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

wwPDB X-ray Structure Validation Summary Report (i)

Aug 28, 2023 – 04:14 AM EDT

PDB ID	:	3K0C
Title	:	Crystal structure of the phosphorylation-site double mutant S431A/T432E of the KaiC circadian clock protein
Authors	:	Pattanayek, R.; Egli, M.; Pattanayek, S.
Deposited on	:	2009-09-24
Resolution	:	3.30 Å(reported)

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

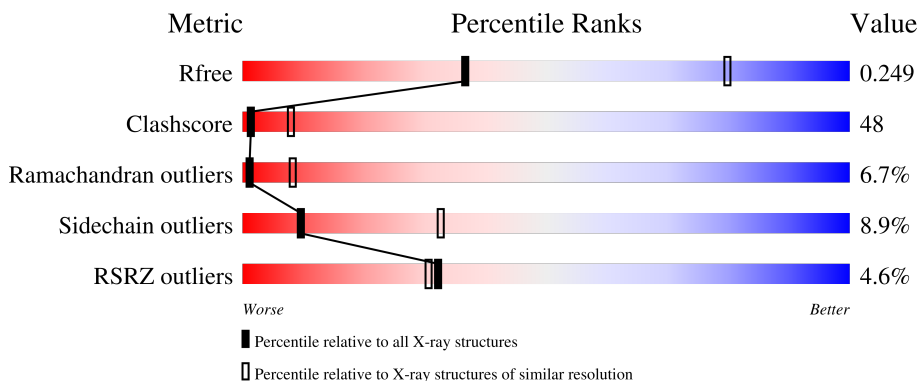|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.30 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		0.249
Clashscore		48
Ramachandran outliers		6.7%
Sidechain outliers		8.9%
RSRZ outliers		4.6%

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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	519	8% 33% 57% 6% · ·
1	B	519	4% 31% 54% 9% 5%
1	E	519	3% 35% 50% 9% · 5%
1	F	519	5% 31% 55% 10% · ·
2	C	519	3% 29% 56% 8% · 6%

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Mol	Chain	Length	Quality of chain
2	D	519	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	A	426	-	-	X	-
1	TPO	B	426	-	-	X	-
1	TPO	F	426	-	-	X	-

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 23919 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total 3990	C 2510	N 701	O 763	P 1	S 15	0	0	0
1	B	491	Total 3875	C 2440	N 678	O 741	P 1	S 15	0	0	0
1	E	492	Total 3883	C 2446	N 679	O 742	P 1	S 15	0	0	0
1	F	506	Total 3990	C 2510	N 701	O 763	P 1	S 15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	431	ALA	SER	engineered mutation	UNP Q79PF4
A	432	GLU	THR	engineered mutation	UNP Q79PF4
B	431	ALA	SER	engineered mutation	UNP Q79PF4
B	432	GLU	THR	engineered mutation	UNP Q79PF4
E	431	ALA	SER	engineered mutation	UNP Q79PF4
E	432	GLU	THR	engineered mutation	UNP Q79PF4
F	431	ALA	SER	engineered mutation	UNP Q79PF4
F	432	GLU	THR	engineered mutation	UNP Q79PF4

- Molecule 2 is a protein called Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	488	Total 3847	C 2426	N 674	O 732	S 15	0	0	0
2	D	485	Total 3823	C 2412	N 671	O 725	S 15	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	431	ALA	SER	engineered mutation	UNP Q79PF4
C	432	GLU	THR	engineered mutation	UNP Q79PF4
D	431	ALA	SER	engineered mutation	UNP Q79PF4
D	432	GLU	THR	engineered mutation	UNP Q79PF4

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

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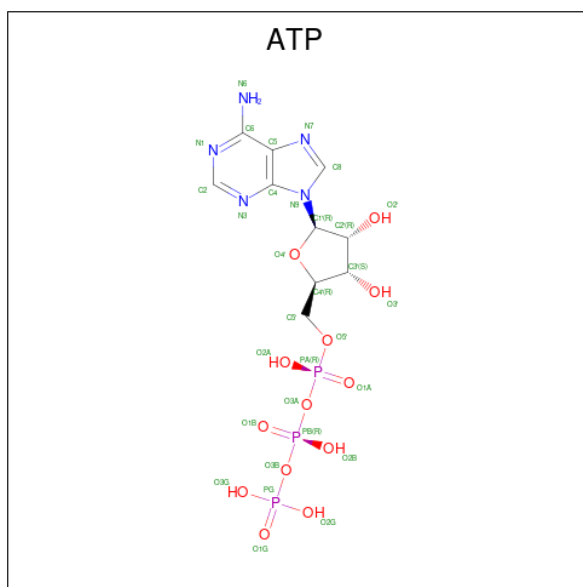
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	B	3	Total	Mg	0	0
			3	3		
4	C	4	Total	Mg	0	0
			4	4		
4	D	4	Total	Mg	0	0
			4	4		
4	E	3	Total	Mg	0	0
			3	3		
4	F	3	Total	Mg	0	0
			3	3		

- Molecule 5 is water.

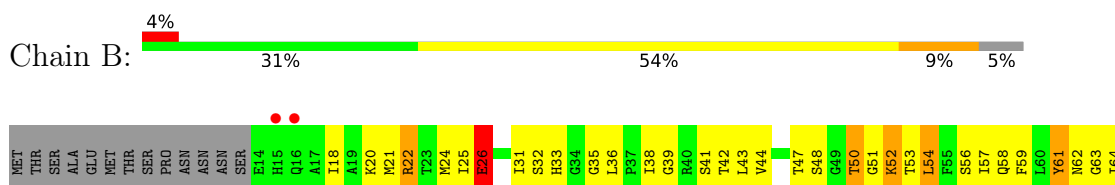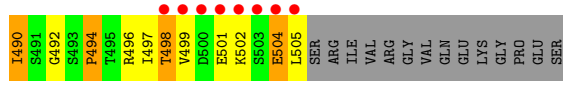| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	18	Total	O	0	0
			18	18		
5	C	22	Total	O	0	0
			22	22		
5	D	31	Total	O	0	0
			31	31		
5	E	13	Total	O	0	0
			13	13		
5	F	21	Total	O	0	0
			21	21		

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.
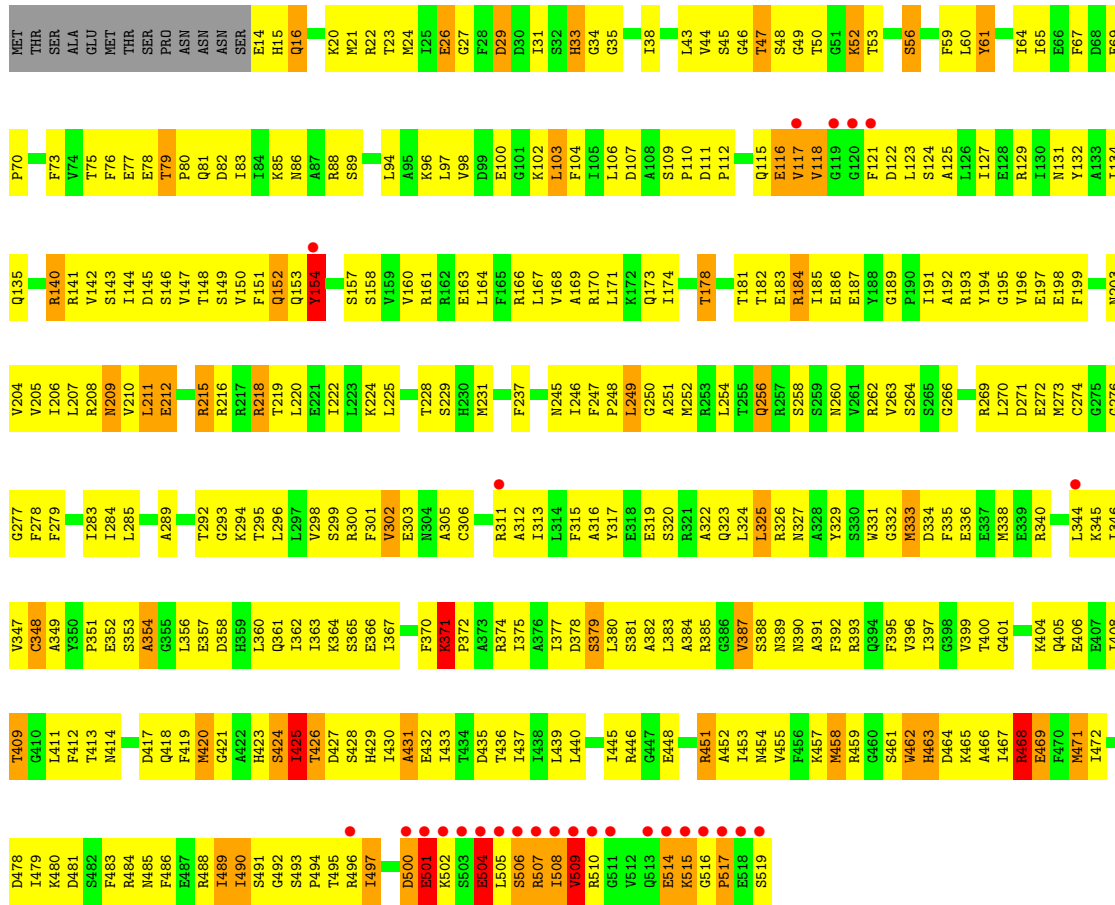
• Molecule 1: Circadian clock protein kinase KaiC

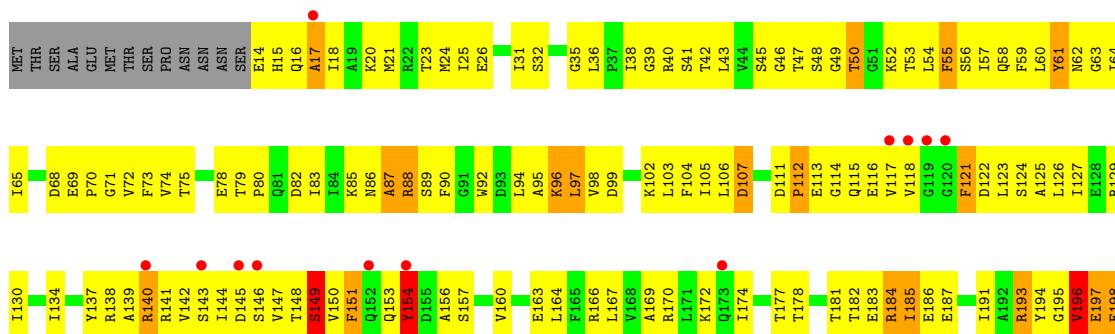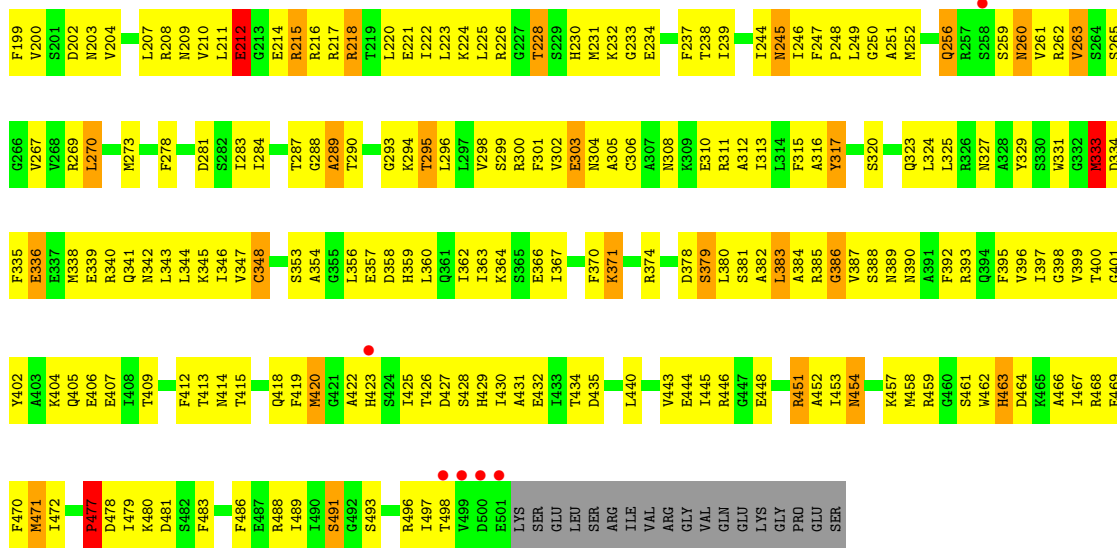• Molecule 1: Circadian clock protein kinase KaiC

● Molecule 1: Circadian clock protein kinase KaiC

I490 S491 G492 S493 P494 T495 R496 I497 T498 V499 D500 E501 K502 S503 E504 L505 SER ARG ILE VAL ARG GLY VAL GLN GLU LYS GLY PRO GLU SER

• Molecule 1: Circadian clock protein kinase KaiC

Chain F:

5%

31% 55% 10%

MET THR SER ALA GLU MET THR SER PRO ASN ASN ASN SER E14 H15 Q16 K20 M21 R22 T23 M24 I25 E26 G27 F28 D29 D30 I31 S32 H33 G34 G35 I38 L43 V44 S45 G46 T47 S48 G49 T50 G51 K52 T53 S56 F59 L60 Y61 I64 I65 E66 F67 D68 E69

P70 F73 V74 T75 F76 E77 E78 T79 P80 Q81 D82 I83 I84 K85 N86 A87 R88 S89 L94 A95 K96 L97 V98 D99 E100 G101 K102 I103 F104 I105 L106 D107 A108 S109 P110 D111 P112 Q115 E116 V117 V118 G119 G120 F121 D122 L123 S124 A125 L126 I127 E128 R129 I130 N131 Y132 A133 I134

Q135 R140 R141 V142 S143 I144 D145 S146 V147 T148 S149 V150 F151 Q152 Q153 Y154 S157 S158 V159 V160 R161 R162 E163 L164 F165 R166 L167 V168 A169 R170 L171 K172 Q173 I174 T178 T181 T182 E183 R184 I185 E186 E187 Y188 G189 P190 I191 A192 R193 Y194 G195 V196 E197 F198 F199 N203

V204 V205 I206 L207 R208 N209 V210 L211 E212 R215 R216 R217 R218 T219 L220 E221 I222 L223 K224 L225 T228 S229 H230 M231 F237 N245 I246 P247 P248 L249 G250 A251 M252 R253 L254 T255 Q256 R257 S258 S259 N260 V261 R262 V263 S264 R265 G266 R269 L270 D271 E272 M273 C274 G275 G276

G277 F278 F279 I283 I284 L285 A289 T292 G293 K294 T295 L296 L297 V298 S299 R300 F301 V302 E303 N304 A305 C306 R311 A312 I313 L314 F315 A316 Y317 E318 E319 S320 R321 A322 Q323 L324 L325 R326 N327 A328 Y329 S330 W331 G332 M333 D334 F335 E336 E337 M338 E339 R340 L344 K345 I346

V347 C348 A349 Y350 P351 E352 S353 A354 G355 L356 E357 D358 H359 L360 Q361 I362 I363 K364 S365 E366 I367 F370 R371 P372 A373 R374 I375 A376 I377 D378 S379 L380 S381 A382 L383 A384 R385 G386 V387 S388 N389 N390 A391 F392 R393 Q394 F395 V396 I397 G398 V399 T400 G401 K404 Q405 E406 E407 I408

T409 G410 L411 F412 T413 N414 D417 Q418 F419 M420 G421 A422 H423 S424 I425 T426 D427 S428 H429 I430 A431 E432 I433 T434 D435 T436 I437 I438 I439 L440 I445 R446 G447 E448 R451 A452 I453 N454 V455 F456 K457 M458 R459 G460 S461 W462 H463 D464 K465 A466 I467 R468 F469 F470 M471 I472

D478 I479 K480 D481 S482 F483 R484 N485 F486 E487 E488 I489 I490 S491 G492 S493 P494 T495 R496 I497 D500 E501 K502 S503 E504 L505 S506 R507 I508 V509 R510 G511 V512 Q513 E514 K515 G516 P517 E518 S519

• Molecule 2: Circadian clock protein kinase KaiC

Chain C:

3%

29% 56% 8% 6%

MET THR SER ALA GLU MET THR SER PRO ASN ASN ASN SER E14 H15 Q16 A17 I18 A19 K20 M21 R22 T23 M24 I25 E26 I31 S32 G35 L36 P37 I38 G39 R40 S41 T42 L43 V44 S45 G46 T47 S48 G49 T50 G51 K52 T53 L54 F55 S56 I57 Q58 F59 L60 Y61 N62 G63 I64

I65 D68 E69 P70 G71 V72 F73 V74 T75 E78 T79 P80 Q81 D82 I83 I84 K85 N86 A87 R88 S89 F90 G91 W92 D93 L94 A95 K96 L97 V98 D99 K102 L103 F104 I105 L106 D107 D111 P112 E113 G114 Q115 E116 V117 V118 G119 G120 F121 D122 L123 S124 A125 L126 I127 E128 R129

I130 I134 Y137 R138 A139 R140 R141 V142 S143 I144 D145 S146 V147 T148 S149 V150 F151 Q152 Q153 Y154 D155 A156 S157 V160 E163 L164 F165 R166 L167 V168 A169 R170 L171 K172 Q173 I174 T177 T178 T181 T182 E183 R184 I185 E186 E187 I191 A192 R193 Y194 G195 V196 E197 E198

• Molecule 2: Circadian clock protein kinase KaiC

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.28Å 135.03Å 204.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (30.00-3.30) 90.8 (30.07-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.269 0.215 , 0.249	Depositor DCC
R_{free} test set	5141 reflections (9.44%)	wwPDB-VP
Wilson B-factor (Å^2)	74.6	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	23919	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, TPO, 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	0.39	0/4044	0.67	0/5446
1	B	0.37	0/3928	0.64	0/5291
1	E	0.48	0/3936	0.72	2/5302 (0.0%)
1	F	0.45	0/4044	0.71	1/5446 (0.0%)
2	C	0.41	0/3912	0.67	0/5273
2	D	0.45	0/3888	0.70	0/5240
All	All	0.43	0/23752	0.69	3/31998 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	16	GLN	N-CA-C	-5.61	95.85	111.00
1	E	332	GLY	N-CA-C	-5.09	100.38	113.10
1	E	380	LEU	N-CA-C	-5.04	97.38	111.00

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	3990	0	3983	403	0
1	B	3875	0	3861	411	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3883	0	3871	375	0
1	F	3990	0	3982	462	0
2	C	3847	0	3839	418	0
2	D	3823	0	3819	359	0
3	A	62	0	24	6	0
3	B	62	0	24	8	0
3	C	62	0	24	8	0
3	D	62	0	24	5	0
3	E	62	0	24	9	0
3	F	62	0	24	4	0
4	A	5	0	0	0	0
4	B	3	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
5	A	12	0	0	1	0
5	B	18	0	0	2	0
5	C	22	0	0	4	0
5	D	31	0	0	6	0
5	E	13	0	0	3	0
5	F	21	0	0	5	0
All	All	23919	0	23499	2276	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 48.

The worst 5 of 2276 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:A:425:ILE:O	1:A:426:TPO:HG22	1.25	1.24
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.26	1.14
1:B:300:ARG:HA	1:B:333:MET:HE1	1.16	1.14
1:A:299:SER:HB3	1:A:333:MET:HE1	1.33	1.10
2:D:379:SER:H	2:D:413:THR:HB	0.97	1.09

There are no symmetry-related clashes.

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	503/519 (97%)	377 (75%)	92 (18%)	34 (7%)	1	8
1	B	488/519 (94%)	365 (75%)	82 (17%)	41 (8%)	1	5
1	E	489/519 (94%)	375 (77%)	79 (16%)	35 (7%)	1	7
1	F	503/519 (97%)	399 (79%)	70 (14%)	34 (7%)	1	8
2	C	486/519 (94%)	373 (77%)	81 (17%)	32 (7%)	1	8
2	D	483/519 (93%)	392 (81%)	69 (14%)	22 (5%)	2	15
All	All	2952/3114 (95%)	2281 (77%)	473 (16%)	198 (7%)	1	8

5 of 198 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	65	ILE
1	A	154	TYR
1	A	212	GLU
1	A	333	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/442 (97%)	400 (93%)	30 (7%)	15	43
1	B	417/442 (94%)	387 (93%)	30 (7%)	14	41
1	E	418/442 (95%)	385 (92%)	33 (8%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	430/442 (97%)	383 (89%)	47 (11%)	6	24
2	C	415/443 (94%)	371 (89%)	44 (11%)	6	25
2	D	412/443 (93%)	372 (90%)	40 (10%)	8	29
All	All	2522/2654 (95%)	2298 (91%)	224 (9%)	9	32

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	209	ASN
1	F	504	GLU
2	D	498	THR
1	F	497	ILE
1	F	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	81	GLN
1	E	81	GLN
1	F	209	ASN
2	D	209	ASN
2	D	441	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	TPO	E	426	1	8,10,11	0.92	0	10,14,16	1.72	2 (20%)
1	TPO	B	426	1	8,10,11	1.54	2 (25%)	10,14,16	2.40	3 (30%)
1	TPO	A	426	1	8,10,11	1.06	1 (12%)	10,14,16	0.87	0
1	TPO	F	426	1	8,10,11	1.46	1 (12%)	10,14,16	2.31	5 (50%)

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
1	TPO	E	426	1	-	3/9/11/13	-
1	TPO	B	426	1	-	4/9/11/13	-
1	TPO	A	426	1	-	2/9/11/13	-
1	TPO	F	426	1	-	2/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	426	TPO	CG2-CB	3.16	1.59	1.51
1	F	426	TPO	CB-CA	3.05	1.60	1.53
1	A	426	TPO	P-OG1	-2.12	1.55	1.59
1	B	426	TPO	P-O1P	-2.03	1.44	1.50

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	426	TPO	P-OG1-CB	-5.53	106.50	123.21
1	B	426	TPO	CG2-CB-CA	-3.92	105.42	113.16
1	E	426	TPO	P-OG1-CB	-3.53	112.55	123.21
1	F	426	TPO	CG2-CB-CA	-3.52	106.22	113.16
1	F	426	TPO	O2P-P-O1P	-3.46	97.14	110.68

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	426	TPO	CG2-CB-OG1-P
1	B	426	TPO	N-CA-CB-CG2
1	B	426	TPO	N-CA-CB-OG1

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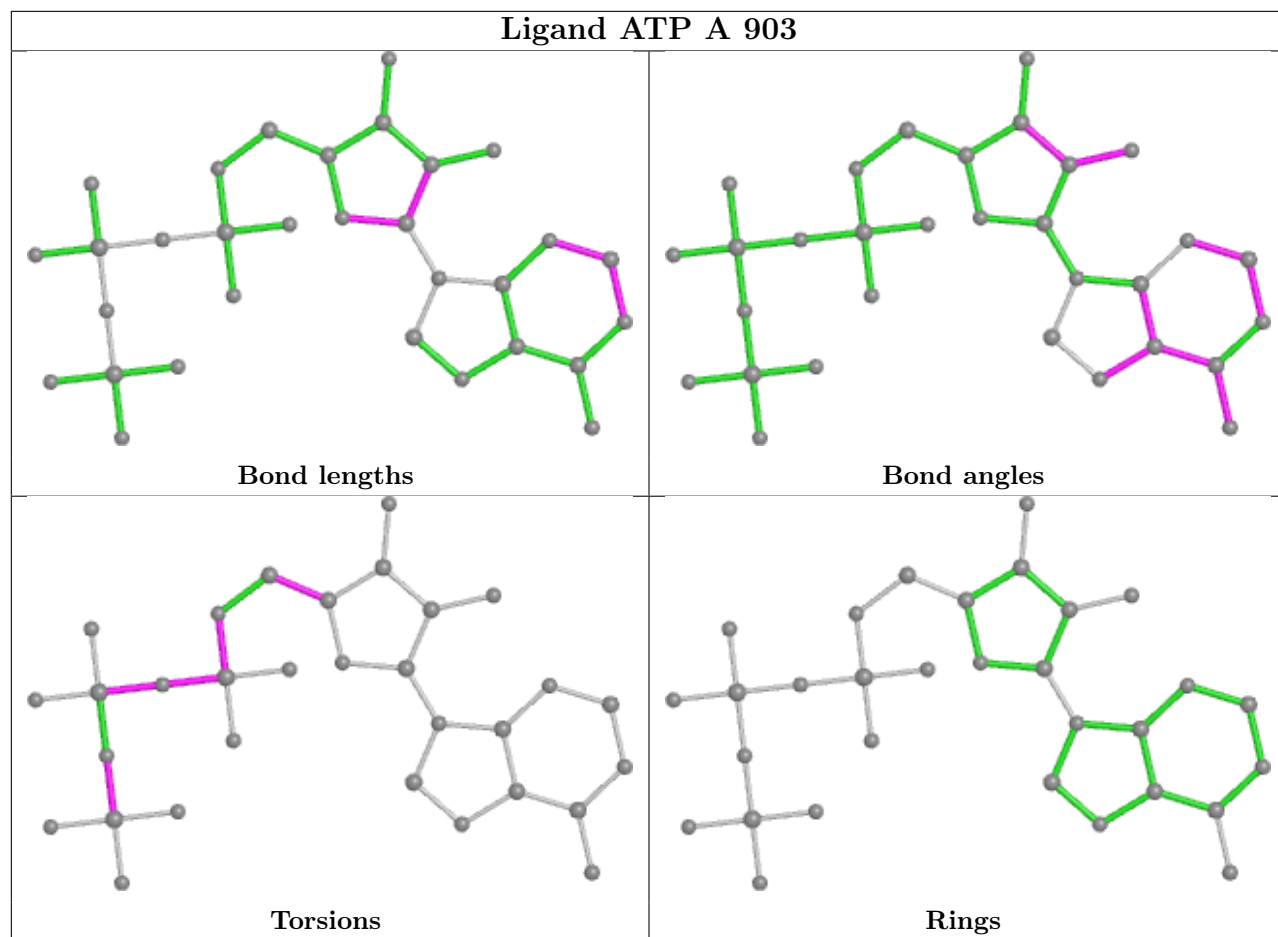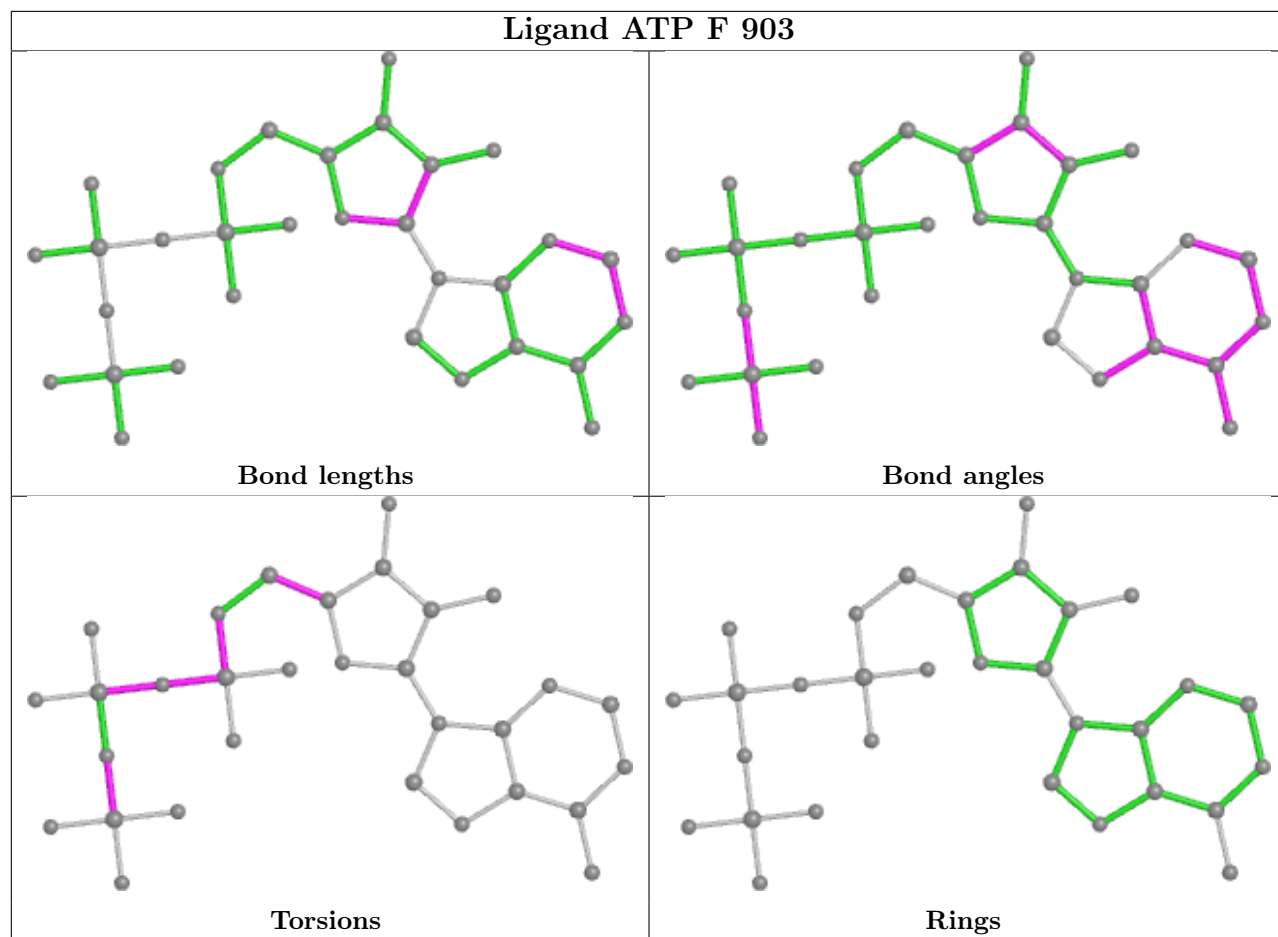| Mol	Chain	Res	Type	Atoms
1	B	426	TPO	C-CA-CB-CG2
1	E	426	TPO	N-CA-CB-CG2

There are no ring outliers.
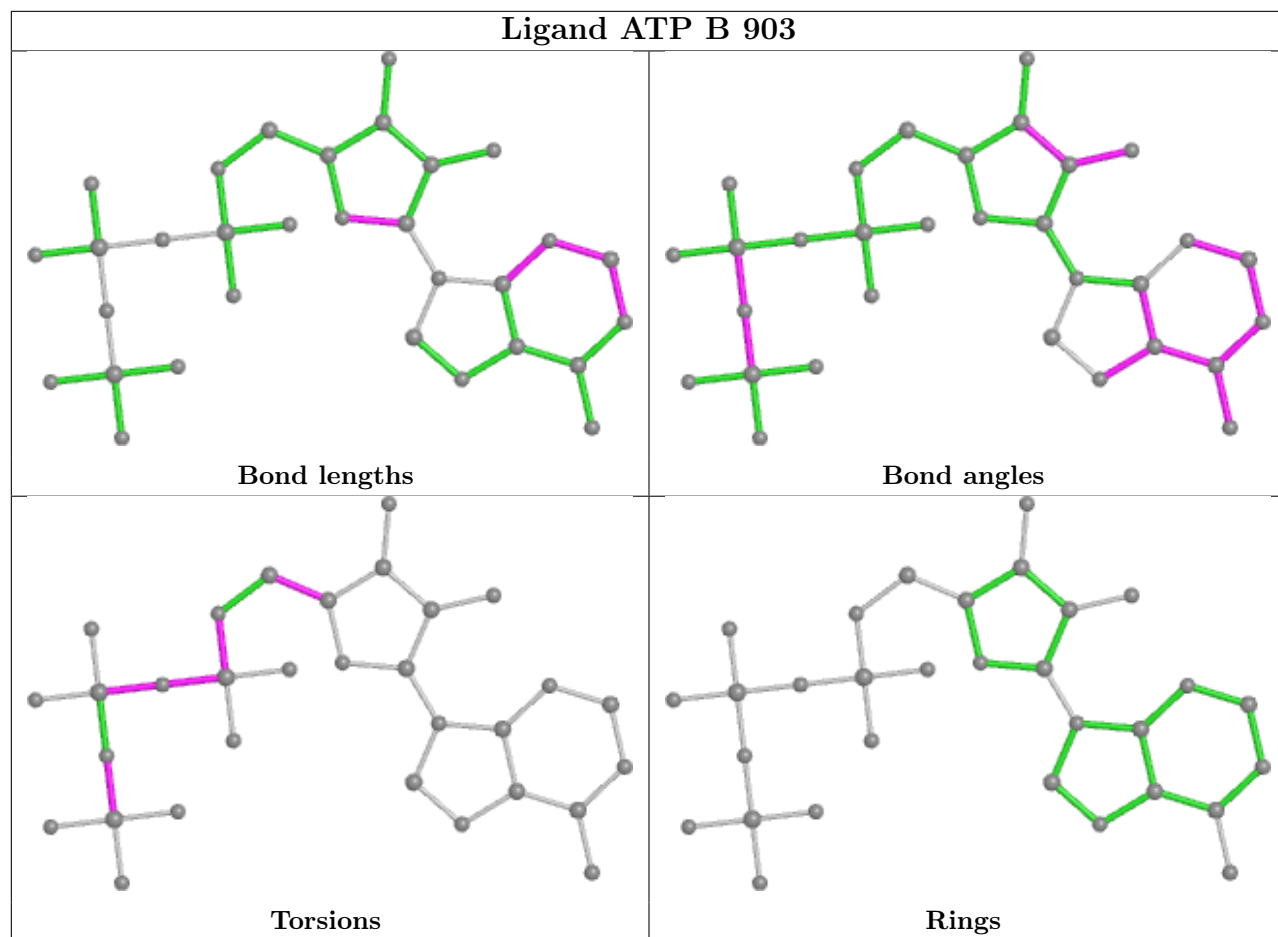
4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	426	TPO	3	0
1	B	426	TPO	7	0
1	A	426	TPO	15	0
1	F	426	TPO	13	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 22 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	ATP	E	903	4	26,33,33	1.17	1 (3%)	31,52,52	1.74	6 (19%)
3	ATP	A	903	4	26,33,33	1.28	4 (15%)	31,52,52	1.73	4 (12%)
3	ATP	F	903	4	26,33,33	1.37	4 (15%)	31,52,52	1.77	6 (19%)
3	ATP	B	903	4	26,33,33	1.31	4 (15%)	31,52,52	1.81	6 (19%)
3	ATP	E	901	4	26,33,33	1.31	2 (7%)	31,52,52	1.81	8 (25%)
3	ATP	C	903	4	26,33,33	1.33	4 (15%)	31,52,52	1.86	5 (16%)
3	ATP	D	901	4	26,33,33	1.42	3 (11%)	31,52,52	1.71	6 (19%)
3	ATP	A	901	4	26,33,33	1.32	3 (11%)	31,52,52	1.81	7 (22%)
3	ATP	F	901	4	26,33,33	1.33	3 (11%)	31,52,52	1.75	5 (16%)

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Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	ATP	B	901	4	26,33,33	1.17	3 (11%)	31,52,52	1.69	3 (9%)
3	ATP	C	901	4	26,33,33	1.33	3 (11%)	31,52,52	1.79	7 (22%)
3	ATP	D	903	4	26,33,33	1.37	4 (15%)	31,52,52	1.76	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	E	903	4	-	7/18/38/38	0/3/3/3
3	ATP	A	903	4	-	7/18/38/38	0/3/3/3
3	ATP	F	903	4	-	7/18/38/38	0/3/3/3
3	ATP	B	903	4	-	9/18/38/38	0/3/3/3
3	ATP	E	901	4	-	9/18/38/38	0/3/3/3
3	ATP	C	903	4	-	9/18/38/38	0/3/3/3
3	ATP	D	901	4	-	7/18/38/38	0/3/3/3
3	ATP	A	901	4	-	6/18/38/38	0/3/3/3
3	ATP	F	901	4	-	6/18/38/38	0/3/3/3
3	ATP	B	901	4	-	5/18/38/38	0/3/3/3
3	ATP	C	901	4	-	8/18/38/38	0/3/3/3
3	ATP	D	903	4	-	7/18/38/38	0/3/3/3

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	901	ATP	C2-N3	4.31	1.39	1.32
3	F	903	ATP	C2-N3	4.29	1.39	1.32
3	C	901	ATP	C2-N3	4.24	1.38	1.32
3	A	901	ATP	C2-N3	4.23	1.38	1.32
3	F	901	ATP	C2-N3	4.14	1.38	1.32

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	901	ATP	N3-C2-N1	-5.56	119.98	128.68
3	E	901	ATP	N3-C2-N1	-5.56	119.99	128.68
3	D	903	ATP	N3-C2-N1	-5.55	120.01	128.68
3	E	903	ATP	N3-C2-N1	-5.51	120.06	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	903	ATP	N3-C2-N1	-5.50	120.08	128.68

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	C5'-O5'-PA-O3A
3	A	901	ATP	C3'-C4'-C5'-O5'
3	A	903	ATP	PB-O3B-PG-O3G
3	A	903	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	903	ATP	3	0
3	A	903	ATP	5	0
3	F	903	ATP	1	0
3	B	903	ATP	4	0
3	E	901	ATP	6	0
3	C	903	ATP	4	0
3	D	901	ATP	4	0
3	A	901	ATP	1	0
3	F	901	ATP	3	0
3	B	901	ATP	4	0
3	C	901	ATP	4	0
3	D	903	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 E 903

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 903

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP F 903

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 903

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP E 901

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 903

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP D 901

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP A 901

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP F 901

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP B 901

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP C 901

Bond lengths

Bond angles

Torsions

Rings

Ligand ATP D 903

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	505/519 (97%)	0.28	39 (7%)	13	12	20, 75, 128, 156	0
1	B	490/519 (94%)	0.14	23 (4%)	31	29	31, 78, 130, 168	0
1	E	491/519 (94%)	-0.16	16 (3%)	46	44	2, 47, 110, 149	0
1	F	505/519 (97%)	-0.01	27 (5%)	26	24	2, 57, 123, 139	0
2	C	488/519 (94%)	-0.03	18 (3%)	41	38	8, 62, 129, 167	0
2	D	485/519 (93%)	-0.26	14 (2%)	51	50	5, 42, 100, 152	0
All	All	2964/3114 (95%)	-0.00	137 (4%)	32	30	2, 62, 126, 168	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	517	PRO	8.2
1	A	518	GLU	7.4
1	E	505	LEU	6.9
1	A	513	GLN	6.5
1	A	517	PRO	6.5

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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
1	TPO	F	426	11/12	0.72	0.35	67,68,79,81	0
1	TPO	E	426	11/12	0.79	0.34	75,89,101,102	0
1	TPO	B	426	11/12	0.83	0.27	79,85,91,92	0
1	TPO	A	426	11/12	0.84	0.28	74,77,78,78	0

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
4	MG	A	701	1/1	0.82	0.80	70,70,70,70	0
4	MG	F	702	1/1	0.88	0.33	62,62,62,62	0
3	ATP	A	903	31/31	0.89	0.24	57,64,69,70	0
3	ATP	B	903	31/31	0.89	0.23	65,69,75,76	0
4	MG	B	701	1/1	0.90	0.47	49,49,49,49	0
3	ATP	A	901	31/31	0.90	0.29	65,80,87,88	0
3	ATP	F	901	31/31	0.91	0.25	53,79,88,88	0
3	ATP	E	901	31/31	0.91	0.25	35,63,67,68	0
4	MG	F	802	1/1	0.92	0.36	21,21,21,21	0
3	ATP	B	901	31/31	0.93	0.20	42,47,53,54	0
3	ATP	C	903	31/31	0.93	0.20	36,41,67,68	0
3	ATP	D	903	31/31	0.93	0.20	15,19,42,44	0
4	MG	E	520	1/1	0.94	0.44	23,23,23,23	0
3	ATP	F	903	31/31	0.94	0.20	31,36,40,40	0
4	MG	C	701	1/1	0.94	0.58	69,69,69,69	0
4	MG	D	702	1/1	0.95	0.57	70,70,70,70	0
3	ATP	E	903	31/31	0.95	0.19	16,24,41,42	0
4	MG	E	702	1/1	0.95	0.33	70,70,70,70	0
3	ATP	C	901	31/31	0.95	0.20	24,28,38,40	0
3	ATP	D	901	31/31	0.95	0.23	38,43,54,55	0
4	MG	B	801	1/1	0.96	0.20	10,10,10,10	0
4	MG	D	801	1/1	0.96	0.38	72,72,72,72	0
4	MG	F	701	1/1	0.96	0.46	29,29,29,29	0
4	MG	A	520	1/1	0.96	0.45	58,58,58,58	0
4	MG	D	701	1/1	0.96	0.37	67,67,67,67	0
4	MG	C	702	1/1	0.97	0.38	67,67,67,67	0
4	MG	B	802	1/1	0.97	0.24	61,61,61,61	0
4	MG	D	802	1/1	0.97	0.24	1,1,1,1	0
4	MG	A	702	1/1	0.97	0.28	76,76,76,76	0
4	MG	A	801	1/1	0.97	0.34	31,31,31,31	0
4	MG	A	802	1/1	0.98	0.48	77,77,77,77	0
4	MG	E	801	1/1	0.98	0.24	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	C	801	1/1	0.98	0.30	6,6,6,6	0
4	MG	C	802	1/1	0.99	0.32	19,19,19,19	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.
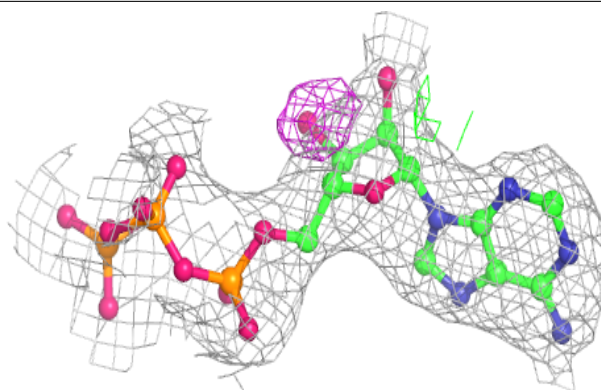

Electron density around ATP A 903:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
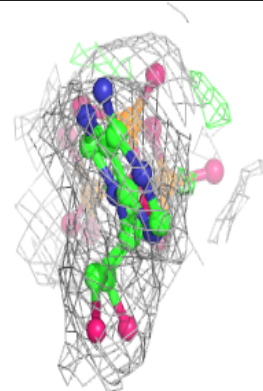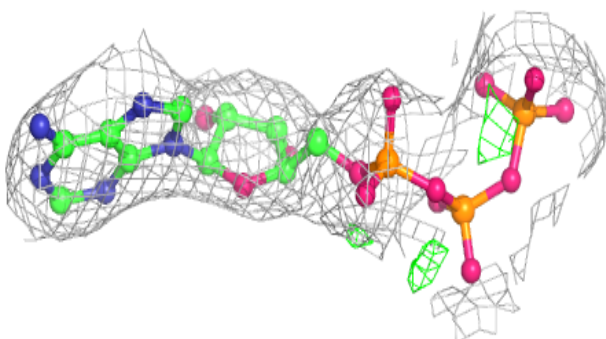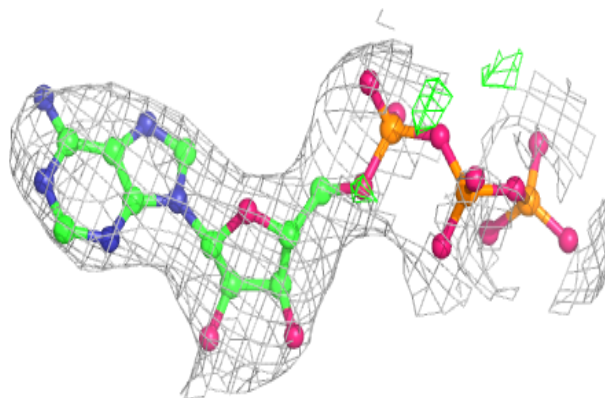$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
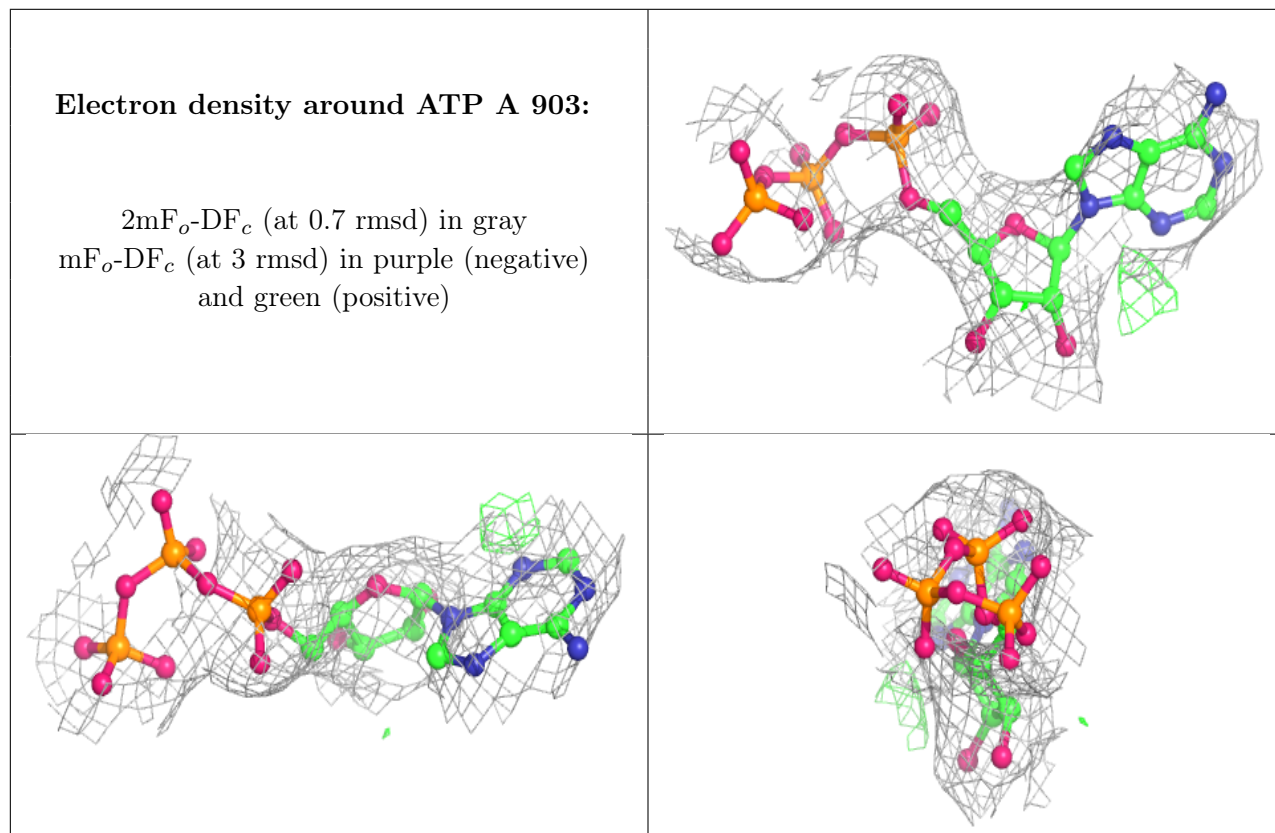
Electron density around ATP B 903:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
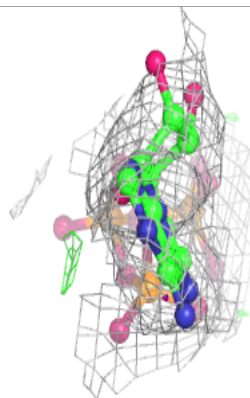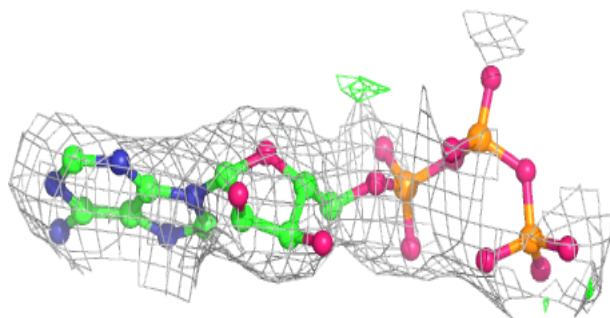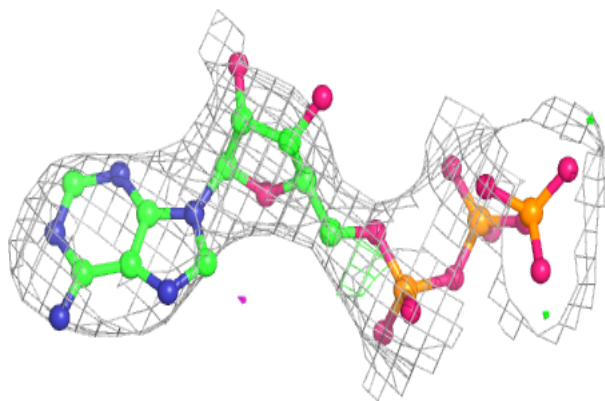
Electron density around ATP A 901:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
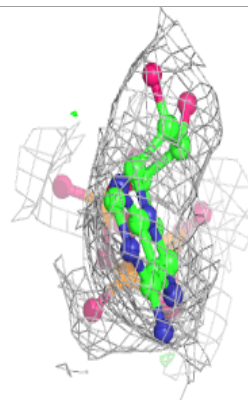$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
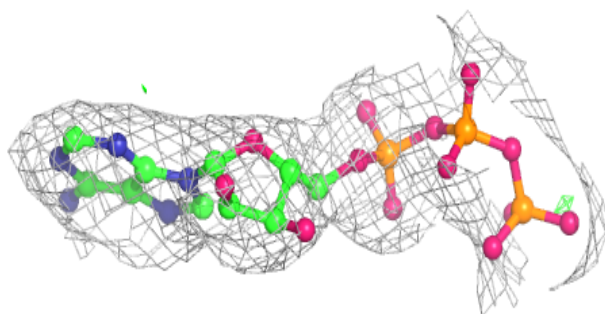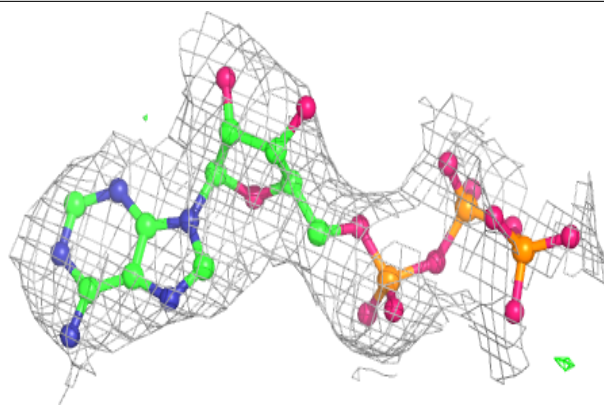and green (positive)
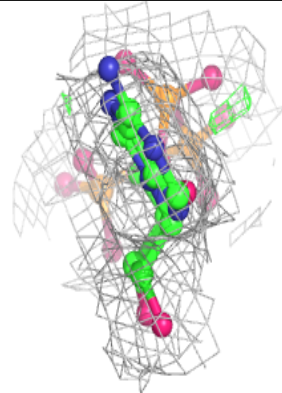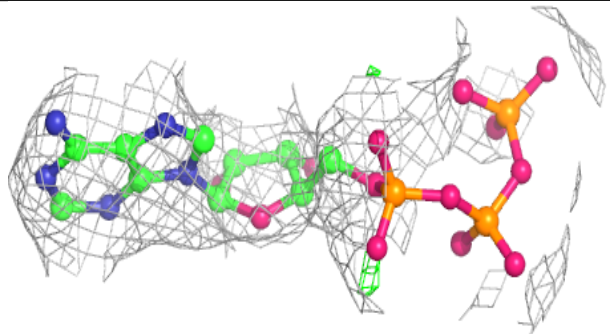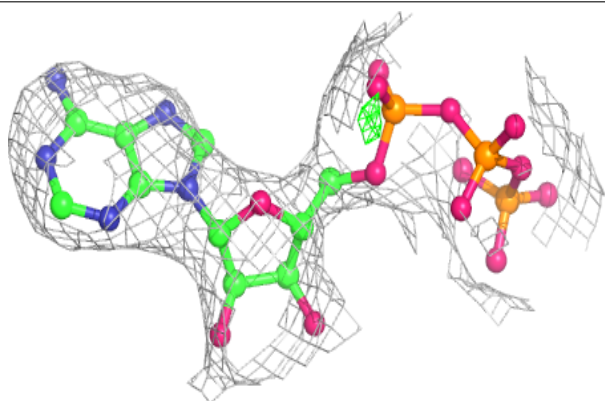
Electron density around ATP F 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
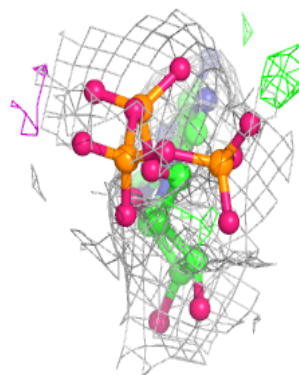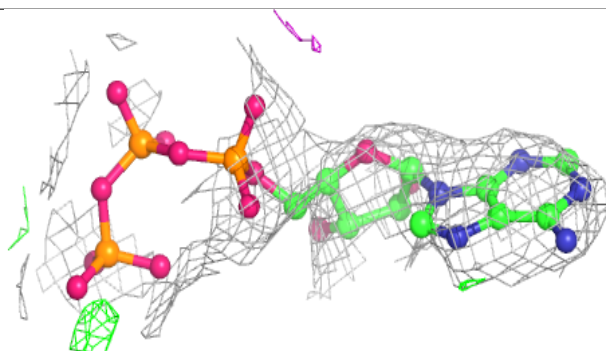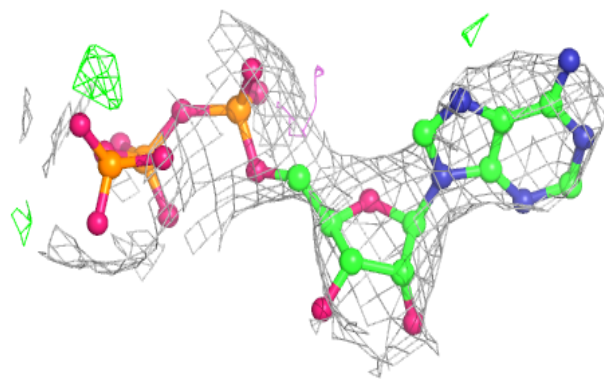
Electron density around ATP E 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
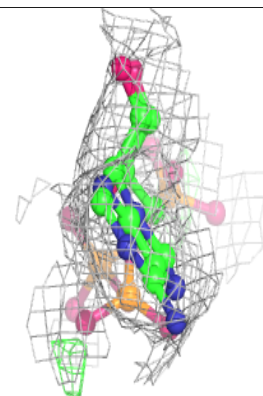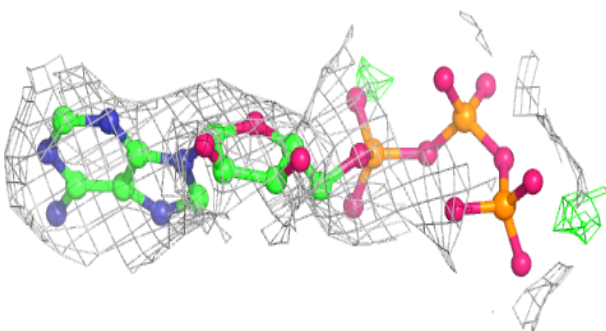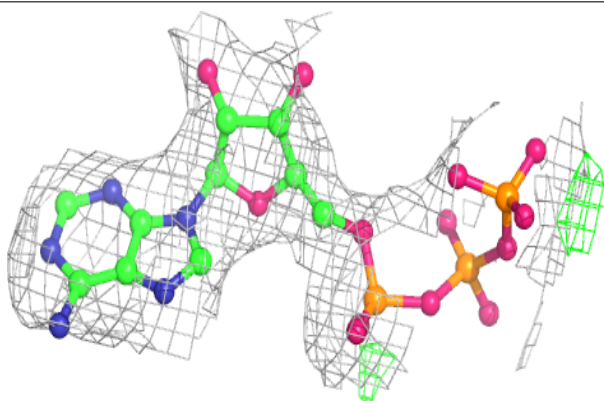
Electron density around ATP B 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
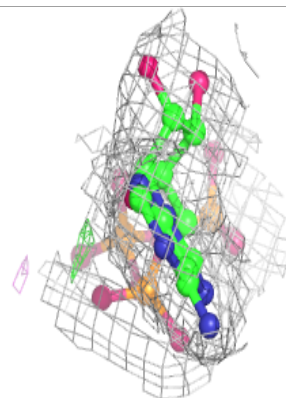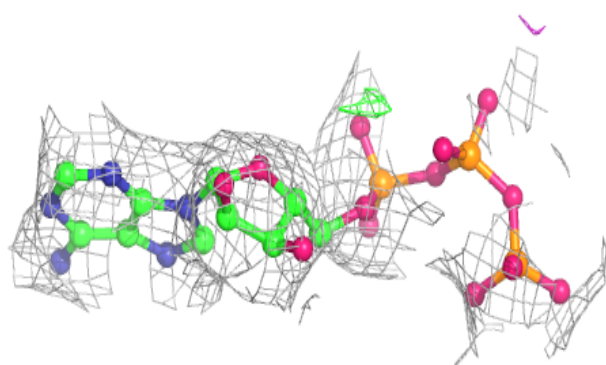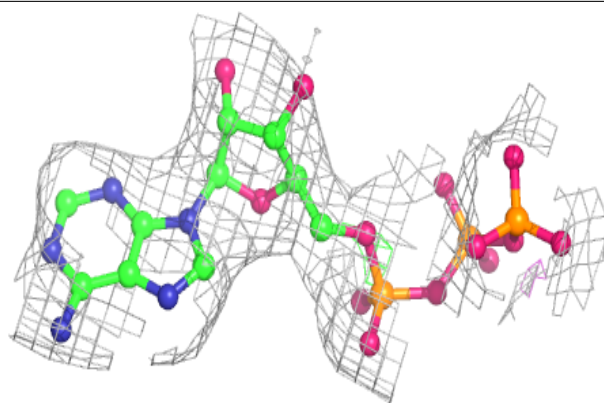
Electron density around ATP C 903:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
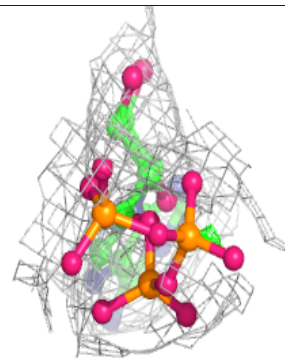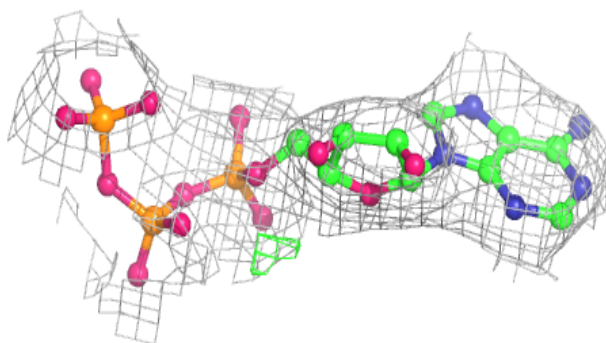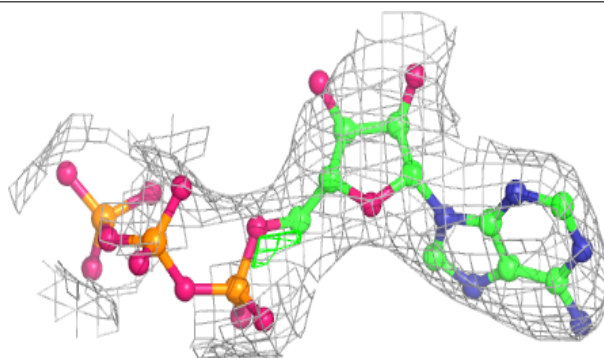
Electron density around ATP D 903:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
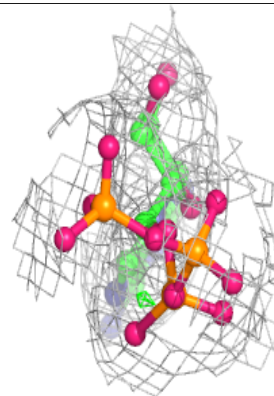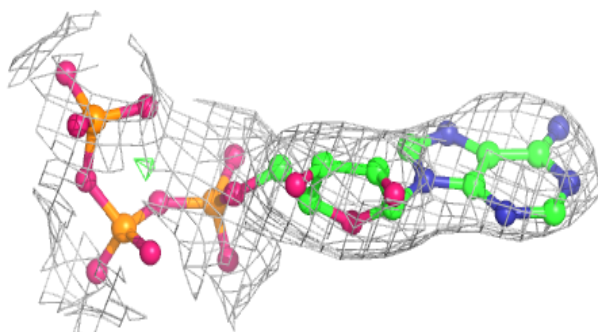mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
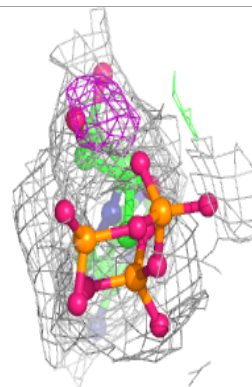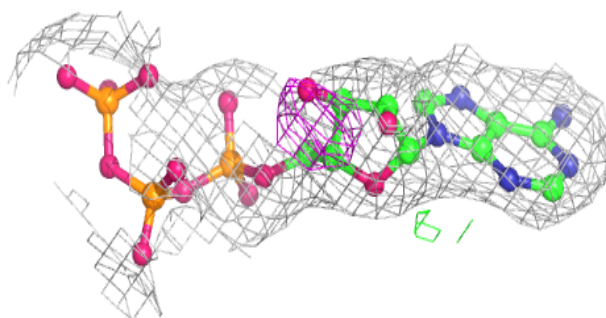
Electron density around ATP F 903:

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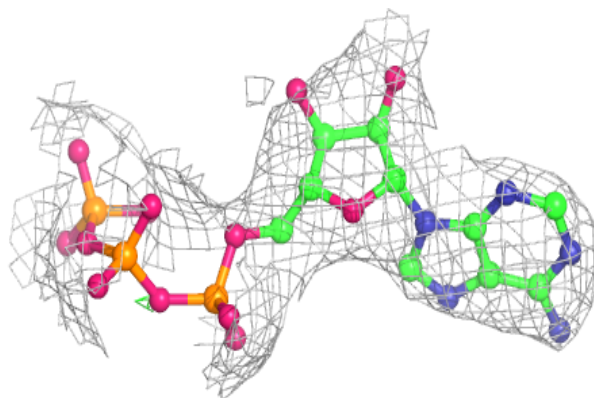and green (positive)

Electron density around ATP E 903:

$2mF_o$-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 901:

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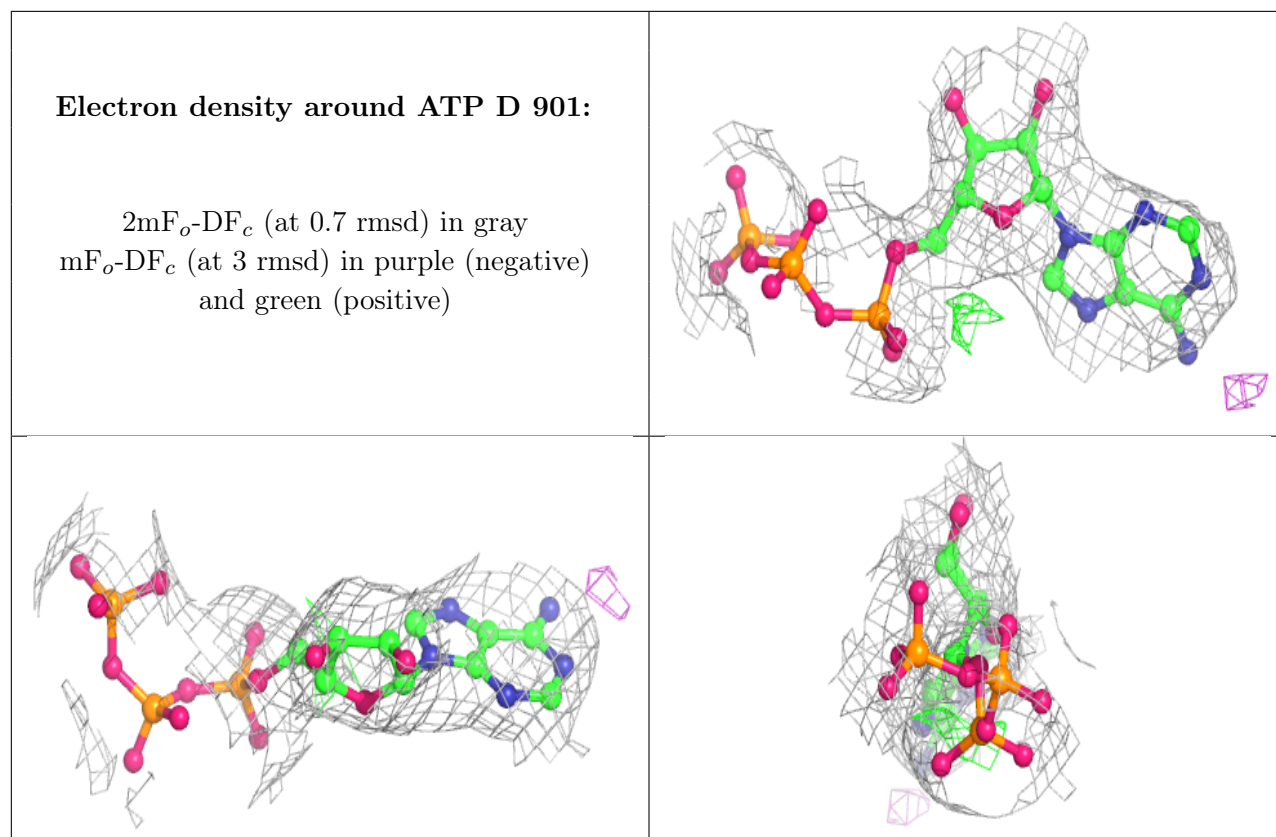mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ATP D 901:

$2mF_o$-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 ⓘ

There are no such residues in this entry.