



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:06 PM UTC

PDB ID : 7RUT / pdb_00007rut
Title : Structure of Human ATP:Cobalamin Adenosyltransferase R190C bound to ATP
Authors : Mascarenhas, R.; Gouda, H.; Koutmos, M.; Banerjee, R.
Deposited on : 2021-08-18
Resolution : 1.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

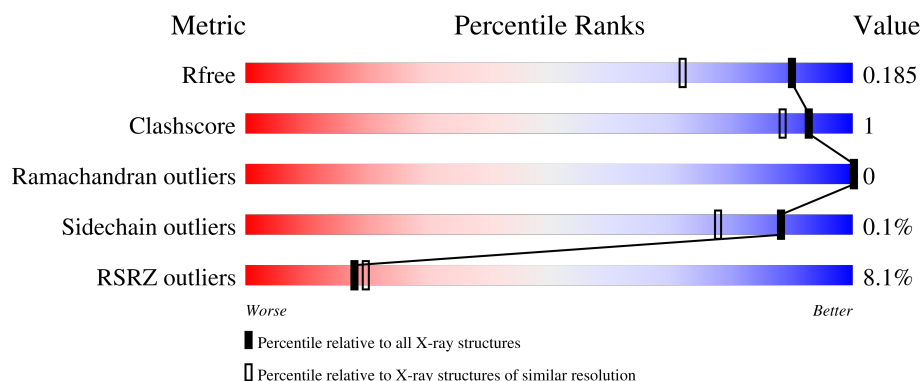
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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

Mol	Chain	Length	Quality of chain
1	A	196	8% 91% 5%
1	B	196	11% 91% 5%
1	C	196	10% 90% 5% 5%
1	D	196	4% 90% 6%
1	E	196	7% 94% 5%

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Mol	Chain	Length	Quality of chain
1	F	196	7% 91% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9572 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 Corrinoid adenosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	187	Total	C	N	O	S	0	1	0
			1427	900	238	281	8			
1	C	186	Total	C	N	O	S	0	4	0
			1426	901	241	275	9			
1	F	186	Total	C	N	O	S	0	3	0
			1436	906	243	279	8			
1	B	187	Total	C	N	O	S	0	4	0
			1440	908	247	276	9			
1	A	186	Total	C	N	O	S	0	5	0
			1458	925	246	279	8			
1	D	185	Total	C	N	O	S	0	4	0
			1456	921	249	278	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	55	MET	-	initiating methionine	UNP Q96EY8
E	190	CYS	ARG	engineered mutation	UNP Q96EY8
C	55	MET	-	initiating methionine	UNP Q96EY8
C	190	CYS	ARG	engineered mutation	UNP Q96EY8
F	55	MET	-	initiating methionine	UNP Q96EY8
F	190	CYS	ARG	engineered mutation	UNP Q96EY8
B	55	MET	-	initiating methionine	UNP Q96EY8
B	190	CYS	ARG	engineered mutation	UNP Q96EY8
A	55	MET	-	initiating methionine	UNP Q96EY8
A	190	CYS	ARG	engineered mutation	UNP Q96EY8
D	55	MET	-	initiating methionine	UNP Q96EY8
D	190	CYS	ARG	engineered mutation	UNP Q96EY8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

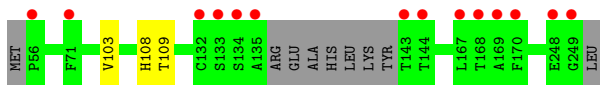
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	105	Total	O	0	0
			105	105		
6	C	109	Total	O	0	0
			109	109		
6	F	127	Total	O	0	0
			127	127		
6	B	128	Total	O	0	0
			128	128		
6	A	123	Total	O	0	0
			123	123		
6	D	125	Total	O	0	0
			125	125		

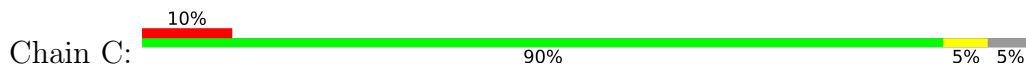
3 Residue-property plots [i](#)

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

- Molecule 1: Corrinoide adenosyltransferase



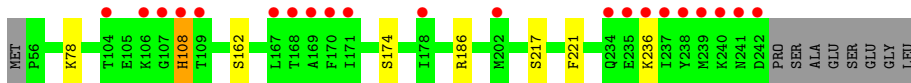
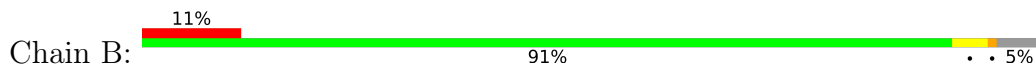
- Molecule 1: Corrinoide adenosyltransferase



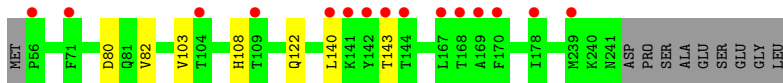
- Molecule 1: Corrinoide adenosyltransferase



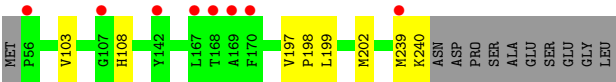
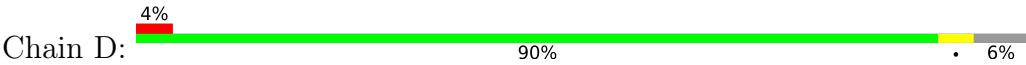
- Molecule 1: Corrinoide adenosyltransferase



- Molecule 1: Corrinoide adenosyltransferase



- Molecule 1: Corrinoide adenosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.15Å 75.77Å 95.84Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	40.49 – 1.50 40.49 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.49-1.50) 99.9 (40.49-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.150 , 0.184 0.151 , 0.185	Depositor DCC
R_{free} test set	8845 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.001 for -k,-h,-l 0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9572	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.25	0/1486	0.44	0/2011
1	B	0.28	0/1467	0.47	1/1983 (0.1%)
1	C	0.23	0/1459	0.39	0/1975
1	D	0.24	0/1484	0.42	0/2005
1	E	0.25	0/1453	0.41	0/1965
1	F	0.24	0/1463	0.41	0/1981
All	All	0.25	0/8812	0.42	1/11920 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	HIS	CA-CB-CG	6.94	120.74	113.80

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	1458	0	1430	5	0
1	B	1440	0	1404	6	0
1	C	1426	0	1396	6	0
1	D	1456	0	1440	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1427	0	1393	2	0
1	F	1436	0	1399	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
4	E	31	0	12	0	0
4	F	31	0	12	0	0
5	A	6	0	8	1	0
6	A	123	0	0	0	0
6	B	128	0	0	1	0
6	C	109	0	0	0	0
6	D	125	0	0	0	0
6	E	105	0	0	0	0
6	F	127	0	0	1	0
All	All	9572	0	8542	26	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 1.

All (26) 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:C:103:VAL:HG13	1:C:108:HIS:HB2	1.72	0.71
1:A:140:LEU:HD23	1:A:143:THR:HG21	1.77	0.67
1:A:103:VAL:HG13	1:A:108:HIS:HB2	1.78	0.65
5:A:501:GOL:O3	5:A:501:GOL:O1	2.22	0.58
1:E:103:VAL:HG13	1:E:108:HIS:HB2	1.86	0.56
1:A:122:GLN:HA	1:A:122:GLN:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:OD2	1:A:82[B]:VAL:HG22	2.08	0.53
1:C:151:LEU:HG	1:C:155:GLN:HE21	1.72	0.53
1:F:61:LYS:NZ	6:F:403:HOH:O	2.42	0.53
1:B:174:SER:HB2	1:B:236:LYS:HZ2	1.75	0.52
1:C:72:THR:HA	1:C:139:HIS:HD2	1.75	0.51
1:C:72:THR:HA	1:C:139:HIS:CD2	2.45	0.51
1:D:197:VAL:HG23	1:D:198:PRO:HD3	1.95	0.48
1:B:217[A]:SER:OG	6:B:401:HOH:O	2.20	0.46
1:B:174:SER:HB2	1:B:236:LYS:NZ	2.31	0.45
1:C:193:GLU:OE2	1:B:78:LYS:NZ	2.43	0.44
1:D:103:VAL:HG13	1:D:108:HIS:HB2	1.99	0.44
1:F:103:VAL:HG13	1:F:108:HIS:HB2	2.00	0.43
1:A:140:LEU:HA	1:A:143:THR:HG23	2.00	0.43
1:B:186:ARG:HD3	1:B:221:PHE:HB2	2.01	0.42
1:F:167:LEU:HD21	1:F:225:ARG:CZ	2.50	0.42
1:C:159:LYS:O	1:C:162:SER:HB2	2.20	0.42
1:D:239:MET:SD	1:D:240:LYS:N	2.93	0.41
1:F:160:TYR:O	1:F:164:LEU:HD12	2.20	0.40
1:D:199:LEU:HD23	1:D:202:MET:CE	2.51	0.40
1:E:109:THR:HA	1:B:162[A]:SER:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	189/196 (96%)	187 (99%)	2 (1%)	0	100	100
1	B	189/196 (96%)	187 (99%)	2 (1%)	0	100	100
1	C	188/196 (96%)	186 (99%)	2 (1%)	0	100	100
1	D	187/196 (95%)	185 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	184/196 (94%)	182 (99%)	2 (1%)	0	100	100
1	F	187/196 (95%)	185 (99%)	2 (1%)	0	100	100
All	All	1124/1176 (96%)	1112 (99%)	12 (1%)	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	154/164 (94%)	154 (100%)	0	100	100
1	B	150/164 (92%)	149 (99%)	1 (1%)	76	57
1	C	151/164 (92%)	151 (100%)	0	100	100
1	D	155/164 (94%)	155 (100%)	0	100	100
1	E	152/164 (93%)	152 (100%)	0	100	100
1	F	151/164 (92%)	151 (100%)	0	100	100
All	All	913/984 (93%)	912 (100%)	1 (0%)	88	78

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	108	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	122	GLN
1	C	139	HIS
1	C	155	GLN
1	C	234	GLN
1	F	233	ASN
1	B	108	HIS

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Mol	Chain	Res	Type
1	B	241	ASN
1	D	163	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 20 are monoatomic - leaving 7 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	$\# Z > 2$
4	ATP	E	303	2,3	32,33,33	1.56	6 (18%)	48,52,52	1.64	8 (16%)
4	ATP	D	306	2,3	32,33,33	1.61	8 (25%)	48,52,52	1.61	7 (14%)
5	GOL	A	501	-	5,5,5	0.94	0	5,5,5	1.04	0
4	ATP	B	304	2,3	32,33,33	1.53	7 (21%)	48,52,52	1.68	10 (20%)
4	ATP	A	505	2,3	32,33,33	1.55	6 (18%)	48,52,52	1.74	10 (20%)
4	ATP	C	305	2,3	32,33,33	1.64	6 (18%)	48,52,52	1.62	9 (18%)
4	ATP	F	304	2,3	32,33,33	1.55	7 (21%)	48,52,52	1.65	7 (14%)

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
4	ATP	E	303	2,3	-	3/22/38/38	0/3/3/3
4	ATP	D	306	2,3	-	1/22/38/38	0/3/3/3
5	GOL	A	501	-	-	0/4/4/4	-
4	ATP	B	304	2,3	-	3/22/38/38	0/3/3/3
4	ATP	A	505	2,3	-	5/22/38/38	0/3/3/3
4	ATP	C	305	2,3	-	3/22/38/38	0/3/3/3
4	ATP	F	304	2,3	-	3/22/38/38	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	304	ATP	C5-C4	4.95	1.47	1.39
4	D	306	ATP	C5-C4	4.85	1.47	1.39
4	A	505	ATP	C5-C4	4.80	1.47	1.39
4	C	305	ATP	C5-C4	4.76	1.47	1.39
4	B	304	ATP	C5-C4	4.73	1.47	1.39
4	E	303	ATP	C5-C4	4.71	1.47	1.39
4	C	305	ATP	PA-O3A	3.85	1.63	1.59
4	E	303	ATP	PB-O3A	3.33	1.63	1.59
4	A	505	ATP	PA-O3A	3.09	1.62	1.59
4	D	306	ATP	PB-O3A	3.06	1.62	1.59
4	D	306	ATP	PA-O3A	3.02	1.62	1.59
4	C	305	ATP	PB-O3B	3.01	1.62	1.59
4	E	303	ATP	PB-O3B	2.97	1.62	1.59
4	B	304	ATP	PB-O3A	2.94	1.62	1.59
4	B	304	ATP	PA-O3A	2.91	1.62	1.59
4	A	505	ATP	PB-O3A	2.89	1.62	1.59
4	F	304	ATP	PA-O3A	2.77	1.62	1.59
4	A	505	ATP	C8-N7	2.69	1.36	1.31
4	B	304	ATP	C8-N7	2.67	1.36	1.31
4	D	306	ATP	PB-O3B	2.65	1.62	1.59
4	C	305	ATP	C8-N7	2.64	1.36	1.31
4	C	305	ATP	PB-O3A	2.61	1.62	1.59
4	D	306	ATP	C8-N7	2.60	1.36	1.31
4	C	305	ATP	C5-C6	2.56	1.48	1.41
4	F	304	ATP	PB-O3A	2.56	1.62	1.59
4	B	304	ATP	C5-C6	2.55	1.48	1.41
4	E	303	ATP	PA-O3A	2.52	1.62	1.59
4	A	505	ATP	C5-C6	2.50	1.47	1.41
4	F	304	ATP	C5-N7	-2.45	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	304	ATP	C8-N7	2.42	1.36	1.31
4	D	306	ATP	C5-C6	2.42	1.47	1.41
4	E	303	ATP	C5-C6	2.36	1.47	1.41
4	F	304	ATP	C5-C6	2.33	1.47	1.41
4	D	306	ATP	C4-N9	-2.32	1.32	1.37
4	E	303	ATP	C8-N7	2.30	1.36	1.31
4	F	304	ATP	PB-O3B	2.30	1.62	1.59
4	D	306	ATP	C5-N7	-2.27	1.34	1.39
4	A	505	ATP	C5-N7	-2.17	1.35	1.39
4	B	304	ATP	C4-N9	-2.15	1.33	1.37
4	B	304	ATP	PB-O3B	2.00	1.61	1.59

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	304	ATP	C5-C4-N3	-5.72	118.84	126.72
4	D	306	ATP	C5-C4-N3	-5.29	119.43	126.72
4	A	505	ATP	C5-C4-N3	-5.25	119.49	126.72
4	E	303	ATP	C5-C4-N3	-5.18	119.58	126.72
4	B	304	ATP	C5-C4-N3	-4.88	120.00	126.72
4	C	305	ATP	C5-C4-N3	-4.68	120.27	126.72
4	F	304	ATP	N3-C4-N9	4.50	134.82	127.17
4	D	306	ATP	N3-C4-N9	4.32	134.51	127.17
4	E	303	ATP	N3-C4-N9	4.19	134.29	127.17
4	A	505	ATP	N3-C4-N9	4.11	134.16	127.17
4	C	305	ATP	N3-C4-N9	3.80	133.63	127.17
4	B	304	ATP	N3-C4-N9	3.55	133.20	127.17
4	B	304	ATP	C2-N3-C4	3.38	120.08	111.83
4	F	304	ATP	C2-N3-C4	3.37	120.06	111.83
4	B	304	ATP	N3-C2-N1	-3.36	123.49	128.58
4	D	306	ATP	C2-N3-C4	3.34	119.99	111.83
4	A	505	ATP	C2-N3-C4	3.31	119.91	111.83
4	C	305	ATP	N3-C2-N1	-3.29	123.60	128.58
4	B	304	ATP	C4-C5-N7	-3.25	106.86	110.58
4	A	505	ATP	C4-C5-N7	-3.25	106.87	110.58
4	E	303	ATP	C2-N3-C4	3.17	119.58	111.83
4	A	505	ATP	N3-C2-N1	-3.17	123.78	128.58
4	E	303	ATP	C4-C5-N7	-3.16	106.97	110.58
4	C	305	ATP	C2-N3-C4	3.02	119.22	111.83
4	D	306	ATP	N3-C2-N1	-2.99	124.06	128.58
4	E	303	ATP	N3-C2-N1	-2.91	124.17	128.58
4	D	306	ATP	C4-C5-N7	-2.89	107.27	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	306	ATP	C4-N9-C8	2.87	108.75	105.74
4	C	305	ATP	C4-N9-C8	2.85	108.73	105.74
4	F	304	ATP	C4-C5-N7	-2.84	107.33	110.58
4	C	305	ATP	C4-C5-N7	-2.84	107.34	110.58
4	F	304	ATP	N3-C2-N1	-2.78	124.38	128.58
4	E	303	ATP	C4-N9-C8	2.77	108.64	105.74
4	A	505	ATP	C4-N9-C8	2.62	108.49	105.74
4	C	305	ATP	C2-N1-C6	2.52	122.87	118.73
4	A	505	ATP	C5-N7-C8	2.47	107.34	103.45
4	F	304	ATP	N6-C6-N1	2.38	123.68	118.38
4	D	306	ATP	O4'-C1'-N9	-2.38	103.52	108.09
4	B	304	ATP	C4-N9-C8	2.35	108.21	105.74
4	F	304	ATP	O4'-C1'-N9	-2.26	103.76	108.09
4	B	304	ATP	O3A-PB-O1B	-2.23	103.98	110.70
4	E	303	ATP	C5-N7-C8	2.23	106.96	103.45
4	B	304	ATP	O4'-C1'-N9	-2.20	103.86	108.09
4	B	304	ATP	C6-C5-N7	2.18	136.29	132.09
4	C	305	ATP	C5-N7-C8	2.18	106.87	103.45
4	A	505	ATP	N9-C8-N7	-2.11	110.94	113.94
4	C	305	ATP	N9-C8-N7	-2.11	110.95	113.94
4	E	303	ATP	O3A-PB-O1B	-2.10	104.39	110.70
4	A	505	ATP	O3A-PB-O1B	-2.06	104.50	110.70
4	B	304	ATP	C5-N7-C8	2.02	106.62	103.45
4	A	505	ATP	C2-N1-C6	2.01	122.04	118.73

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	306	ATP	C5'-O5'-PA-O2A
4	C	305	ATP	PB-O3B-PG-O1G
4	B	304	ATP	PB-O3B-PG-O1G
4	A	505	ATP	PB-O3B-PG-O1G
4	E	303	ATP	PG-O3B-PB-O1B
4	C	305	ATP	PG-O3B-PB-O1B
4	F	304	ATP	PG-O3B-PB-O1B
4	E	303	ATP	C5'-O5'-PA-O2A
4	B	304	ATP	PG-O3B-PB-O1B
4	A	505	ATP	PG-O3B-PB-O1B
4	A	505	ATP	PB-O3A-PA-O2A
4	F	304	ATP	PB-O3B-PG-O2G
4	E	303	ATP	PG-O3B-PB-O2B

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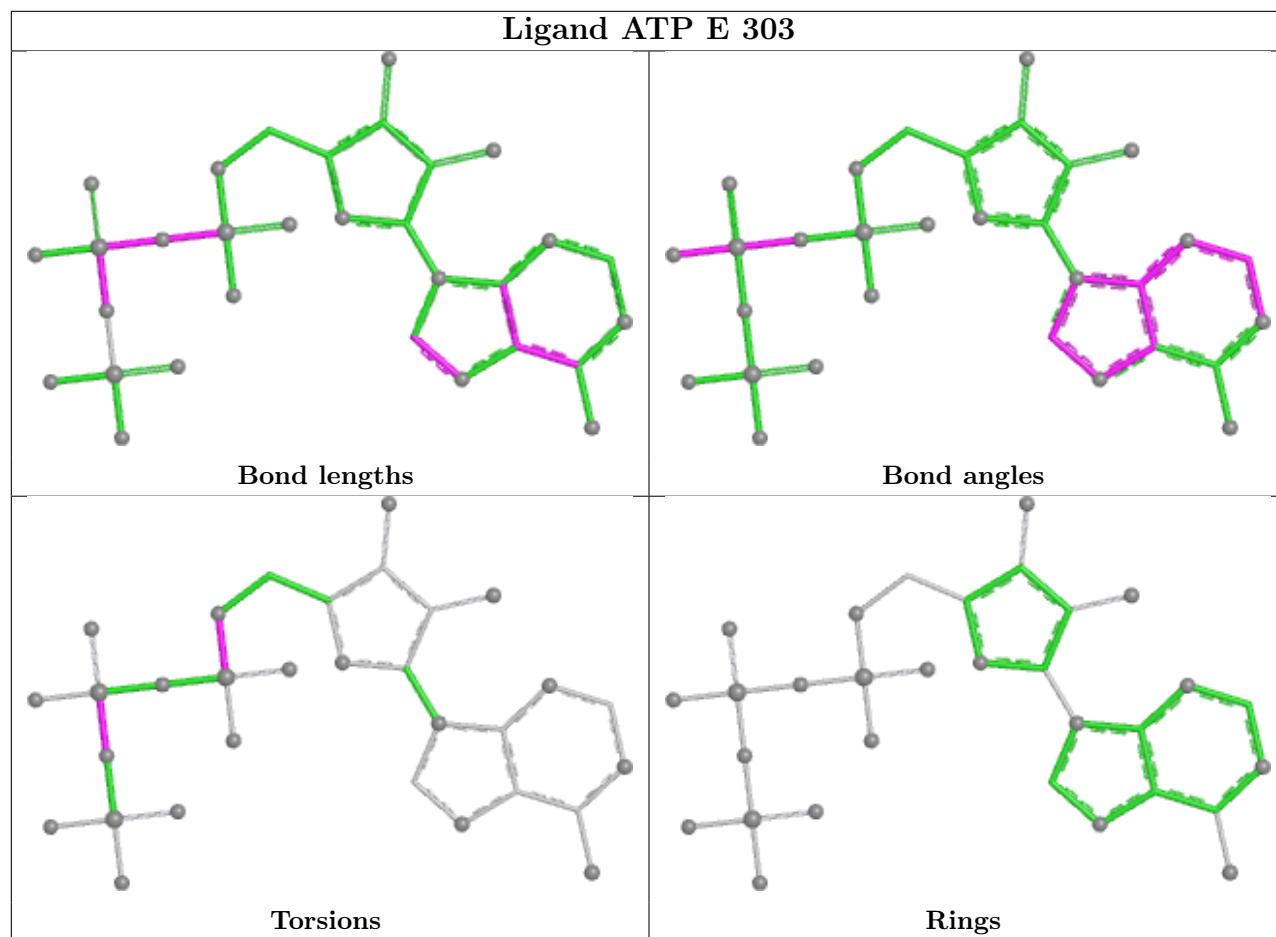
Mol	Chain	Res	Type	Atoms
4	C	305	ATP	PG-O3B-PB-O2B
4	F	304	ATP	PG-O3B-PB-O2B
4	A	505	ATP	PG-O3B-PB-O2B
4	B	304	ATP	PG-O3B-PB-O2B
4	A	505	ATP	PB-O3A-PA-O1A

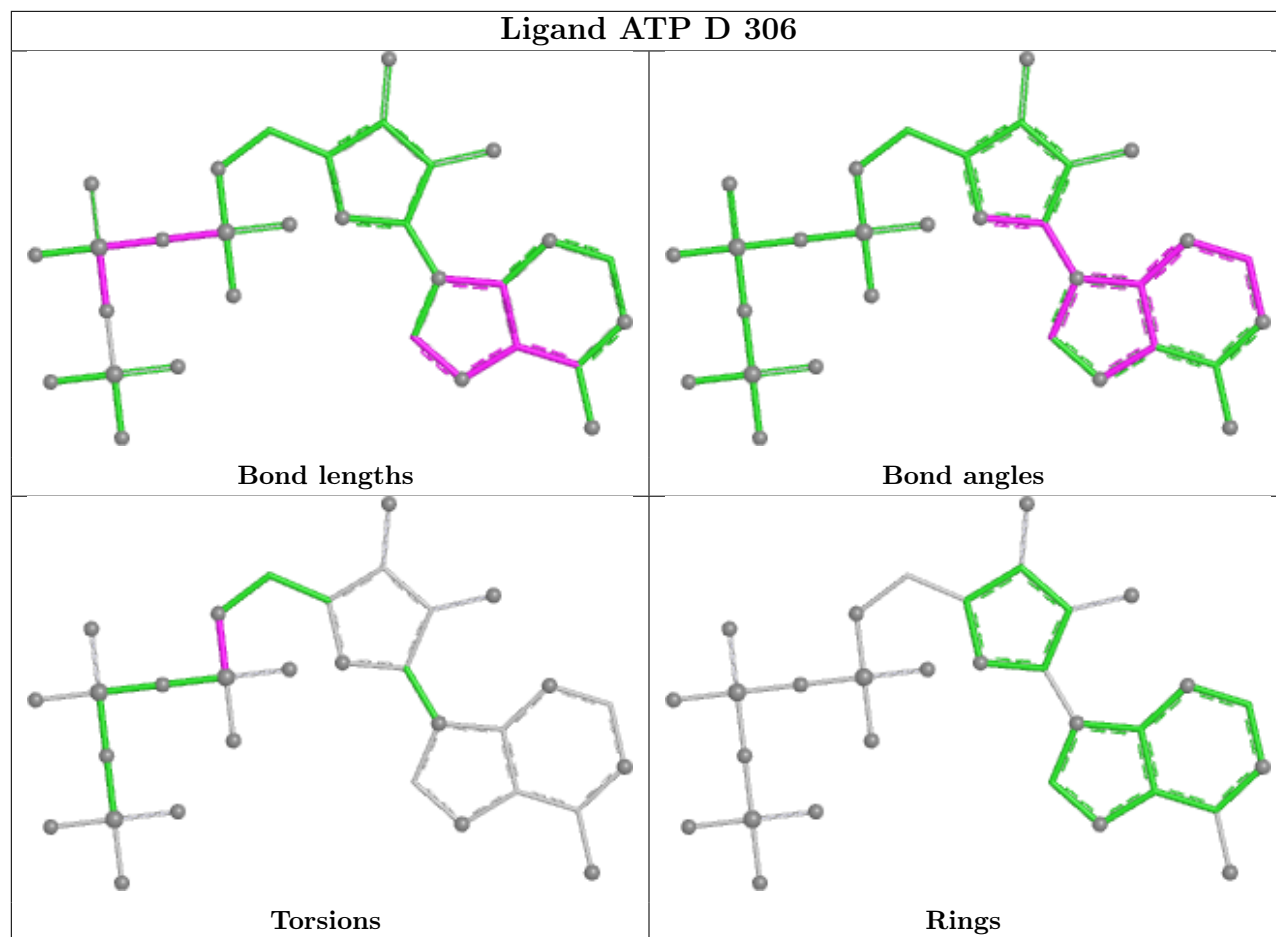
There are no ring outliers.

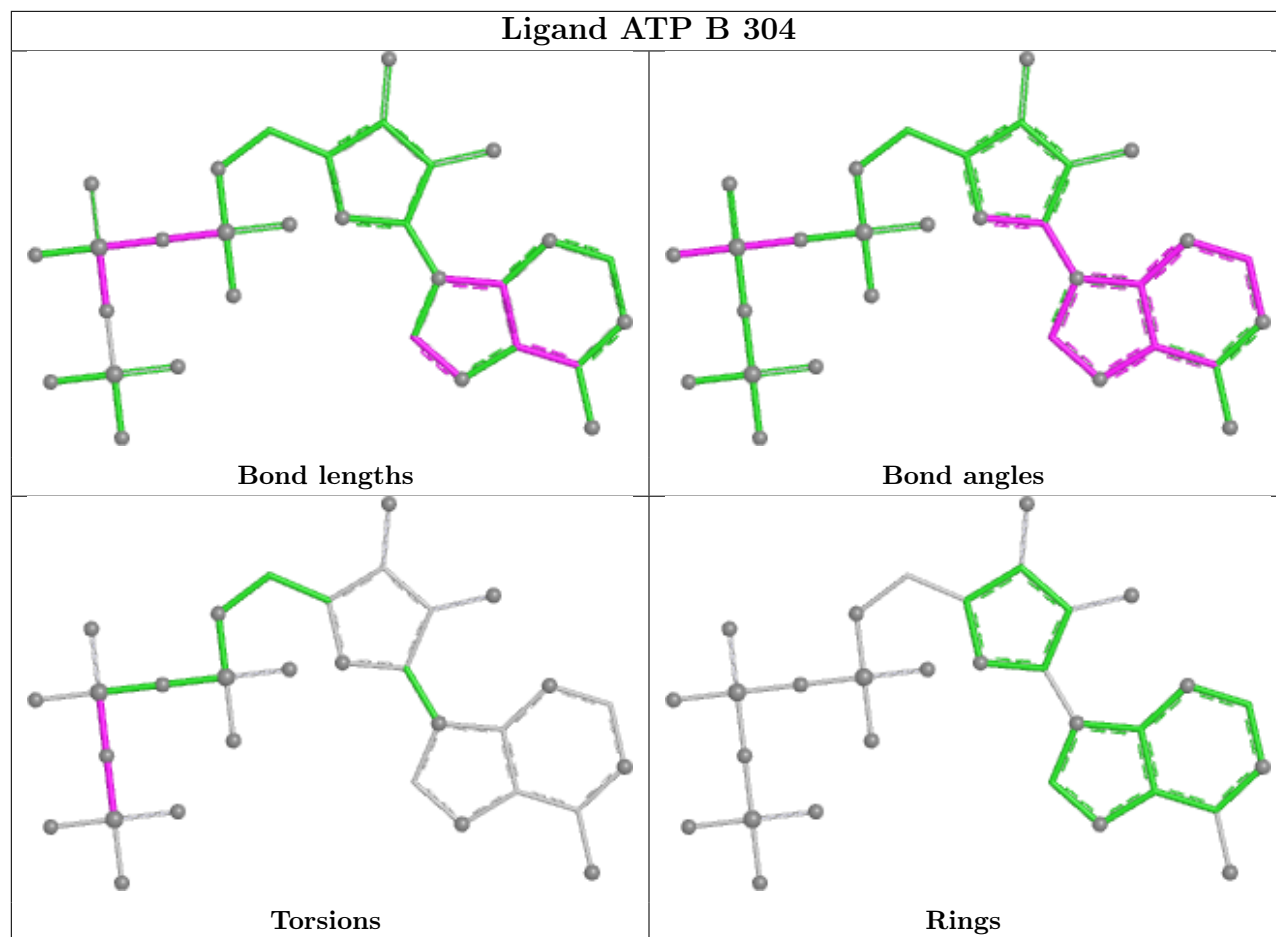
1 monomer is involved in 1 short contact:

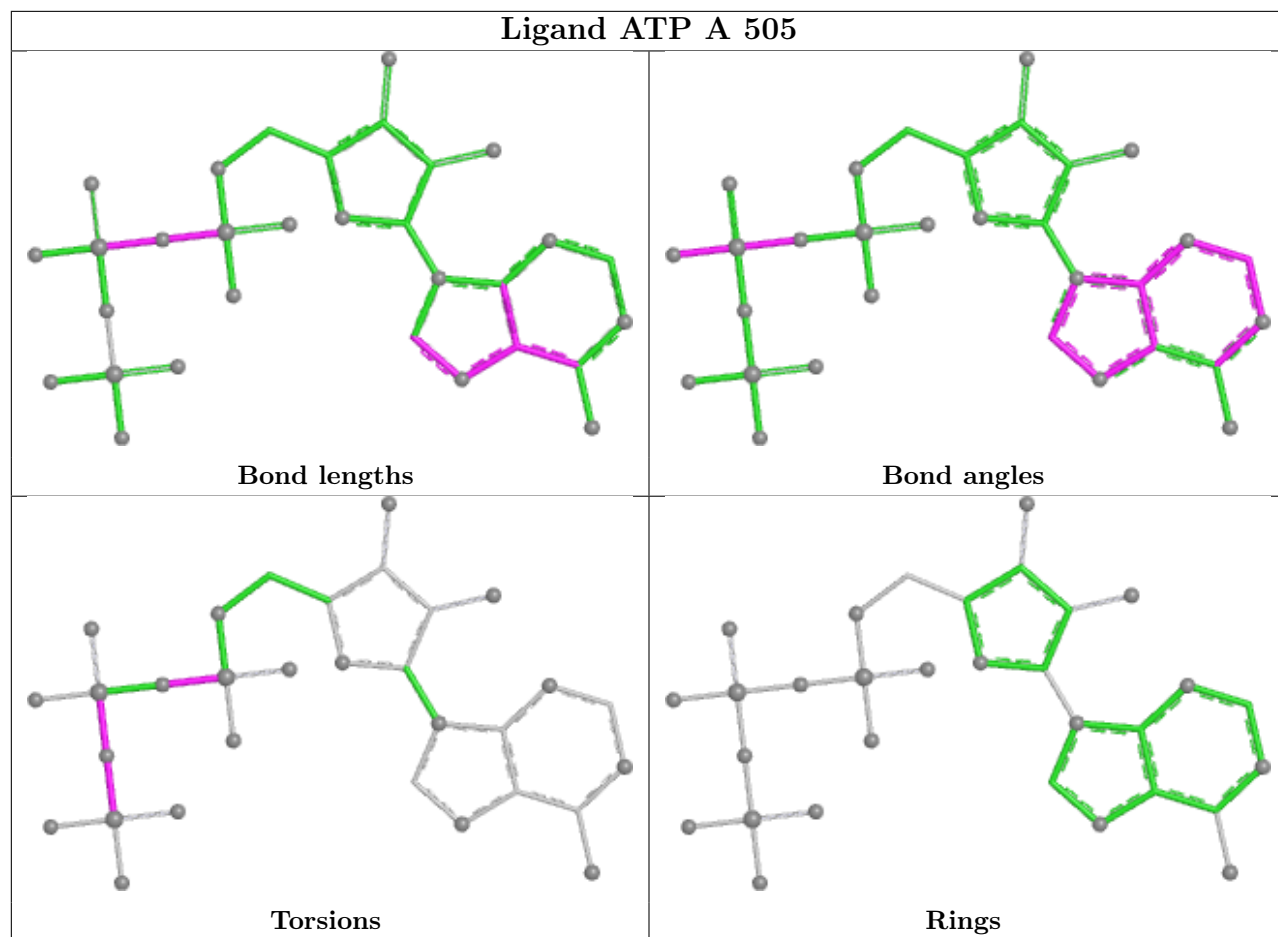
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GOL	1	0

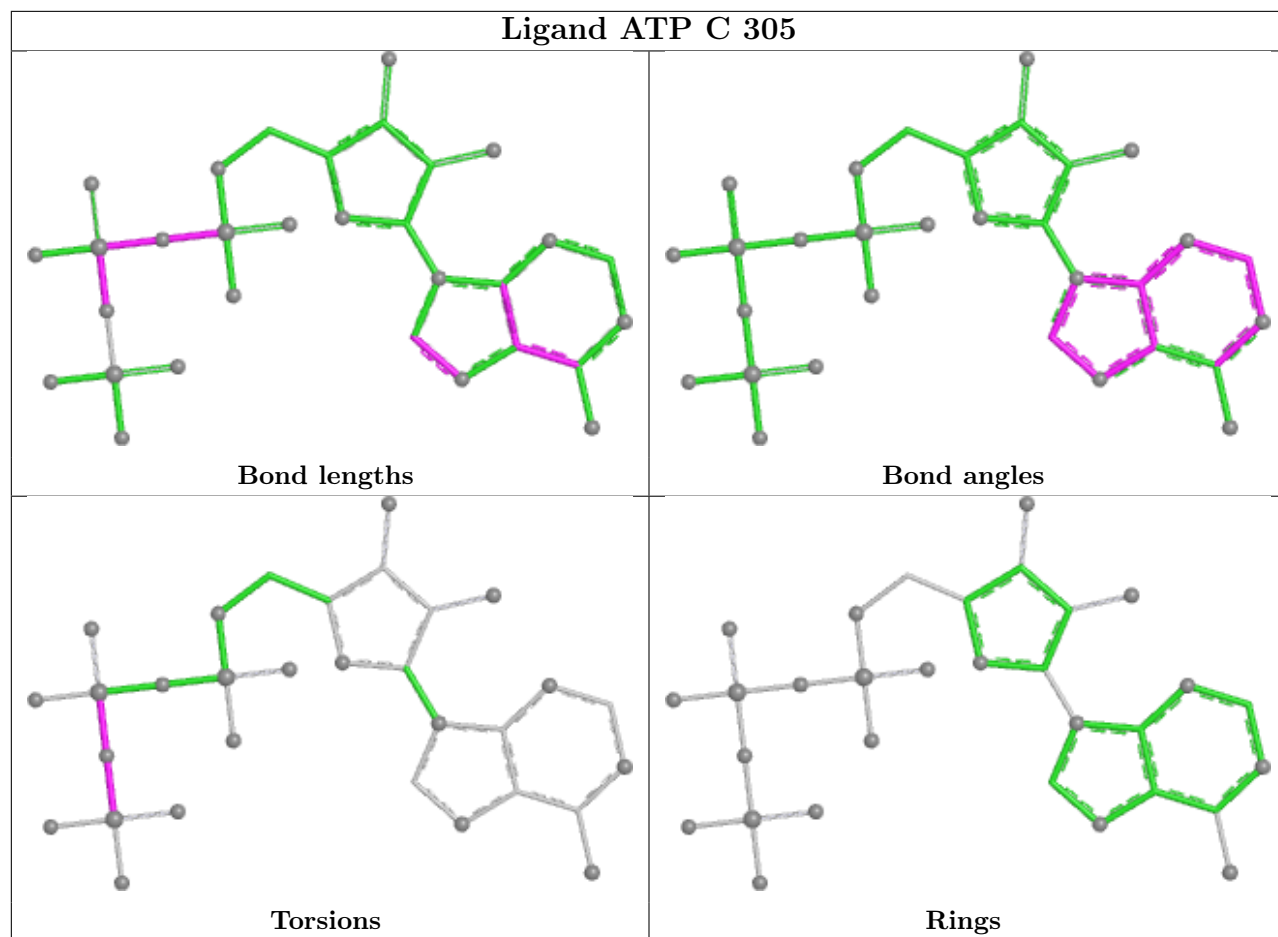
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

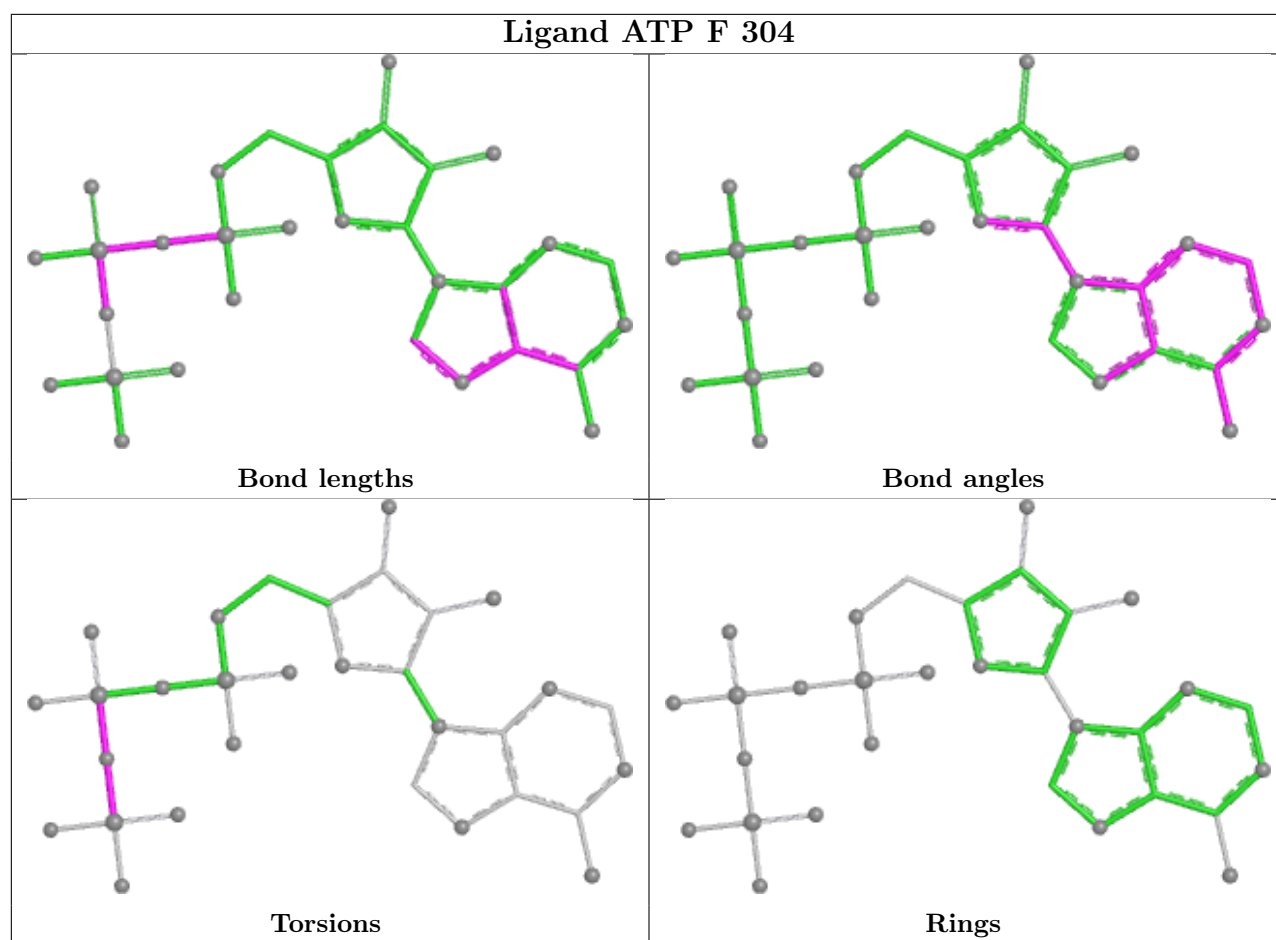












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	186/196 (94%)	0.17	15 (8%)	18 20	9, 25, 61, 83	5 (2%)
1	B	187/196 (95%)	0.21	21 (11%)	10 10	10, 24, 77, 142	4 (2%)
1	C	186/196 (94%)	0.20	19 (10%)	12 12	12, 27, 67, 92	4 (2%)
1	D	185/196 (94%)	0.02	8 (4%)	40 44	10, 25, 52, 79	4 (2%)
1	E	187/196 (95%)	0.13	14 (7%)	20 22	16, 29, 61, 91	1 (0%)
1	F	186/196 (94%)	0.05	13 (6%)	22 24	10, 25, 59, 87	3 (1%)
All	All	1117/1176 (94%)	0.13	90 (8%)	18 20	9, 26, 64, 142	21 (1%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	HIS	8.1
1	D	56	PRO	5.4
1	A	142	TYR	5.2
1	B	170	PHE	4.9
1	C	167	LEU	4.4
1	C	107	GLY	4.3
1	A	104	THR	4.3
1	A	167	LEU	4.2
1	F	164	LEU	4.2
1	B	237	ILE	4.1
1	C	138	ALA	4.1
1	B	239	MET	4.1
1	B	107	GLY	4.1
1	E	167	LEU	4.0
1	F	241	ASN	4.0
1	C	140	LEU	3.8
1	C	139	HIS	3.7
1	E	71	PHE	3.7
1	C	142	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	238	TYR	3.7
1	A	168	THR	3.7
1	E	168	THR	3.5
1	B	169	ALA	3.5
1	D	169	ALA	3.5
1	C	168	THR	3.4
1	A	71[A]	PHE	3.4
1	E	135	ALA	3.4
1	B	109	THR	3.3
1	D	168	THR	3.2
1	D	239	MET	3.2
1	F	168	THR	3.1
1	E	132	CYS	3.1
1	C	170	PHE	3.0
1	B	167	LEU	3.0
1	F	142	TYR	3.0
1	F	233	ASN	3.0
1	D	170	PHE	3.0
1	B	171	ILE	2.9
1	E	248	GLU	2.9
1	A	170	PHE	2.9
1	A	143	THR	2.9
1	E	249	GLY	2.8
1	F	169	ALA	2.8
1	E	170	PHE	2.8
1	E	143	THR	2.8
1	B	236	LYS	2.8
1	F	239	MET	2.7
1	A	178	ILE	2.7
1	A	141	LYS	2.7
1	C	169	ALA	2.7
1	C	239	MET	2.7
1	C	56	PRO	2.7
1	F	140	LEU	2.6
1	A	239	MET	2.6
1	E	169	ALA	2.6
1	A	169	ALA	2.6
1	A	140	LEU	2.6
1	C	103	VAL	2.6
1	B	241	ASN	2.6
1	D	167	LEU	2.6
1	D	107	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	104	THR	2.5
1	B	168	THR	2.5
1	B	235	GLU	2.4
1	F	167	LEU	2.4
1	E	144	THR	2.4
1	C	105	GLU	2.4
1	C	108	HIS	2.4
1	F	170	PHE	2.4
1	E	56	PRO	2.3
1	B	234	GLN	2.3
1	A	109	THR	2.3
1	C	106	LYS	2.3
1	B	242	ASP	2.3
1	F	237	ILE	2.3
1	E	134	SER	2.3
1	B	240	LYS	2.2
1	A	144	THR	2.2
1	B	202	MET	2.2
1	B	106	LYS	2.2
1	C	144	THR	2.2
1	C	71	PHE	2.1
1	F	234	GLN	2.1
1	C	151	LEU	2.0
1	B	178	ILE	2.0
1	D	142	TYR	2.0
1	F	144	THR	2.0
1	A	56	PRO	2.0
1	E	133	SER	2.0
1	C	162	SER	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

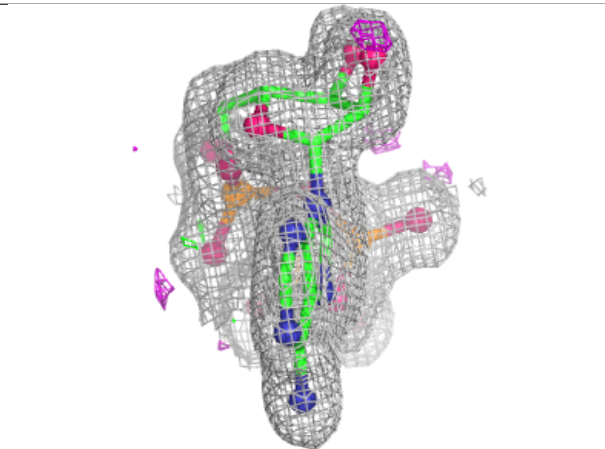
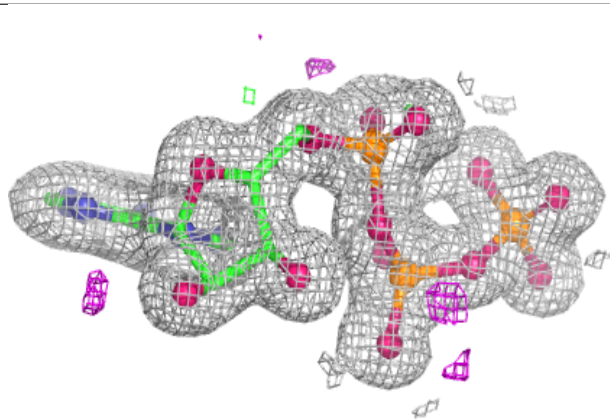
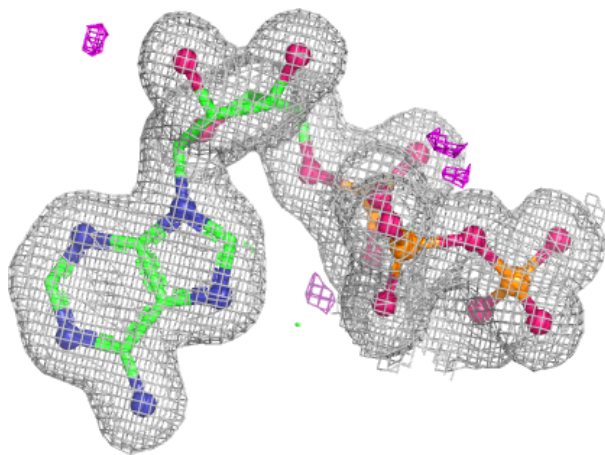
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	C	302	1/1	0.84	0.12	57,57,57,57	0
2	MG	E	301	1/1	0.87	0.20	71,71,71,71	0
5	GOL	A	501	6/6	0.87	0.15	66,67,67,67	0
2	MG	F	302	1/1	0.88	0.11	50,50,50,50	0
3	K	C	304	1/1	0.97	0.07	54,54,54,54	0
3	K	E	302	1/1	0.98	0.25	40,40,40,40	0
2	MG	D	301	1/1	0.99	0.03	18,18,18,18	0
2	MG	D	302	1/1	0.99	0.04	19,19,19,19	0
2	MG	F	301	1/1	0.99	0.04	18,18,18,18	0
2	MG	B	301	1/1	0.99	0.03	18,18,18,18	0
3	K	A	504	1/1	0.99	0.03	24,24,24,24	0
3	K	D	304	1/1	0.99	0.08	24,24,24,24	0
3	K	D	305	1/1	0.99	0.07	48,48,48,48	0
4	ATP	E	303	31/31	0.99	0.04	17,20,24,25	0
4	ATP	C	305	31/31	0.99	0.04	16,19,22,23	0
4	ATP	F	304	31/31	0.99	0.04	16,20,24,26	0
4	ATP	B	304	31/31	0.99	0.04	16,19,23,24	0
4	ATP	A	505	31/31	0.99	0.04	17,21,23,25	0
4	ATP	D	306	31/31	0.99	0.04	17,21,25,27	0
2	MG	A	502	1/1	0.99	0.02	20,20,20,20	0
3	K	B	302	1/1	1.00	0.02	23,23,23,23	0
3	K	B	303	1/1	1.00	0.08	24,24,24,24	0
3	K	A	503	1/1	1.00	0.04	26,26,26,26	0
3	K	C	303	1/1	1.00	0.03	25,25,25,25	0
3	K	D	303	1/1	1.00	0.05	25,25,25,25	0
2	MG	C	301	1/1	1.00	0.02	18,18,18,18	0
3	K	F	303	1/1	1.00	0.05	24,24,24,24	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.

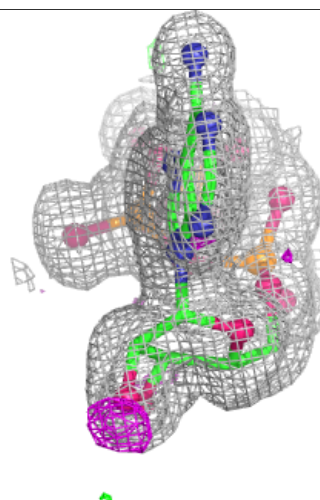
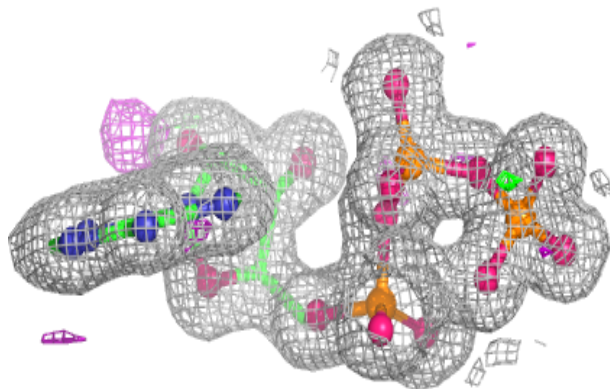
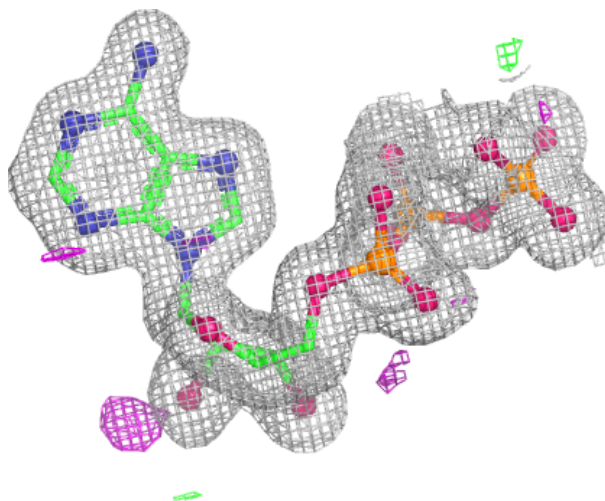
Electron density around ATP E 303:

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



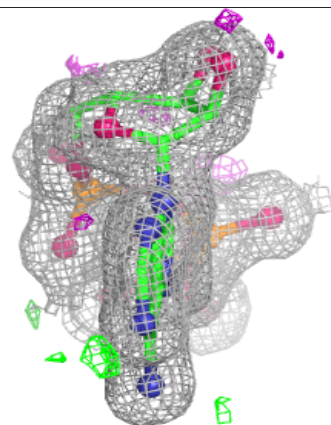
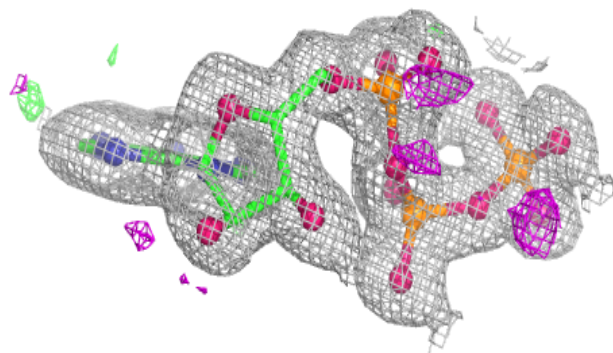
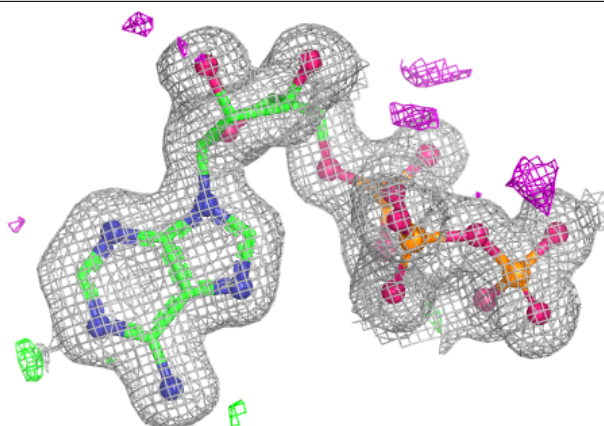
Electron density around ATP C 305:

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



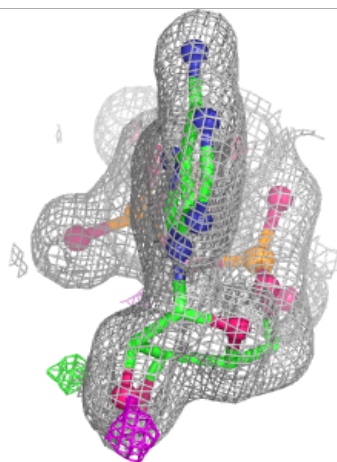
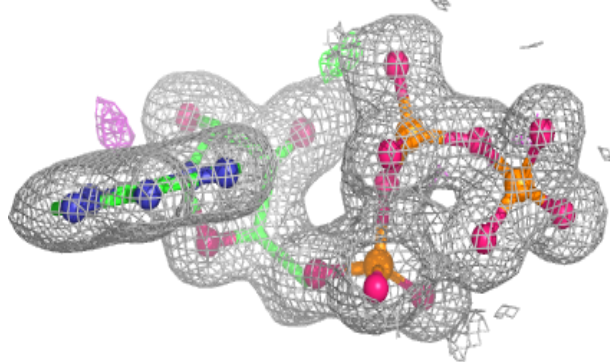
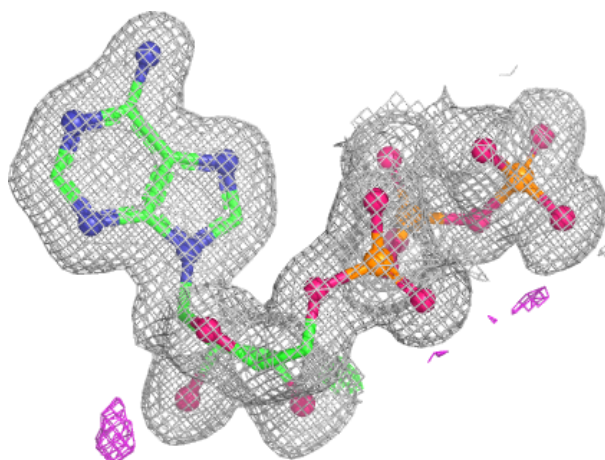
Electron density around ATP F 304:

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



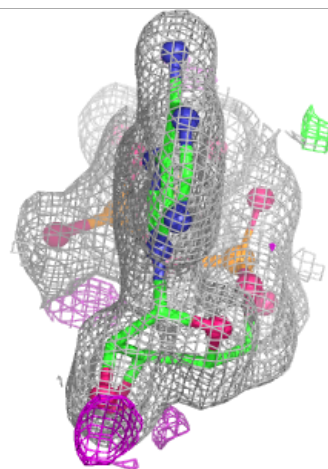
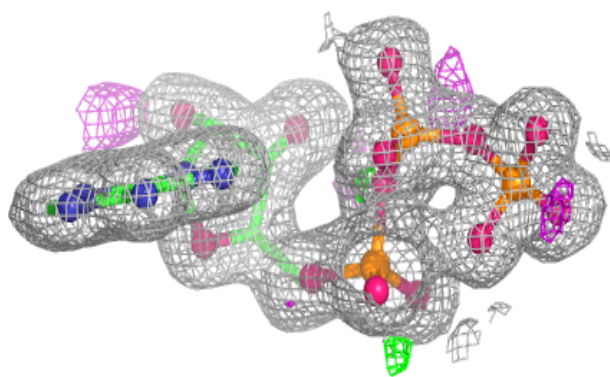
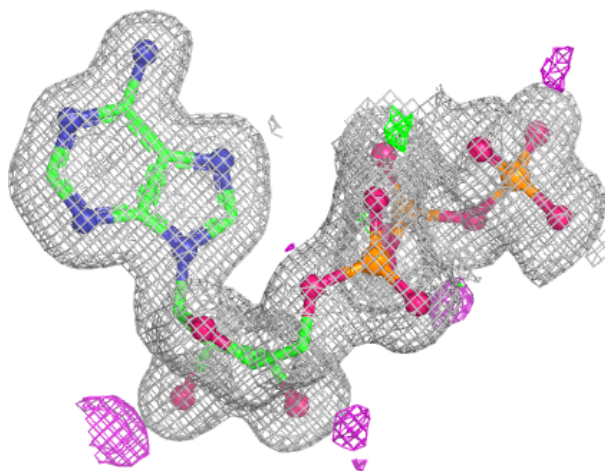
Electron density around ATP B 304:

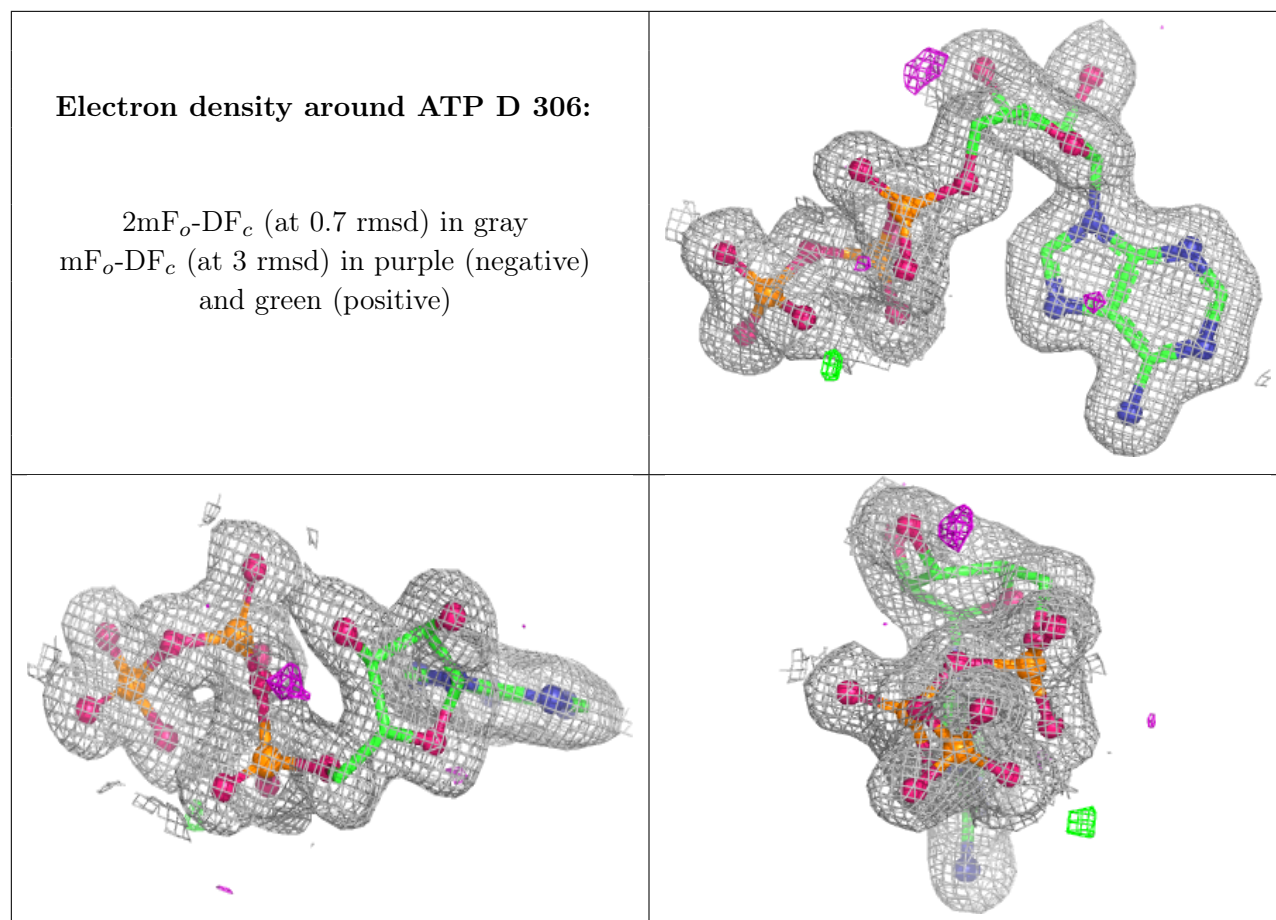
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP A 505:

$2mF_o-DF_c$ (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.