



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:36 PM UTC

PDB ID : 5ETL / pdb_00005etl
Title : E. coli 6-hydroxymethyl-7,8-dihydropterin pyrophosphokinase complexed with AMPCPP and inhibitor at 1.82 angstrom resolution
Authors : Dennis, M.L.; Peat, T.S.; Swarbrick, J.D.
Deposited on : 2015-11-17
Resolution : 1.82 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

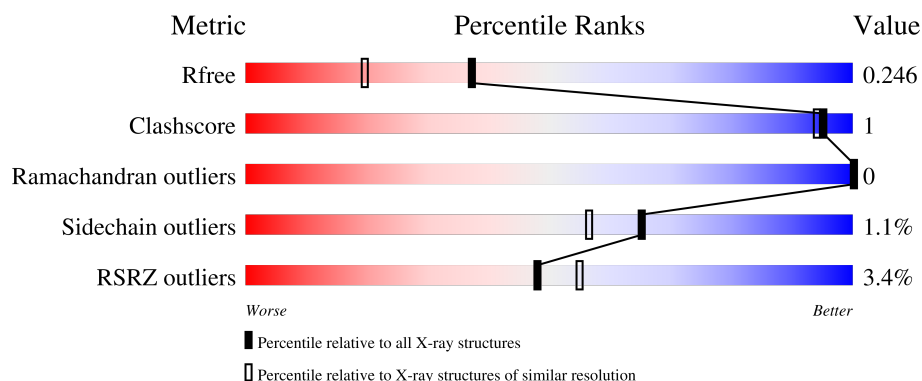
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	162	3% 91% • •
1	B	162	4% 89% 6% • •
1	C	162	4% 94% • •
1	D	162	2% 96% • • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5768 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 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	1	0
			1243	795	213	230	5			
1	B	155	Total	C	N	O	S	0	2	0
			1249	799	213	232	5			
1	C	156	Total	C	N	O	S	0	0	0
			1242	795	213	229	5			
1	D	160	Total	C	N	O	S	0	2	0
			1287	825	219	238	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P26281
A	-2	SER	-	expression tag	UNP P26281
A	-1	ALA	-	expression tag	UNP P26281
B	-3	GLY	-	expression tag	UNP P26281
B	-2	SER	-	expression tag	UNP P26281
B	-1	ALA	-	expression tag	UNP P26281
C	-3	GLY	-	expression tag	UNP P26281
C	-2	SER	-	expression tag	UNP P26281
C	-1	ALA	-	expression tag	UNP P26281
D	-3	GLY	-	expression tag	UNP P26281
D	-2	SER	-	expression tag	UNP P26281
D	-1	ALA	-	expression tag	UNP P26281

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

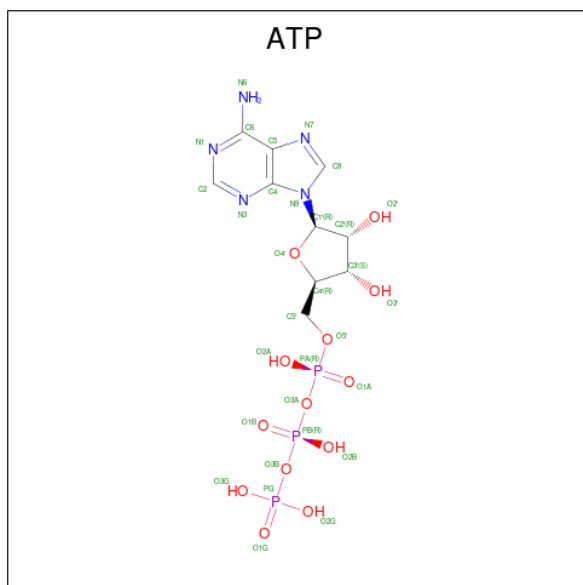
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

Continued on next page...

Continued from previous page...

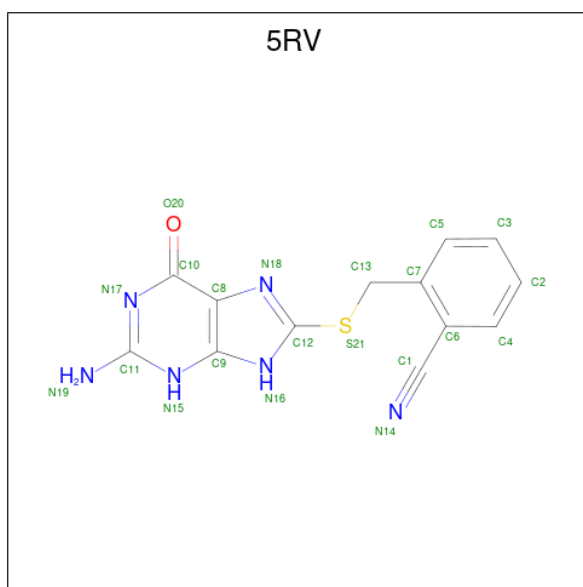
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	C	3	Total	Ca	0	0
			3	3		
2	D	2	Total	Ca	0	0
			2	2		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	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		

- Molecule 4 is 2-[(2-azanyl-6-oxidanylidene-3,9-dihydropurin-8-yl)sulfanylmethyl]benzenecarbonitrile (CCD ID: 5RV) (formula: $C_{13}H_{10}N_6OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			21	13	6	1	1		
4	B	1	Total	C	N	O	S	0	0
			21	13	6	1	1		
4	C	1	Total	C	N	O	S	0	0
			21	13	6	1	1		
4	D	1	Total	C	N	O	S	0	0
			21	13	6	1	1		

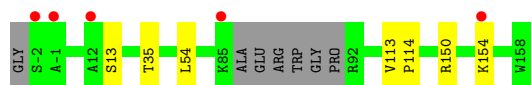
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	132	Total	O	0	0
			132	132		
5	B	109	Total	O	0	0
			109	109		
5	C	140	Total	O	0	0
			140	140		
5	D	147	Total	O	0	0
			147	147		

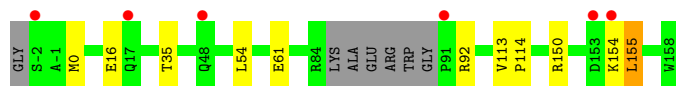
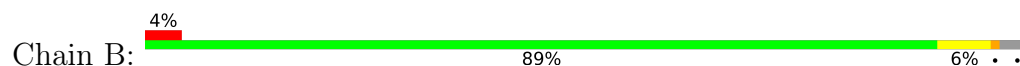
3 Residue-property plots [i](#)

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.

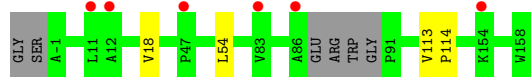
- Molecule 1: 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase



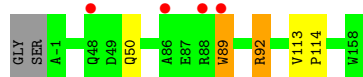
- Molecule 1: 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase



- Molecule 1: 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase



- Molecule 1: 2-amino-4-hydroxy-6-hydroxymethyldihydropteridine pyrophosphokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.45Å 36.18Å 121.33Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	45.81 – 1.82 45.81 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.81-1.82) 99.6 (45.81-1.82)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.202 , 0.241 0.209 , 0.246	Depositor DCC
R_{free} test set	2709 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5768	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6057e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA, ATP, 5RV

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	0.89	1/1270 (0.1%)	0.92	2/1726 (0.1%)
1	B	0.88	1/1280 (0.1%)	0.94	2/1739 (0.1%)
1	C	0.91	0/1270	0.86	0/1726
1	D	0.95	1/1321 (0.1%)	0.94	2/1799 (0.1%)
All	All	0.91	3/5141 (0.1%)	0.91	6/6990 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	GLN	C-O	-6.40	1.18	1.24
1	A	150	ARG	C-O	-5.48	1.17	1.23
1	B	92	ARG	C-O	-5.04	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	SER	CA-C-N	6.36	127.79	119.84
1	A	13	SER	C-N-CA	6.36	127.79	119.84
1	B	16	GLU	N-CA-C	5.75	117.62	111.36
1	D	92	ARG	N-CA-C	5.48	117.59	108.99
1	B	155	LEU	N-CA-C	5.23	118.01	109.59
1	D	89	TRP	N-CA-C	-5.20	100.42	108.90

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	1243	0	1250	2	0
1	B	1249	0	1255	7	0
1	C	1242	0	1250	2	0
1	D	1287	0	1285	1	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	21	0	0	0	0
4	B	21	0	0	0	0
4	C	21	0	0	0	0
4	D	21	0	0	0	0
5	A	132	0	0	0	0
5	B	109	0	0	0	0
5	C	140	0	0	0	0
5	D	147	0	0	0	0
All	All	5768	0	5088	12	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 (12) 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:B:0:MET:HB3	1:B:61:GLU:HG2	1.85	0.57
1:B:154:LYS:HG2	1:B:155:LEU:H	1.72	0.55
1:B:154:LYS:CG	1:B:155:LEU:H	2.21	0.53
1:D:113:VAL:HA	1:D:114:PRO:C	2.38	0.48
1:C:113:VAL:HA	1:C:114:PRO:C	2.39	0.47
1:B:154:LYS:HG2	1:B:155:LEU:N	2.32	0.45
1:B:113:VAL:HA	1:B:114:PRO:C	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:HA	1:A:114:PRO:C	2.43	0.44
1:B:154:LYS:CG	1:B:155:LEU:N	2.81	0.43
1:C:18:VAL:HG21	1:C:54:LEU:HD22	2.02	0.41
1:A:54:LEU:HD23	1:A:54:LEU:C	2.46	0.40
1:B:54:LEU:HD23	1:B:54:LEU:C	2.47	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	152/162 (94%)	150 (99%)	2 (1%)	0	100	100
1	B	153/162 (94%)	150 (98%)	3 (2%)	0	100	100
1	C	152/162 (94%)	151 (99%)	1 (1%)	0	100	100
1	D	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
All	All	617/648 (95%)	608 (98%)	9 (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	136/139 (98%)	134 (98%)	2 (2%)	57	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	137/139 (99%)	135 (98%)	2 (2%)	57	46
1	C	135/139 (97%)	135 (100%)	0	100	100
1	D	139/139 (100%)	137 (99%)	2 (1%)	59	49
All	All	547/556 (98%)	541 (99%)	6 (1%)	65	56

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	A	154	LYS
1	B	35	THR
1	B	150	ARG
1	D	89	TRP
1	D	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	145	GLN
1	C	145	GLN
1	C	156	ASN
1	D	145	GLN
1	D	156	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 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	C	204	2	32,33,33	2.10	7 (21%)	48,52,52	1.88	13 (27%)
4	5RV	A	206	-	23,23,23	2.07	5 (21%)	27,32,32	1.81	6 (22%)
3	ATP	A	205	2	32,33,33	2.04	7 (21%)	48,52,52	1.94	11 (22%)
3	ATP	B	203	2	32,33,33	1.98	5 (15%)	48,52,52	1.94	14 (29%)
4	5RV	B	204	-	23,23,23	2.18	6 (26%)	27,32,32	1.94	7 (25%)
4	5RV	C	205	-	23,23,23	2.10	5 (21%)	27,32,32	2.24	7 (25%)
3	ATP	D	203	2	32,33,33	2.79	15 (46%)	48,52,52	1.58	8 (16%)
4	5RV	D	204	-	23,23,23	1.99	6 (26%)	27,32,32	1.86	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	C	204	2	-	1/22/38/38	0/3/3/3
4	5RV	A	206	-	-	3/7/7/7	0/3/3/3
3	ATP	A	205	2	-	2/22/38/38	0/3/3/3
3	ATP	B	203	2	-	2/22/38/38	0/3/3/3
4	5RV	B	204	-	-	3/7/7/7	0/3/3/3
4	5RV	C	205	-	-	3/7/7/7	0/3/3/3
3	ATP	D	203	2	-	1/22/38/38	0/3/3/3
4	5RV	D	204	-	-	3/7/7/7	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	203	ATP	PA-O3A	8.42	1.68	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	204	5RV	O20-C10	7.19	1.36	1.23
4	C	205	5RV	O20-C10	7.08	1.36	1.23
3	C	204	ATP	PA-O3A	7.05	1.67	1.59
4	A	206	5RV	O20-C10	6.87	1.36	1.23
4	D	204	5RV	O20-C10	6.70	1.35	1.23
3	B	203	ATP	PB-O3A	6.31	1.66	1.59
3	A	205	ATP	PA-O3A	6.26	1.66	1.59
3	A	205	ATP	PB-O3A	6.11	1.66	1.59
3	C	204	ATP	PB-O3A	5.75	1.65	1.59
3	B	203	ATP	PA-O3A	5.61	1.65	1.59
3	A	205	ATP	C5-C4	4.59	1.47	1.39
3	D	203	ATP	C5-C4	4.57	1.47	1.39
3	B	203	ATP	C5-C4	4.56	1.47	1.39
3	D	203	ATP	C5-N7	-4.53	1.30	1.39
3	C	204	ATP	C5-C4	4.42	1.47	1.39
3	D	203	ATP	PG-O1G	-4.31	1.37	1.50
3	D	203	ATP	PB-O1B	-4.21	1.36	1.50
3	D	203	ATP	PA-O2A	-3.87	1.37	1.55
3	D	203	ATP	C4-N9	-3.82	1.29	1.37
3	D	203	ATP	PG-O2G	-3.81	1.40	1.54
4	A	206	5RV	C12-N18	3.69	1.37	1.31
4	B	204	5RV	C12-N18	3.60	1.36	1.31
3	D	203	ATP	C8-N9	-3.23	1.32	1.37
4	C	205	5RV	C12-N18	3.23	1.36	1.31
3	D	203	ATP	PG-O3G	-3.18	1.43	1.54
4	D	204	5RV	C12-N18	3.04	1.36	1.31
4	C	205	5RV	C10-C8	-2.96	1.37	1.45
4	A	206	5RV	C10-C8	-2.87	1.37	1.45
4	B	204	5RV	C10-C8	-2.75	1.37	1.45
3	A	205	ATP	PB-O3B	2.74	1.62	1.59
3	D	203	ATP	PA-O1A	-2.71	1.41	1.50
4	A	206	5RV	C11-N19	2.71	1.40	1.34
4	D	204	5RV	C10-C8	-2.70	1.37	1.45
4	D	204	5RV	C11-N19	2.59	1.40	1.34
3	B	203	ATP	C5-C6	2.59	1.48	1.41
4	C	205	5RV	C11-N19	2.50	1.40	1.34
4	B	204	5RV	C12-S21	-2.49	1.72	1.75
3	C	204	ATP	C5-C6	2.49	1.47	1.41
4	B	204	5RV	C11-N19	2.46	1.39	1.34
3	C	204	ATP	C8-N7	2.39	1.36	1.31
3	D	203	ATP	O4'-C4'	-2.39	1.39	1.45
4	D	204	5RV	C10-N17	-2.38	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	203	ATP	C5-N7	-2.36	1.34	1.39
3	C	204	ATP	C5-N7	-2.33	1.34	1.39
4	B	204	5RV	C10-N17	-2.31	1.34	1.38
4	A	206	5RV	C10-N17	-2.21	1.34	1.38
4	C	205	5RV	C12-N16	-2.20	1.31	1.36
3	D	203	ATP	PB-O3B	-2.16	1.57	1.59
4	D	204	5RV	C12-N16	-2.15	1.31	1.36
3	A	205	ATP	C5-C6	2.13	1.46	1.41
3	D	203	ATP	O5'-C5'	-2.11	1.36	1.44
3	A	205	ATP	C8-N7	2.08	1.35	1.31
3	D	203	ATP	PB-O2B	-2.07	1.45	1.55
3	C	204	ATP	PB-O3B	2.07	1.61	1.59
3	A	205	ATP	C4-N9	-2.02	1.33	1.37

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	205	ATP	C5-C4-N3	-6.13	118.27	126.72
4	C	205	5RV	C9-C8-N18	-5.78	104.41	111.34
3	B	203	ATP	C5-C4-N3	-5.56	119.07	126.72
3	A	205	ATP	N3-C4-N9	5.49	136.50	127.17
3	C	204	ATP	C5-C4-N3	-5.35	119.34	126.72
3	B	203	ATP	N3-C4-N9	5.08	135.80	127.17
4	B	204	5RV	C9-C8-N18	-5.05	105.29	111.34
4	D	204	5RV	C9-C8-N18	-4.97	105.38	111.34
3	C	204	ATP	N3-C4-N9	4.78	135.29	127.17
3	D	203	ATP	C5-C4-N3	-4.48	120.55	126.72
4	A	206	5RV	C9-C8-N18	-4.30	106.19	111.34
4	D	204	5RV	C7-C13-S21	4.24	125.76	110.75
3	D	203	ATP	N3-C4-N9	4.17	134.26	127.17
3	A	205	ATP	C2-N3-C4	4.03	121.66	111.83
4	C	205	5RV	C7-C6-C1	3.99	123.87	120.16
3	C	204	ATP	C2-N3-C4	3.98	121.55	111.83
3	C	204	ATP	N3-C2-N1	-3.92	122.65	128.58
3	A	205	ATP	N3-C2-N1	-3.83	122.78	128.58
4	C	205	5RV	C13-C7-C6	3.75	125.24	121.14
4	C	205	5RV	C10-C8-N18	3.67	136.25	127.76
3	B	203	ATP	C2-N3-C4	3.59	120.60	111.83
4	B	204	5RV	C7-C13-S21	3.56	123.37	110.75
3	B	203	ATP	C4-N9-C8	3.54	109.45	105.74
4	C	205	5RV	C7-C13-S21	3.43	122.90	110.75
4	D	204	5RV	C10-C8-N18	3.42	135.66	127.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	206	5RV	C7-C13-S21	3.35	122.61	110.75
4	C	205	5RV	C4-C6-C1	-3.32	113.61	119.36
3	D	203	ATP	N6-C6-N1	3.32	125.78	118.38
3	B	203	ATP	N3-C2-N1	-3.32	123.56	128.58
3	A	205	ATP	C4-N9-C8	3.26	109.16	105.74
4	B	204	5RV	C13-C7-C6	3.22	124.66	121.14
4	A	206	5RV	C13-C7-C6	3.19	124.62	121.14
4	A	206	5RV	C10-C8-N18	3.17	135.09	127.76
3	C	204	ATP	C4-N9-C8	3.13	109.03	105.74
4	B	204	5RV	C10-C8-N18	3.06	134.83	127.76
3	D	203	ATP	C2'-C1'-N9	3.03	120.83	113.30
3	B	203	ATP	C4-C5-N7	-2.91	107.25	110.58
3	C	204	ATP	C2'-C1'-N9	2.90	120.50	113.30
4	C	205	5RV	C6-C1-N14	-2.82	173.26	177.90
3	B	203	ATP	O3B-PB-O1B	-2.65	102.73	110.70
3	D	203	ATP	C2-N3-C4	2.62	118.23	111.83
3	D	203	ATP	C4-C5-N7	-2.59	107.62	110.58
3	A	205	ATP	C2'-C1'-N9	2.57	119.69	113.30
3	C	204	ATP	O4'-C1'-C2'	-2.54	101.17	106.62
3	D	203	ATP	C5-C6-N6	-2.53	117.02	123.29
3	A	205	ATP	O3G-PG-O2G	2.53	117.28	107.80
4	D	204	5RV	C13-C7-C6	2.53	123.90	121.14
4	B	204	5RV	N19-C11-N17	-2.51	114.77	119.67
3	B	203	ATP	C5-N7-C8	2.51	107.39	103.45
3	A	205	ATP	N6-C6-N1	2.50	123.94	118.38
3	B	203	ATP	C2'-C1'-N9	2.46	119.41	113.30
3	C	204	ATP	C5-C6-N6	-2.44	117.25	123.29
4	A	206	5RV	N19-C11-N17	-2.43	114.92	119.67
3	B	203	ATP	C4'-O4'-C1'	-2.41	104.14	109.47
3	D	203	ATP	C4-N9-C8	2.39	108.24	105.74
3	A	205	ATP	C1'-N9-C8	-2.38	121.81	127.09
3	C	204	ATP	N6-C6-N1	2.38	123.67	118.38
3	A	205	ATP	C4-C5-N7	-2.36	107.89	110.58
3	C	204	ATP	C4-C5-N7	-2.34	107.91	110.58
3	C	204	ATP	O4'-C4'-C3'	-2.34	100.52	105.15
4	B	204	5RV	S21-C12-N18	-2.33	120.47	125.97
3	B	203	ATP	C1'-N9-C8	-2.32	121.94	127.09
3	B	203	ATP	O2B-PB-O3B	2.27	113.42	107.27
3	B	203	ATP	N9-C8-N7	-2.25	110.74	113.94
3	A	205	ATP	C5-C6-N6	-2.25	117.73	123.29
3	B	203	ATP	O3G-PG-O2G	2.17	115.93	107.80
4	D	204	5RV	C11-N15-C9	-2.16	113.58	119.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	204	ATP	C6-C5-N7	2.11	136.15	132.09
4	A	206	5RV	C11-N15-C9	-2.07	113.86	119.75
4	D	204	5RV	N19-C11-N17	-2.04	115.69	119.67
3	C	204	ATP	C3'-C2'-C1'	2.04	105.32	101.46
4	B	204	5RV	N15-C11-N17	2.01	127.00	123.32

There are no chirality outliers.

All (18) torsion outliers are listed below:

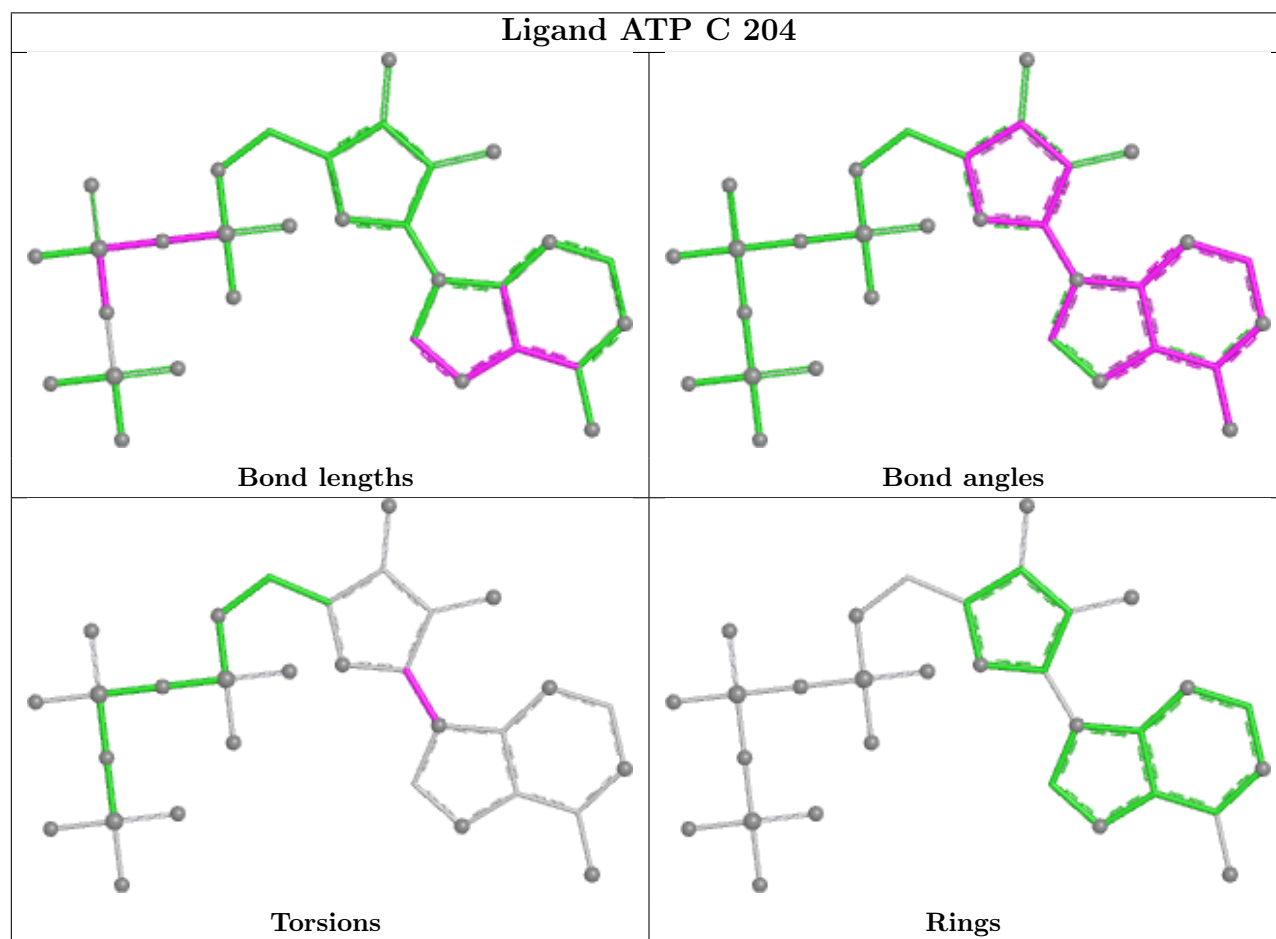
Mol	Chain	Res	Type	Atoms
4	C	205	5RV	C7-C13-S21-C12
4	D	204	5RV	C7-C13-S21-C12
4	A	206	5RV	C7-C13-S21-C12
4	B	204	5RV	C7-C13-S21-C12
4	A	206	5RV	N16-C12-S21-C13
4	B	204	5RV	N16-C12-S21-C13
4	C	205	5RV	N16-C12-S21-C13
4	D	204	5RV	N16-C12-S21-C13
4	A	206	5RV	N18-C12-S21-C13
4	B	204	5RV	N18-C12-S21-C13
4	C	205	5RV	N18-C12-S21-C13
4	D	204	5RV	N18-C12-S21-C13
3	D	203	ATP	O4'-C1'-N9-C8
3	A	205	ATP	O4'-C1'-N9-C8
3	B	203	ATP	PG-O3B-PB-O2B
3	A	205	ATP	C2'-C1'-N9-C8
3	B	203	ATP	O4'-C1'-N9-C8
3	C	204	ATP	O4'-C1'-N9-C8

There are no ring outliers.

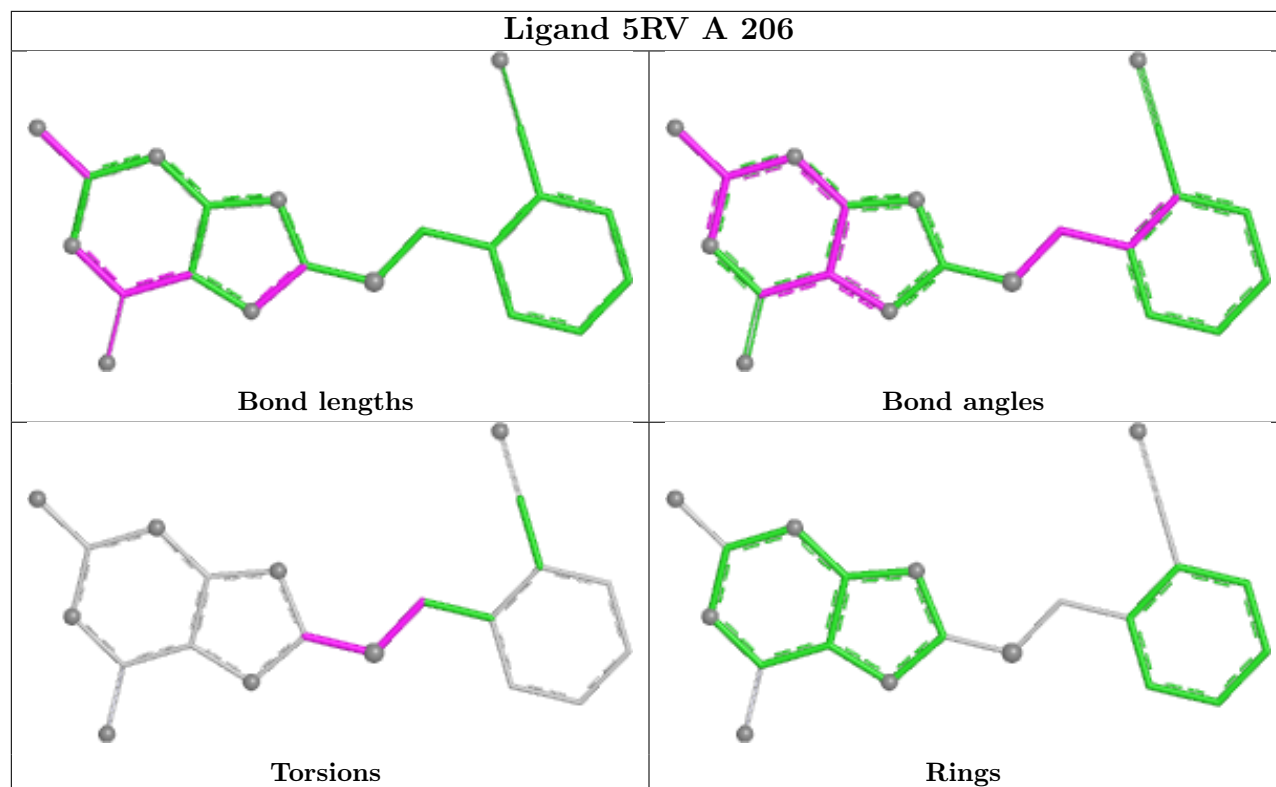
No monomer is involved in short contacts.

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.

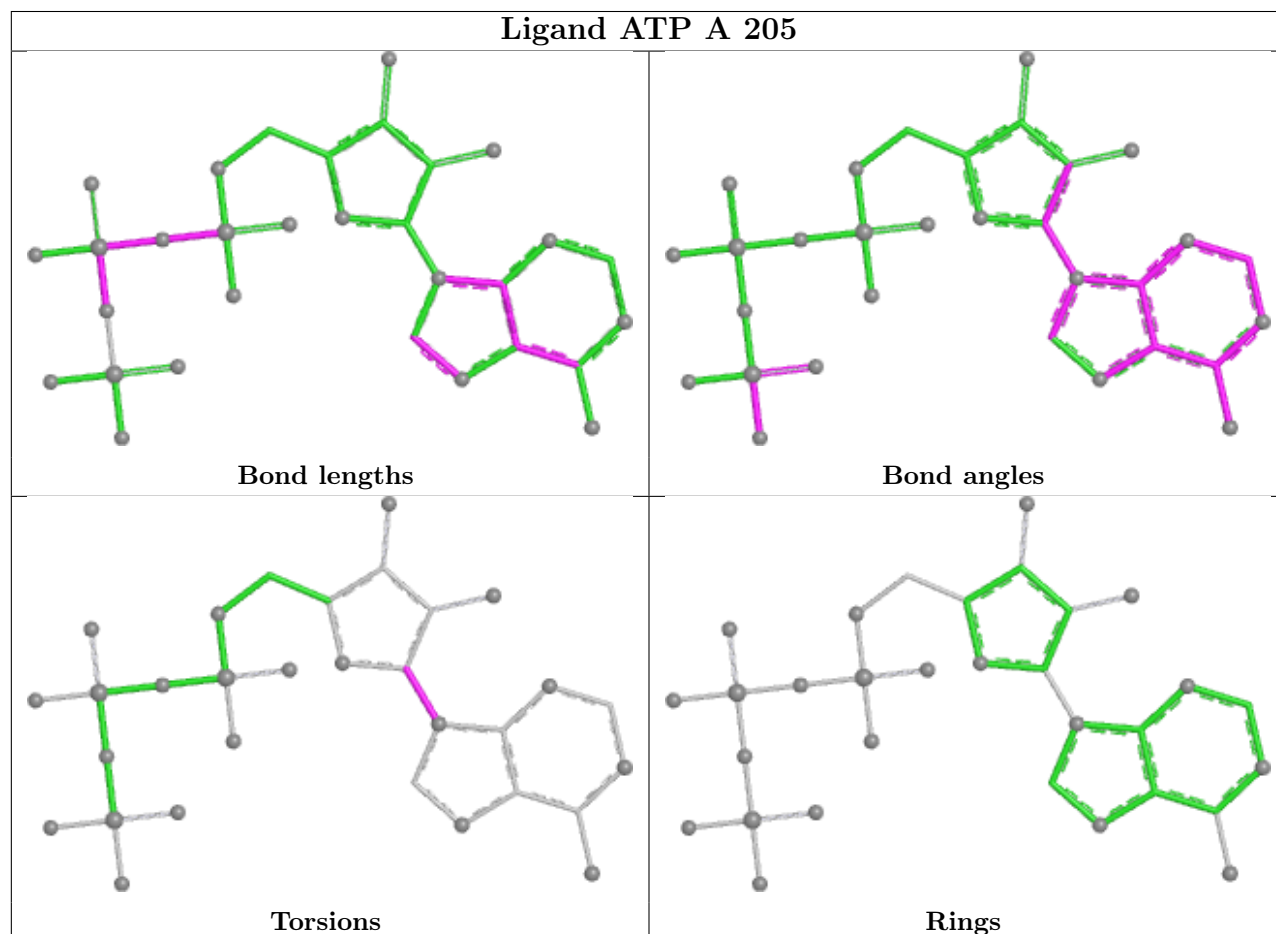
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



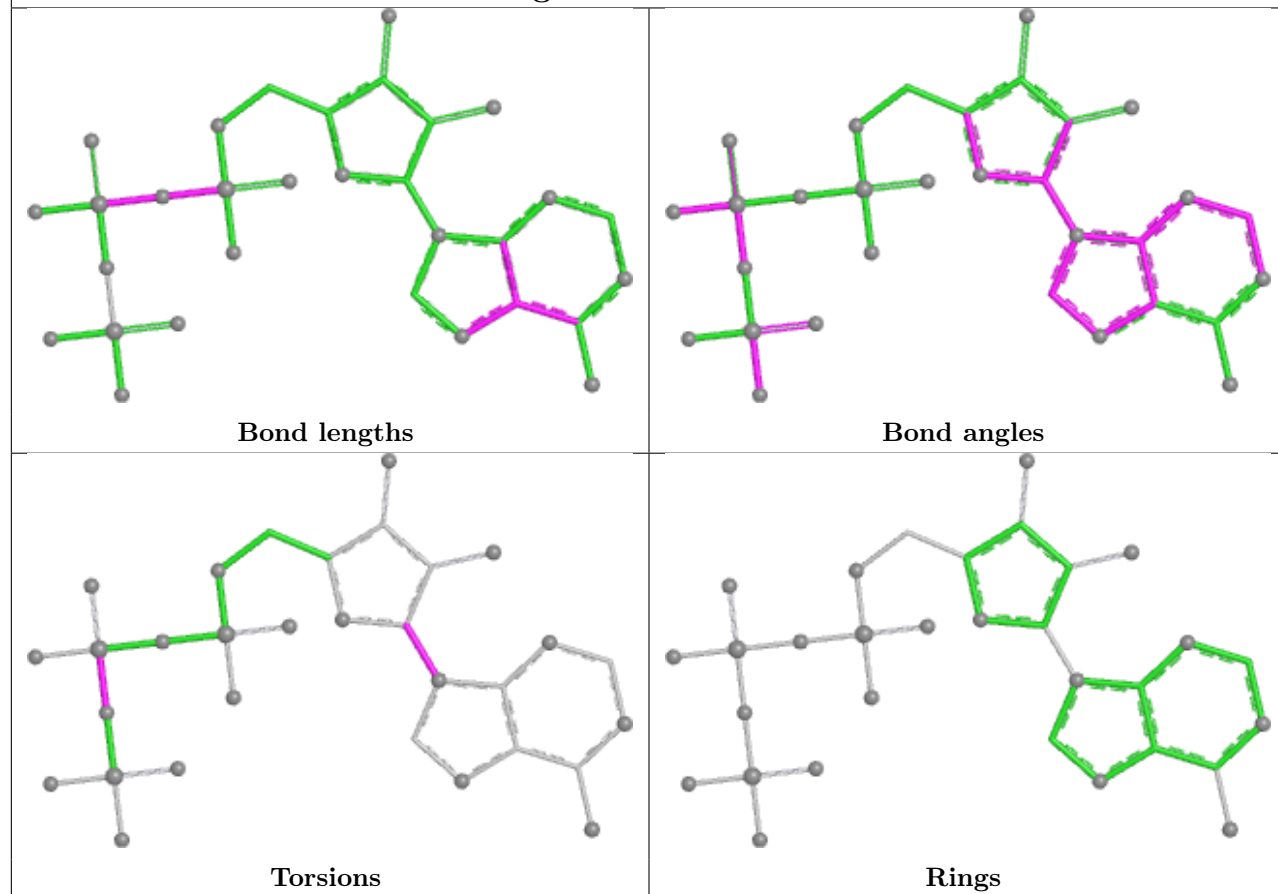
Ligand 5RV A 206



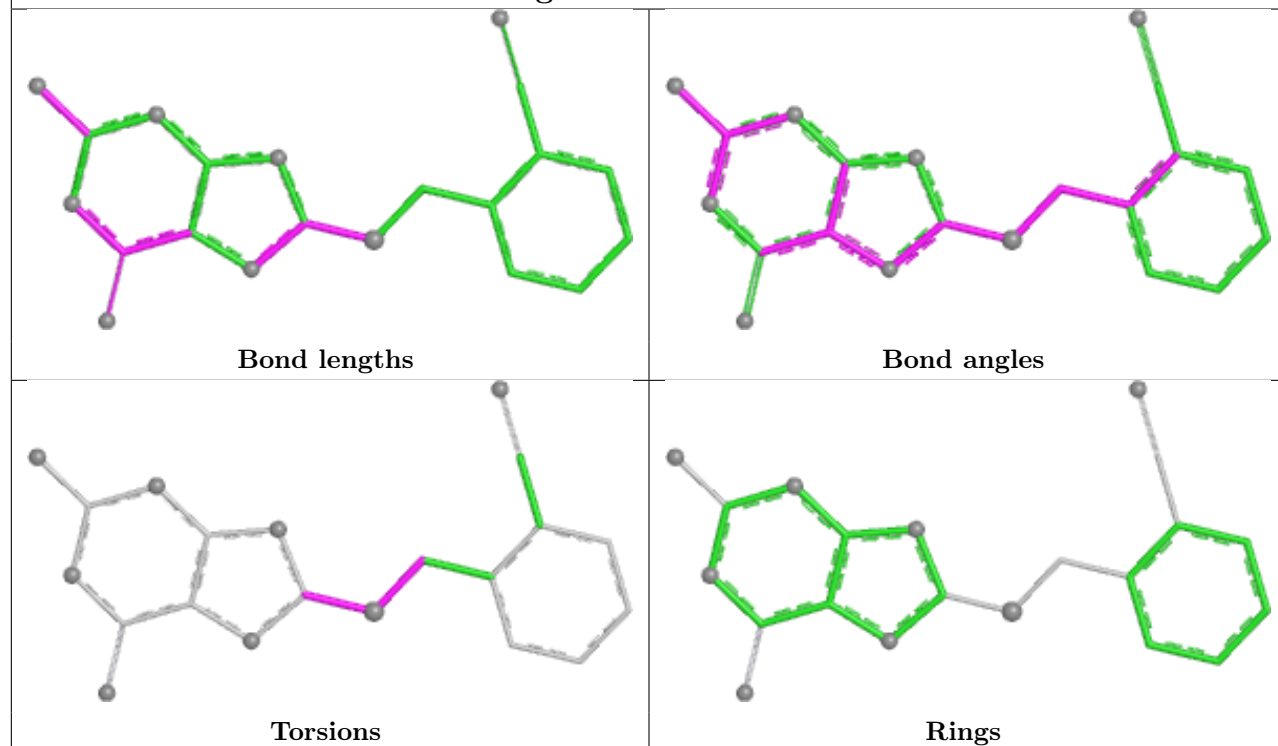
Ligand ATP A 205



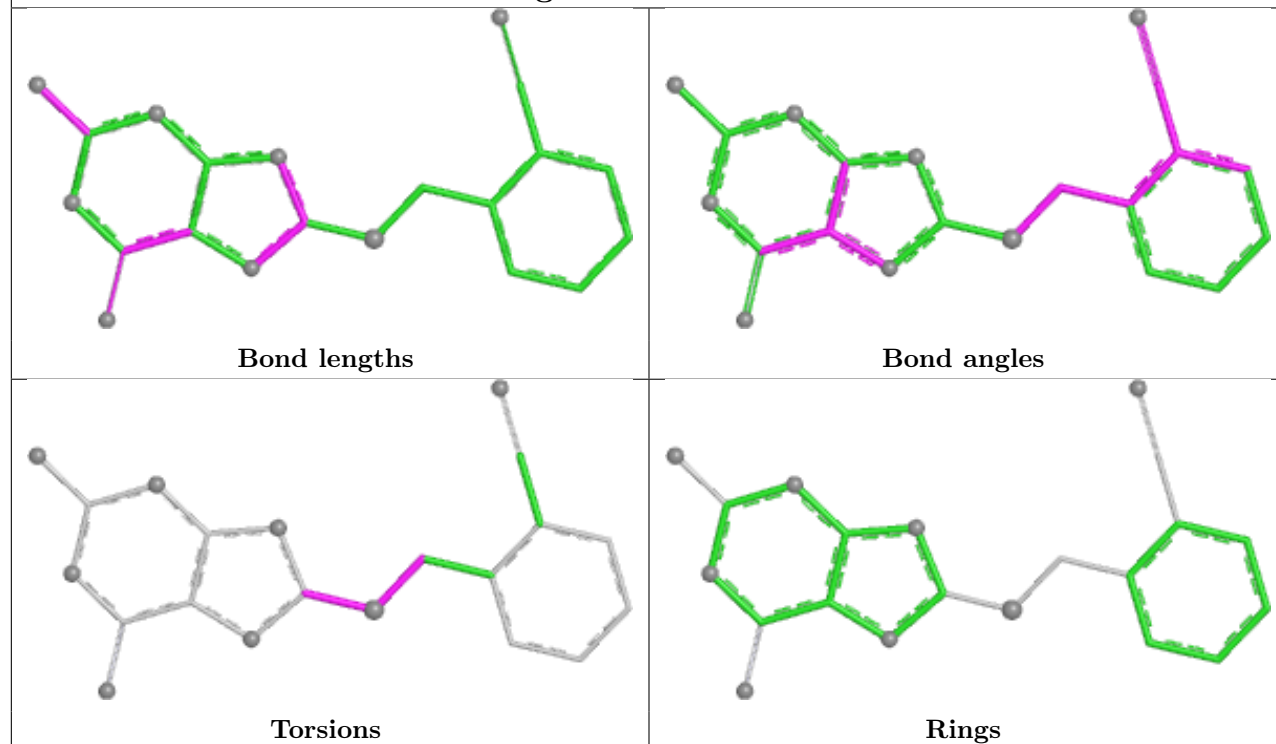
Ligand ATP B 203



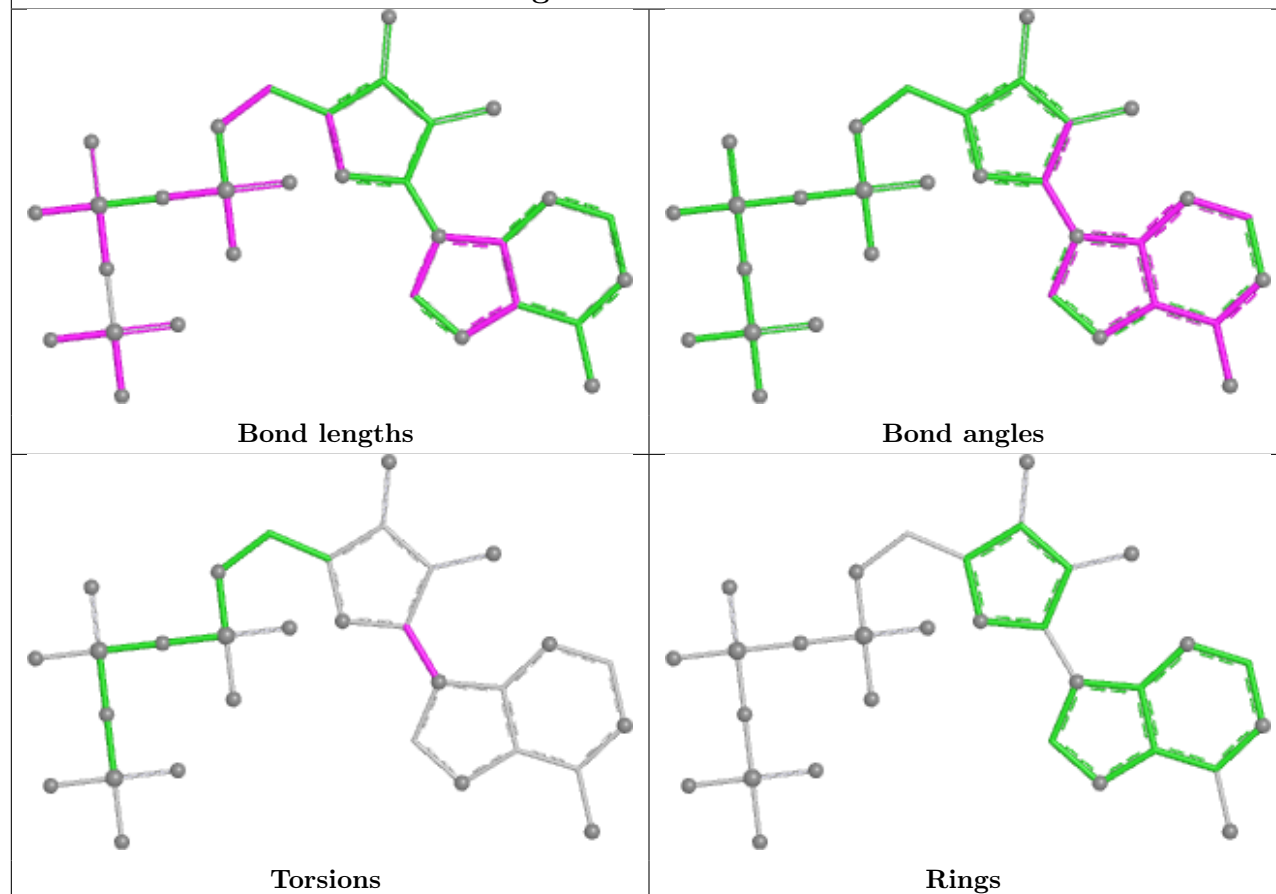
Ligand 5RV B 204

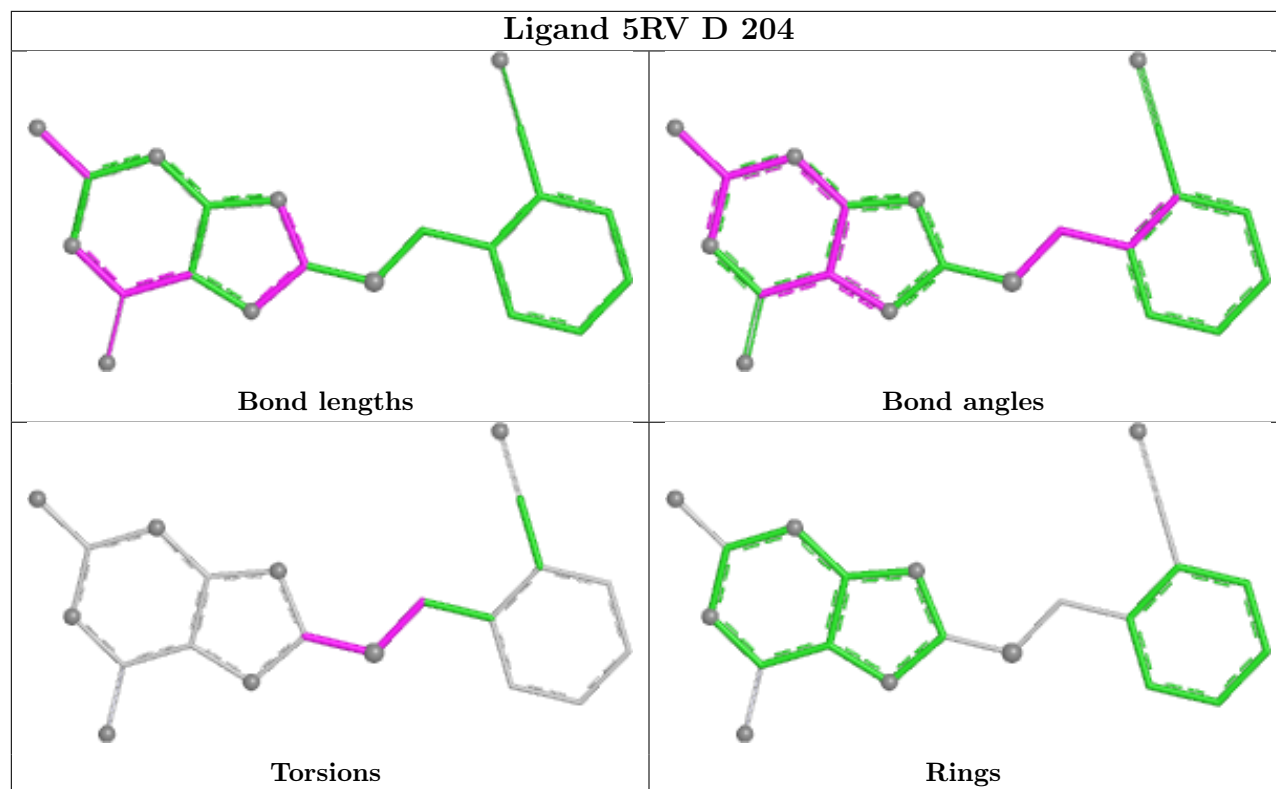


Ligand 5RV C 205



Ligand ATP D 203





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	155/162 (95%)	0.03	5 (3%)	50	57	4, 11, 25, 38	1 (0%)
1	B	155/162 (95%)	0.14	6 (3%)	43	49	5, 11, 29, 62	2 (1%)
1	C	156/162 (96%)	0.14	6 (3%)	44	50	5, 11, 25, 38	0
1	D	160/162 (98%)	0.08	4 (2%)	58	64	5, 11, 29, 54	2 (1%)
All	All	626/648 (96%)	0.10	21 (3%)	48	55	4, 11, 28, 62	5 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	89	TRP	6.0
1	D	48	GLN	4.9
1	B	91	PRO	4.1
1	D	88	ARG	3.8
1	B	153	ASP	3.8
1	C	86	ALA	3.6
1	C	154	LYS	3.2
1	B	48	GLN	3.2
1	D	86	ALA	3.0
1	B	-2	SER	3.0
1	B	154	LYS	2.9
1	A	85	LYS	2.7
1	A	-2	SER	2.7
1	A	-1	ALA	2.5
1	C	47	PRO	2.5
1	A	12	ALA	2.4
1	B	17	GLN	2.4
1	C	11	LEU	2.3
1	A	154	LYS	2.1
1	C	12	ALA	2.1
1	C	83	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

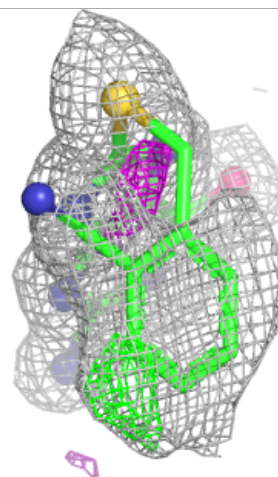
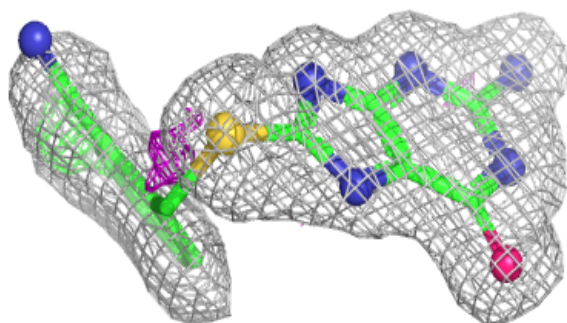
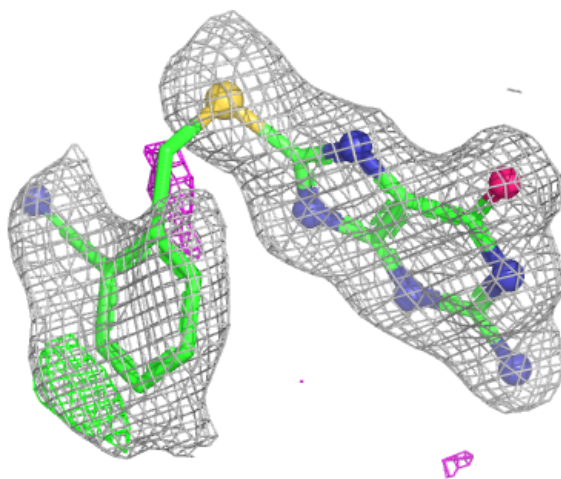
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	5RV	B	204	21/21	0.90	0.14	17,23,51,66	0
4	5RV	A	206	21/21	0.91	0.12	15,21,39,42	0
4	5RV	C	205	21/21	0.92	0.13	12,22,43,54	0
4	5RV	D	204	21/21	0.94	0.11	10,15,36,49	0
3	ATP	D	203	31/31	0.96	0.07	9,13,19,22	0
3	ATP	C	204	31/31	0.97	0.07	8,16,23,26	0
3	ATP	A	205	31/31	0.97	0.06	11,16,18,22	0
3	ATP	B	203	31/31	0.97	0.07	12,17,23,31	0
2	CA	A	201	1/1	0.98	0.07	13,13,13,13	0
2	CA	A	203	1/1	0.98	0.04	23,23,23,23	0
2	CA	D	202	1/1	0.99	0.06	14,14,14,14	0
2	CA	A	202	1/1	0.99	0.06	18,18,18,18	0
2	CA	A	204	1/1	0.99	0.04	28,28,28,28	0
2	CA	B	201	1/1	0.99	0.06	15,15,15,15	0
2	CA	B	202	1/1	0.99	0.05	17,17,17,17	0
2	CA	C	201	1/1	0.99	0.08	14,14,14,14	0
2	CA	C	202	1/1	0.99	0.04	15,15,15,15	0
2	CA	C	203	1/1	0.99	0.03	18,18,18,18	0
2	CA	D	201	1/1	0.99	0.09	12,12,12,12	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.

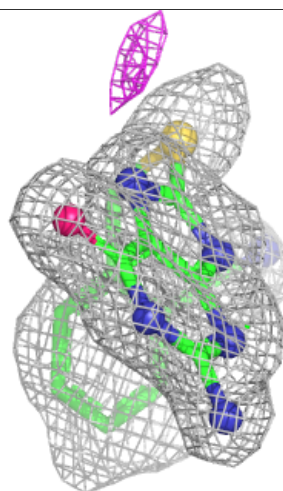
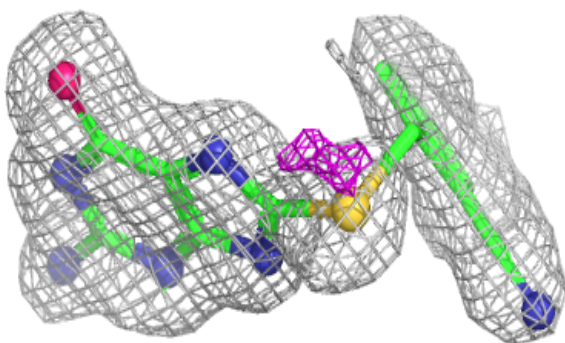
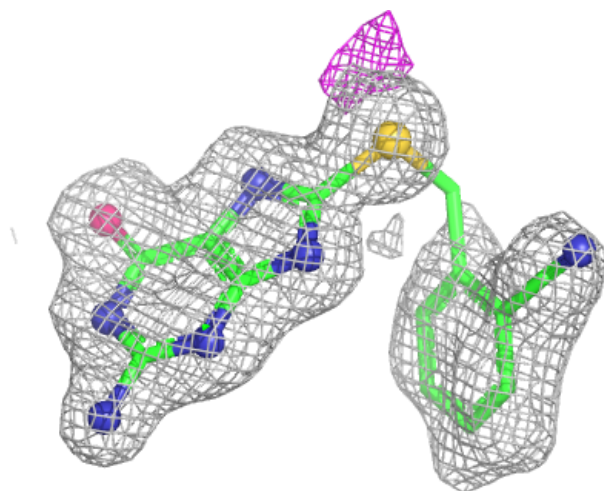
Electron density around 5RV B 204:

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



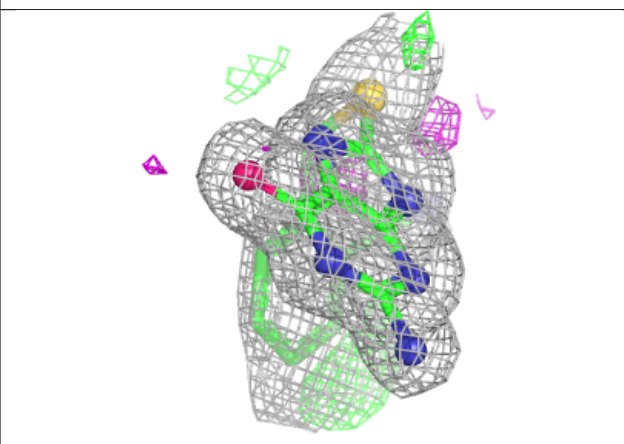
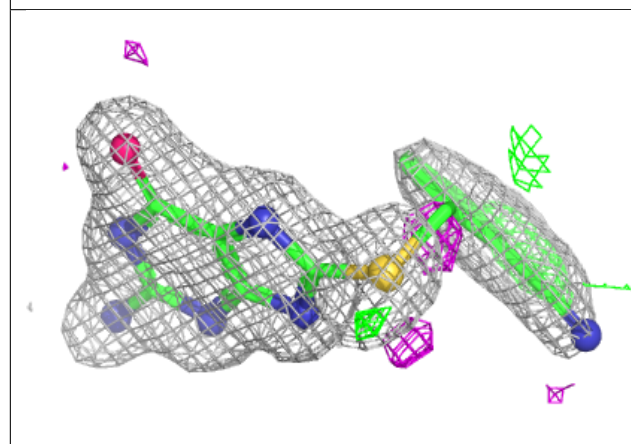
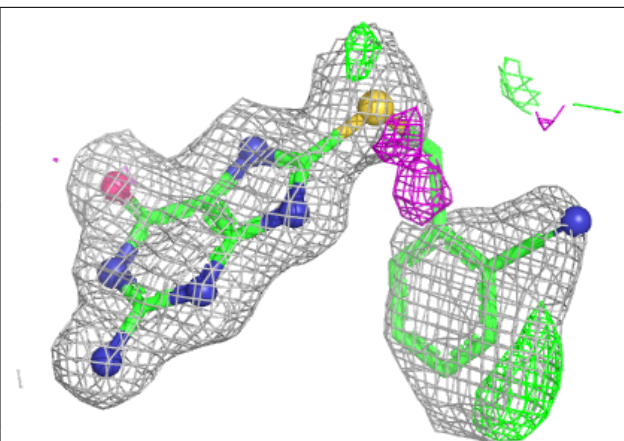
Electron density around 5RV A 206:

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

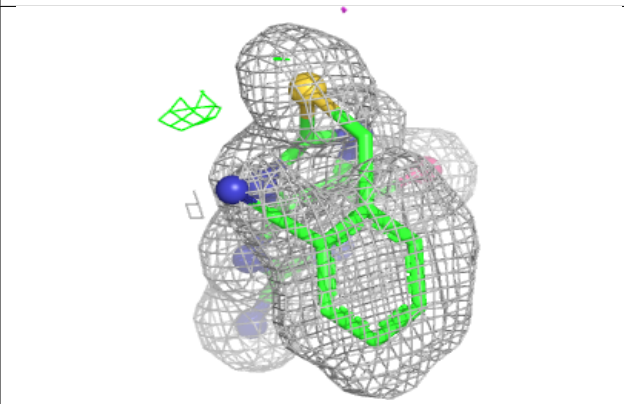
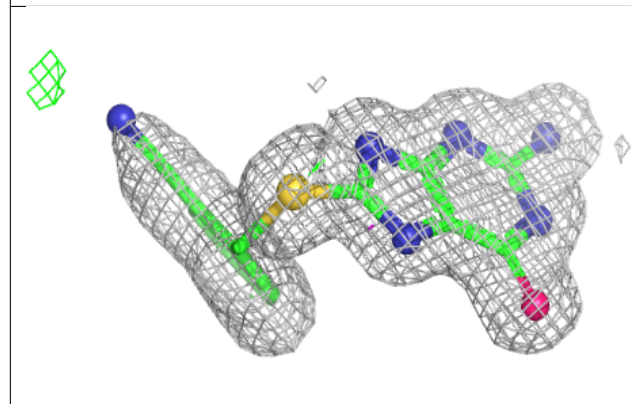
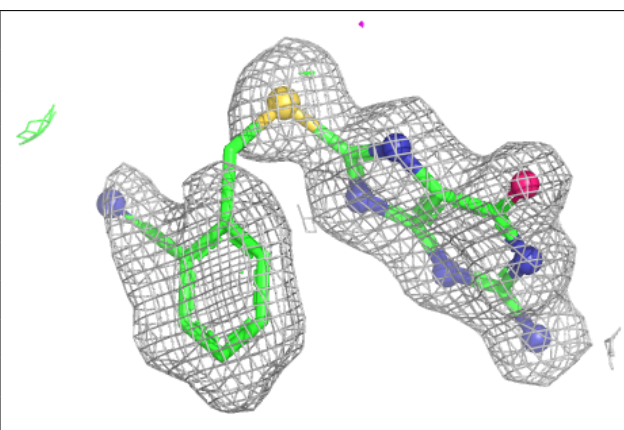


Electron density around 5RV C 205:

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

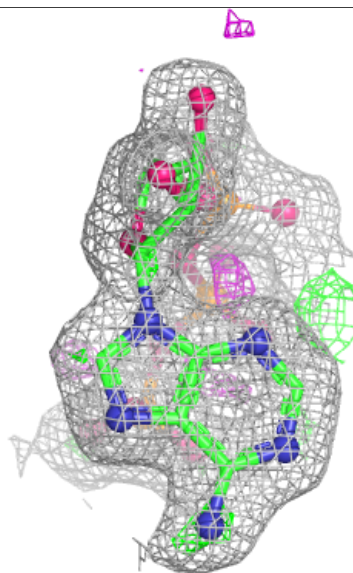
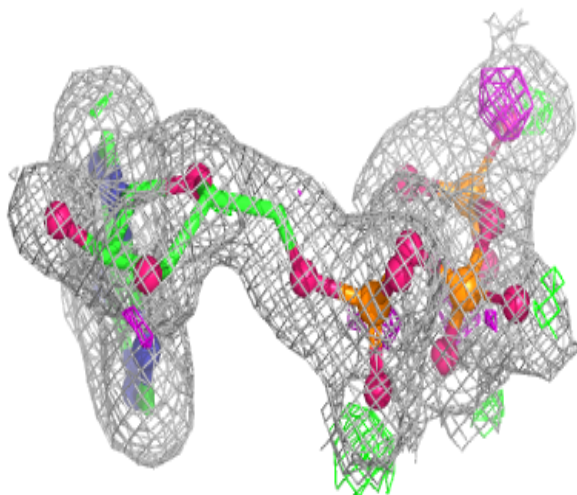
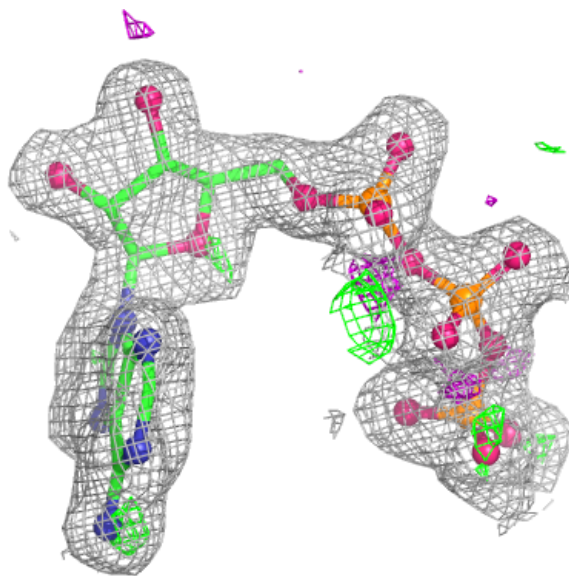
**Electron density around 5RV D 204:**

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



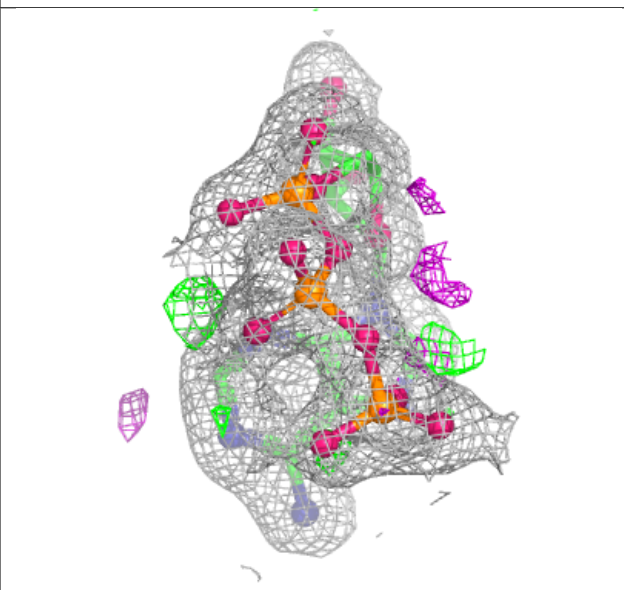
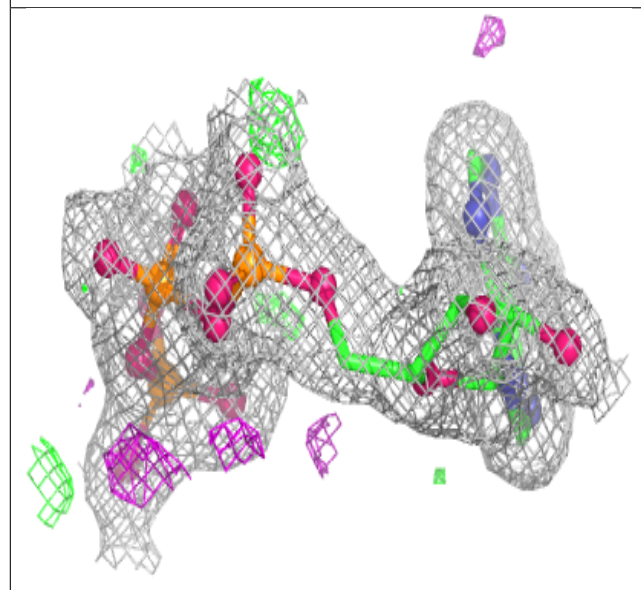
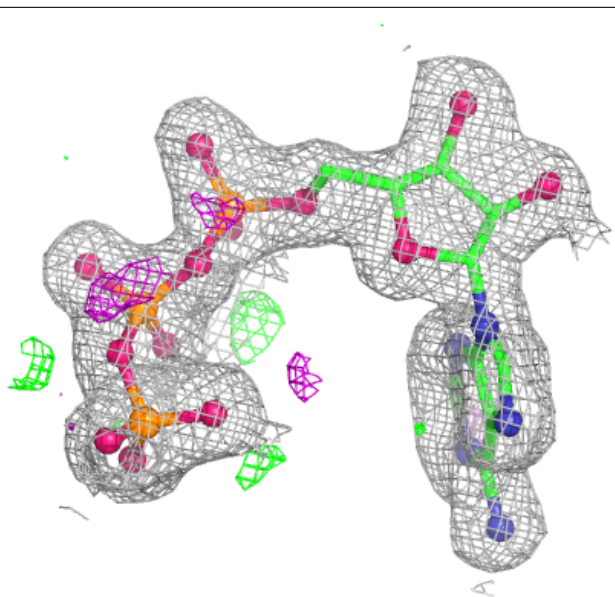
Electron density around ATP D 203:

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



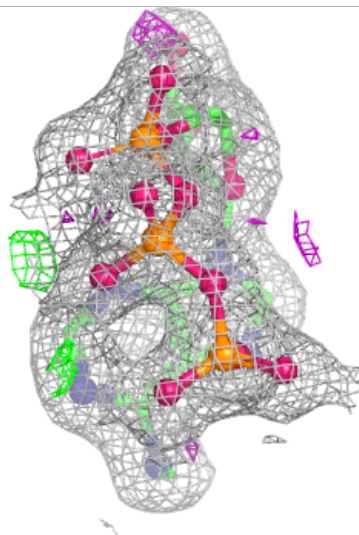
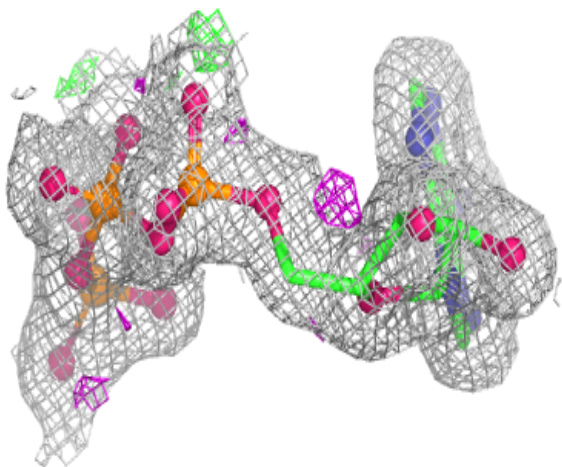
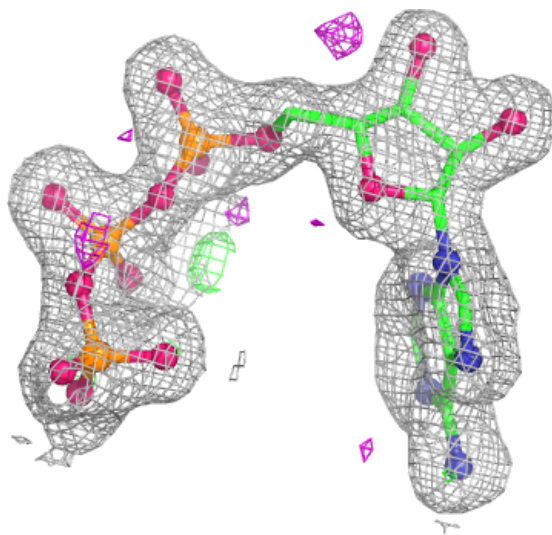
Electron density around ATP C 204:

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



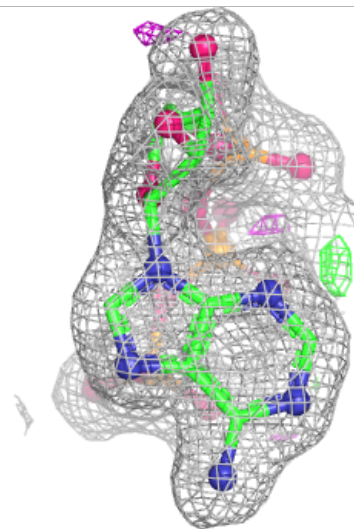
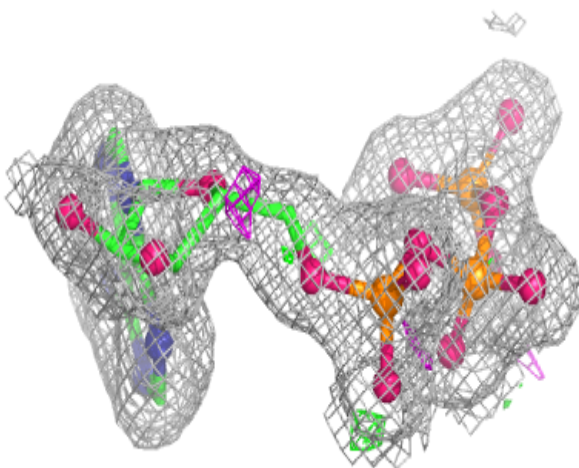
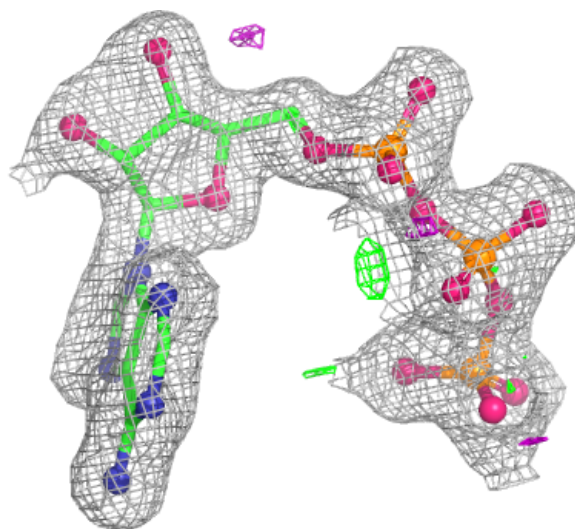
Electron density around ATP A 205:

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 203:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.