2	1:F:203:ASN:OD1	2.39	0.54
1:H:77:GLU:OE2	1:H:149:ARG:HD3	2.07	0.54
1:D:232:ARG:HH12	1:D:236:ARG:HE	1.56	0.54
1:C:263:ARG:HG2	1:C:265:TRP:CZ2	2.44	0.53
1:B:137:PRO:HG3	1:D:22:THR:HG22	1.89	0.53
1:C:172:MET:HB3	1:C:176:GLN:HG3	1.90	0.53
1:C:28:VAL:HG21	1:C:104:MET:HG3	1.89	0.53
1:E:263:ARG:HG2	1:E:265:TRP:CZ2	2.44	0.52
1:G:28:VAL:HG21	1:G:104:MET:HG3	1.92	0.52
1:D:179:GLN:HA	1:D:182:MET:HE2	1.92	0.52
1:F:263:ARG:HG2	1:F:265:TRP:CZ2	2.44	0.52
1:B:16:ASN:OD1	1:C:14:LYS:NZ	2.42	0.52
1:F:77:GLU:OE2	1:F:149:ARG:HD3	2.10	0.51
1:C:218:PHE:HZ	1:C:241:ARG:HG3	1.74	0.51
1:G:169:LYS:HD2	1:G:197:CYS:HB3	1.91	0.51
1:G:165:ASN:O	1:G:169:LYS:HB2	2.11	0.50
1:G:99:LEU:HD22	1:H:31:LYS:HD2	1.93	0.50
1:C:92:ARG:HH22	2:D:402:ATP:PG	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:ASN:ND2	1:H:93:GLU:OE1	2.34	0.50
1:A:3:ASN:HA	1:B:151:VAL:HG11	1.95	0.49
1:C:217:GLU:HG3	1:C:247:LYS:HD2	1.94	0.49
1:E:162:THR:HA	1:E:193:LEU:HD21	1.93	0.49
1:F:25:ILE:HD13	1:F:145:TYR:CD2	2.47	0.49
1:G:166:LEU:HD23	1:G:170:LEU:HD22	1.94	0.48
1:B:263:ARG:HG2	1:B:265:TRP:CZ2	2.49	0.48
1:D:25:ILE:HD13	1:D:145:TYR:CD2	2.49	0.48
1:F:218:PHE:HZ	1:F:241:ARG:HG3	1.79	0.48
1:C:139:PHE:CG	1:C:267:LYS:HG2	2.48	0.48
1:E:239:LYS:HD3	1:E:242:LYS:HD2	1.95	0.47
2:A:402:ATP:O3G	1:B:92:ARG:NH2	2.43	0.47
1:C:230:SER:HA	1:C:234:VAL:HG23	1.97	0.47
1:D:221:TYR:CZ	1:D:223:THR:HA	2.49	0.47
1:A:173:THR:OG1	1:A:176:GLN:HG2	2.14	0.47
1:B:170:LEU:HD11	1:B:196:GLU:O	2.14	0.47
1:G:34[A]:HIS:CD2	2:G:401:ATP:H4'	2.50	0.47
1:C:222:GLU:O	1:C:224:GLU:N	2.44	0.47
1:A:162:THR:HA	1:A:193:LEU:HD21	1.97	0.47
1:A:60:LYS:HE3	1:B:123:ILE:HG13	1.97	0.47
1:D:218:PHE:HZ	1:D:241:ARG:HG3	1.80	0.46
1:E:33:PHE:HA	1:E:36:PHE:HB3	1.97	0.46
1:E:71:ALA:HA	1:E:79:SER:O	2.15	0.46
1:E:16:ASN:OD1	1:H:14:LYS:NZ	2.42	0.46
1:C:139:PHE:CD2	1:C:267:LYS:HG2	2.51	0.46
1:D:232:ARG:HH12	1:D:236:ARG:NE	2.12	0.46
1:G:263:ARG:HG2	1:G:265:TRP:CZ2	2.51	0.46
1:A:83:ARG:NH1	1:A:85:ASN:HB2	2.31	0.45
1:C:34[A]:HIS:NE2	2:C:401:ATP:O3'	2.43	0.45
1:F:33:PHE:HA	1:F:36:PHE:HB3	1.96	0.45
1:C:263:ARG:HB3	1:C:266:LEU:HD22	1.97	0.45
1:E:54:MET:HE2	1:E:108:TYR:HE2	1.80	0.45
1:A:33:PHE:HA	1:A:36:PHE:HB3	1.99	0.45
1:B:5:LYS:HE3	1:B:6:TYR:CZ	2.52	0.45
1:H:223:THR:HG22	1:H:268:ASP:OD2	2.16	0.45
1:A:99:LEU:HA	1:A:99:LEU:HD23	1.85	0.45
1:E:77:GLU:CD	1:E:149:ARG:HH21	2.19	0.45
1:G:88:LEU:HG	1:G:89:TYR:CD2	2.52	0.45
1:H:231:LYS:HB3	1:H:232:ARG:H	1.46	0.45
1:B:143:ARG:HD3	1:B:260:TRP:CD2	2.52	0.44
1:C:64:LYS:NZ	1:C:65:TYR:OH	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:27:ARG:HD3	1:G:145:TYR:OH	2.17	0.44
1:B:64:LYS:HB3	1:B:65:TYR:CD1	2.53	0.44
1:G:162:THR:HA	1:G:193:LEU:HD21	2.00	0.44
1:A:218:PHE:CE2	1:A:244:ALA:HB2	2.53	0.44
1:E:218:PHE:HZ	1:E:241:ARG:HG3	1.81	0.44
1:H:66:SER:HB3	1:H:242:LYS:HA	1.99	0.44
1:F:162:THR:HA	1:F:193:LEU:HD21	1.98	0.43
1:H:263:ARG:HG2	1:H:265:TRP:CZ2	2.53	0.43
1:B:35:LYS:HE2	1:B:125:HIS:NE2	2.33	0.43
1:E:54:MET:HG2	4:E:523:HOH:O	2.18	0.43
1:H:172:MET:HB3	1:H:176:GLN:HG3	1.99	0.43
1:B:28:VAL:HG21	1:B:104:MET:HG3	2.00	0.43
1:D:109:MET:HG2	1:D:121:LEU:CD1	2.49	0.43
1:C:174:PRO:HG2	1:H:175:GLN:HG3	2.01	0.43
1:E:237:LEU:HD23	1:E:237:LEU:HA	1.82	0.42
1:B:5:LYS:HE3	1:B:6:TYR:OH	2.19	0.42
1:A:124:ASP:OD1	1:B:64:LYS:HE3	2.20	0.42
1:G:172:MET:HB3	1:G:176:GLN:HG3	2.01	0.42
1:D:22:THR:OG1	1:D:135:LEU:HD22	2.19	0.42
1:H:33:PHE:HA	1:H:36:PHE:HB3	2.01	0.42
1:D:230:SER:HA	1:D:234:VAL:HG23	2.00	0.42
1:E:222:GLU:O	1:E:224:GLU:N	2.49	0.42
1:B:19:LEU:HD23	1:B:22:THR:HG21	2.01	0.42
1:H:173:THR:OG1	1:H:176:GLN:HG2	2.20	0.42
1:H:142:ILE:HA	1:H:142:ILE:HD13	1.89	0.42
1:H:72:TYR:HD1	1:H:213:ILE:HG13	1.84	0.42
1:G:34[A]:HIS:ND1	2:G:401:ATP:O2B	2.52	0.42
1:H:238:GLU:O	1:H:242:LYS:HG3	2.19	0.41
1:D:109:MET:HG2	1:D:121:LEU:HD13	2.01	0.41
1:E:116:PHE:HB3	1:E:119:LYS:HB2	2.01	0.41
1:G:43:GLU:HB2	1:G:47:ASP:HA	2.01	0.41
1:B:14:LYS:HE2	4:C:507:HOH:O	2.20	0.41
1:D:28:VAL:HG21	1:D:104:MET:HG3	2.01	0.41
1:H:218:PHE:HZ	1:H:241:ARG:HG3	1.85	0.41
1:E:19:LEU:HA	1:E:20:PRO:HD3	1.93	0.41
1:E:16:ASN:ND2	1:E:93:GLU:OE1	2.43	0.41
1:F:28:VAL:HG21	1:F:104:MET:HG3	2.01	0.41
1:C:31:LYS:HZ3	1:D:89:TYR:HH	1.58	0.41
1:E:187:SER:O	1:E:191:GLU:HG3	2.20	0.41
1:E:238:GLU:HB3	1:E:242:LYS:HE3	2.03	0.41
1:A:3:ASN:HB3	1:A:4:SER:H	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:THR:OG1	1:G:135:LEU:HD22	2.21	0.41
1:G:99:LEU:HD23	1:G:99:LEU:HA	1.98	0.41
1:A:16:ASN:OD1	1:D:14:LYS:HE2	2.21	0.41
1:A:88:LEU:HG	1:A:89:TYR:CD2	2.55	0.41
1:E:27:ARG:O	1:E:131:ALA:HA	2.21	0.41
1:E:28:VAL:HG21	1:E:104:MET:HG3	2.03	0.41
1:A:216:ARG:O	1:A:265:TRP:NE1	2.49	0.40
1:D:165:ASN:O	1:D:169:LYS:HB2	2.22	0.40
1:E:170:LEU:HD11	1:E:196:GLU:O	2.21	0.40
1:D:231:LYS:HA	1:D:231:LYS:HD3	1.88	0.40
1:H:258:SER:HA	1:H:261:LYS:HB3	2.02	0.40
1:B:33:PHE:HA	1:B:36:PHE:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	240/271 (89%)	235 (98%)	5 (2%)	0	100	100
1	B	239/271 (88%)	233 (98%)	6 (2%)	0	100	100
1	C	264/271 (97%)	256 (97%)	8 (3%)	0	100	100
1	D	264/271 (97%)	255 (97%)	9 (3%)	0	100	100
1	E	267/271 (98%)	259 (97%)	8 (3%)	0	100	100
1	F	251/271 (93%)	243 (97%)	8 (3%)	0	100	100
1	G	240/271 (89%)	234 (98%)	6 (2%)	0	100	100
1	H	255/271 (94%)	246 (96%)	9 (4%)	0	100	100
All	All	2020/2168 (93%)	1961 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/252 (91%)	226 (99%)	3 (1%)	69	84
1	B	228/252 (90%)	225 (99%)	3 (1%)	69	84
1	C	250/252 (99%)	248 (99%)	2 (1%)	81	91
1	D	250/252 (99%)	248 (99%)	2 (1%)	81	91
1	E	252/252 (100%)	249 (99%)	3 (1%)	71	85
1	F	240/252 (95%)	238 (99%)	2 (1%)	81	91
1	G	229/252 (91%)	226 (99%)	3 (1%)	69	84
1	H	244/252 (97%)	239 (98%)	5 (2%)	55	74
All	All	1922/2016 (95%)	1899 (99%)	23 (1%)	71	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	A	190	ASN
1	A	246	LEU
1	B	78	TYR
1	B	114	GLN
1	B	158	LEU
1	C	78	TYR
1	C	266	LEU
1	D	78	TYR
1	D	99	LEU
1	E	78	TYR
1	E	226	GLU
1	E	229	LEU
1	F	78	TYR
1	F	166	LEU
1	G	11	LEU
1	G	78	TYR
1	G	171	LYS
1	H	9	VAL

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Mol	Chain	Res	Type
1	H	78	TYR
1	H	99	LEU
1	H	236	ARG
1	H	237	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	46	ASN
1	D	157	ASN
1	E	179	GLN
1	F	128	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 40 ligands modelled in this entry, 24 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ATP	D	401	3	26,33,33	0.94	1 (3%)	31,52,52	1.38	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ATP	B	401	3	26,33,33	0.87	1 (3%)	31,52,52	1.29	2 (6%)
2	ATP	F	402	3	26,33,33	0.96	1 (3%)	31,52,52	1.31	2 (6%)
2	ATP	E	402	3	26,33,33	0.94	2 (7%)	31,52,52	1.39	3 (9%)
2	ATP	G	402	3	26,33,33	0.98	1 (3%)	31,52,52	1.39	5 (16%)
2	ATP	B	402	3	26,33,33	0.96	1 (3%)	31,52,52	1.40	5 (16%)
2	ATP	A	402	3	26,33,33	0.93	1 (3%)	31,52,52	1.31	3 (9%)
2	ATP	C	402	3	26,33,33	0.99	1 (3%)	31,52,52	1.27	2 (6%)
2	ATP	E	401	3	26,33,33	1.04	2 (7%)	31,52,52	1.35	4 (12%)
2	ATP	H	401	3	26,33,33	0.94	1 (3%)	31,52,52	1.46	6 (19%)
2	ATP	C	401	3	26,33,33	1.01	1 (3%)	31,52,52	1.28	3 (9%)
2	ATP	A	401	3	26,33,33	0.85	0	31,52,52	1.37	5 (16%)
2	ATP	D	402	3	26,33,33	0.92	1 (3%)	31,52,52	1.40	3 (9%)
2	ATP	H	402	3	26,33,33	0.91	1 (3%)	31,52,52	1.29	3 (9%)
2	ATP	G	401	3	26,33,33	0.95	1 (3%)	31,52,52	1.42	5 (16%)
2	ATP	F	401	3	26,33,33	0.91	1 (3%)	31,52,52	1.38	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	D	401	3	-	4/18/38/38	0/3/3/3
2	ATP	B	401	3	-	4/18/38/38	0/3/3/3
2	ATP	F	402	3	-	10/18/38/38	0/3/3/3
2	ATP	E	402	3	-	11/18/38/38	0/3/3/3
2	ATP	G	402	3	-	6/18/38/38	0/3/3/3
2	ATP	B	402	3	-	8/18/38/38	0/3/3/3
2	ATP	A	402	3	-	10/18/38/38	0/3/3/3
2	ATP	C	402	3	-	4/18/38/38	0/3/3/3
2	ATP	E	401	3	-	5/18/38/38	0/3/3/3
2	ATP	H	401	3	-	8/18/38/38	0/3/3/3
2	ATP	C	401	3	-	5/18/38/38	0/3/3/3
2	ATP	A	401	3	-	6/18/38/38	0/3/3/3
2	ATP	D	402	3	-	6/18/38/38	0/3/3/3
2	ATP	H	402	3	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	G	401	3	-	7/18/38/38	0/3/3/3
2	ATP	F	401	3	-	6/18/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	ATP	C5-C4	2.65	1.47	1.40
2	B	402	ATP	C5-C4	2.64	1.47	1.40
2	D	401	ATP	C5-C4	2.58	1.47	1.40
2	F	401	ATP	C5-C4	2.53	1.47	1.40
2	G	401	ATP	C5-C4	2.50	1.47	1.40
2	C	402	ATP	C5-C4	2.50	1.47	1.40
2	D	402	ATP	C5-C4	2.48	1.47	1.40
2	A	402	ATP	C5-C4	2.42	1.47	1.40
2	H	402	ATP	C5-C4	2.42	1.47	1.40
2	C	401	ATP	C5-C4	2.40	1.47	1.40
2	E	402	ATP	C5-C4	2.40	1.47	1.40
2	G	402	ATP	C5-C4	2.39	1.47	1.40
2	F	402	ATP	C5-C4	2.38	1.47	1.40
2	E	401	ATP	C5-C4	2.32	1.47	1.40
2	E	401	ATP	O4'-C1'	2.26	1.44	1.41
2	B	401	ATP	C5-C4	2.24	1.46	1.40
2	E	402	ATP	C2-N3	2.03	1.35	1.32

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	ATP	N3-C2-N1	-3.68	122.93	128.68
2	H	401	ATP	N3-C2-N1	-3.64	123.00	128.68
2	E	402	ATP	N3-C2-N1	-3.56	123.11	128.68
2	D	402	ATP	N3-C2-N1	-3.37	123.41	128.68
2	B	402	ATP	N3-C2-N1	-3.34	123.45	128.68
2	E	401	ATP	N3-C2-N1	-3.28	123.55	128.68
2	F	402	ATP	N3-C2-N1	-3.24	123.61	128.68
2	H	402	ATP	N3-C2-N1	-3.22	123.64	128.68
2	F	401	ATP	C3'-C2'-C1'	3.22	105.82	100.98
2	D	402	ATP	C4-C5-N7	-3.17	106.09	109.40
2	G	402	ATP	N3-C2-N1	-3.16	123.74	128.68
2	F	401	ATP	C4-C5-N7	-3.16	106.11	109.40
2	A	402	ATP	N3-C2-N1	-3.16	123.75	128.68
2	G	401	ATP	PA-O3A-PB	-3.14	122.06	132.83
2	C	401	ATP	N3-C2-N1	-3.14	123.78	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	ATP	C4-C5-N7	-3.10	106.17	109.40
2	F	402	ATP	C4-C5-N7	-3.06	106.21	109.40
2	C	402	ATP	N3-C2-N1	-3.05	123.91	128.68
2	E	402	ATP	C4-C5-N7	-3.05	106.22	109.40
2	A	401	ATP	N3-C2-N1	-3.01	123.98	128.68
2	F	401	ATP	N3-C2-N1	-2.92	124.12	128.68
2	G	401	ATP	N3-C2-N1	-2.90	124.14	128.68
2	G	401	ATP	C3'-C2'-C1'	2.90	105.34	100.98
2	G	402	ATP	PB-O3B-PG	-2.87	122.99	132.83
2	A	401	ATP	C3'-C2'-C1'	2.84	105.25	100.98
2	C	401	ATP	C3'-C2'-C1'	2.83	105.25	100.98
2	E	401	ATP	C4-C5-N7	-2.82	106.46	109.40
2	B	402	ATP	PA-O3A-PB	-2.79	123.25	132.83
2	B	401	ATP	N3-C2-N1	-2.77	124.35	128.68
2	D	401	ATP	C3'-C2'-C1'	2.74	105.10	100.98
2	G	402	ATP	C4-C5-N7	-2.71	106.58	109.40
2	H	401	ATP	C2-N1-C6	2.66	123.31	118.75
2	C	402	ATP	C4-C5-N7	-2.65	106.64	109.40
2	D	401	ATP	C4-C5-N7	-2.63	106.66	109.40
2	B	402	ATP	C4-C5-N7	-2.62	106.67	109.40
2	H	402	ATP	C4-C5-N7	-2.59	106.70	109.40
2	B	402	ATP	C3'-C2'-C1'	2.52	104.78	100.98
2	A	402	ATP	C4-C5-N7	-2.52	106.77	109.40
2	G	402	ATP	C3'-C2'-C1'	2.48	104.72	100.98
2	H	401	ATP	C4-C5-N7	-2.48	106.81	109.40
2	A	401	ATP	C4-C5-N7	-2.42	106.88	109.40
2	G	401	ATP	PB-O3B-PG	-2.41	124.56	132.83
2	G	401	ATP	C4-C5-N7	-2.41	106.89	109.40
2	A	401	ATP	O2'-C2'-C3'	-2.37	104.15	111.82
2	H	401	ATP	PB-O3B-PG	-2.35	124.76	132.83
2	E	401	ATP	O5'-PA-O1A	-2.34	99.93	109.07
2	C	401	ATP	C4-C5-N7	-2.31	106.99	109.40
2	F	401	ATP	O3G-PG-O2G	2.29	116.38	107.64
2	H	401	ATP	C3'-C2'-C1'	2.27	104.39	100.98
2	H	402	ATP	O3G-PG-O2G	2.24	116.19	107.64
2	H	401	ATP	PA-O3A-PB	-2.18	125.33	132.83
2	E	401	ATP	O3G-PG-O2G	2.17	115.94	107.64
2	A	401	ATP	O3G-PG-O2G	2.16	115.90	107.64
2	G	402	ATP	PA-O3A-PB	-2.12	125.55	132.83
2	B	402	ATP	O3B-PG-O1G	-2.10	99.53	111.19
2	E	402	ATP	O3B-PG-O1G	-2.08	99.64	111.19
2	A	402	ATP	O3G-PG-O2G	2.06	115.50	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	402	ATP	PA-O3A-PB	-2.05	125.78	132.83
2	D	401	ATP	C2-N1-C6	2.03	122.22	118.75

There are no chirality outliers.

All (106) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	402	ATP	C5'-O5'-PA-O1A
2	G	402	ATP	C5'-O5'-PA-O2A
2	C	401	ATP	PB-O3B-PG-O2G
2	C	401	ATP	PB-O3B-PG-O3G
2	G	401	ATP	PB-O3B-PG-O2G
2	G	401	ATP	PB-O3A-PA-O5'
2	G	401	ATP	C3'-C4'-C5'-O5'
2	E	402	ATP	PB-O3B-PG-O2G
2	E	402	ATP	C5'-O5'-PA-O1A
2	A	402	ATP	PB-O3B-PG-O2G
2	A	402	ATP	C5'-O5'-PA-O1A
2	A	402	ATP	C5'-O5'-PA-O2A
2	C	402	ATP	C5'-O5'-PA-O1A
2	C	402	ATP	C5'-O5'-PA-O2A
2	D	402	ATP	PB-O3B-PG-O3G
2	D	402	ATP	C5'-O5'-PA-O1A
2	D	402	ATP	C5'-O5'-PA-O2A
2	F	402	ATP	PB-O3B-PG-O2G
2	F	402	ATP	C5'-O5'-PA-O1A
2	H	401	ATP	PB-O3B-PG-O2G
2	H	401	ATP	C5'-O5'-PA-O1A
2	E	401	ATP	PB-O3B-PG-O2G
2	A	401	ATP	PB-O3B-PG-O2G
2	F	401	ATP	PB-O3B-PG-O2G
2	B	402	ATP	C5'-O5'-PA-O1A
2	H	402	ATP	O4'-C4'-C5'-O5'
2	F	402	ATP	C3'-C4'-C5'-O5'
2	G	401	ATP	O4'-C4'-C5'-O5'
2	F	402	ATP	O4'-C4'-C5'-O5'
2	B	402	ATP	O4'-C4'-C5'-O5'
2	B	402	ATP	C3'-C4'-C5'-O5'
2	H	402	ATP	C3'-C4'-C5'-O5'
2	H	401	ATP	O4'-C4'-C5'-O5'
2	G	402	ATP	O4'-C4'-C5'-O5'
2	E	402	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	G	402	ATP	C3'-C4'-C5'-O5'
2	A	402	ATP	PB-O3A-PA-O1A
2	H	402	ATP	PB-O3B-PG-O3G
2	C	402	ATP	PB-O3B-PG-O3G
2	G	402	ATP	C5'-O5'-PA-O3A
2	F	402	ATP	C5'-O5'-PA-O3A
2	H	401	ATP	C5'-O5'-PA-O3A
2	B	402	ATP	C5'-O5'-PA-O3A
2	E	402	ATP	C3'-C4'-C5'-O5'
2	E	401	ATP	O4'-C4'-C5'-O5'
2	C	401	ATP	PA-O3A-PB-O1B
2	H	402	ATP	PB-O3A-PA-O1A
2	D	402	ATP	PA-O3A-PB-O1B
2	B	401	ATP	PB-O3A-PA-O1A
2	F	402	ATP	PB-O3A-PA-O2A
2	A	401	ATP	PA-O3A-PB-O2B
2	F	401	ATP	PA-O3A-PB-O1B
2	B	402	ATP	PG-O3B-PB-O2B
2	E	402	ATP	C5'-O5'-PA-O2A
2	F	402	ATP	C5'-O5'-PA-O2A
2	H	401	ATP	C5'-O5'-PA-O2A
2	B	402	ATP	C5'-O5'-PA-O2A
2	D	401	ATP	PA-O3A-PB-O2B
2	E	402	ATP	PA-O3A-PB-O1B
2	A	402	ATP	PB-O3A-PA-O2A
2	B	401	ATP	PB-O3A-PA-O2A
2	H	401	ATP	PA-O3A-PB-O2B
2	E	401	ATP	PA-O3A-PB-O2B
2	E	401	ATP	PB-O3B-PG-O1G
2	A	401	ATP	PB-O3B-PG-O1G
2	B	402	ATP	PB-O3B-PG-O1G
2	D	401	ATP	PG-O3B-PB-O2B
2	D	401	ATP	PA-O3A-PB-O1B
2	G	402	ATP	PA-O3A-PB-O1B
2	E	402	ATP	PB-O3A-PA-O1A
2	A	402	ATP	PA-O3A-PB-O1B
2	B	401	ATP	PG-O3B-PB-O1B
2	B	401	ATP	O4'-C4'-C5'-O5'
2	H	401	ATP	C3'-C4'-C5'-O5'
2	A	401	ATP	O4'-C4'-C5'-O5'
2	F	402	ATP	PB-O3B-PG-O1G
2	F	401	ATP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
2	D	401	ATP	O4'-C4'-C5'-O5'
2	A	402	ATP	O4'-C4'-C5'-O5'
2	G	401	ATP	PB-O3B-PG-O3G
2	E	402	ATP	PB-O3B-PG-O3G
2	A	402	ATP	PB-O3B-PG-O3G
2	F	402	ATP	PB-O3B-PG-O3G
2	H	401	ATP	PB-O3B-PG-O3G
2	F	401	ATP	PB-O3B-PG-O3G
2	E	402	ATP	C5'-O5'-PA-O3A
2	A	402	ATP	C5'-O5'-PA-O3A
2	C	402	ATP	C5'-O5'-PA-O3A
2	D	402	ATP	C5'-O5'-PA-O3A
2	A	401	ATP	C5'-O5'-PA-O3A
2	E	401	ATP	C3'-C4'-C5'-O5'
2	F	401	ATP	O4'-C4'-C5'-O5'
2	C	401	ATP	PA-O3A-PB-O2B
2	H	402	ATP	PB-O3A-PA-O2A
2	E	402	ATP	PA-O3A-PB-O2B
2	E	402	ATP	PB-O3A-PA-O2A
2	D	402	ATP	PA-O3A-PB-O2B
2	F	402	ATP	PB-O3A-PA-O1A
2	F	401	ATP	PA-O3A-PB-O2B
2	B	402	ATP	PG-O3B-PB-O1B
2	G	401	ATP	C5'-O5'-PA-O1A
2	H	402	ATP	C5'-O5'-PA-O1A
2	A	401	ATP	C5'-O5'-PA-O1A
2	C	401	ATP	O4'-C4'-C5'-O5'
2	A	402	ATP	C3'-C4'-C5'-O5'
2	G	401	ATP	PB-O3B-PG-O1G

There are no ring outliers.

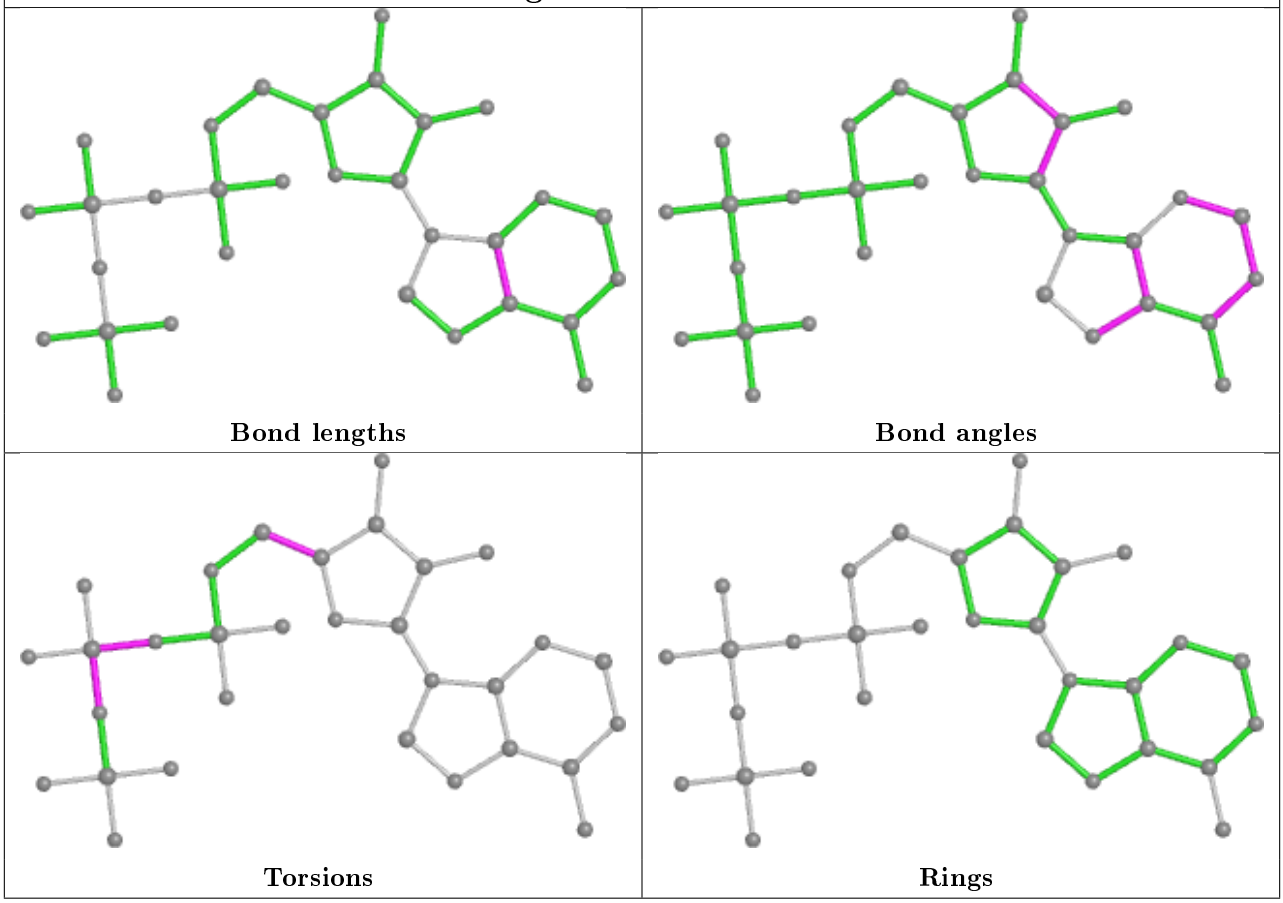
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	ATP	1	0
2	C	402	ATP	2	0
2	C	401	ATP	1	0
2	D	402	ATP	2	0
2	G	401	ATP	2	0

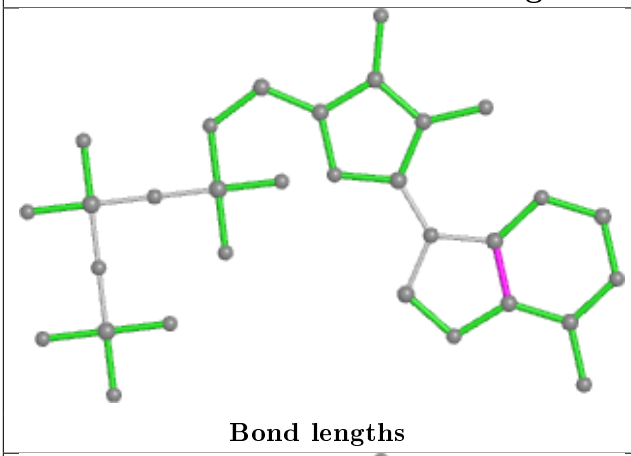
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

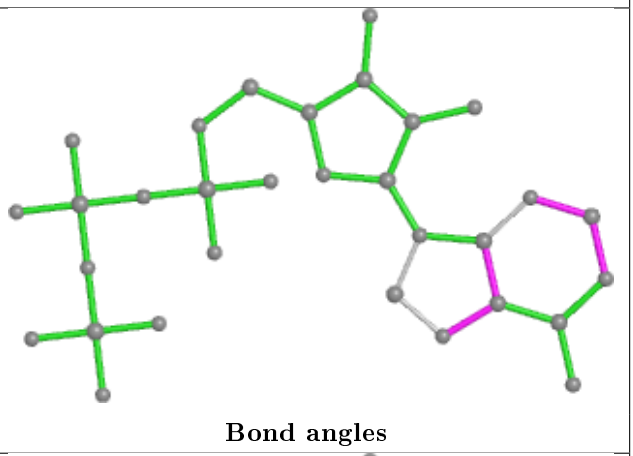
Ligand ATP D 401



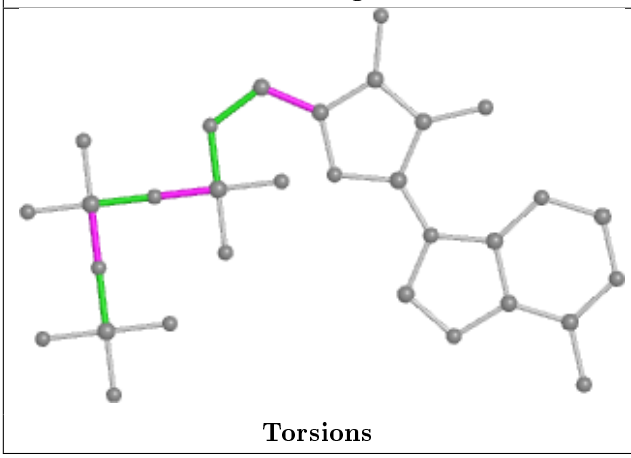
Ligand ATP B 401



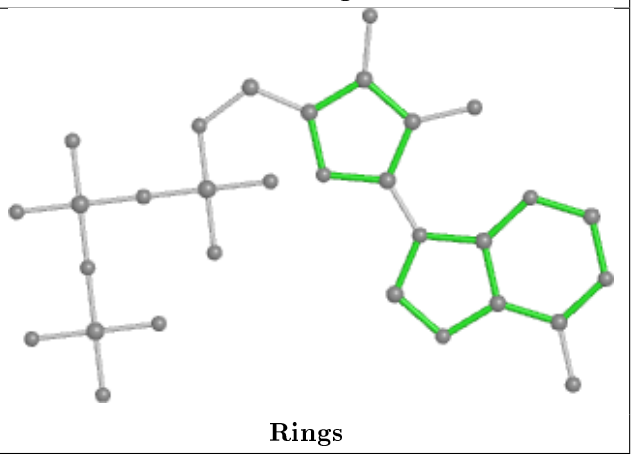
Bond lengths



Bond angles

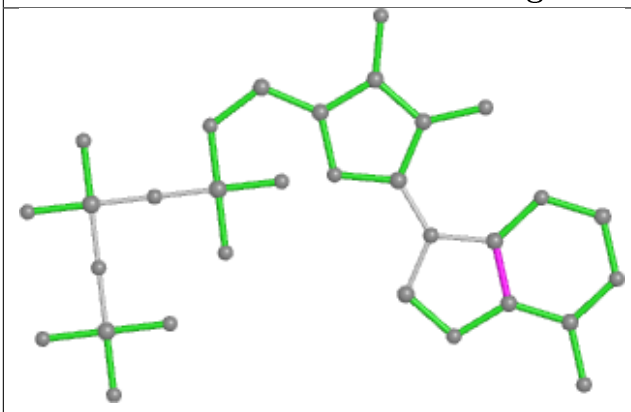


Torsions



Rings

Ligand ATP F 402



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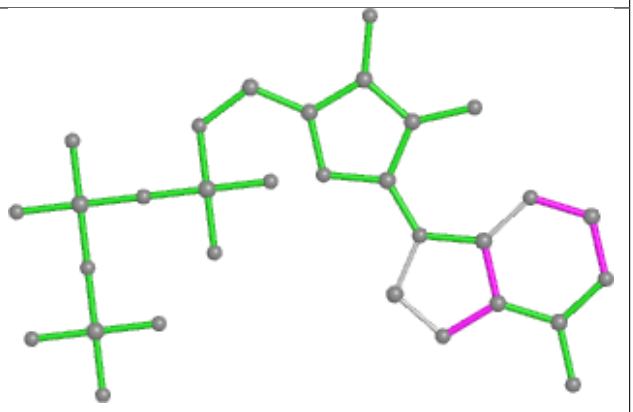

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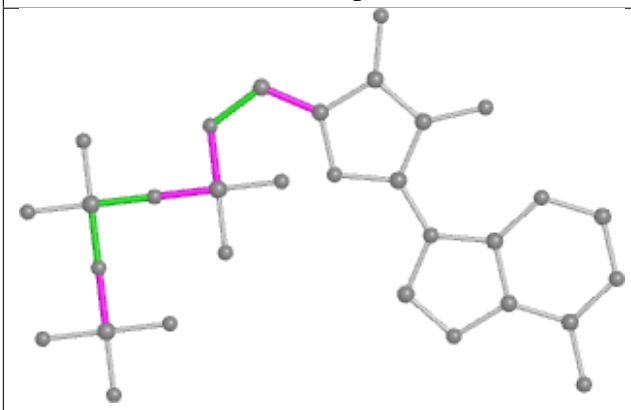

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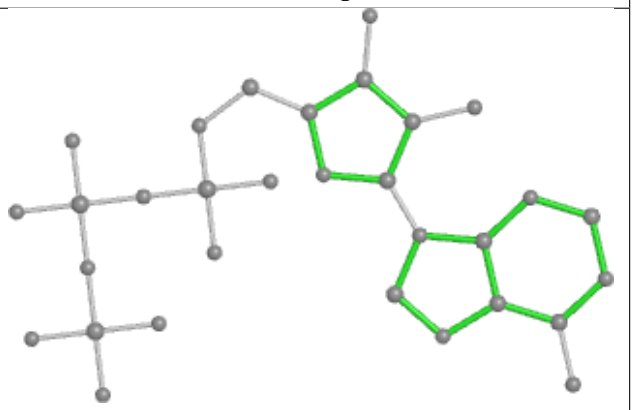
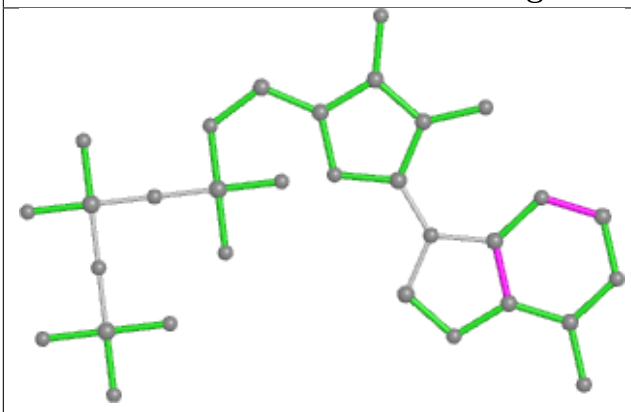


Rings

Ligand ATP E 402



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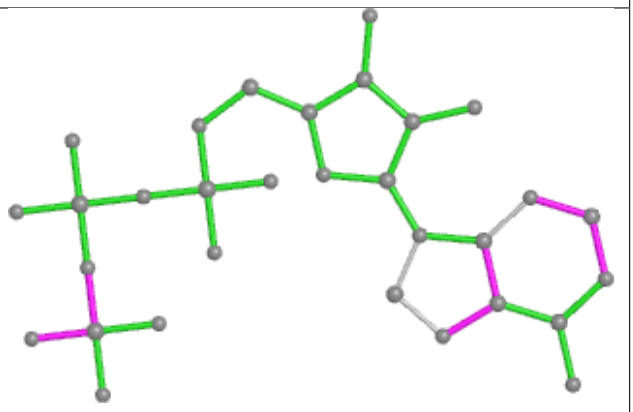

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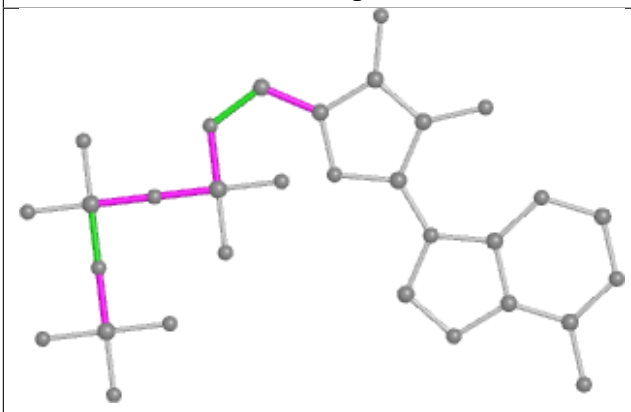

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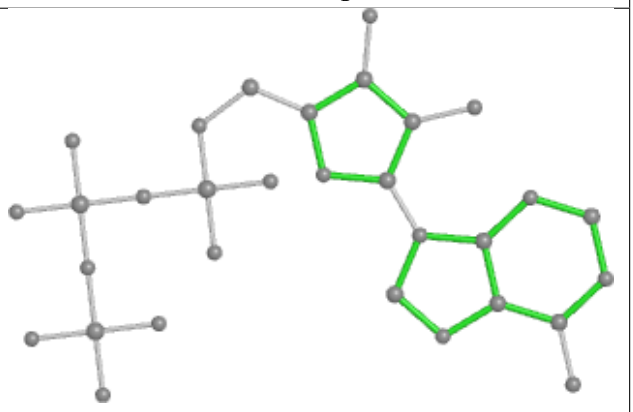
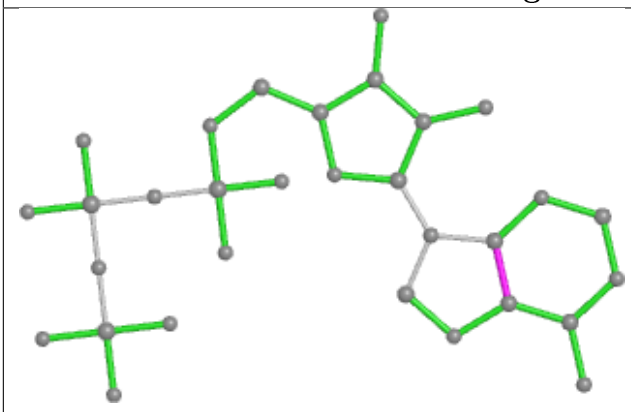


Rings

Ligand ATP G 402



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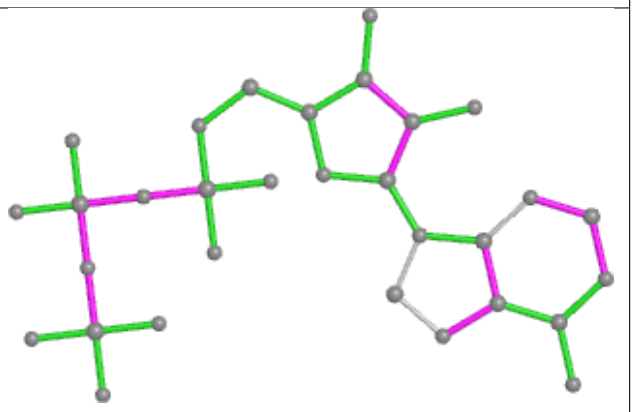

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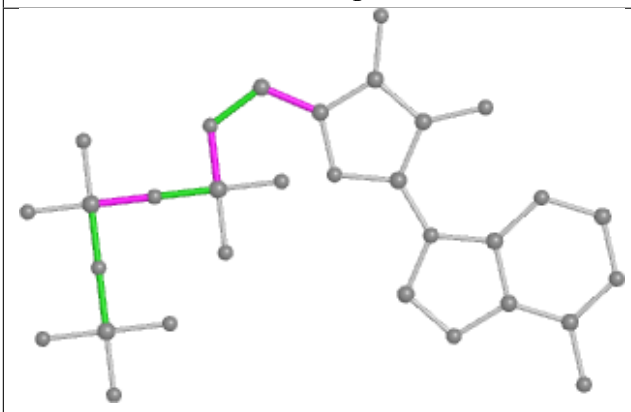

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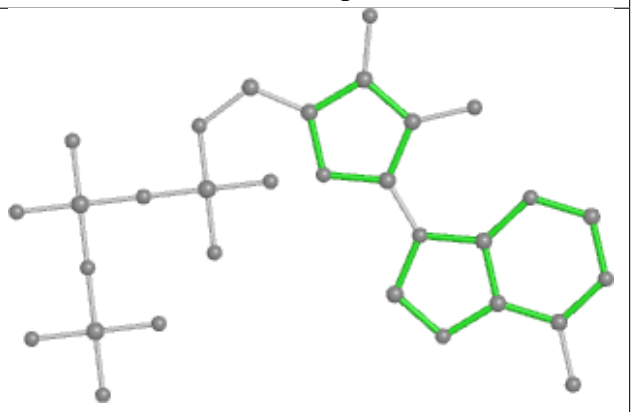
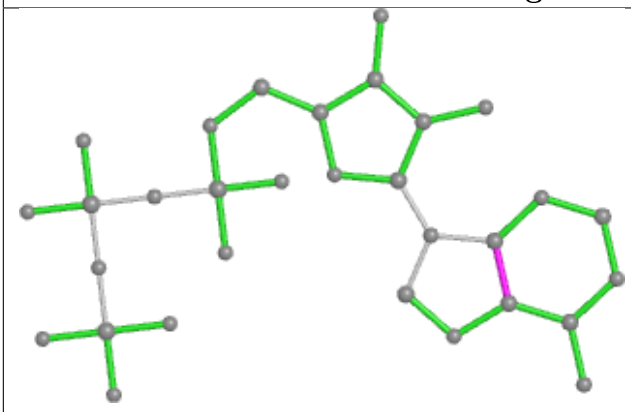


Rings

Ligand ATP B 402



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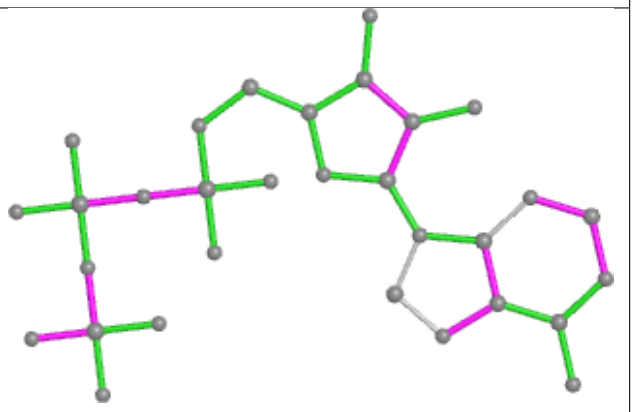
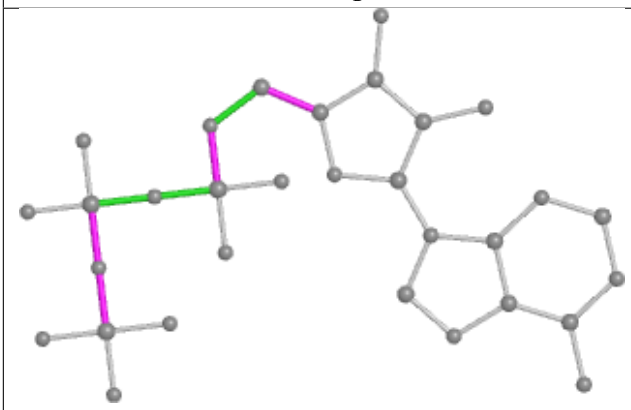


Bond angles



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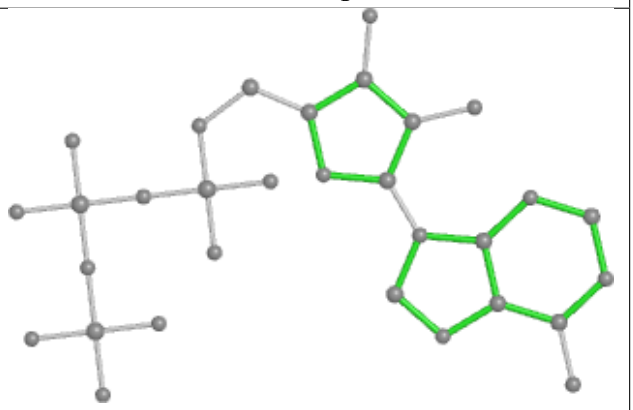

Rings

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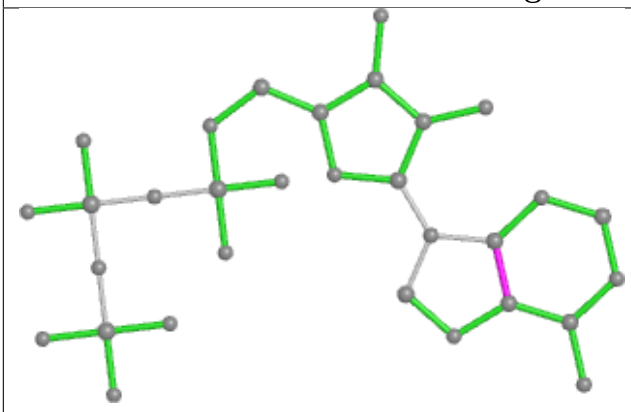

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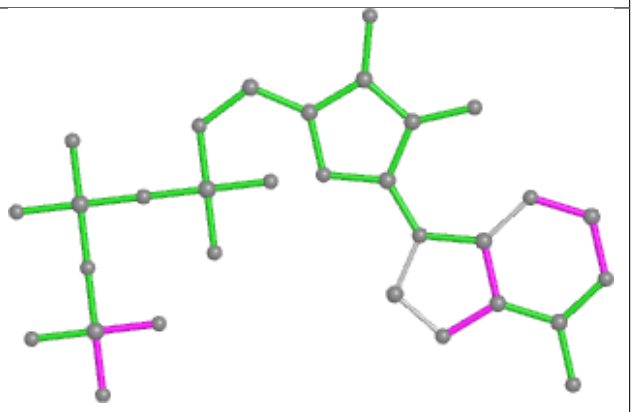

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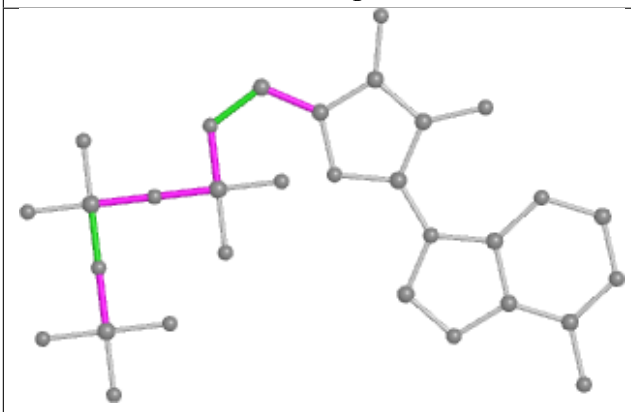

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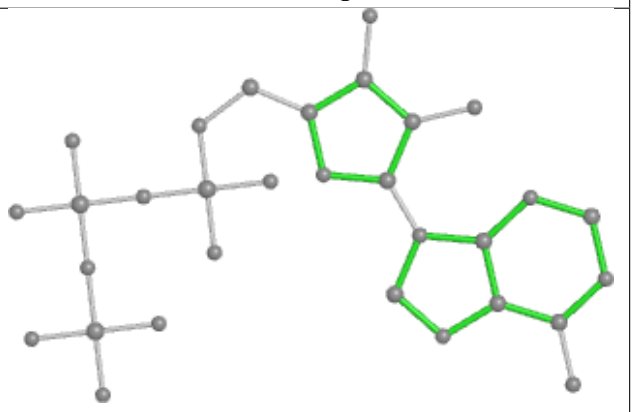

Rings

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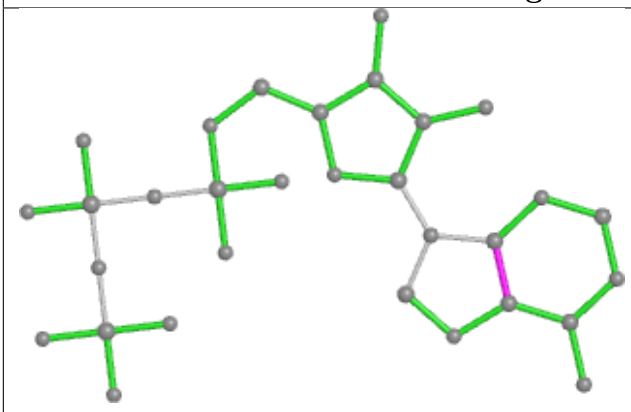

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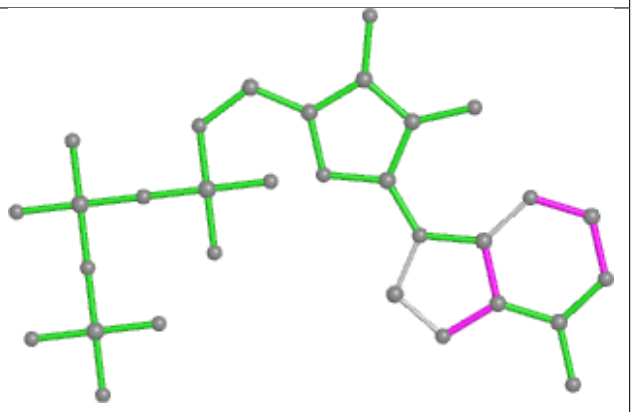

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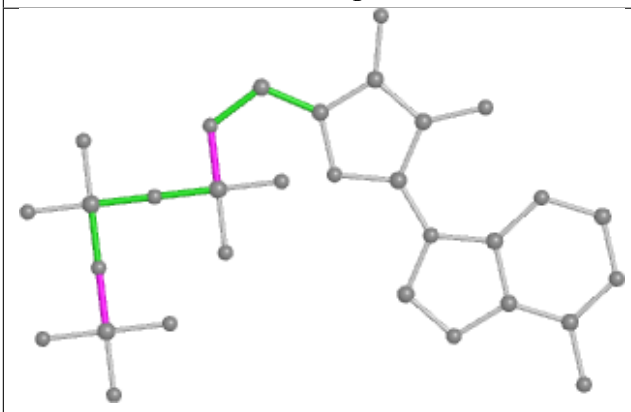

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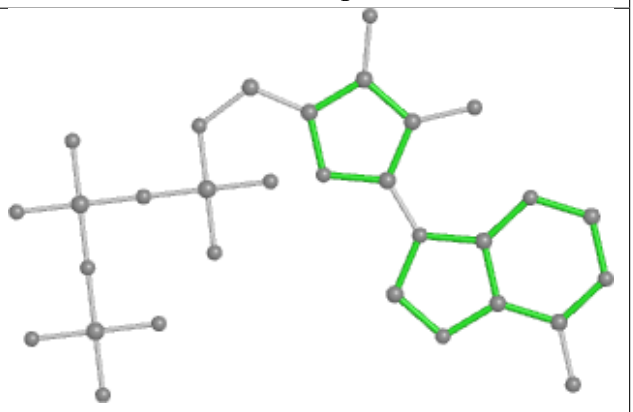

Rings

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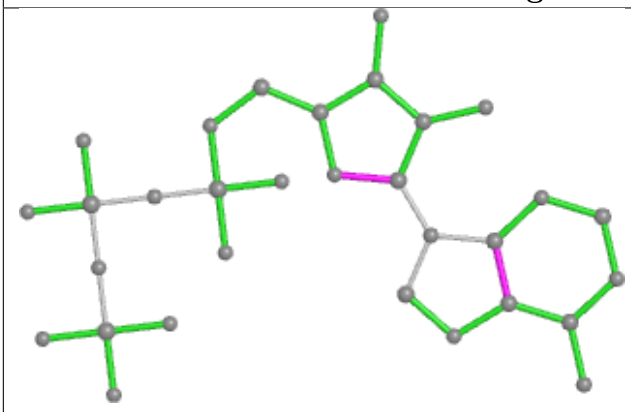

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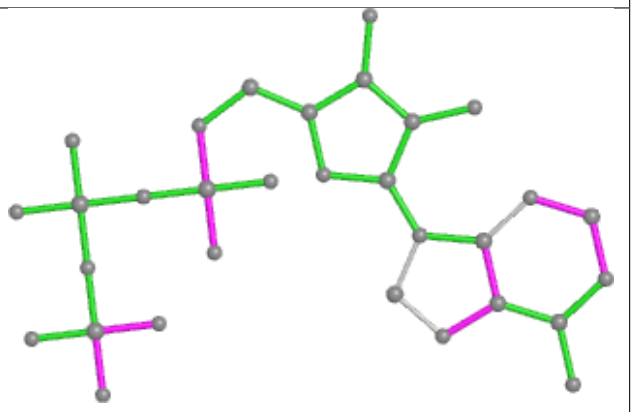

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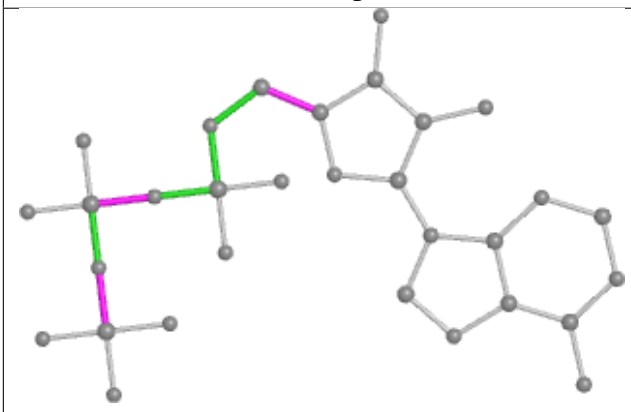

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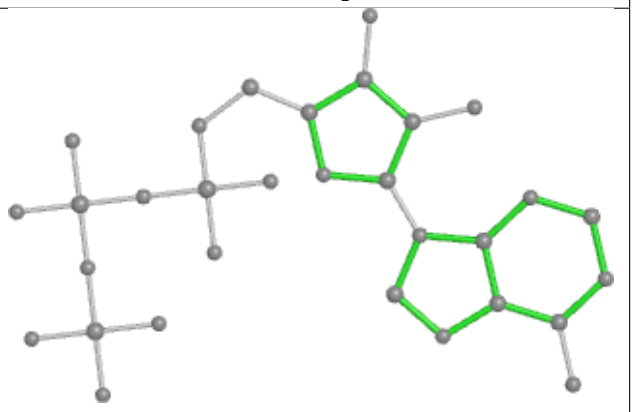
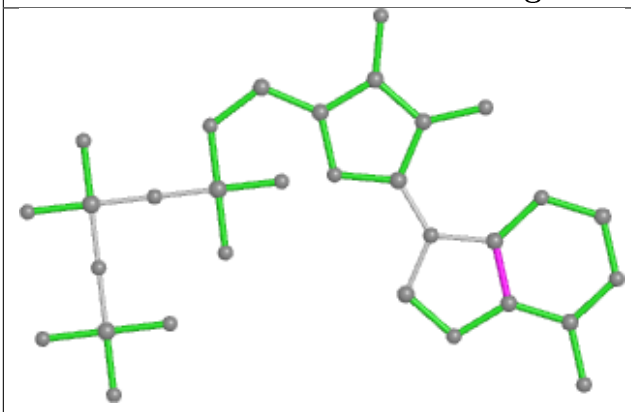
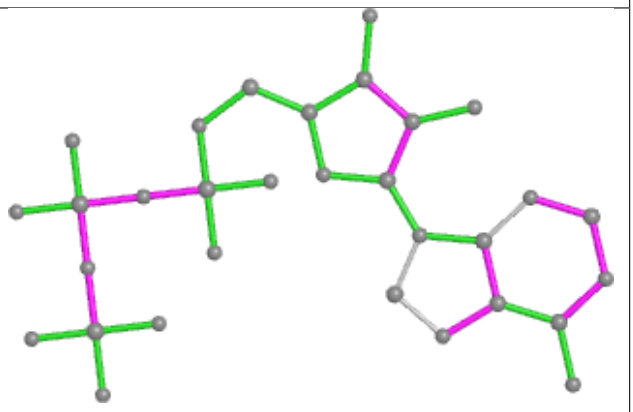


Rings

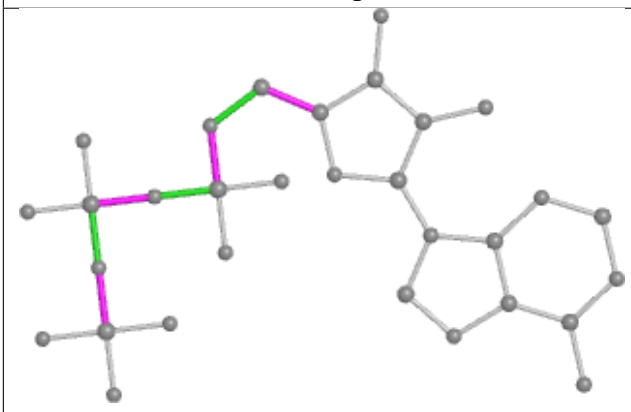
Ligand ATP H 401



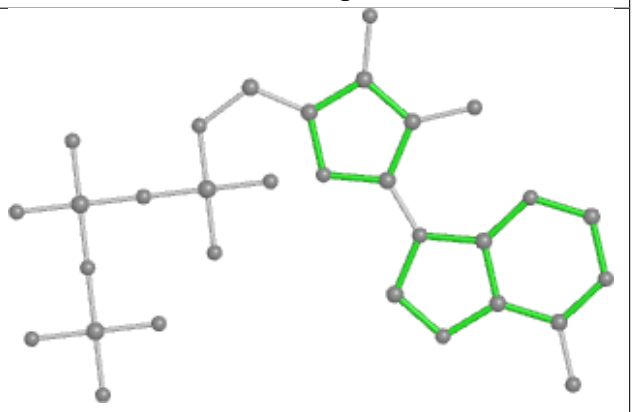
Bond lengths



Bond angles

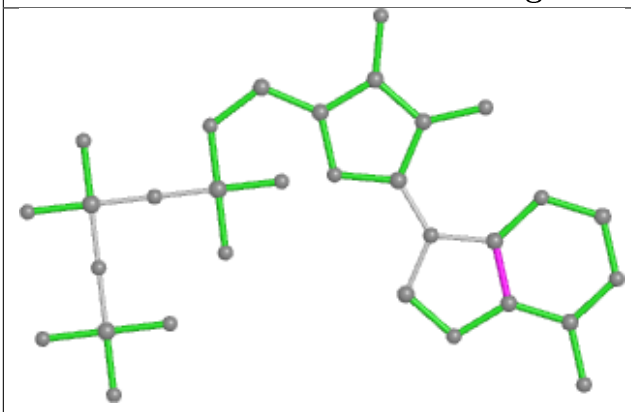


Torsions

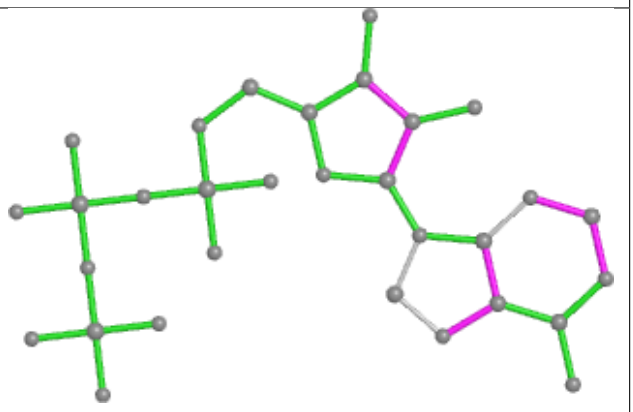


Rings

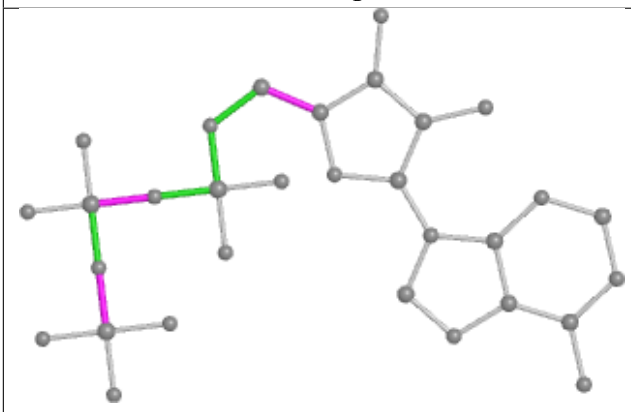
Ligand ATP C 401



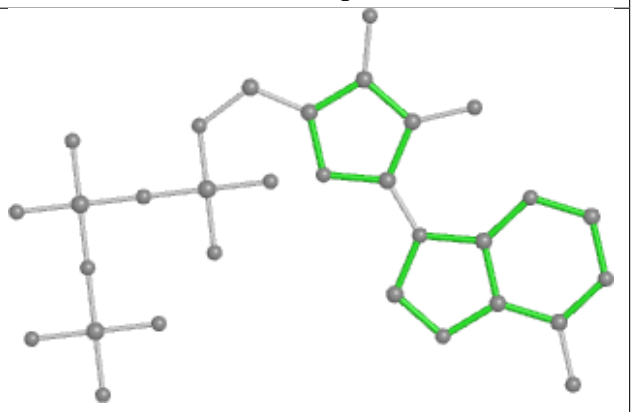
Bond lengths



Bond angles

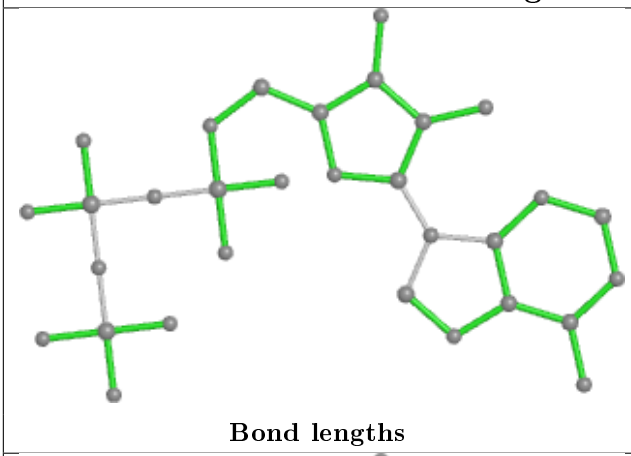


Torsions

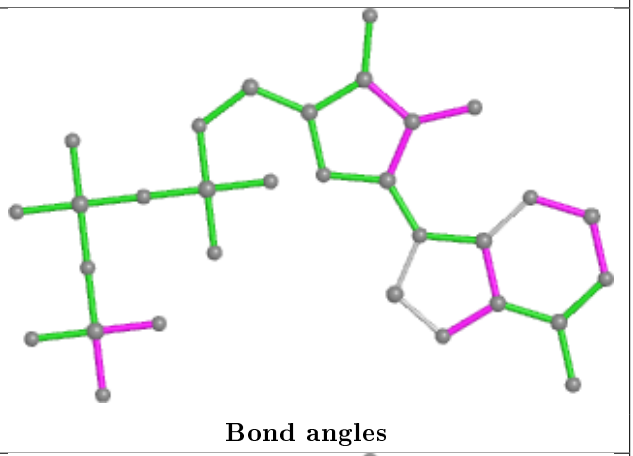


Rings

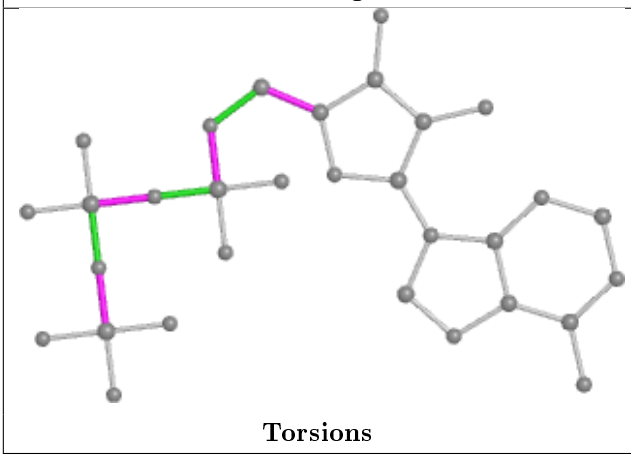
Ligand ATP A 401



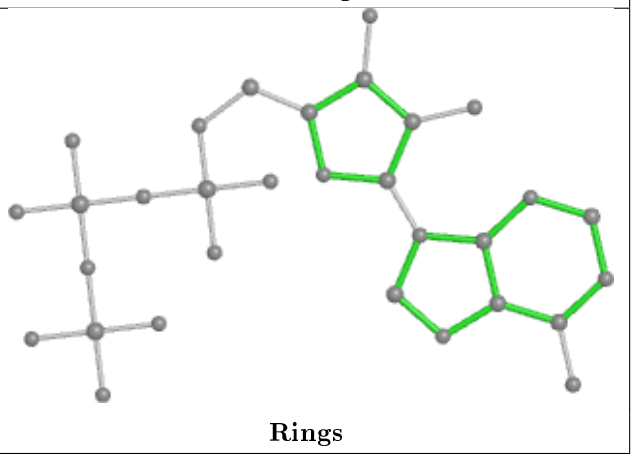
Bond lengths



Bond angles

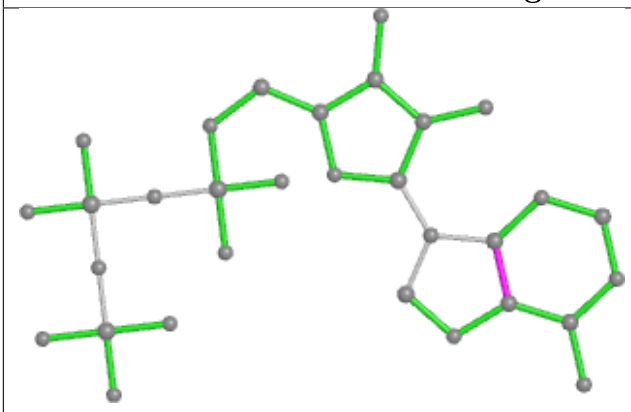


Torsions

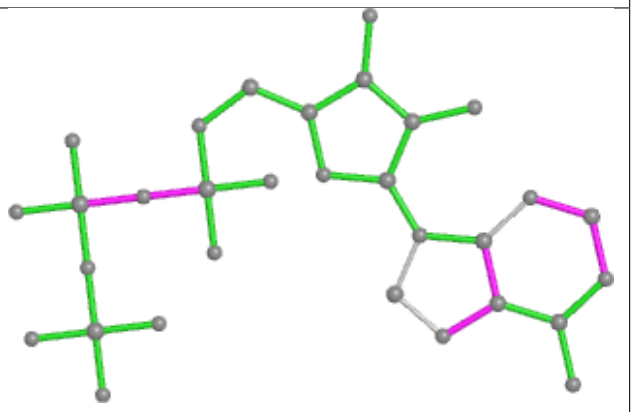


Rings

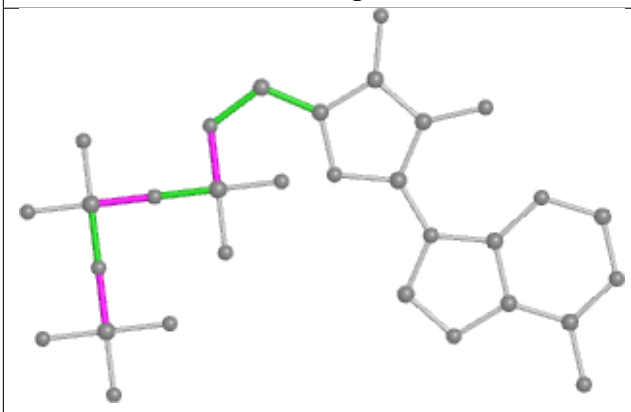
Ligand ATP D 402



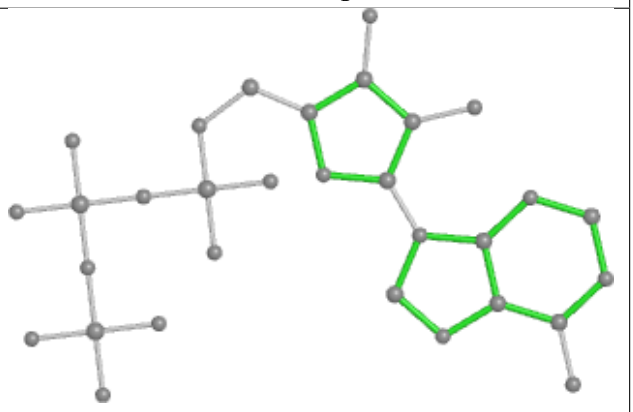
Bond lengths



Bond angles

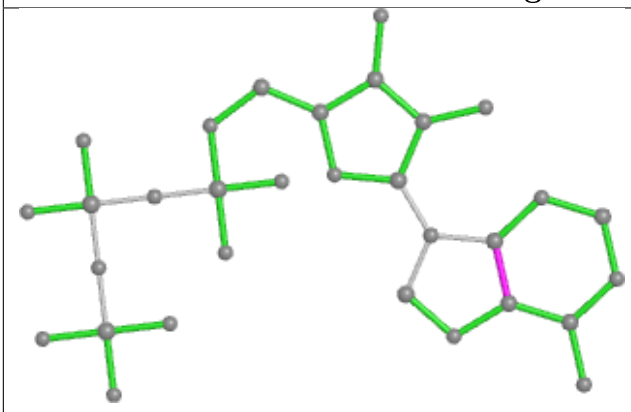


Torsions

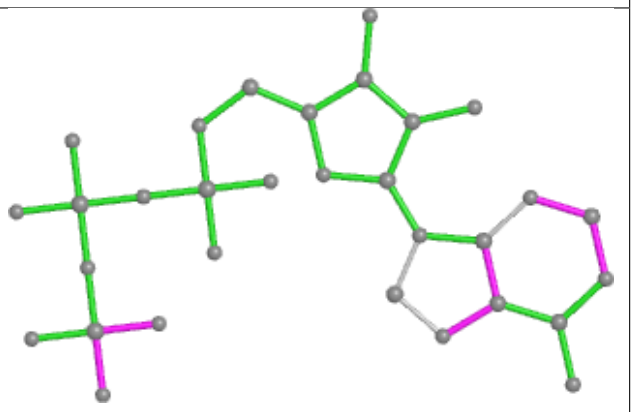


Rings

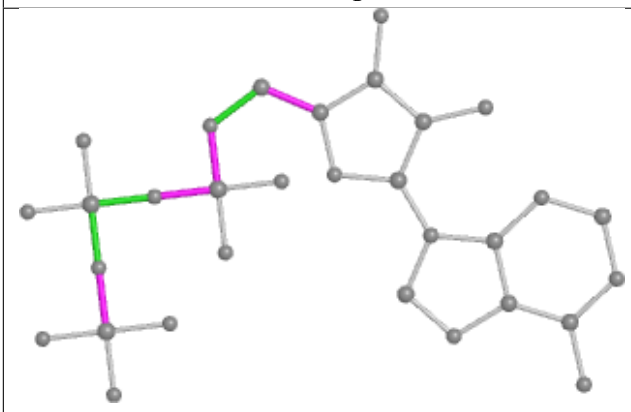
Ligand ATP H 402



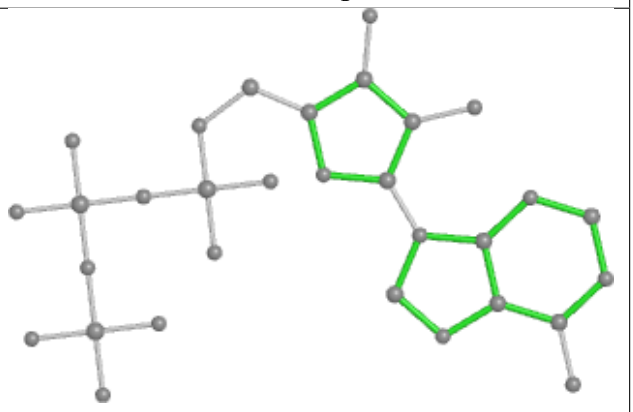
Bond lengths



Bond angles

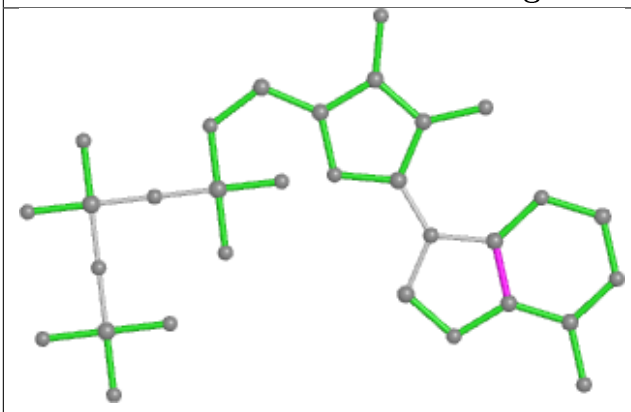


Torsions

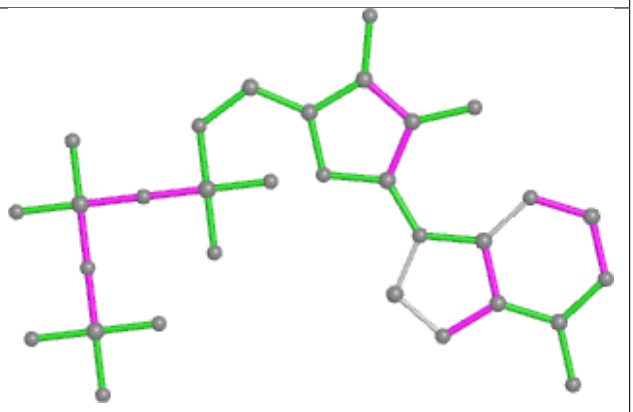


Rings

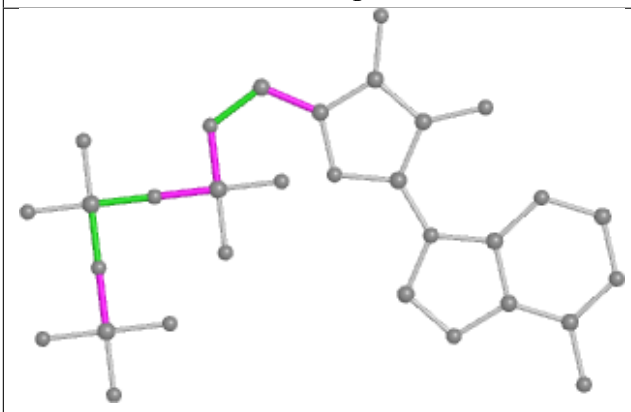
Ligand ATP G 401



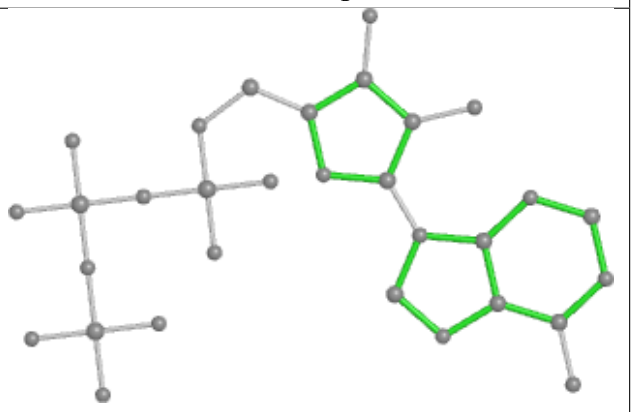
Bond lengths



Bond angles

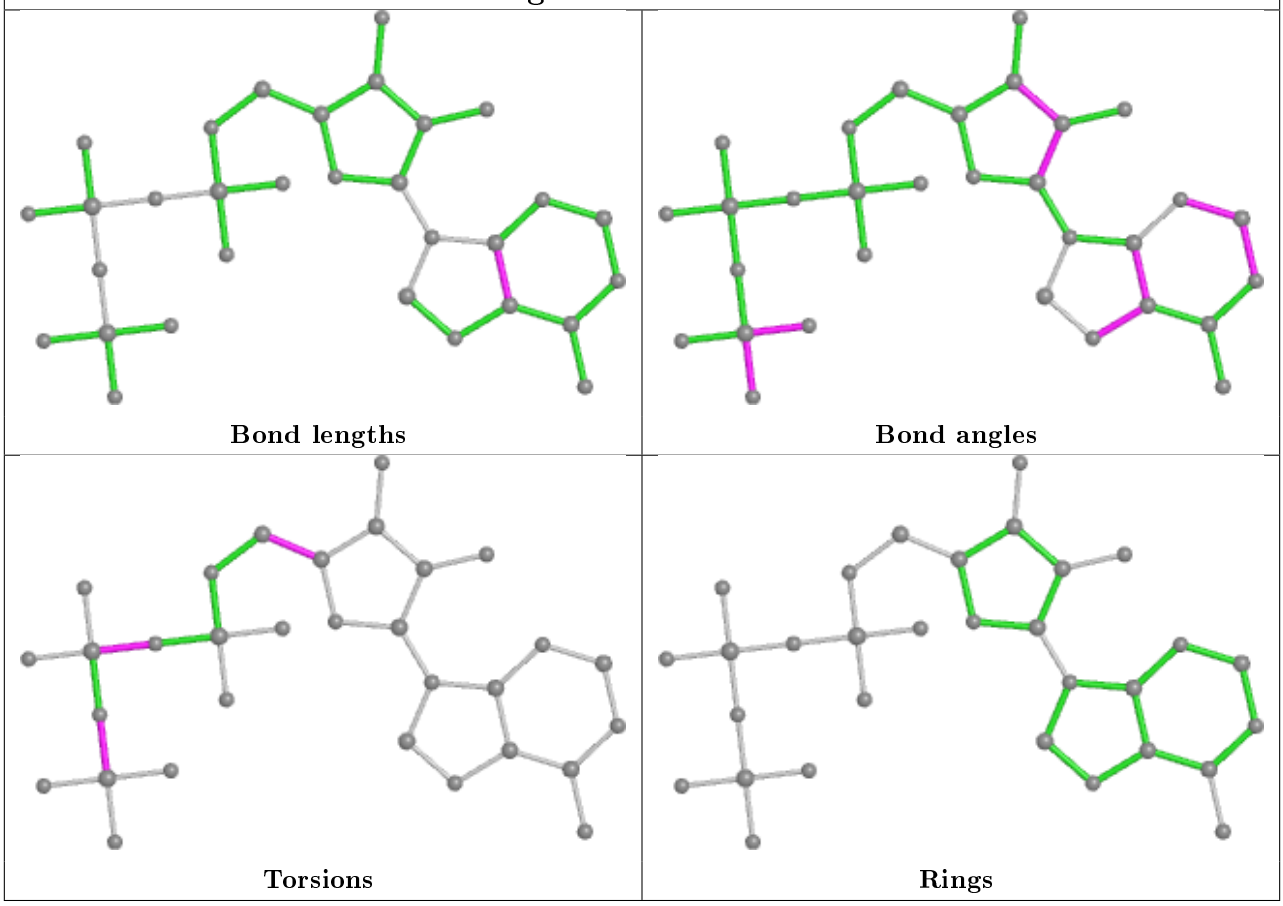


Torsions



Rings

Ligand ATP F 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	244/271 (90%)	0.47	16 (6%) 18 17	19, 37, 65, 88	0
1	B	243/271 (89%)	0.26	9 (3%) 41 41	20, 34, 50, 83	0
1	C	265/271 (97%)	0.66	23 (8%) 10 9	23, 43, 85, 114	0
1	D	266/271 (98%)	0.75	28 (10%) 6 5	23, 46, 95, 118	0
1	E	268/271 (98%)	0.59	27 (10%) 7 6	25, 41, 88, 114	0
1	F	255/271 (94%)	0.76	26 (10%) 6 6	26, 50, 93, 109	0
1	G	243/271 (89%)	0.78	31 (12%) 3 3	31, 59, 101, 114	0
1	H	259/271 (95%)	0.61	24 (9%) 8 8	32, 57, 99, 118	0
All	All	2043/2168 (94%)	0.61	184 (9%) 9 8	19, 45, 92, 118	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	GLU	11.1
1	C	227	ALA	10.7
1	D	225	ASP	9.8
1	F	234	VAL	9.7
1	D	227	ALA	9.1
1	F	237	LEU	8.8
1	E	229	LEU	8.5
1	C	237	LEU	8.0
1	D	228	GLU	8.0
1	A	221	TYR	6.9
1	D	220	ASN	6.9
1	D	232	ARG	6.7
1	C	231	LYS	6.6
1	F	235	GLN	6.5
1	H	233	GLN	6.4
1	C	232	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	229	LEU	5.9
1	F	233	GLN	5.7
1	E	228	GLU	5.6
1	D	229	LEU	5.5
1	D	231	LYS	5.5
1	E	225	ASP	5.4
1	H	221	TYR	5.4
1	F	194	PHE	5.2
1	F	236	ARG	5.2
1	C	235	GLN	5.1
1	E	227	ALA	5.0
1	A	244	ALA	5.0
1	D	234	VAL	4.9
1	D	219	GLU	4.8
1	C	226	GLU	4.8
1	H	222	GLU	4.8
1	D	223	THR	4.7
1	D	230	SER	4.7
1	C	230	SER	4.6
1	E	232	ARG	4.6
1	A	219	GLU	4.6
1	C	225	ASP	4.6
1	E	224	GLU	4.4
1	D	224	GLU	4.4
1	F	239	LYS	4.4
1	G	168	LEU	4.3
1	G	179	GLN	4.3
1	F	243	LYS	4.2
1	H	234	VAL	4.2
1	B	221	TYR	4.1
1	E	231	LYS	4.0
1	A	220	ASN	4.0
1	F	240	LYS	4.0
1	D	3	ASN	4.0
1	G	175	GLN	4.0
1	C	224	GLU	4.0
1	C	234	VAL	4.0
1	D	236	ARG	3.9
1	C	242	LYS	3.9
1	H	223	THR	3.7
1	B	220	ASN	3.6
1	G	201	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	237	LEU	3.6
1	A	218	PHE	3.6
1	D	218	PHE	3.5
1	D	235	GLN	3.5
1	C	236	ARG	3.5
1	G	167	VAL	3.5
1	B	182	MET	3.5
1	G	164	TRP	3.5
1	B	218	PHE	3.4
1	H	230	SER	3.4
1	D	191	GLU	3.3
1	G	197	CYS	3.3
1	E	1	MET	3.3
1	D	183	GLY	3.2
1	G	174	PRO	3.2
1	E	194	PHE	3.2
1	E	236	ARG	3.2
1	A	3	ASN	3.2
1	F	174	PRO	3.2
1	F	168	LEU	3.1
1	F	218	PHE	3.1
1	F	238	GLU	3.1
1	G	35	LYS	3.1
1	A	174	PRO	3.1
1	G	221	TYR	3.1
1	H	232	ARG	3.1
1	G	218	PHE	3.1
1	F	166	LEU	3.1
1	E	235	GLN	3.0
1	H	186	ALA	3.0
1	C	240	LYS	3.0
1	E	226	GLU	3.0
1	H	236	ARG	3.0
1	D	268	ASP	3.0
1	F	221	TYR	3.0
1	B	164	TRP	3.0
1	G	172	MET	3.0
1	F	241	ARG	3.0
1	H	240	LYS	3.0
1	H	235	GLN	3.0
1	E	242	LYS	2.9
1	G	173	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	240	LYS	2.9
1	A	118	ASP	2.9
1	D	238	GLU	2.9
1	H	220	ASN	2.9
1	C	238	GLU	2.8
1	H	244	ALA	2.8
1	G	171	LYS	2.8
1	F	167	VAL	2.8
1	C	179	GLN	2.7
1	G	34[A]	HIS	2.7
1	F	222	GLU	2.7
1	D	237	LEU	2.7
1	H	180	ARG	2.7
1	C	34[A]	HIS	2.7
1	A	195	LYS	2.7
1	E	238	GLU	2.7
1	C	174	PRO	2.7
1	E	203	ASN	2.7
1	G	194	PHE	2.6
1	C	233	GLN	2.6
1	B	244	ALA	2.6
1	G	186	ALA	2.6
1	F	220	ASN	2.6
1	H	243	LYS	2.6
1	H	242	LYS	2.5
1	E	241	ARG	2.5
1	G	184	THR	2.5
1	F	244	ALA	2.5
1	E	230	SER	2.5
1	D	233	GLN	2.5
1	H	231	LYS	2.5
1	G	205	SER	2.4
1	G	163	PHE	2.4
1	G	178	GLU	2.4
1	E	239	LYS	2.4
1	H	5	LYS	2.4
1	H	193	LEU	2.4
1	G	45	PRO	2.4
1	F	175	GLN	2.4
1	G	181	LEU	2.4
1	F	177	ALA	2.4
1	F	219	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	241	ARG	2.4
1	E	240	LYS	2.4
1	H	218	PHE	2.4
1	G	219	GLU	2.4
1	E	233	GLN	2.4
1	G	190	ASN	2.4
1	A	166	LEU	2.3
1	C	182	MET	2.3
1	F	242	LYS	2.3
1	G	176	GLN	2.3
1	H	174	PRO	2.3
1	D	195	LYS	2.3
1	E	2	ALA	2.3
1	C	243	LYS	2.3
1	E	268	ASP	2.3
1	H	264	PRO	2.3
1	D	222	GLU	2.2
1	G	182	MET	2.2
1	G	193	LEU	2.2
1	F	172	MET	2.2
1	H	219	GLU	2.2
1	E	234	VAL	2.2
1	A	26	ILE	2.2
1	G	198	GLY	2.2
1	F	171	LYS	2.2
1	B	219	GLU	2.1
1	A	168	LEU	2.1
1	B	268	ASP	2.1
1	A	170	LEU	2.1
1	A	265	TRP	2.1
1	D	243	LYS	2.1
1	G	49	LYS	2.1
1	E	202	ASN	2.1
1	G	247	LYS	2.1
1	H	251	VAL	2.1
1	A	178	GLU	2.0
1	E	243	LYS	2.0
1	D	221	TYR	2.0
1	D	197	CYS	2.0
1	E	3	ASN	2.0
1	B	168	LEU	2.0
1	A	182	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	MG	G	404	1/1	0.87	0.07	38,38,38,38	0
3	MG	D	405	1/1	0.91	0.15	30,30,30,30	0
3	MG	B	405	1/1	0.92	0.12	27,27,27,27	0
3	MG	C	403	1/1	0.93	0.07	33,33,33,33	0
3	MG	F	403	1/1	0.93	0.08	39,39,39,39	0
3	MG	A	403	1/1	0.95	0.06	33,33,33,33	0
3	MG	C	405	1/1	0.95	0.05	24,24,24,24	0
2	ATP	B	402	31/31	0.96	0.20	21,104,107,109	0
3	MG	D	404	1/1	0.96	0.12	28,28,28,28	0
3	MG	F	405	1/1	0.96	0.10	30,30,30,30	0
2	ATP	G	401	31/31	0.96	0.15	42,79,81,82	0
2	ATP	H	402	31/31	0.97	0.14	27,66,72,74	0
3	MG	H	403	1/1	0.97	0.11	43,43,43,43	0
3	MG	H	405	1/1	0.97	0.12	29,29,29,29	0
2	ATP	F	401	31/31	0.97	0.13	22,41,53,57	0
3	MG	C	404	1/1	0.97	0.09	32,32,32,32	0
3	MG	A	404	1/1	0.97	0.11	24,24,24,24	0
2	ATP	F	402	31/31	0.97	0.12	24,57,61,66	0
2	ATP	G	402	31/31	0.97	0.14	34,61,70,72	0
3	MG	E	405	1/1	0.97	0.10	22,22,22,22	0
3	MG	G	405	1/1	0.98	0.04	43,43,43,43	0
3	MG	F	404	1/1	0.98	0.10	31,31,31,31	0
2	ATP	H	401	31/31	0.98	0.13	32,47,55,57	0
3	MG	D	403	1/1	0.98	0.16	39,39,39,39	0
3	MG	E	404	1/1	0.98	0.12	26,26,26,26	0
2	ATP	A	402	31/31	0.98	0.13	21,54,62,65	0
3	MG	E	403	1/1	0.98	0.07	31,31,31,31	0

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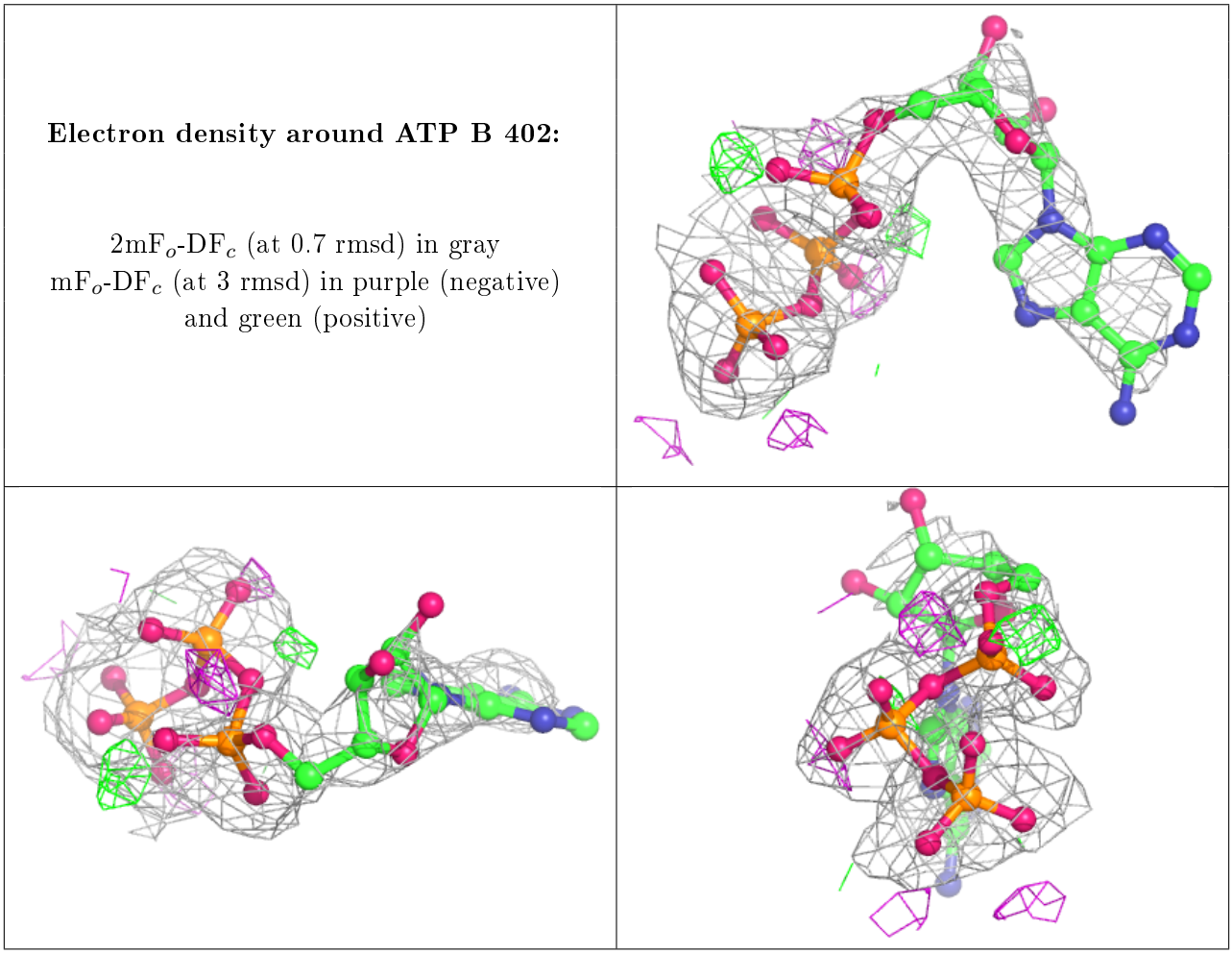
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ATP	C	402	31/31	0.98	0.15	24,50,54,55	0
3	MG	B	404	1/1	0.98	0.14	22,22,22,22	0
3	MG	A	405	1/1	0.98	0.14	20,20,20,20	0
2	ATP	D	402	31/31	0.98	0.13	23,50,55,56	0
3	MG	H	404	1/1	0.98	0.09	33,33,33,33	0
3	MG	B	403	1/1	0.98	0.08	33,33,33,33	0
2	ATP	D	401	31/31	0.98	0.14	26,34,40,43	0
2	ATP	C	401	31/31	0.98	0.14	22,40,46,47	0
3	MG	G	403	1/1	0.98	0.05	45,45,45,45	0
2	ATP	E	402	31/31	0.99	0.13	19,44,51,57	0
2	ATP	E	401	31/31	0.99	0.13	25,36,40,41	0
2	ATP	A	401	31/31	0.99	0.13	20,27,36,38	0
2	ATP	B	401	31/31	0.99	0.14	15,27,34,35	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.

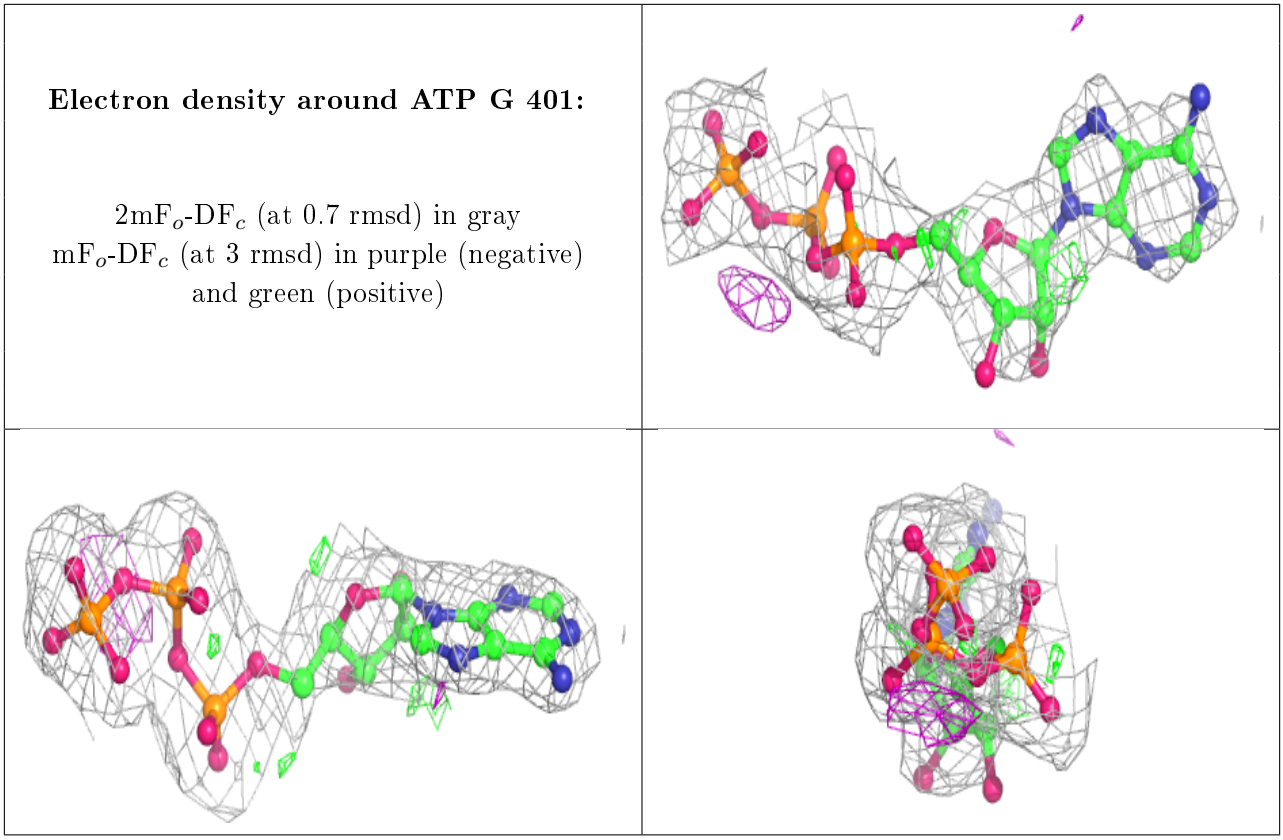
Electron density around ATP B 402:

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



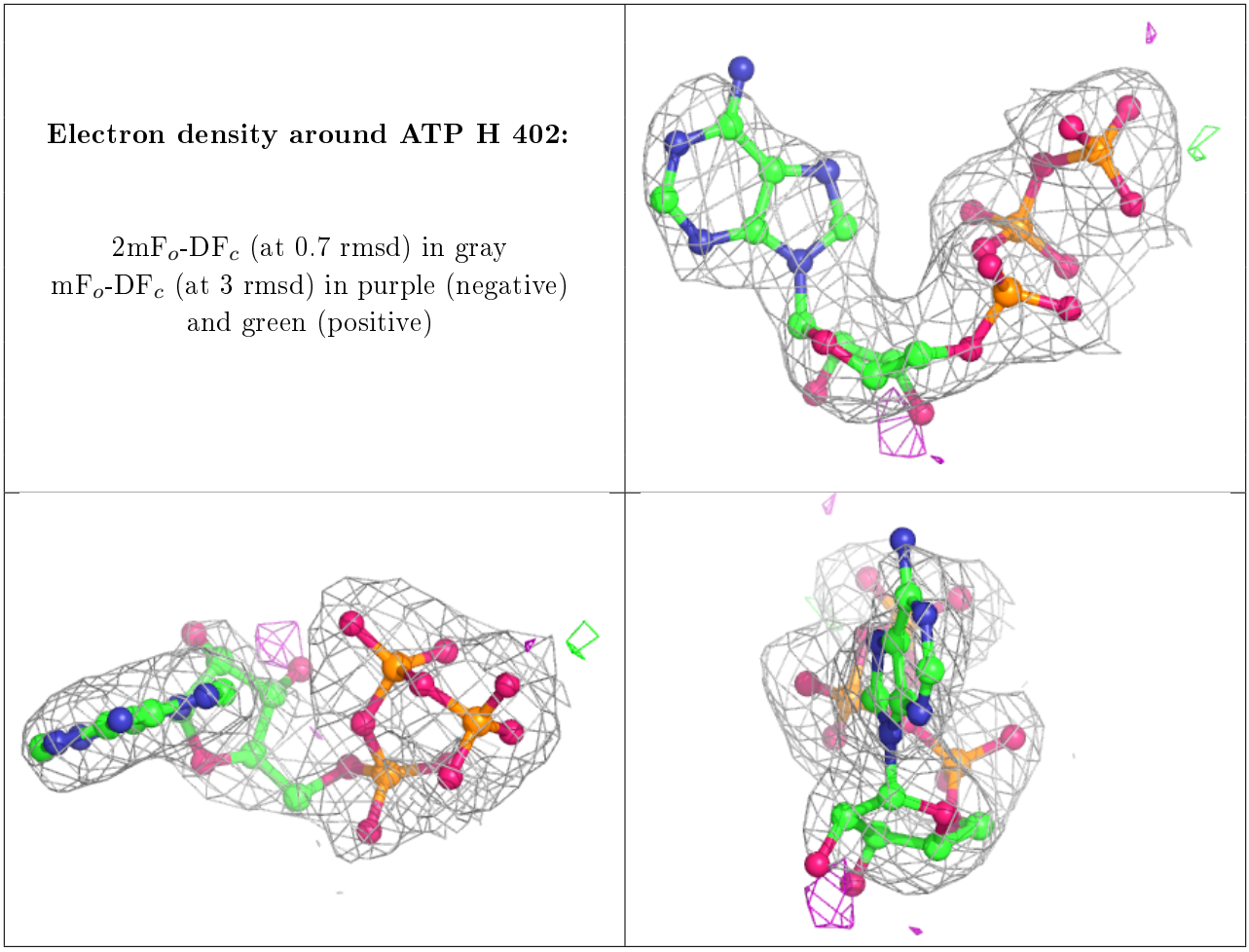
Electron density around ATP G 401:

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



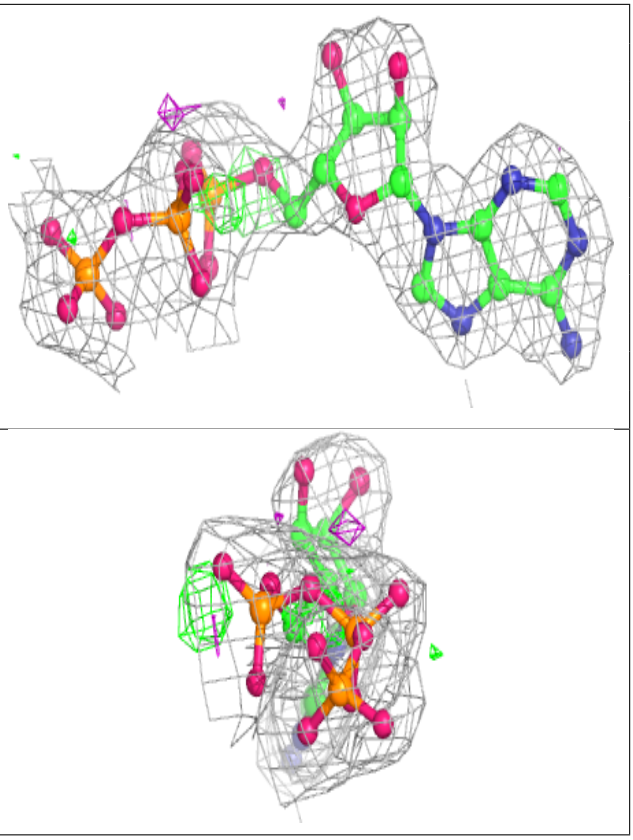
Electron density around ATP H 402:

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



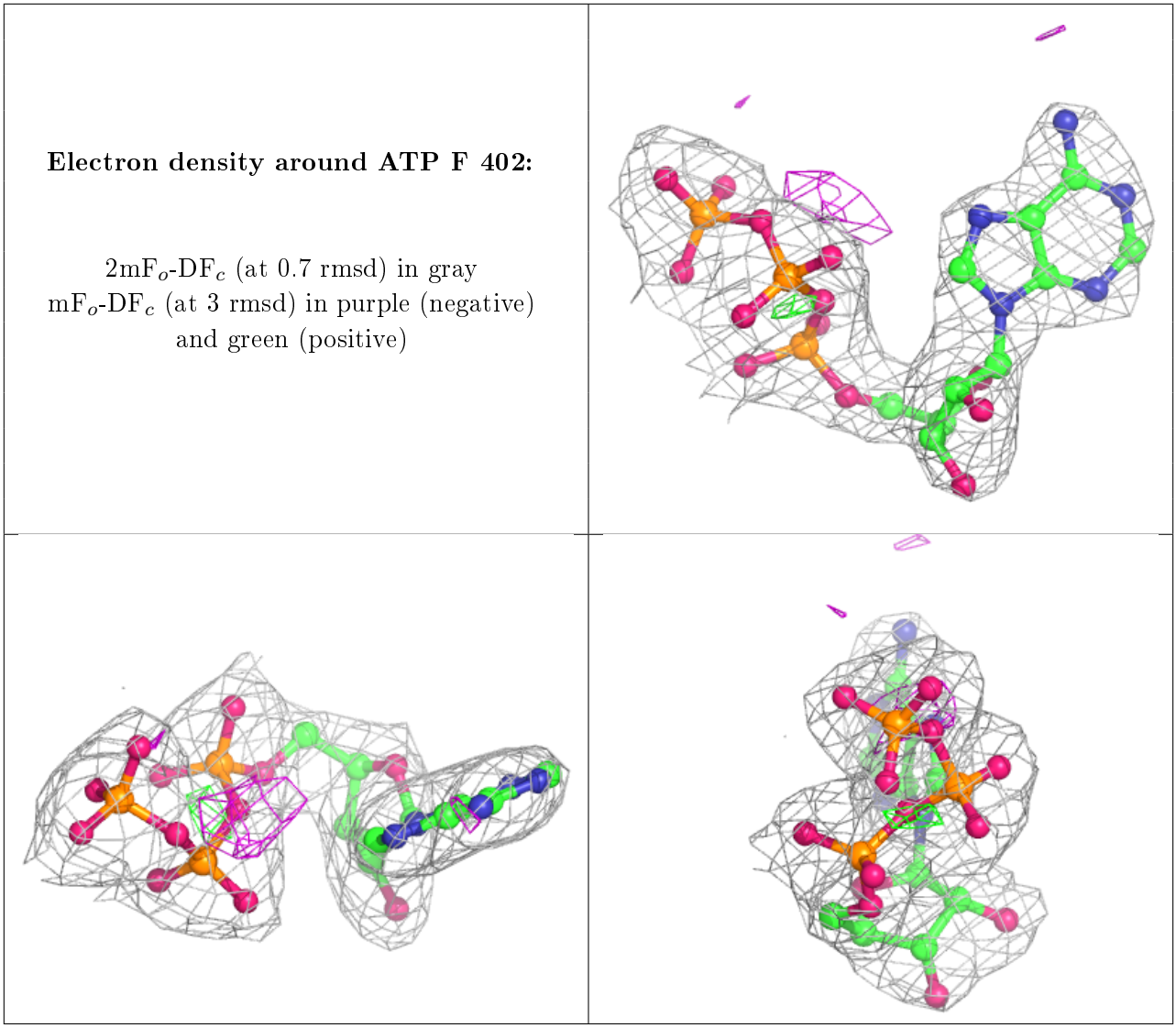
Electron density around ATP F 401:

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



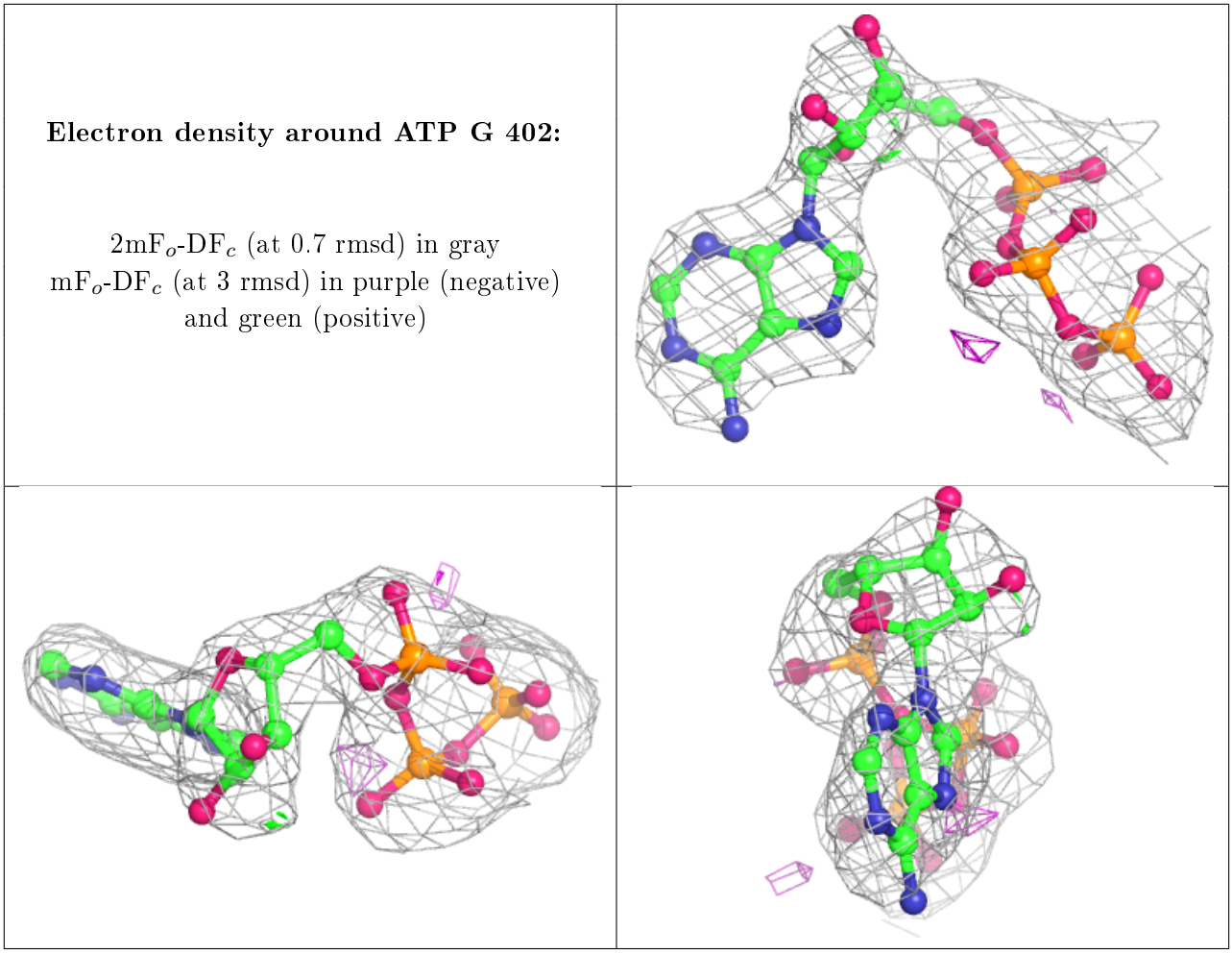
Electron density around ATP F 402:

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



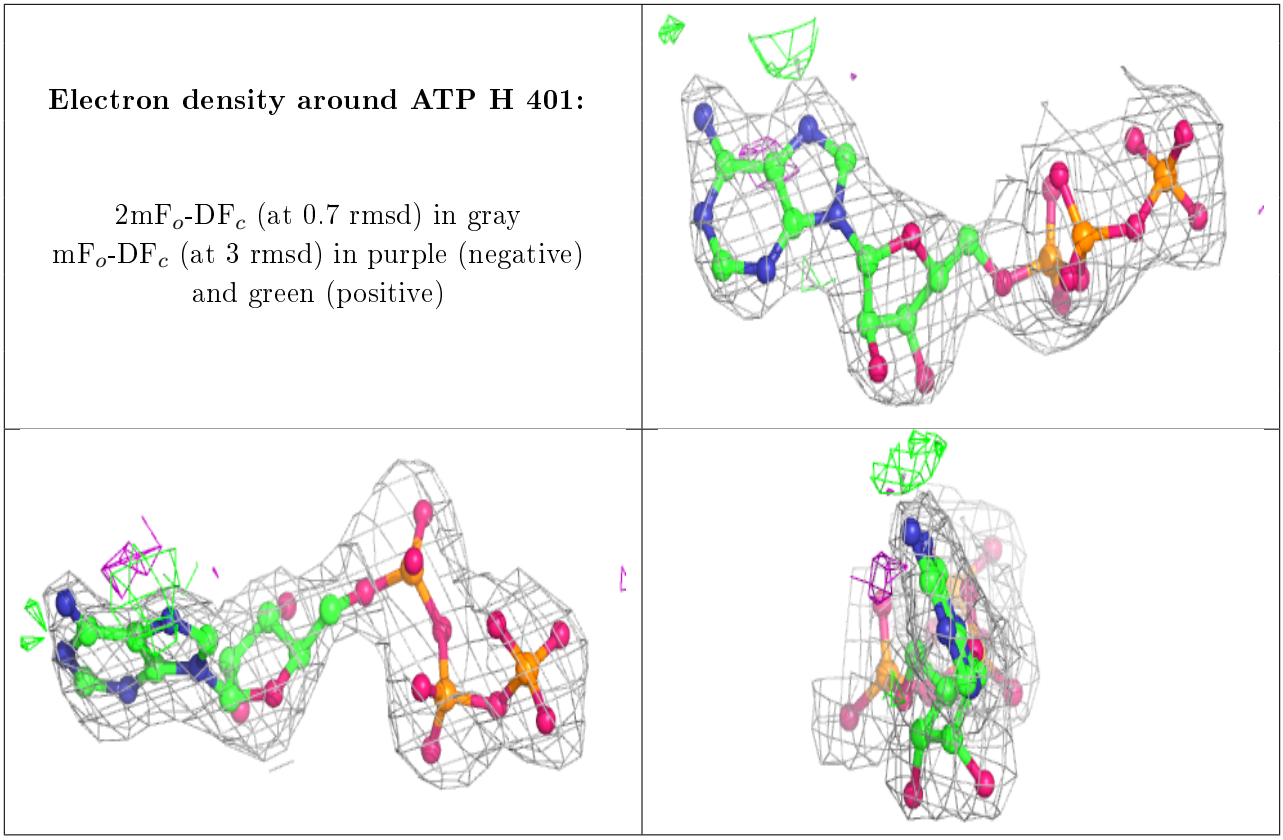
Electron density around ATP G 402:

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



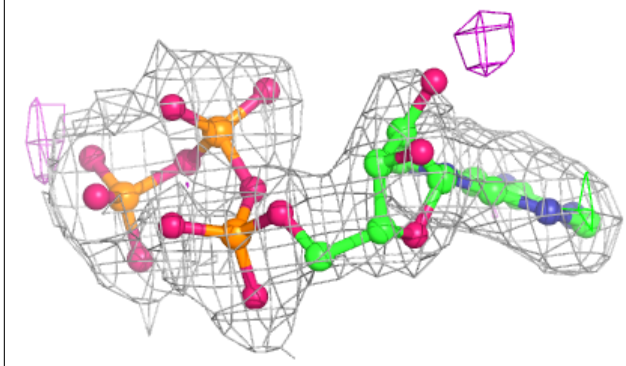
Electron density around ATP H 401:

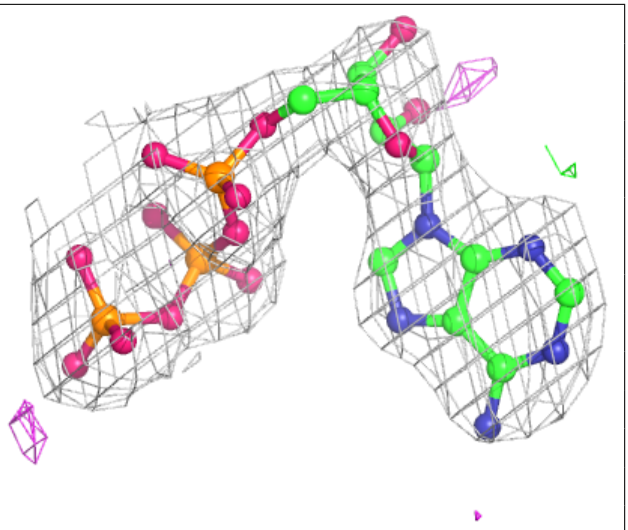
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

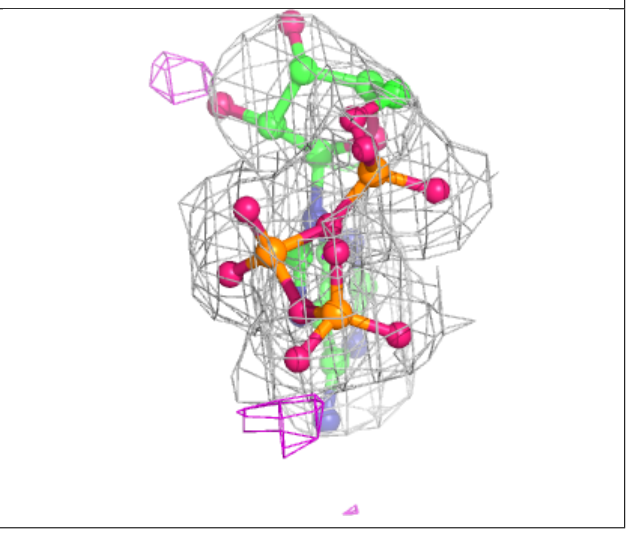


Electron density around ATP A 402:

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

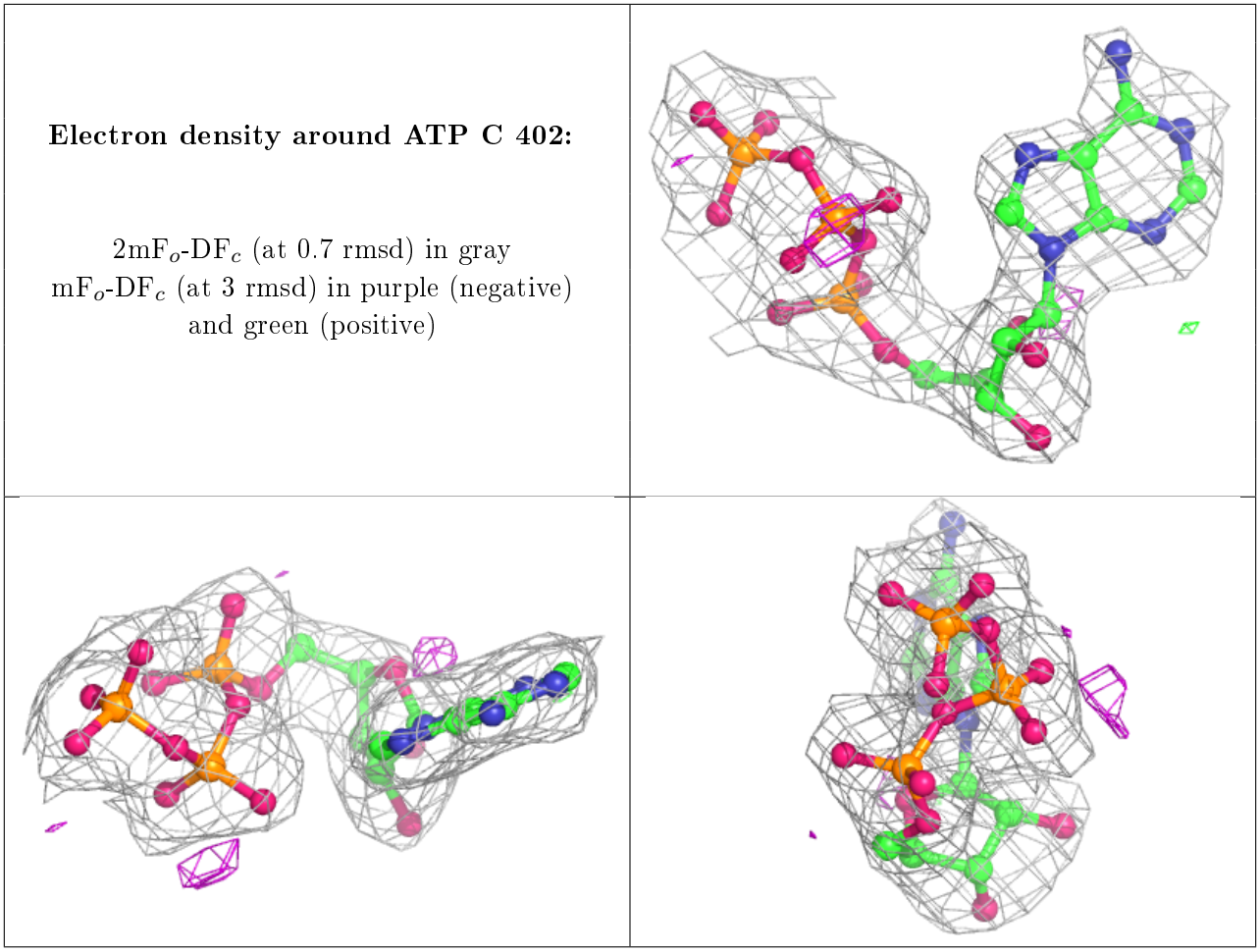






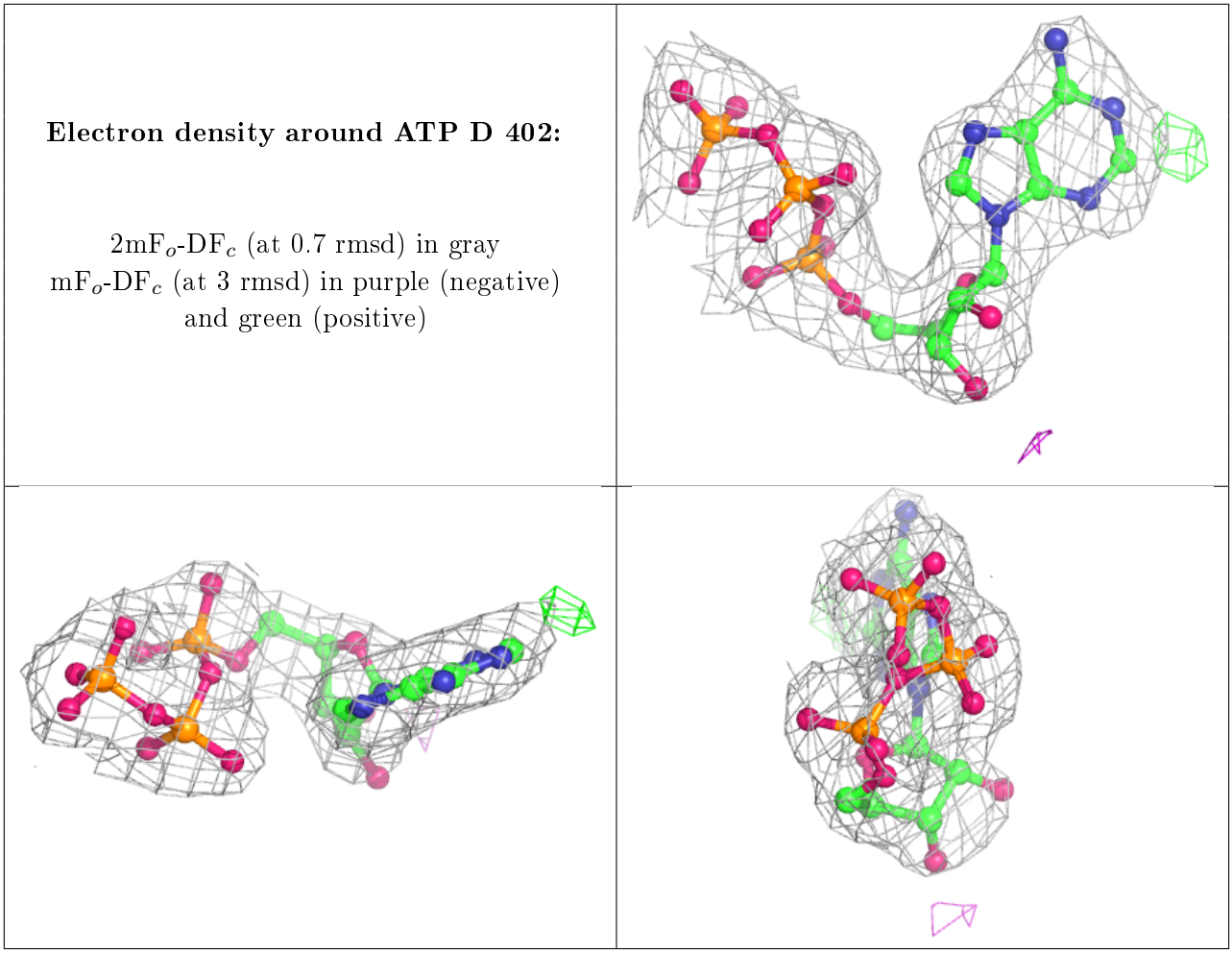
Electron density around ATP C 402:

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



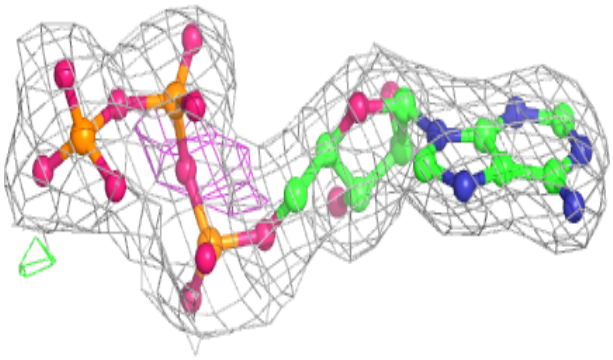
Electron density around ATP D 402:

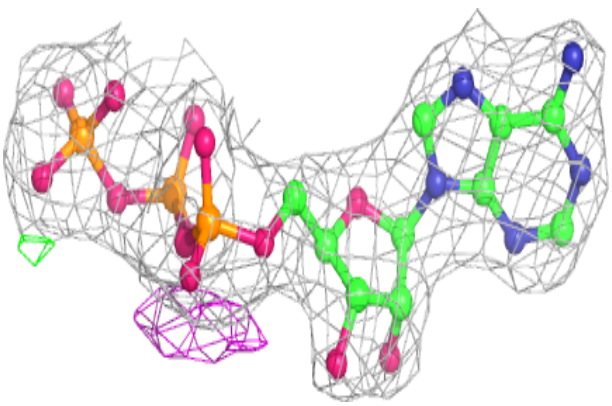
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

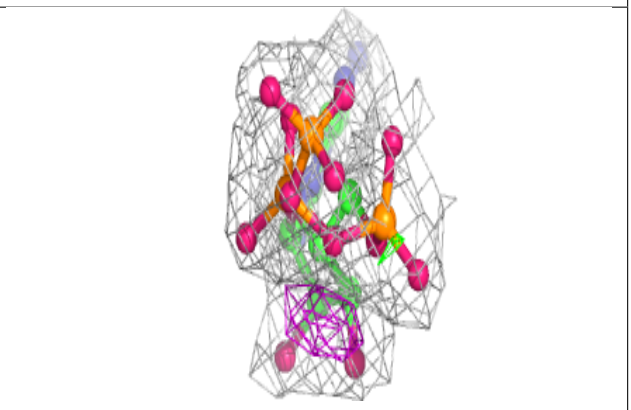


Electron density around ATP D 401:

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

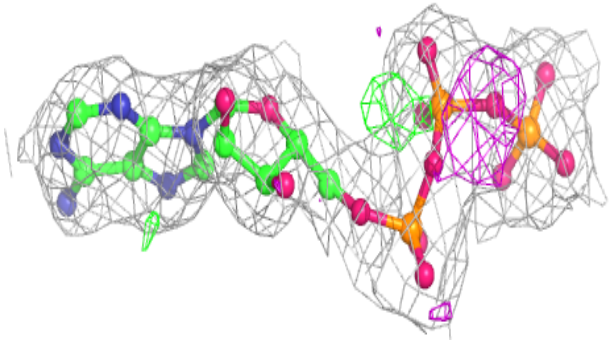


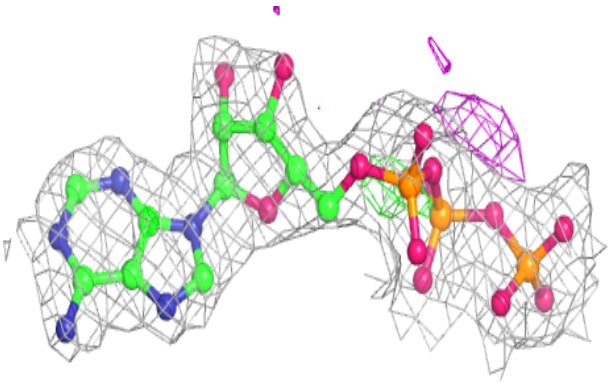


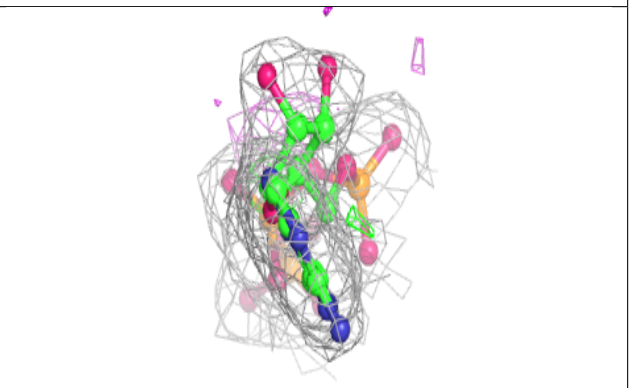


Electron density around ATP C 401:

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

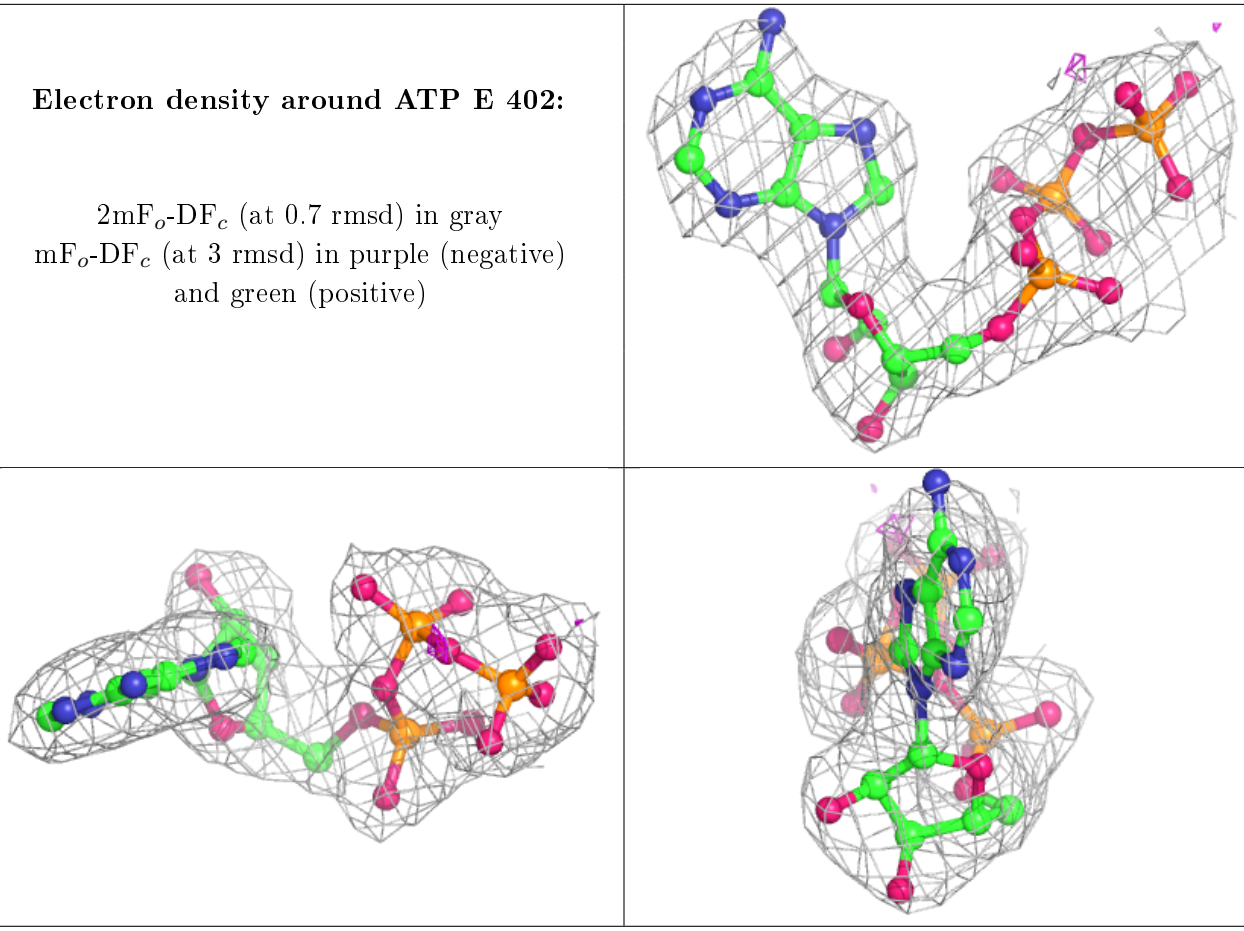






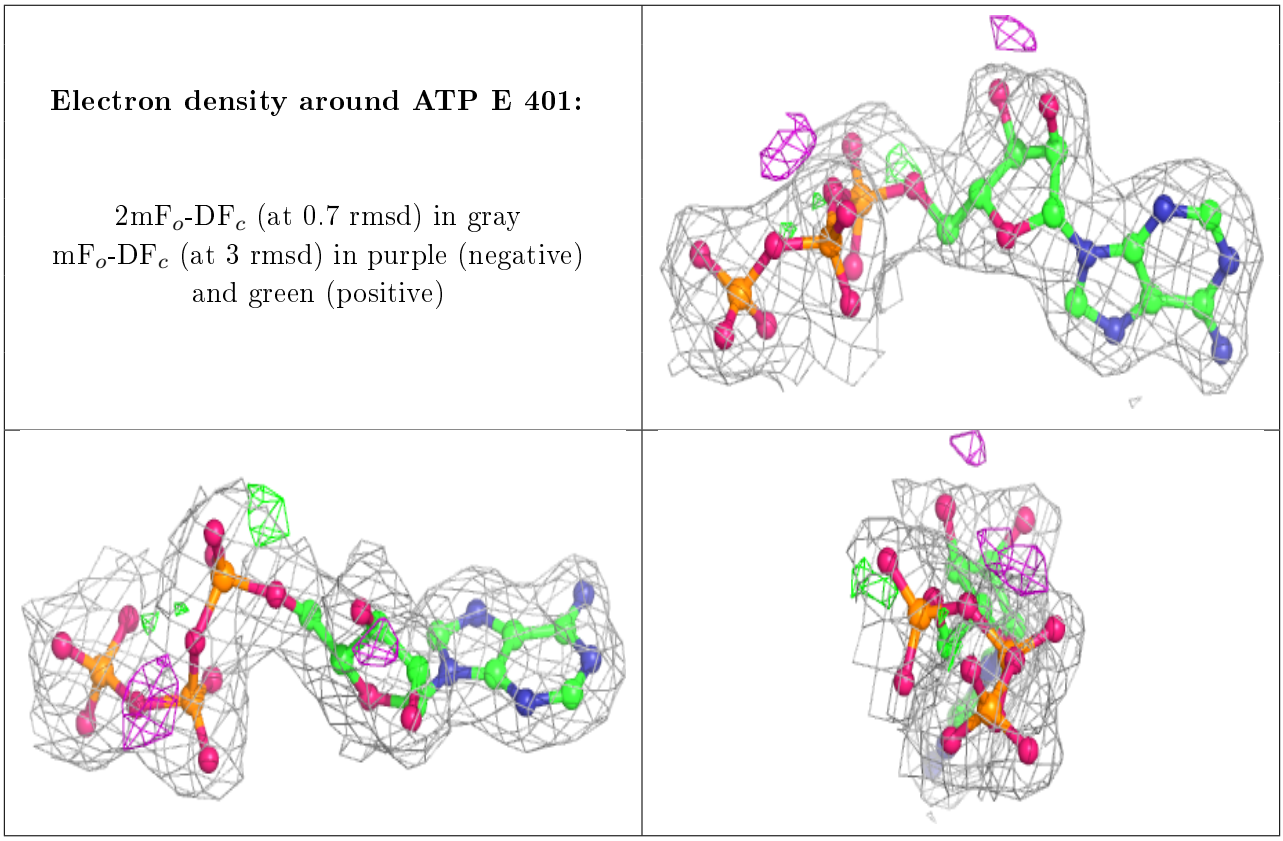
Electron density around ATP E 402:

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



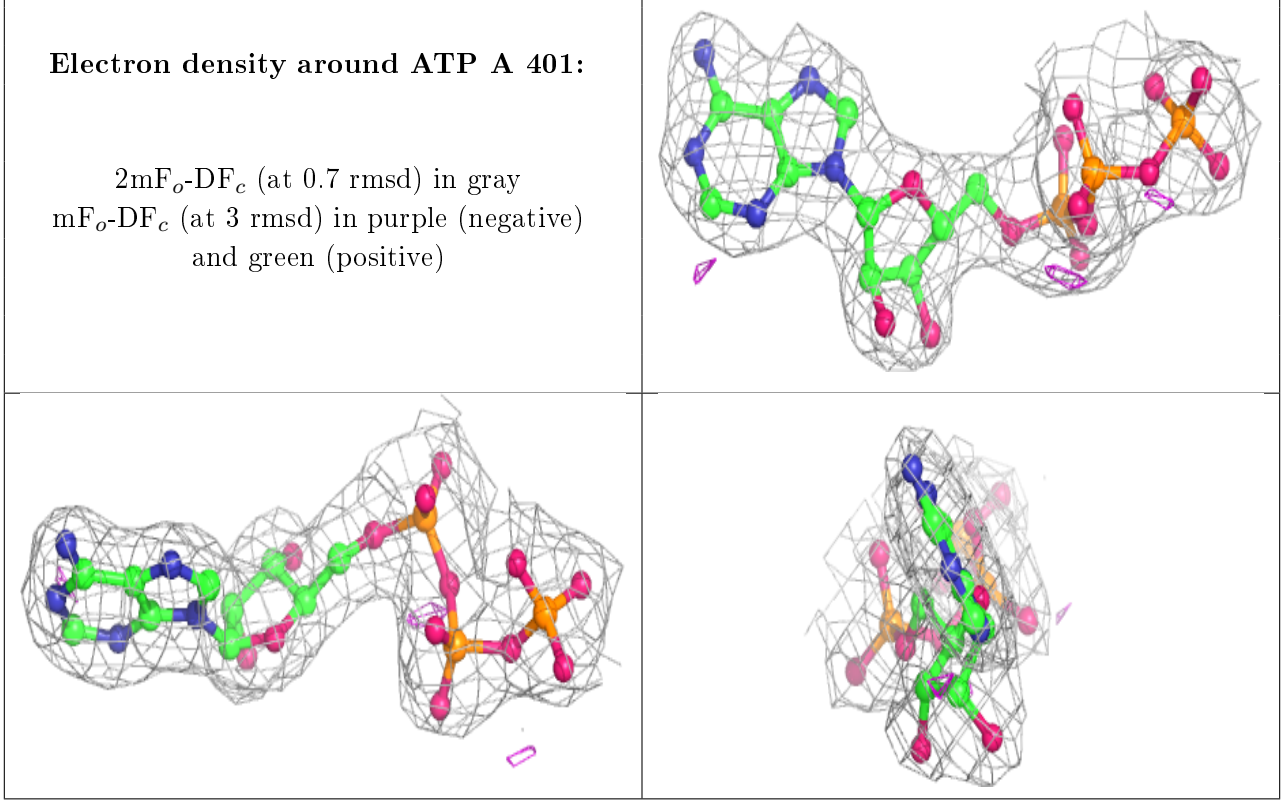
Electron density around ATP E 401:

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



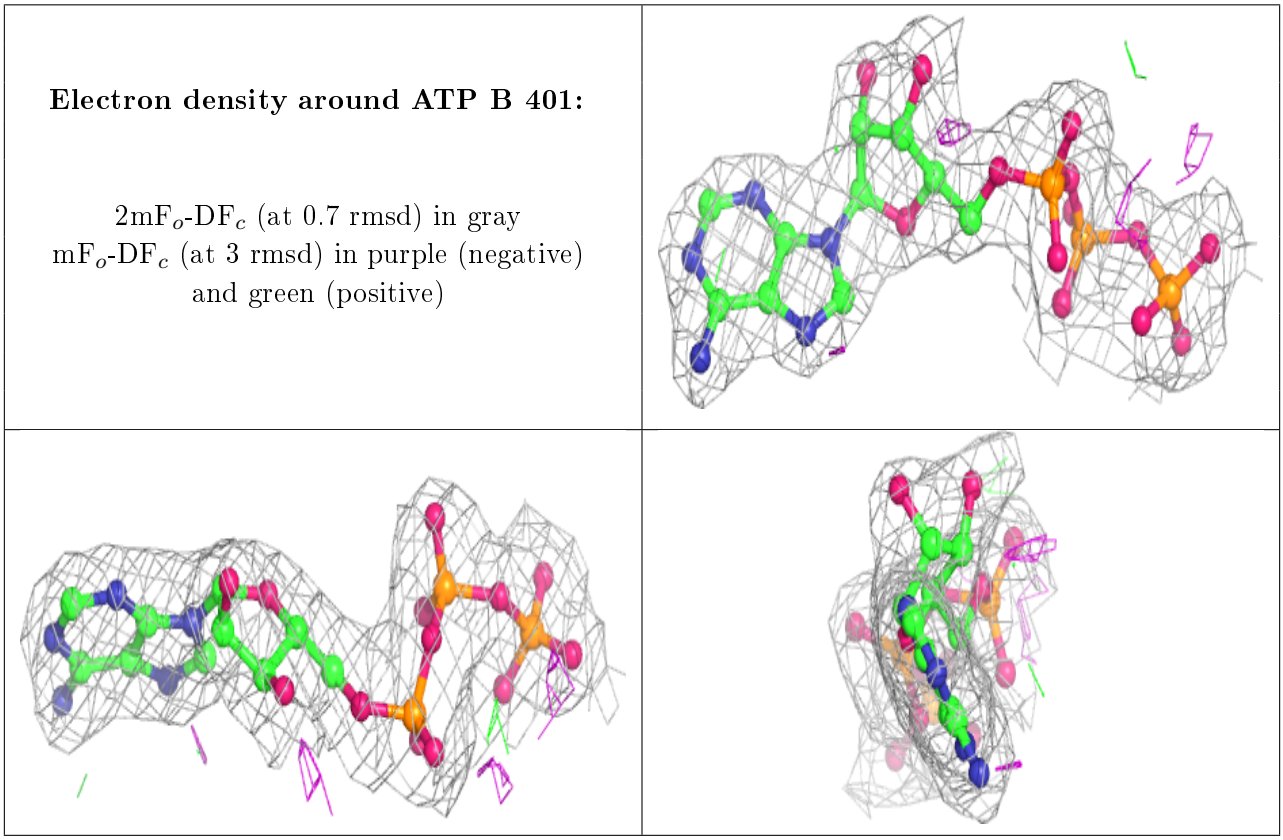
Electron density around ATP A 401:

$2mF_o$-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 401:

$2mF_o$-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.