W O R L D W I D E
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P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 6, 2024 – 11:40 pm GMT

PDB ID	:	5MCP
Title	:	Structure of IMP dehydrogenase from Ashbya gossypii bound to ATP
Authors	:	Winter, G.; Fernandez-Justel, D.; de Pereda, J.M.; Revuelta, J.L.; Buey, R.M.
Deposited on	:	2016-11-10
Resolution	:	2.40 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

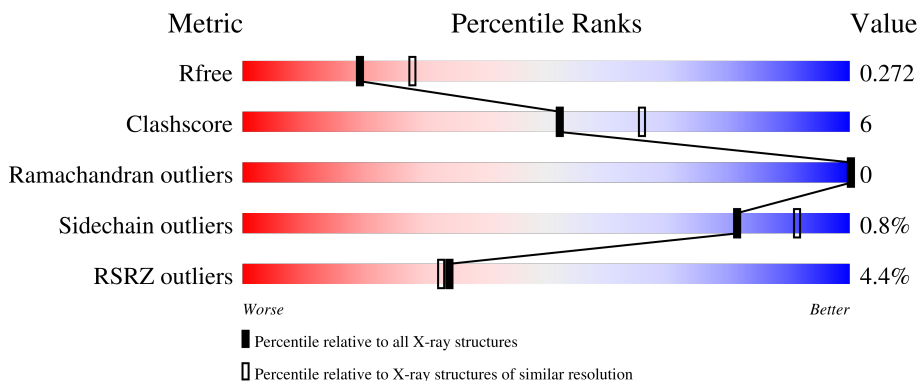|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.40 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.
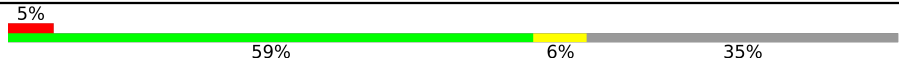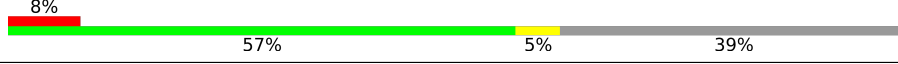
Metric	Percentile Ranks	Value
Rfree		0.272
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		4.4%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 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	523	·% ▬ 77% 7% 16%
1	B	523	2% ▬ 76% 8% 15%
1	C	523	79% 6% 15%
1	D	523	·% ▬ 76% 9% 15%
1	E	523	3% ▬ 66% 8% 26%

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Mol	Chain	Length	Quality of chain
1	F	523	5% 59% 6% 35%
1	G	523	7% 64% 9% 27%
1	H	523	8% 57% 5% 39%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 45606 atoms, of which 21090 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.
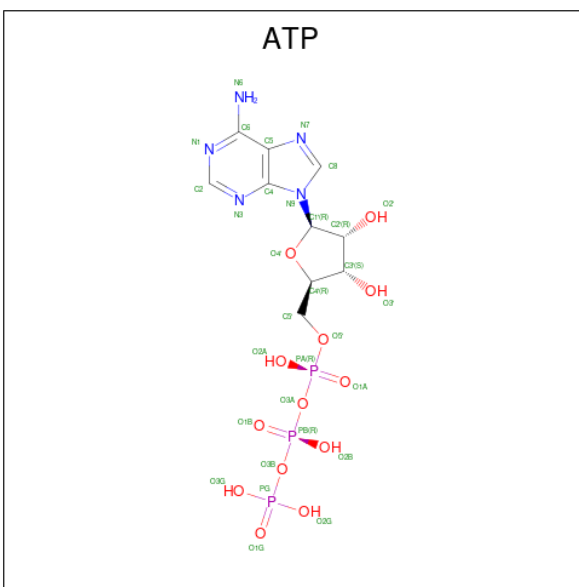
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	440	Total	C	H	N	O	S	0	0	0
			6568	2057	3293	563	632	23			
1	B	444	Total	C	H	N	O	S	0	0	0
			6442	2039	3187	564	631	21			
1	C	446	Total	C	H	N	O	S	0	1	0
			6556	2068	3260	567	637	24			
1	D	443	Total	C	H	N	O	S	0	1	0
			6541	2060	3267	566	625	23			
1	E	387	Total	C	H	N	O	S	0	0	0
			5039	1659	2384	464	517	15			
1	F	342	Total	C	H	N	O	S	0	1	0
			4054	1379	1832	407	423	13			
1	G	382	Total	C	H	N	O	S	0	0	0
			4580	1561	2066	455	484	14			
1	H	321	Total	C	H	N	O	S	0	0	0
			3526	1225	1529	374	387	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q756Z6
B	0	HIS	-	expression tag	UNP Q756Z6
C	0	HIS	-	expression tag	UNP Q756Z6
D	0	HIS	-	expression tag	UNP Q756Z6
E	0	HIS	-	expression tag	UNP Q756Z6
F	0	HIS	-	expression tag	UNP Q756Z6
G	0	HIS	-	expression tag	UNP Q756Z6
H	0	HIS	-	expression tag	UNP Q756Z6

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

ATP

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	A	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	C	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	D	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	E	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	E	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	E	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	F	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	G	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	G	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	G	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		
2	H	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	H	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
2	H	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		
3	E	2	Total	Mg	0	0
			2	2		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	277	Total	O	0	0
			277	277		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	283	Total 283	O 283	0	0
4	C	301	Total 301	O 301	0	0
4	D	285	Total 285	O 285	0	0
4	E	51	Total 51	O 51	0	0
4	F	38	Total 38	O 38	0	0
4	G	24	Total 24	O 24	0	0
4	H	17	Total 17	O 17	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Inosine-5'-monophosphate dehydrogenase

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F499 R500 T501 A504 E507 GLY GLY VAL HIS ASN LEU HIS SER TYR GLU LYS ARG LEU PHE ASP

• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain D:

HIS MET T2 D29 S30 K31 T32 G35 D40 F41 L42 S58 C101 V127 G128 P129 D130 M139 K140 F143 G144 V150 T151 D152 D153 P156 Q170 F171 V172 GLU D174 L178 A199 L203 K210 L211 L224 S225 R226 T227 S234 Q261

R262 S279 Q280 D299 L300 Q301 D322 G329 S330 GLY SER ILE CYS ILE THR GLN GLU V339 M340 A341 Q359 I373 G383 A384 P400 GLU TYR PHE PHE ARG ASP GLY LYS ARG LEU LYS THR TYR ARG GLY MET GLY SER ILE ASP ALA MET GLN LYS THR ASP

VAL LYS GLY ASN ALA ALA THR SER ARG PHE SER GLU SER ASP LYS VAL LEU VAL ALA GLN GLY VAL THR GLY SER VAL I455 G470 R481 F486 R487 R500 T501 P502 S503 A504 Q505 L506 E507 GLY GLY VAL HIS ASN LEU HIS SER TYR GLU LYS ARG LEU PHE ASP

• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain E:

HIS MET THR TYR R4 A17 E18 K19 L22 M28 R33 GLY G35 L36 L61 K64 I65 T66 F71 S74 V79 T80 E81 K114 LYS V116 N122 ALA PRO VAL V126 P129 ASP ALA THR V133 V136 M139 G144 F145 A146 GLY F148 D152

ASP GLY LYS PRO THR GLY LYS LEU GLN GLY I163 Q170 V179 SER GLU I182 T189 GLY TYR ARG GLY MET GLY SER ILE ASP ALA MET GLN LYS THR ASP

E398 S399 P400 GLY TYR PHE ARG ASP GLY LYS ARG LEU LYS THR TYR ARG GLY MET GLY SER ILE ASP ALA MET GLN LYS THR ASP VAL LYS GLY ASN ALA ALA THR SER ARG PHE SER GLU SER ASP LYS VAL LEU VAL ALA GLN GLY VAL THR GLY SER VAL LEU VAL ALA GLN GLY LYS VAL LEU VAL ALA LEU ALA GLN GLY LYS VAL LEU VAL ALA GLY SER VAL LEU VAL ALA GLY LYS VAL LEU K457

L467 I478 R487 D491 F499 ARG THR PRO SER ALA GLN LEU GLU GLY GLY VAL ASN LEU SER TYR GLU LYS ARG LEU PHE ASP

• Molecule 1: Inosine-5'-monophosphate dehydrogenase

Chain F:

HIS MET THR TYR R4 A9 A14 T15 Y16 A17 E18 K19 D20 S30 R33 G34 GLY L36 T37 Y38 F41 S53 GLU VAL V56 L57 L61 T66 L67 ASN A69 H87 M88 A89 L90 LEU GLY ILE GLY G95 E117 ASN GLY F120 ILE ASN ALA P124 V125 V126

V127 G128 P129 ASP ALA THR V133 F143 GLY F145 P149 V150 THR ASP ASP GLY LYS PRO THR GLY LYS LEU GLN GLY I163 D168 F171 VAL GLU ASP E175 M183 THR K185 I188 THR GLY LYS GLN ILE ASN L196 K207 K208 GLY LYS LEU PRO ILE VAL ASP GLU

ALA GLY CYS LEU VAL SER MET LEU SER SER ARG THR ASP MET LEU MET K231 A238 S239 LYS SER ALA ASP THR K245 L248 T255 V275 Q280 G281 Q286 D299 I303 E311 Q312 G320 G327 M328 GLY SER GLY SER ILE CYS ILE THR GLN GLU VAL MET A341

Q346 A349 V350 Y351 A366 ASP GLY GLY VAL Q371 H375 I376 T377 K378 A379 L382 L393 ALA GLY THR GLU SER PRO GLY GLU TYR PHE ARG ASP GLY LYS ARG LEU LYS THR TYR ARG GLY MET GLY SER ILE ASP ALA MET GLN LYS THR ASP VAL LYS GLY

ASN ALA ALA THR SER ARG TYR PHE SER SER GLU SER ASP LYS VAL LEU VAL ALA GLN GLY VAL THR GLY SER VAL ASP LYS SER ILE LYS LYS TYR I464 S474 V480 R481 SER L483 F486 R487 S494 F499 ARG THR PRO SER ALA GLN LYS THR ASP VAL GLY GLY VAL HIS

ASN LEU HIS TYR GLU ARG LEU PHE ASP

• **Molecule 1:** Inosine-5'-monophosphate dehydrogenase

Chain G:

7%

64%   9%   27%

HIS MET THR Y3 R4 D5 Q26 L27 M28 R33 GLY GLY LEU T37 Y38 N39 D40 F41 F50 S53 L61 F71 S74 E81 A82 D83 H87 M88 A89 I97 H98 H99 V110 F120 ILE ASN ALA PRO VAL VAL VAL GLY PRO ASP A131 T132 V133

K140 G144 F145 V150 THR ASP ASP G154 L160 I163 I164 E173 E175 T176 L177 L178 V179 M183 T189 GLY LYS GLN ILE ASN L196 E197 E198 K207 P212 I213 VAL ASP GLU ALA GLY CYS LEU VAL SER MET LEU S225 R226 THR ASP LEU MET LYS ASN

GLN S234 Y235 P236 L237 A238 S239 K240 S241 ALA ASP T244 A252 I253 G254 THR I256 V275 D277 S278 S279 GLN G281 A304 A313 A314 S315 L316 A319 G320 G329 SER GLY SER ILE CYS ILE THR GLN GLU VAL MET ALA CYS GLY R344 V350 V353 T354 Q355 F356

G368 G369 A381 M388 M389 G390 G391 M392 LEU ALA G395 E398 S399 P400 GLY GLU TYR PHE PHE ARG ASP GLY LYS ARG LEU LYS THR TYR ARG GLY MET GLY SER ILE ASP ALA MET GLN LYS ASP VAL LYS ASN ALA ALA THR SER ARG TYR PHE SER GLU SER ASP

LYS VAL LEU VAL ALA GLN GLY VAL THR GLY SER VAL ILE ASP K457 G458 S459 I460 P465 Y466 L467 N469 G470 L471 Q472 Q476 G479 V480 R481 R487 R500 T501 PRO SER ALA GLN LEU GLU GLY GLY VAL HIS ASN LEU HIS SER TYR GLU LYS ARG LEU PHE ASP

• **Molecule 1:** Inosine-5'-monophosphate dehydrogenase

Chain H:

8%

57%   5%   39%

HIS MET THR Y3 A6 A9 L10 E11 H12 L13 A14 T15 Y16 ALA E18 G21 L22 M28 ASP SER LYS THR ARG GLY GLY LEU T37 Y38 F41 P45 GLY LYS ILE ASP F50 S53 GLU VAL V56 V72 S73 S74 A89 G93 I94 I97 H98 HIS ASN

CYS T102 V110 K114 K115 Y116 GLU ASN GLY PHE ILE ASN ALA P124 P129 ASP ALA T132 M139 F143 GLY F145 F148 P149 V150 T151 ASP GLY LYS PRO THR GLY LYS LEU GLN G162 I163 T176 I188 THR GLY LYS GLN GLY ILE ASN LEU GLU GLU ALA ASN

Q201 I202 L203 K204 N205 K210 LEU PRO ILE VAL ASP GLU ALA GLY CYS LEU VAL SER M223 D228 LEU MET LYS ASN GLN S234 A238 S241 A242 ASP T244 L247 L248 C249 GLY ALA ALA ILE GLY THR ILE ASP ALA ASP R260 A269 G270 L271 ASP VAL VAL VAL LEU ASP

SER SER Q280 G281 N282 SER V284 K291 T296 L300 I303 A304 G305 N306 V307 V308 T309 R310 A313 A321 D322 G323 L324 R325 I326 G327 M328 GLY SER GLY SER ILE CYS ILE THR GLN GLU VAL MET A341 F360 D367 GLY GLY VAL Q371 A384 S385 THR V387 M388

M389 GLY GLY MET LEU ALA GLY THR THR GLU SER PRO GLY GLU TYR PHE PHE ARG ASP GLY LYS ARG LEU LYS THR TYR ARG GLY MET GLY SER ILE ASP ALA MET GLN LYS THR ASP VAL LYS GLY ASN ALA ALA THR SER ARG TYR PHE SER GLU SER ASP LYS VAL LEU VAL LEU VAL ALA GLN

GLY VAL THR GLY SER VAL ILE ASP LYS GLY SER ILE LYS LYS Y463 L467 F486 R487 F499 ARG THR PRO SER ALA GLN LEU GLU GLY GLY VAL HIS ASN LEU HIS SER TYR GLU LYS ARG LEU PHE ASP

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	127.89Å 152.09Å 152.25Å 90.00° 93.03° 90.00°	Depositor
Resolution (Å)	152.04 – 2.40 152.04 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (152.04-2.40) 92.3 (152.04-2.40)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.11_2567: ???)	Depositor
R, R_{free}	0.249 , 0.271 0.250 , 0.272	Depositor DCC
R_{free} test set	11359 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.0	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	45606	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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

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	0.36	2/3318 (0.1%)	0.48	0/4484
1	B	0.32	0/3300	0.49	0/4469
1	C	0.36	0/3345	0.51	0/4526
1	D	0.30	0/3322	0.48	0/4493
1	E	0.38	0/2678	0.51	0/3629
1	F	0.27	0/2241	0.44	0/3038
1	G	0.36	0/2544	0.50	0/3459
1	H	0.32	0/2004	0.46	0/2716
All	All	0.34	2/22752 (0.0%)	0.49	0/30814

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	ARG	CZ-NH2	7.18	1.42	1.33
1	A	33	ARG	CZ-NH1	6.72	1.41	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	305	GLY	Peptide

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	3275	3293	3286	38	0
1	B	3255	3187	3194	39	0
1	C	3296	3260	3260	25	0
1	D	3274	3267	3262	40	0
1	E	2655	2384	2365	42	0
1	F	2222	1832	1816	21	0
1	G	2514	2066	2057	38	0
1	H	1997	1529	1508	15	0
2	A	93	34	36	6	0
2	B	155	56	60	4	0
2	C	93	34	36	3	0
2	D	93	34	36	4	0
2	E	93	34	36	1	0
2	F	31	12	12	1	0
2	G	93	34	36	4	0
2	H	93	34	36	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	277	0	0	11	0
4	B	283	0	0	7	0
4	C	301	0	0	9	2
4	D	285	0	0	8	2
4	E	51	0	0	5	0
4	F	38	0	0	4	0
4	G	24	0	0	3	0
4	H	17	0	0	0	0
All	All	24516	21090	21036	244	2

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 6.

The worst 5 of 244 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:PHE:CD1	1:E:389:MET:HE3	1.74	1.22
1:G:133:VAL:HG23	1:G:177:LEU:O	1.38	1.22
1:E:64:LYS:HB2	1:E:301:GLN:NE2	1.54	1.20
1:E:71:PHE:CD1	1:E:389:MET:CE	2.26	1.18
1:E:71:PHE:HD1	1:E:389:MET:CE	1.57	1.14

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:705:HOH:O	4:D:802:HOH:O[2_554]	2.09	0.11
4:C:975:HOH:O	4:D:873:HOH:O[2_554]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	430/523 (82%)	421 (98%)	9 (2%)	0	100	100
1	B	436/523 (83%)	430 (99%)	6 (1%)	0	100	100
1	C	441/523 (84%)	432 (98%)	9 (2%)	0	100	100
1	D	436/523 (83%)	426 (98%)	10 (2%)	0	100	100
1	E	356/523 (68%)	343 (96%)	13 (4%)	0	100	100
1	F	306/523 (58%)	295 (96%)	11 (4%)	0	100	100
1	G	354/523 (68%)	346 (98%)	8 (2%)	0	100	100
1	H	279/523 (53%)	272 (98%)	7 (2%)	0	100	100
All	All	3038/4184 (73%)	2965 (98%)	73 (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	350/430 (81%)	347 (99%)	3 (1%)	78	90
1	B	337/430 (78%)	334 (99%)	3 (1%)	78	90
1	C	345/430 (80%)	342 (99%)	3 (1%)	78	90
1	D	343/430 (80%)	339 (99%)	4 (1%)	71	85
1	E	234/430 (54%)	234 (100%)	0	100	100
1	F	165/430 (38%)	164 (99%)	1 (1%)	86	94
1	G	191/430 (44%)	190 (100%)	1 (0%)	88	95
1	H	128/430 (30%)	127 (99%)	1 (1%)	81	91
All	All	2093/3440 (61%)	2077 (99%)	16 (1%)	81	91

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	487	ARG
1	F	487	ARG
1	C	487	ARG
1	D	487	ARG
1	C	486	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	359	GLN
1	E	286	GLN
1	E	301	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	ATP	B	602	3	26,33,33	1.81	3 (11%)	31,52,52	2.33	8 (25%)
2	ATP	C	602	3	26,33,33	1.73	2 (7%)	31,52,52	2.36	10 (32%)
2	ATP	A	601	3	26,33,33	1.77	4 (15%)	31,52,52	2.34	10 (32%)
2	ATP	H	602	3	26,33,33	1.91	5 (19%)	31,52,52	2.30	10 (32%)
2	ATP	E	601	3	26,33,33	1.98	3 (11%)	31,52,52	2.18	9 (29%)
2	ATP	D	602	3	26,33,33	1.81	3 (11%)	31,52,52	2.27	10 (32%)
2	ATP	E	603	-	26,33,33	1.91	5 (19%)	31,52,52	2.26	7 (22%)
2	ATP	E	602	3	26,33,33	1.84	3 (11%)	31,52,52	2.35	9 (29%)
2	ATP	C	603	-	26,33,33	1.83	4 (15%)	31,52,52	2.28	8 (25%)
2	ATP	G	601	3	26,33,33	1.84	4 (15%)	31,52,52	2.35	9 (29%)
2	ATP	B	605	3	26,33,33	1.86	4 (15%)	31,52,52	2.37	8 (25%)
2	ATP	G	602	3	26,33,33	1.94	4 (15%)	31,52,52	2.32	8 (25%)
2	ATP	B	606	3	26,33,33	1.86	3 (11%)	31,52,52	2.33	9 (29%)
2	ATP	G	603	-	26,33,33	1.86	4 (15%)	31,52,52	2.20	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	ATP	F	601	-	26,33,33	1.92	3 (11%)	31,52,52	2.28	9 (29%)
2	ATP	D	603	-	26,33,33	1.86	4 (15%)	31,52,52	2.36	9 (29%)
2	ATP	A	603	-	26,33,33	1.85	4 (15%)	31,52,52	2.34	9 (29%)
2	ATP	H	601	3	26,33,33	1.85	4 (15%)	31,52,52	2.38	10 (32%)
2	ATP	C	601	3	26,33,33	1.87	4 (15%)	31,52,52	2.35	10 (32%)
2	ATP	A	602	3	26,33,33	1.86	2 (7%)	31,52,52	2.31	10 (32%)
2	ATP	B	603	-	26,33,33	1.79	3 (11%)	31,52,52	2.32	10 (32%)
2	ATP	D	601	3	26,33,33	1.73	3 (11%)	31,52,52	2.37	10 (32%)
2	ATP	H	603	-	26,33,33	1.84	3 (11%)	31,52,52	2.30	9 (29%)
2	ATP	B	601	3	26,33,33	1.84	4 (15%)	31,52,52	2.35	9 (29%)

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	B	602	3	-	0/18/38/38	0/3/3/3
2	ATP	C	602	3	-	5/18/38/38	0/3/3/3
2	ATP	A	601	3	-	1/18/38/38	0/3/3/3
2	ATP	H	602	3	-	6/18/38/38	0/3/3/3
2	ATP	E	601	3	-	1/18/38/38	0/3/3/3
2	ATP	D	602	3	-	6/18/38/38	0/3/3/3
2	ATP	E	603	-	-	2/18/38/38	0/3/3/3
2	ATP	E	602	3	-	3/18/38/38	0/3/3/3
2	ATP	C	603	-	-	0/18/38/38	0/3/3/3
2	ATP	G	601	3	-	2/18/38/38	0/3/3/3
2	ATP	B	605	3	-	4/18/38/38	0/3/3/3
2	ATP	G	602	3	-	1/18/38/38	0/3/3/3
2	ATP	B	606	3	-	3/18/38/38	0/3/3/3
2	ATP	G	603	-	-	4/18/38/38	0/3/3/3
2	ATP	F	601	-	-	5/18/38/38	0/3/3/3
2	ATP	D	603	-	-	2/18/38/38	0/3/3/3
2	ATP	A	603	-	-	0/18/38/38	0/3/3/3
2	ATP	H	601	3	-	2/18/38/38	0/3/3/3
2	ATP	C	601	3	-	4/18/38/38	0/3/3/3
2	ATP	A	602	3	-	4/18/38/38	0/3/3/3

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W O R L D W I D E
PDB
PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	B	603	-	-	3/18/38/38	0/3/3/3
2	ATP	D	601	3	-	2/18/38/38	0/3/3/3
2	ATP	H	603	-	-	2/18/38/38	0/3/3/3
2	ATP	B	601	3	-	1/18/38/38	0/3/3/3

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	ATP	PA-O5'	8.38	1.93	1.59
2	F	601	ATP	PA-O5'	7.81	1.90	1.59
2	H	602	ATP	PA-O5'	7.73	1.90	1.59
2	A	602	ATP	PA-O5'	7.70	1.90	1.59
2	G	602	ATP	PA-O5'	7.63	1.90	1.59

The worst 5 of 219 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	603	ATP	PA-O3A-PB	-7.02	108.74	132.83
2	B	606	ATP	PA-O3A-PB	-6.91	109.12	132.83
2	H	601	ATP	PA-O3A-PB	-6.85	109.31	132.83
2	G	601	ATP	PA-O3A-PB	-6.82	109.41	132.83
2	A	601	ATP	PA-O3A-PB	-6.81	109.47	132.83

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	ATP	C5'-O5'-PA-O1A
2	A	602	ATP	C5'-O5'-PA-O2A
2	B	601	ATP	PB-O3B-PG-O3G
2	B	605	ATP	C5'-O5'-PA-O3A
2	C	602	ATP	PB-O3B-PG-O2G

There are no ring outliers.

15 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	ATP	1	0
2	C	602	ATP	1	0
2	A	601	ATP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	601	ATP	1	0
2	D	602	ATP	3	0
2	C	603	ATP	1	0
2	B	605	ATP	2	0
2	G	602	ATP	1	0
2	G	603	ATP	3	0
2	F	601	ATP	1	0
2	D	603	ATP	1	0
2	A	603	ATP	2	0
2	C	601	ATP	2	0
2	A	602	ATP	2	0
2	B	603	ATP	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 ATP B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP H 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP E 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP D 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP E 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP E 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP G 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 605

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP G 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 606

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP G 603

Bond lengths

Bond angles

Torsions

Rings

wwPDB X-ray Structure Validation Summary Report

Ligand ATP F 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP D 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP H 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 602

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP D 601

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP H 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 601

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	440/523 (84%)	-0.10	3 (0%)	87	86	19, 36, 92, 167	0
1	B	444/523 (84%)	-0.09	11 (2%)	57	55	22, 37, 100, 144	0
1	C	446/523 (85%)	-0.11	0	100	100	20, 36, 95, 159	0
1	D	443/523 (84%)	-0.07	7 (1%)	72	70	20, 35, 91, 124	0
1	E	387/523 (73%)	0.23	18 (4%)	31	30	23, 99, 141, 182	0
1	F	342/523 (65%)	0.42	26 (7%)	13	12	71, 110, 146, 183	0
1	G	382/523 (73%)	0.52	36 (9%)	8	7	30, 106, 152, 182	0
1	H	321/523 (61%)	0.62	40 (12%)	3	3	80, 114, 153, 183	0
All	All	3205/4184 (76%)	0.15	141 (4%)	34	33	19, 77, 137, 183	0

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	320	GLY	5.6
1	G	38	TYR	5.4
1	H	9	ALA	4.8
1	H	326	ILE	4.8
1	F	38	TYR	4.5

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	605	1/1	0.54	0.17	113,113,113,113	0
3	MG	B	604	1/1	0.60	0.13	79,79,79,79	0
3	MG	C	604	1/1	0.69	0.37	89,89,89,89	0
2	ATP	G	603	31/31	0.74	0.26	100,106,122,125	43
3	MG	E	605	1/1	0.76	0.17	93,93,93,93	0
2	ATP	B	606	31/31	0.77	0.19	97,103,121,123	0
2	ATP	E	603	31/31	0.80	0.20	133,141,164,166	0
2	ATP	H	603	31/31	0.80	0.19	101,111,126,129	43
2	ATP	E	602	31/31	0.84	0.17	100,102,121,124	0
2	ATP	F	601	31/31	0.84	0.13	118,133,146,153	0
2	ATP	H	602	31/31	0.86	0.14	92,97,112,117	0
2	ATP	G	602	31/31	0.86	0.15	98,105,122,123	0
2	ATP	E	601	31/31	0.87	0.13	83,90,105,109	0
3	MG	G	604	1/1	0.87	0.28	64,64,64,64	0
2	ATP	H	601	31/31	0.88	0.13	89,97,114,119	0
2	ATP	C	601	31/31	0.89	0.16	64,69,81,82	0
2	ATP	C	602	31/31	0.89	0.16	46,54,70,93	0
2	ATP	B	603	31/31	0.90	0.13	54,62,72,72	0
2	ATP	B	605	31/31	0.91	0.12	92,100,118,127	0
2	ATP	G	601	31/31	0.91	0.12	81,89,103,108	0
2	ATP	A	603	31/31	0.91	0.13	47,57,71,71	0
2	ATP	D	603	31/31	0.91	0.14	53,59,73,74	0
3	MG	F	602	1/1	0.92	0.24	95,95,95,95	0
2	ATP	C	603	31/31	0.92	0.14	50,59,70,73	0
2	ATP	D	602	31/31	0.93	0.13	45,49,63,68	0
2	ATP	A	601	31/31	0.93	0.16	50,58,67,70	0
2	ATP	A	602	31/31	0.94	0.15	49,55,64,68	0
2	ATP	B	601	31/31	0.94	0.14	63,67,80,84	0
2	ATP	B	602	31/31	0.94	0.12	49,59,67,68	0
2	ATP	D	601	31/31	0.95	0.13	49,51,61,75	0
3	MG	D	604	1/1	0.95	0.18	87,87,87,87	0
3	MG	E	604	1/1	0.95	0.34	86,86,86,86	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 G 603:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
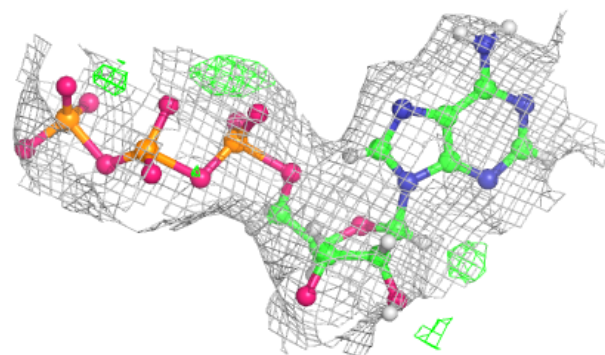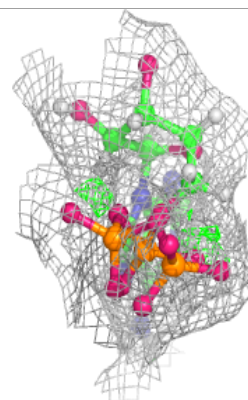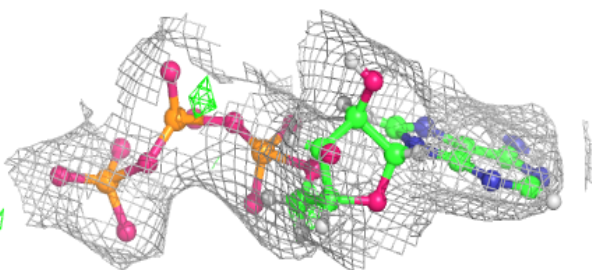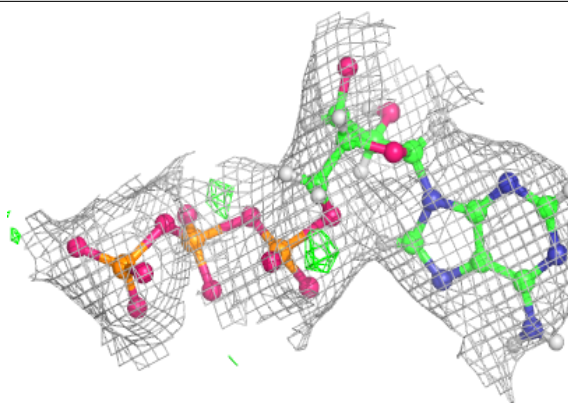and green (positive)
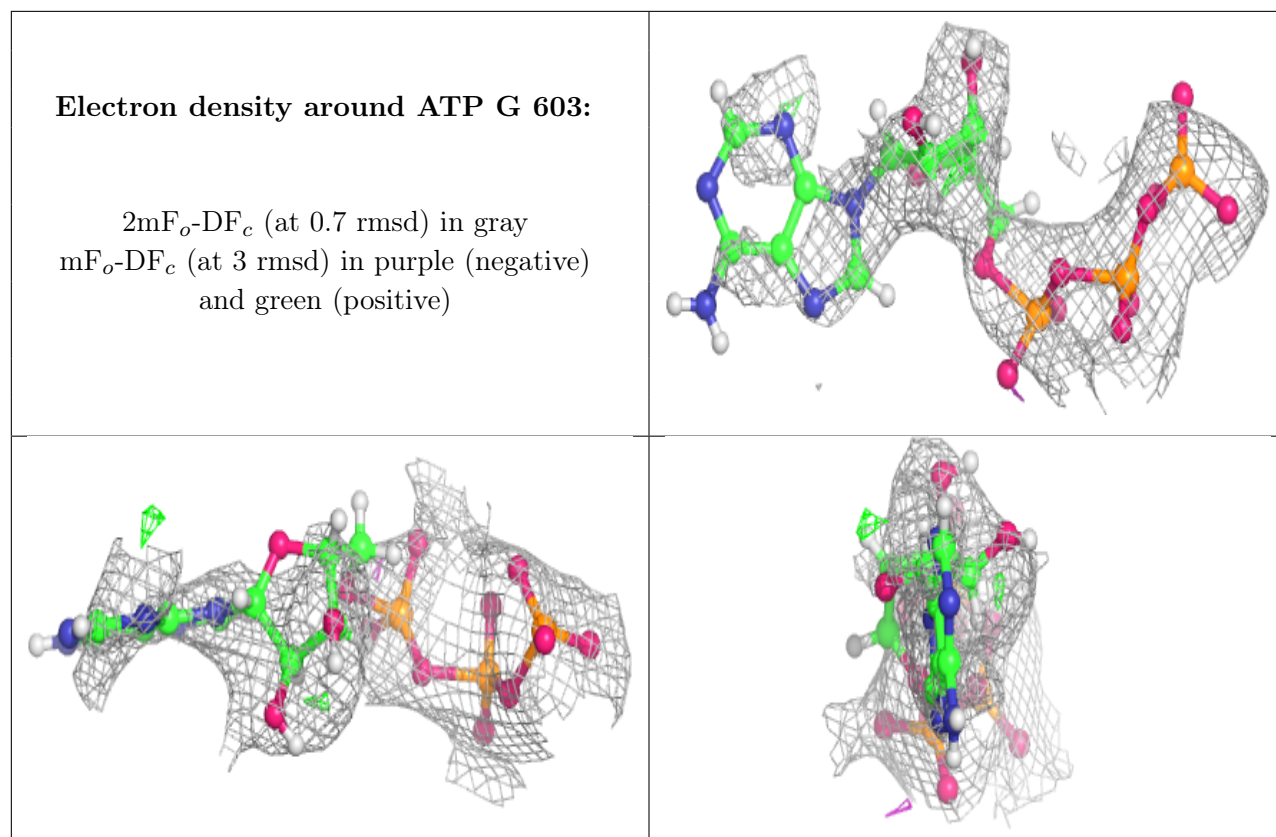
Electron density around ATP B 606:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
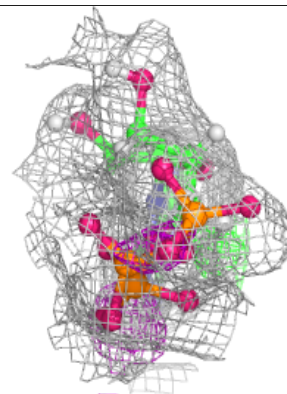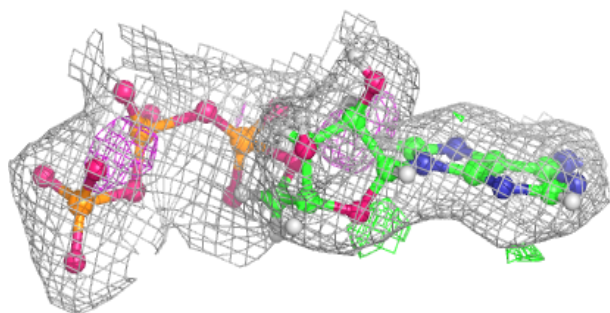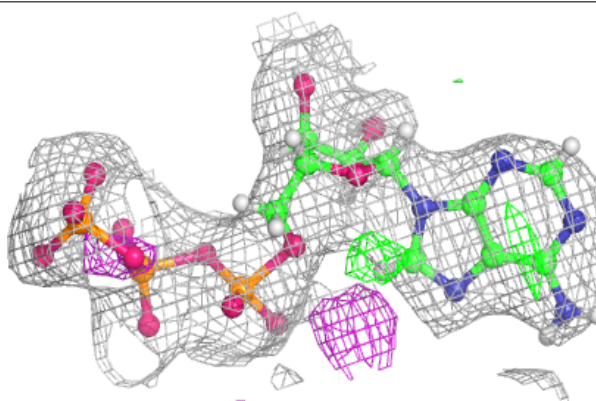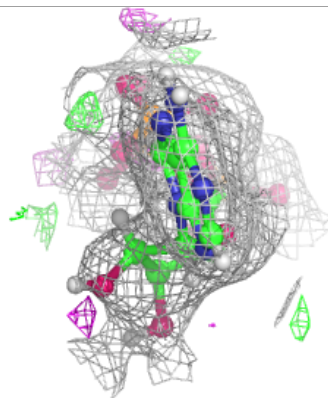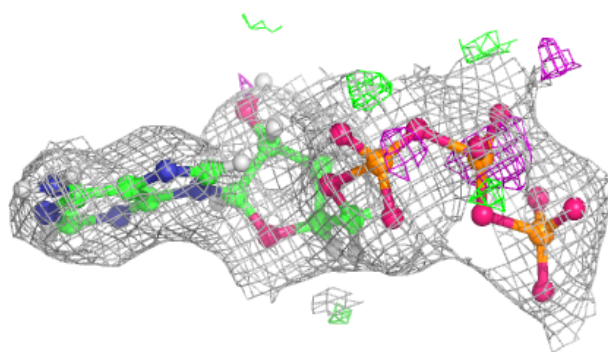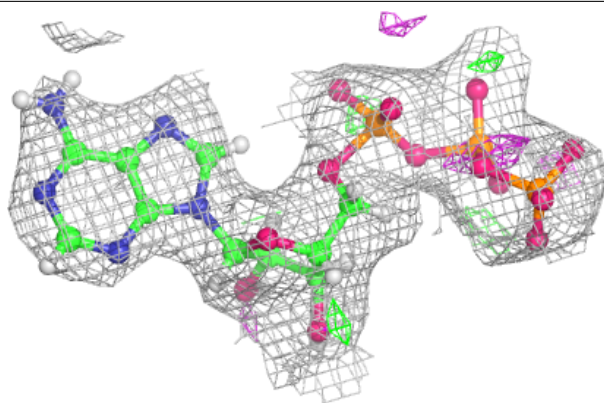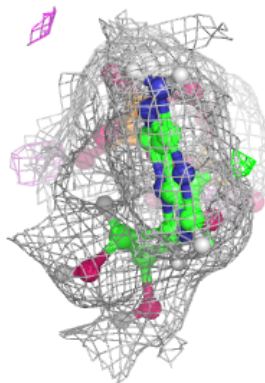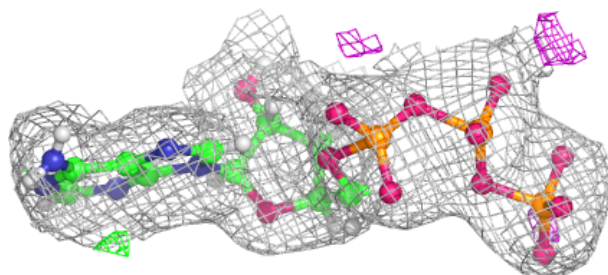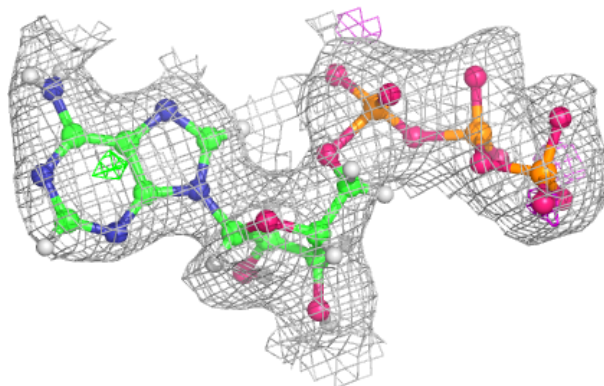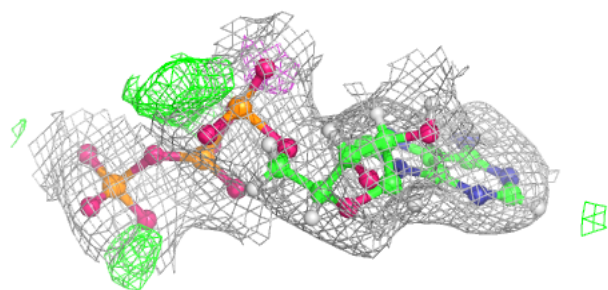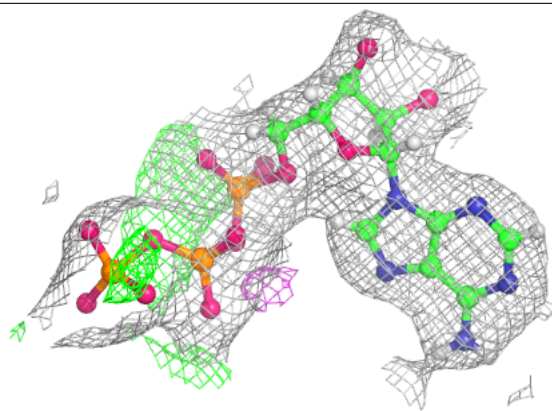mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
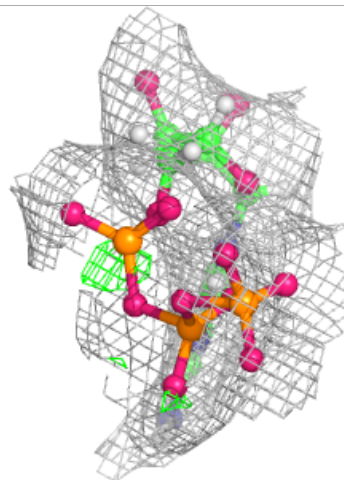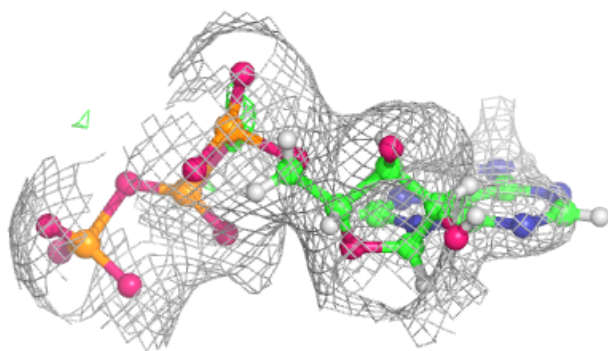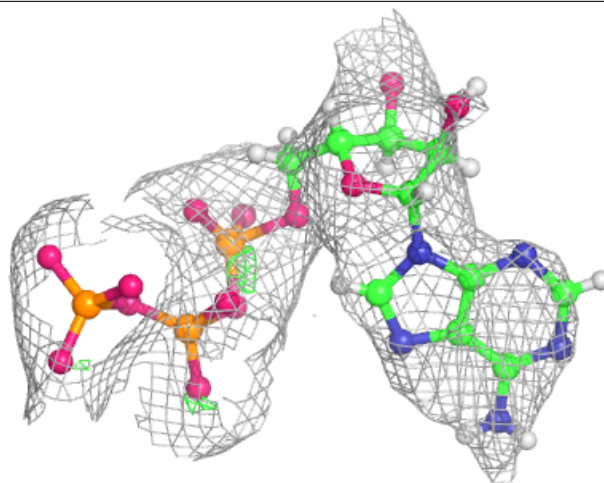
Electron density around ATP E 603:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
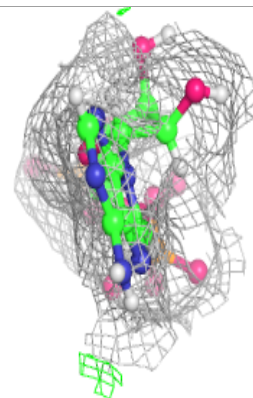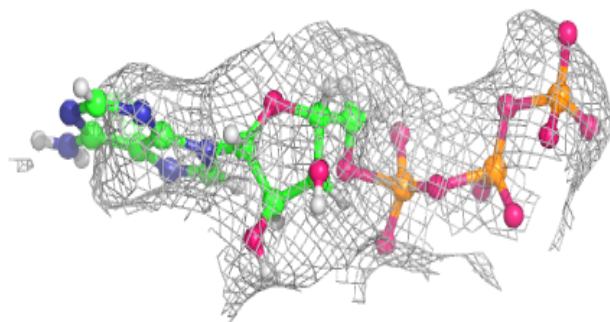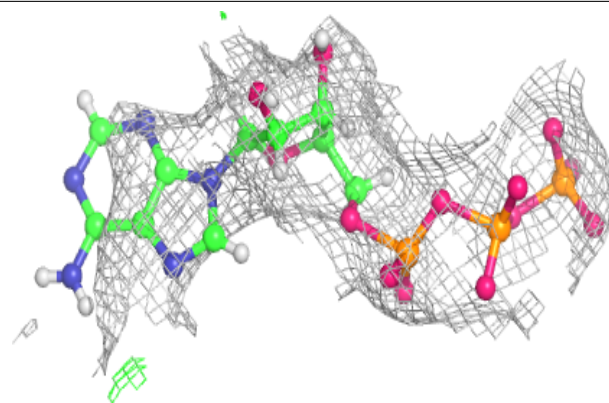
Electron density around ATP H 603:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
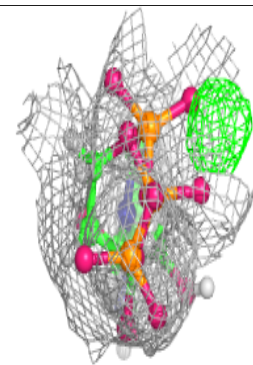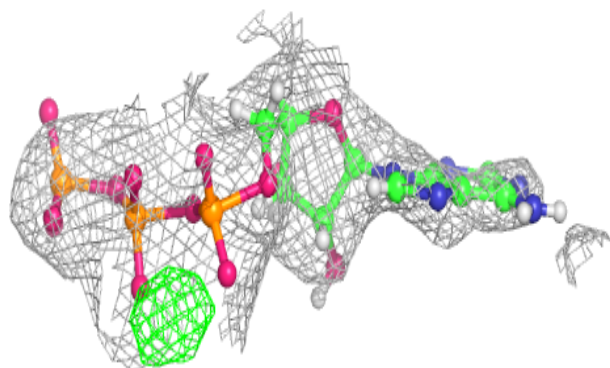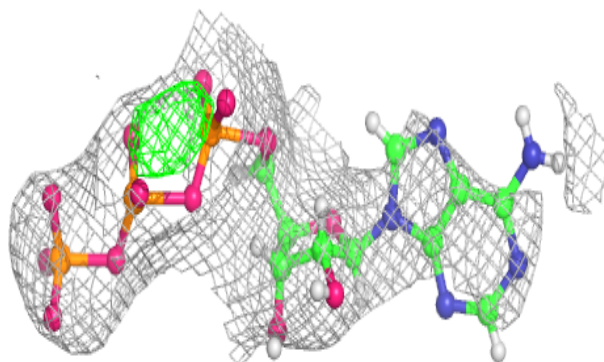
Electron density around ATP E 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
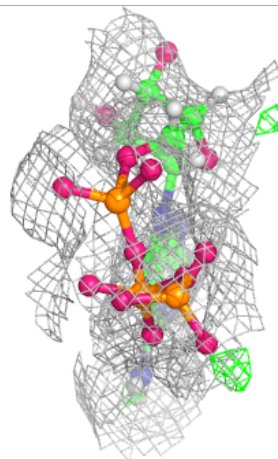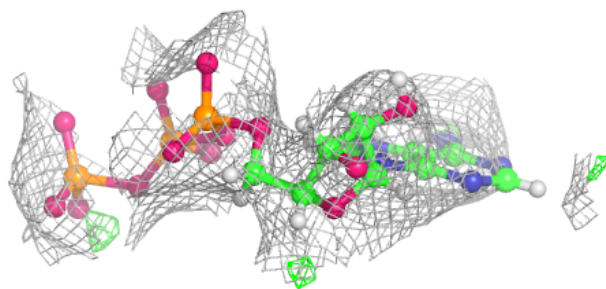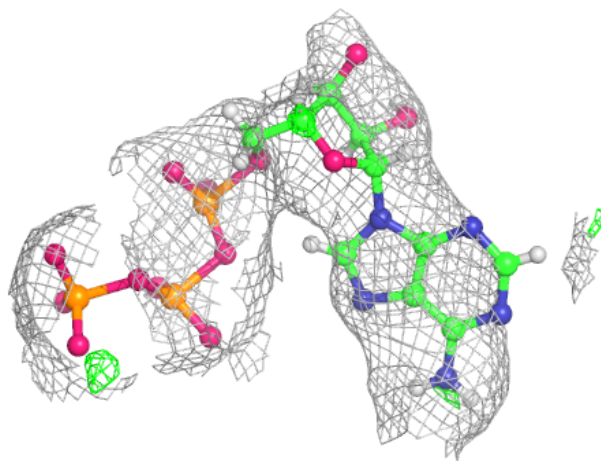
Electron density around ATP F 601:

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

Electron density around ATP H 602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
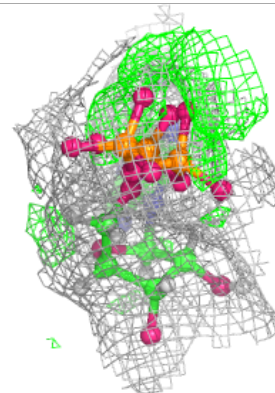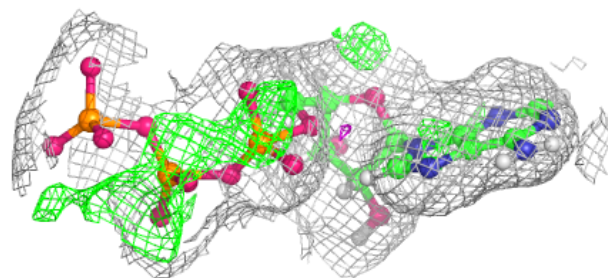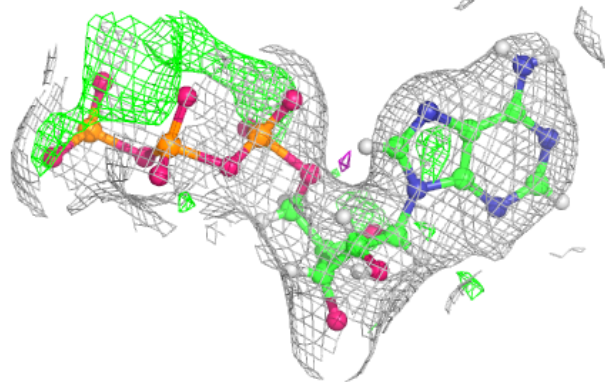and green (positive)
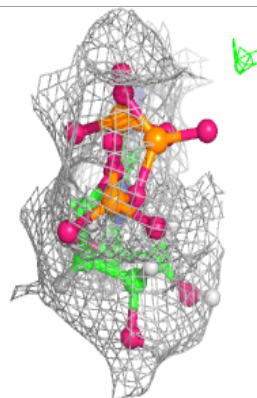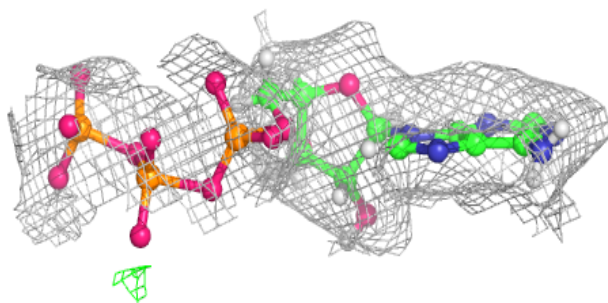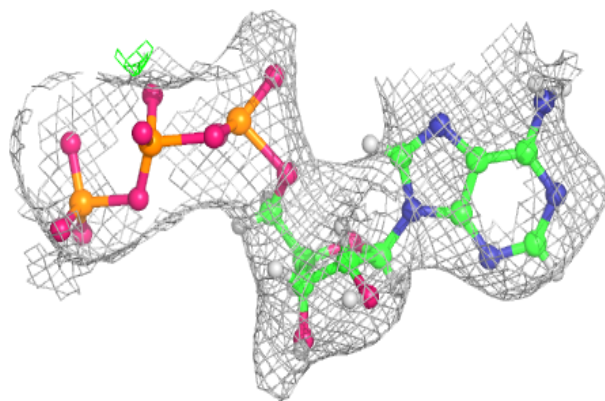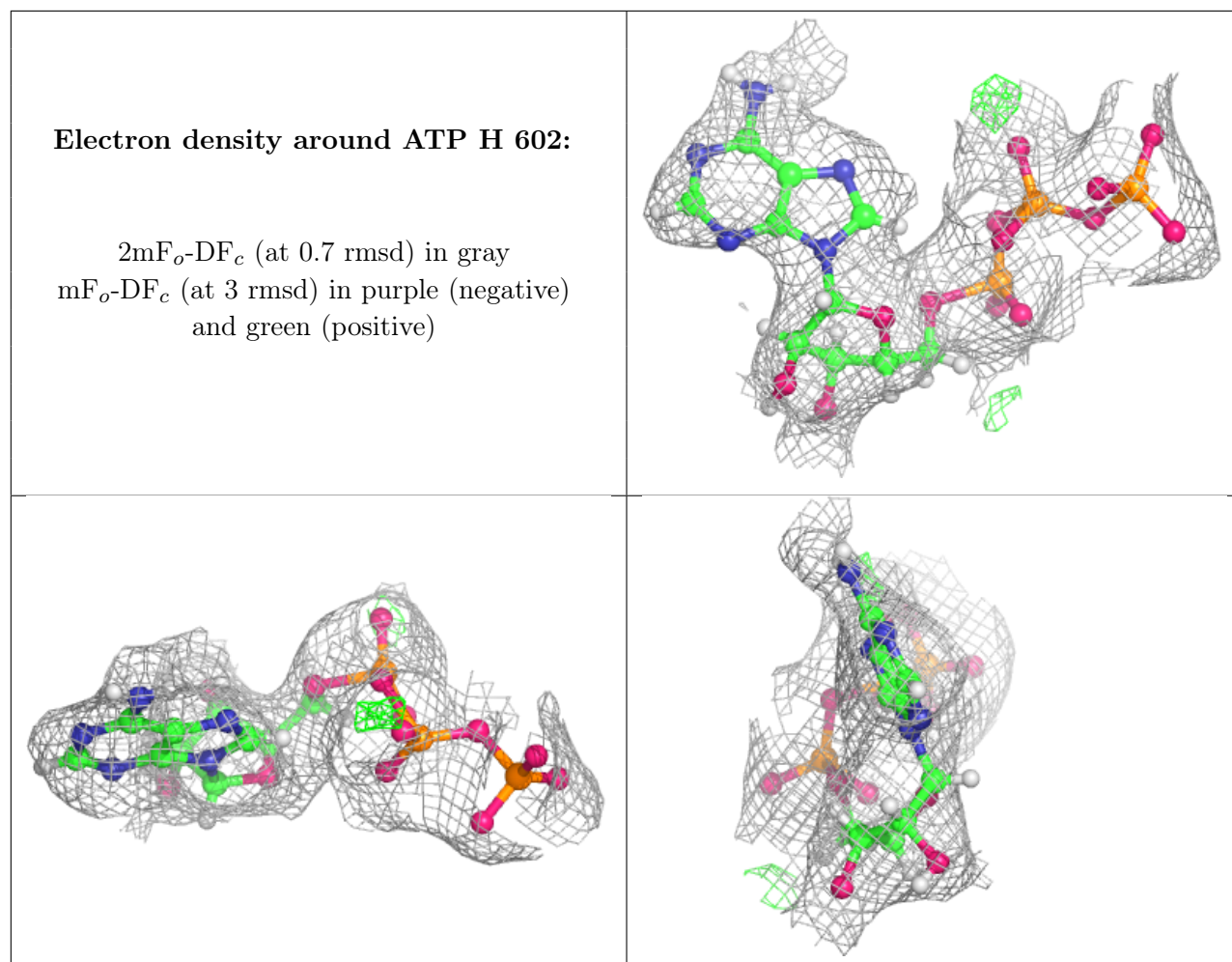
Electron density around ATP G 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
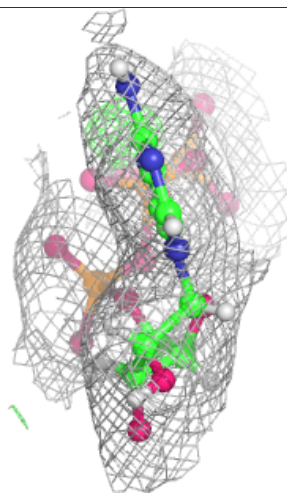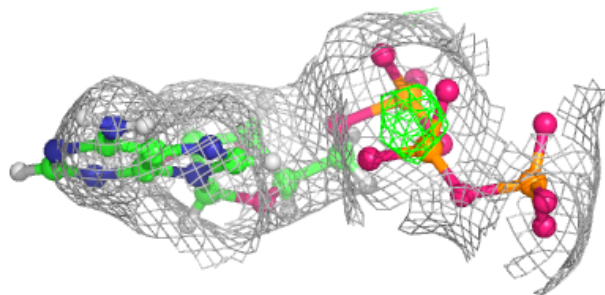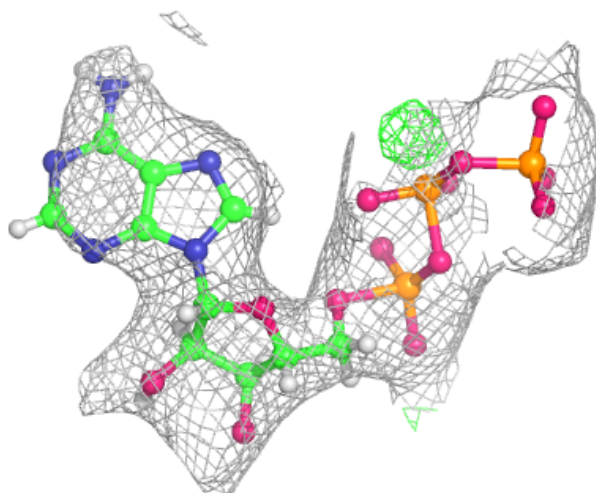
Electron density around ATP E 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
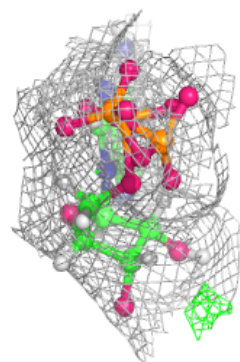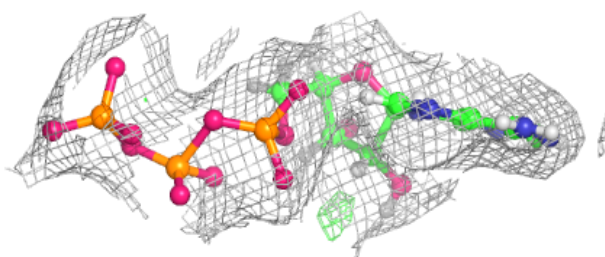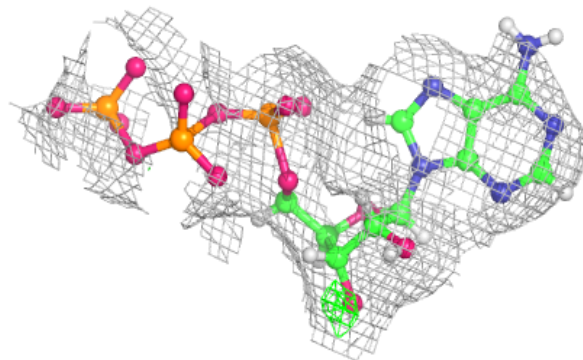
Electron density around ATP H 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
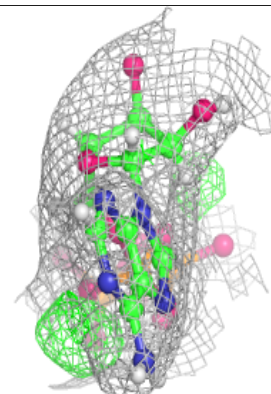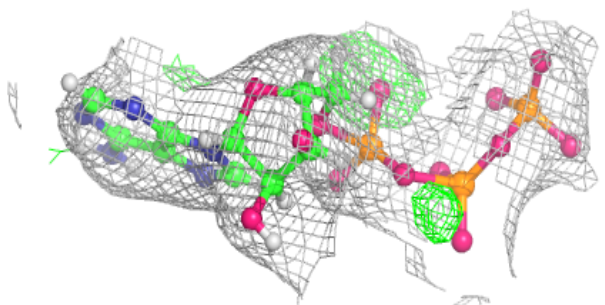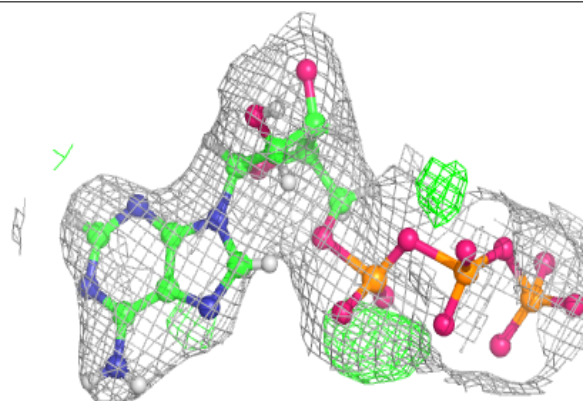
Electron density around ATP C 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
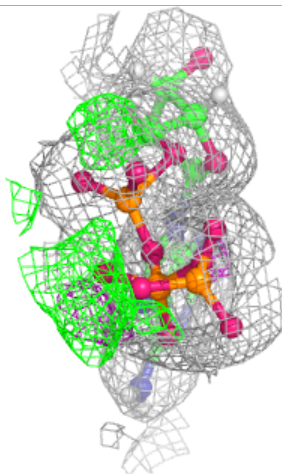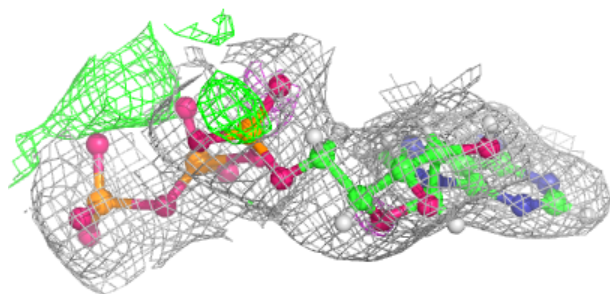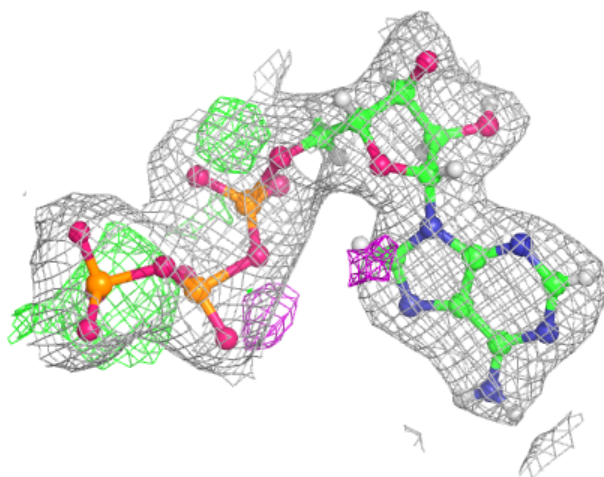and green (positive)
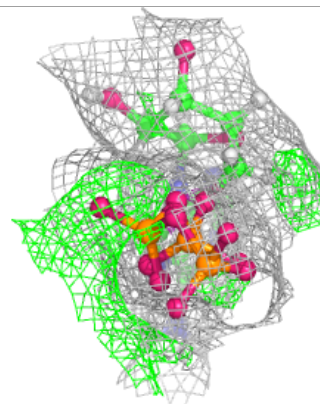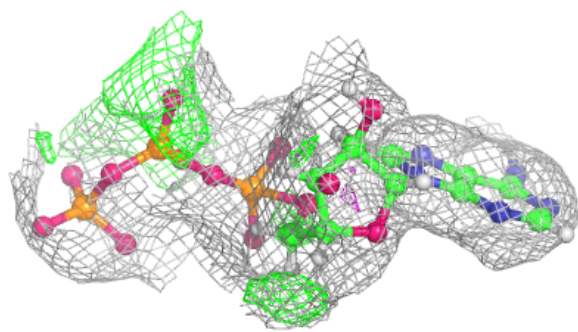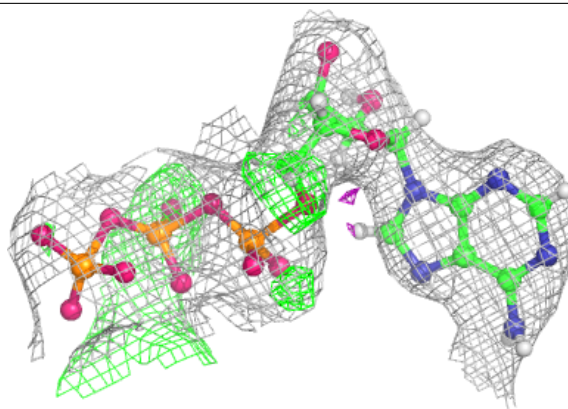
Electron density around ATP C 602:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
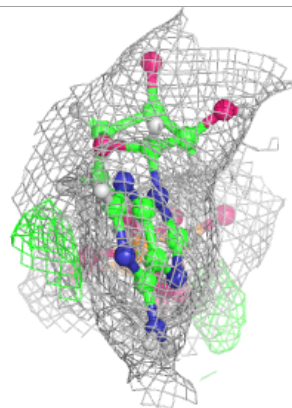and green (positive)
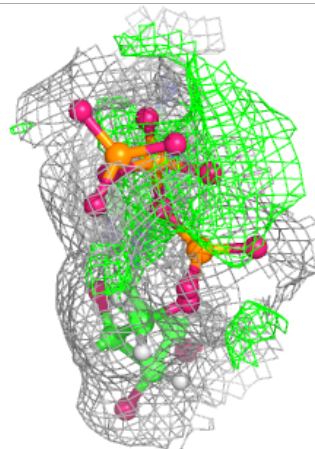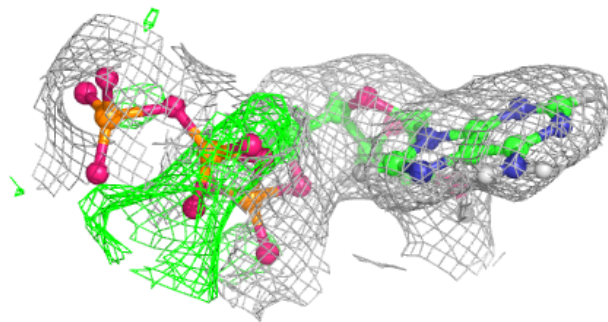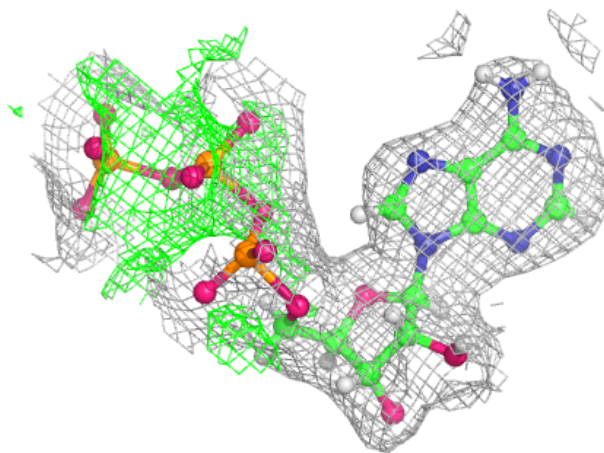
Electron density around ATP B 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
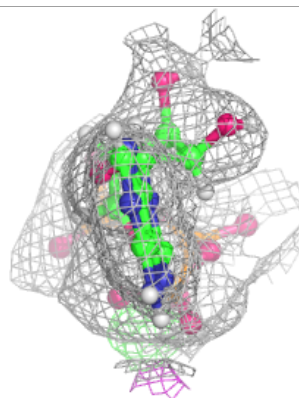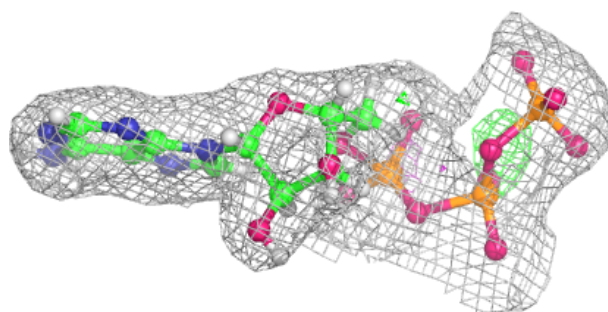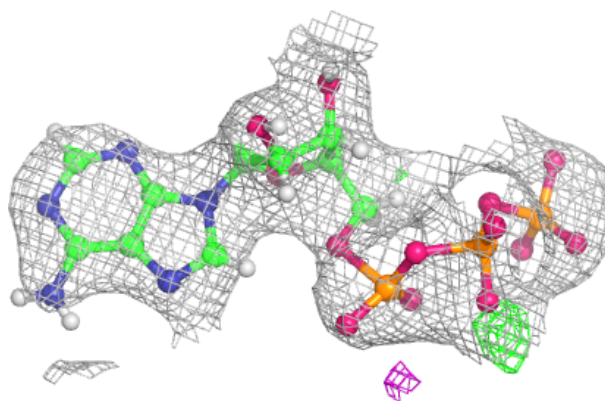
Electron density around ATP B 605:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
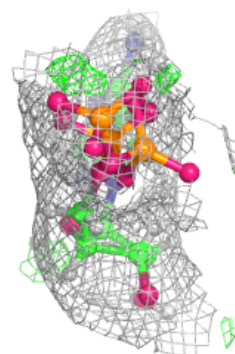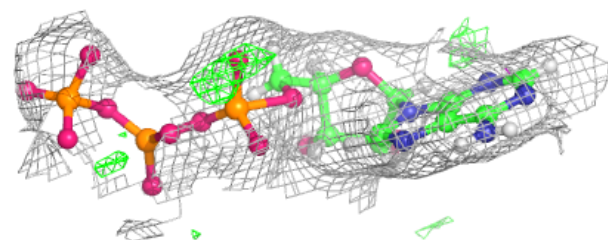
Electron density around ATP G 601:

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

Electron density around ATP A 603:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
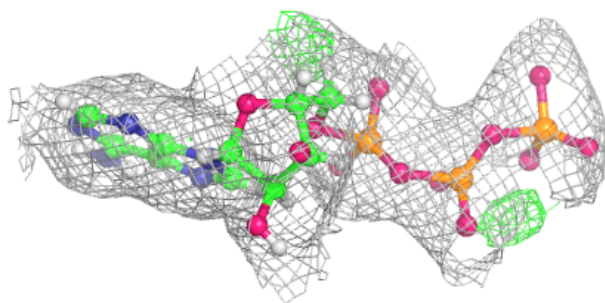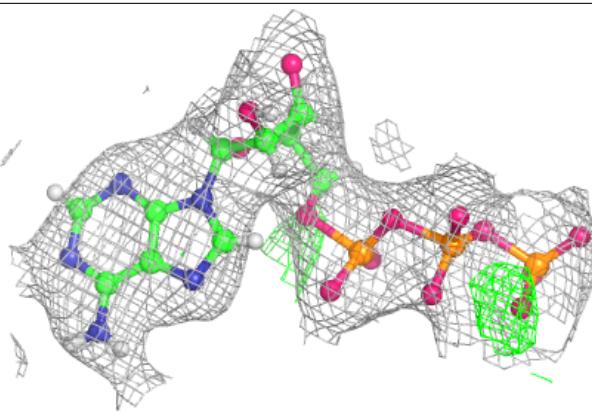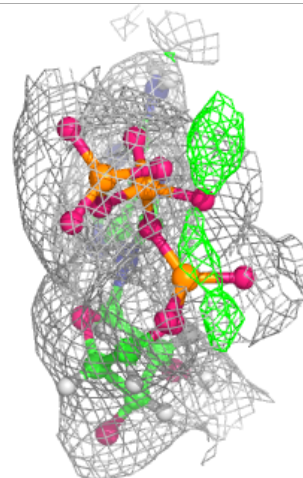
Electron density around ATP D 603:

$2mF_o$-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 603:

$2mF_o$-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 602:

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

Electron density around ATP A 601:

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

Electron density around ATP A 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
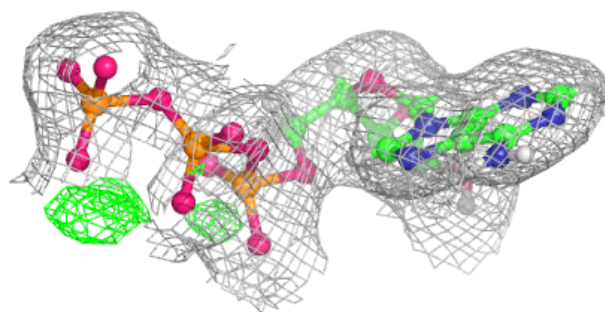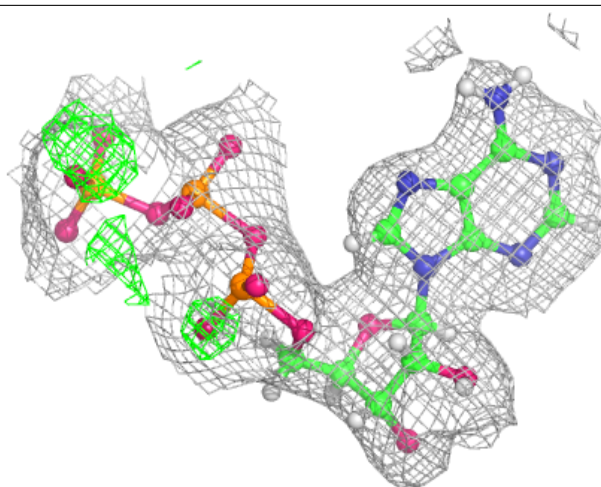mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ATP B 601:

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

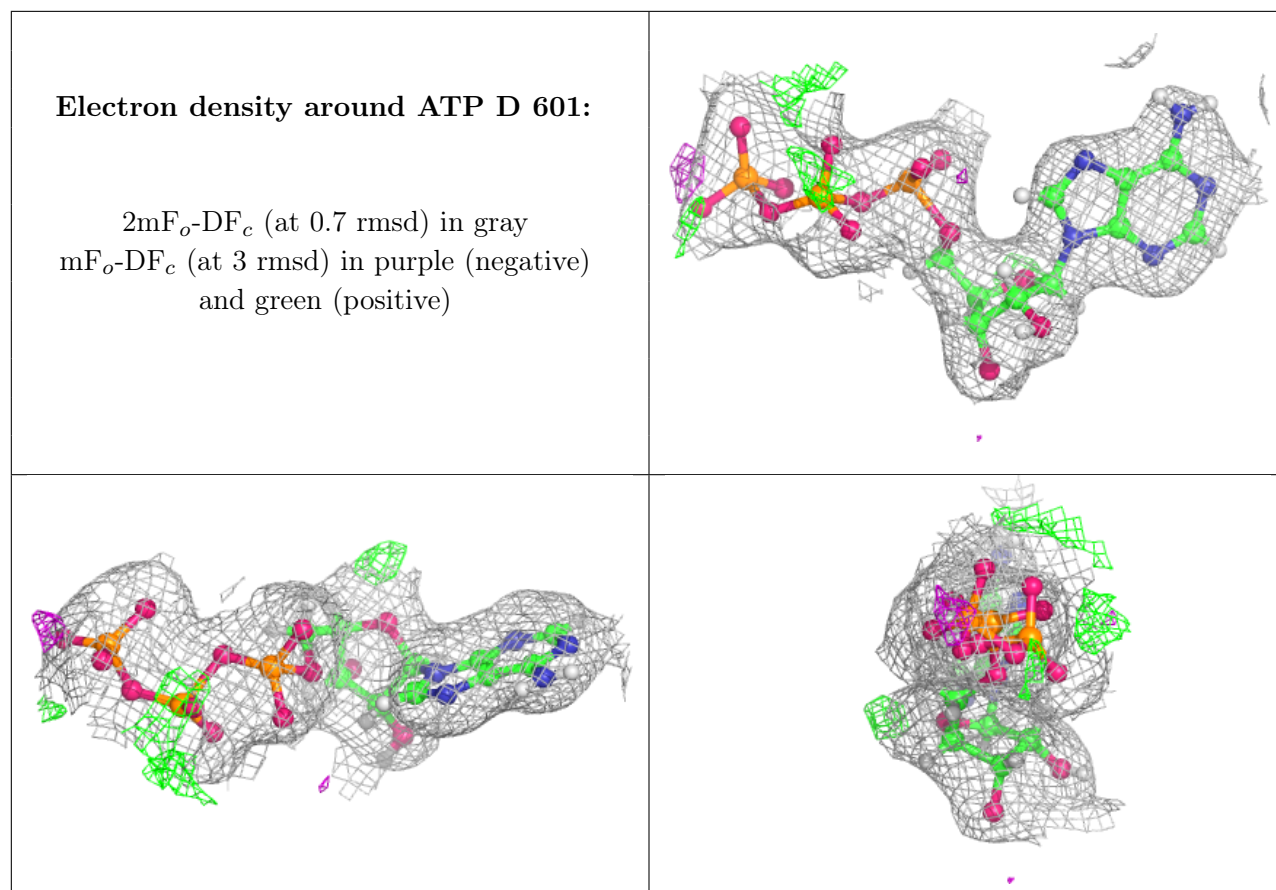**Electron density around ATP B 602:**

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

Electron density around ATP D 601:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.