



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:54 pm BST

PDB ID : 2WWI  
Title : Plasmodium falciparum thymidylate kinase in complex with AZTMP and ADP  
Authors : Whittingham, J.L.; Carrero-Lerida, J.; Brannigan, J.A.; Ruiz-Perez, L.M.; Silva, A.P.G.; Fogg, M.J.; Wilkinson, A.J.; Gilbert, I.H.; Wilson, K.S.; Gonzalez-Pacanowska, D.  
Deposited on : 2009-10-23  
Resolution : 2.99 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](mailto: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.

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

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

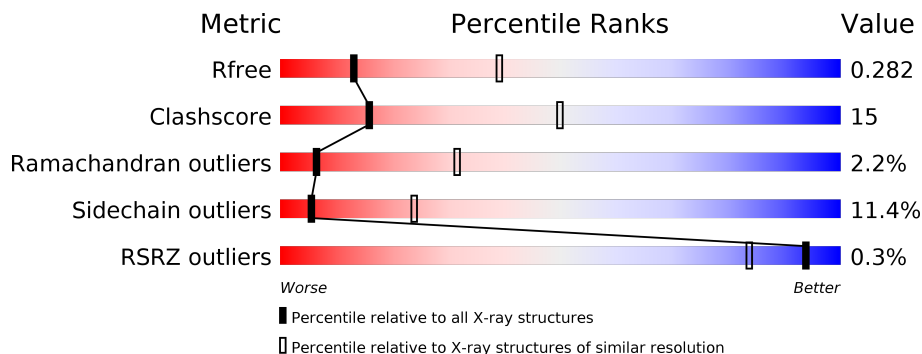
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	212	
1	B	212	
1	C	212	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5244 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 THYMIDILATE KINASE, PUTATIVE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	Total 1728	C 1110	N 287	O 325	S 6	63	0	0
1	B	197	Total 1637	C 1056	N 269	O 306	S 6	99	0	0
1	C	205	Total 1705	C 1095	N 283	O 321	S 6	112	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP Q8I4S1
A	0	HIS	-	expression tag	UNP Q8I4S1
B	-1	SER	-	expression tag	UNP Q8I4S1
B	0	HIS	-	expression tag	UNP Q8I4S1
C	-1	SER	-	expression tag	UNP Q8I4S1
C	0	HIS	-	expression tag	UNP Q8I4S1

- Molecule 2 is 3'-AZIDO-3'-DEOXYTHYMIDINE-5'-MONOPHOSPHATE (three-letter code: ATM) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

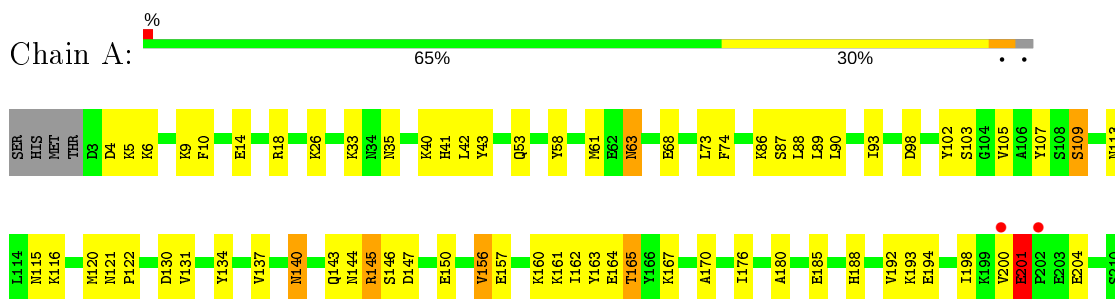
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	7	Total	O	0	0
			7	7		
4	C	3	Total	O	0	0
			3	3		

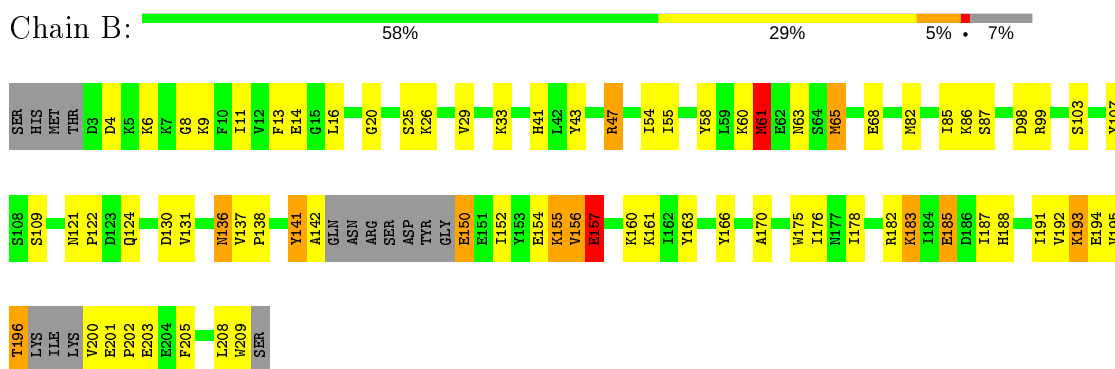
### 3 Residue-property plots [i](#)

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

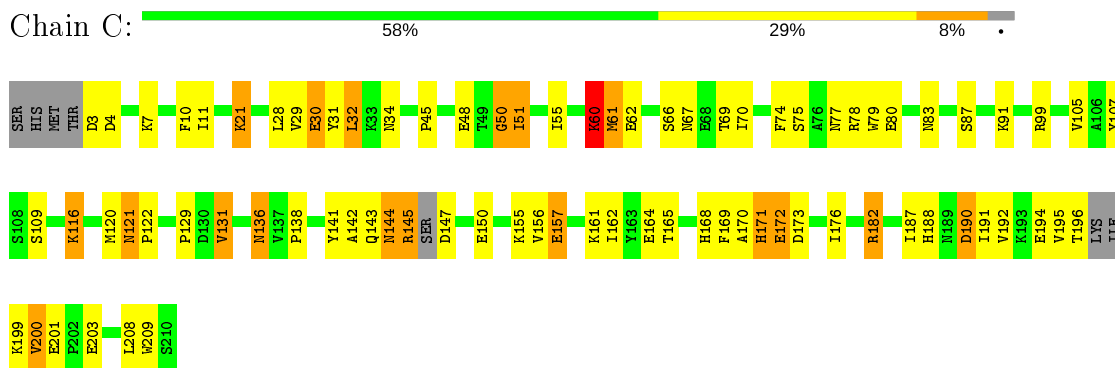
- Molecule 1: THYMIDILATE KINASE, PUTATIVE



- Molecule 1: THYMIDILATE KINASE, PUTATIVE



- Molecule 1: THYMIDILATE KINASE, PUTATIVE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.34Å 110.34Å 119.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.35 – 2.99 34.56 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (95.35-2.99) 99.1 (34.56-2.99)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.50 (at 3.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.199 , 0.287 0.199 , 0.282	Depositor DCC
$R_{free}$ test set	869 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtrriage
Anisotropy	0.503	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ATM, ADP

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	0.99	9/1770 (0.5%)	0.82	3/2389 (0.1%)
1	B	0.84	5/1676 (0.3%)	0.95	8/2263 (0.4%)
1	C	0.86	8/1745 (0.5%)	0.84	5/2353 (0.2%)
All	All	0.90	22/5191 (0.4%)	0.87	16/7005 (0.2%)

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

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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	GLU	CB-CG	-13.84	1.25	1.52
1	A	193	LYS	CB-CG	-12.52	1.18	1.52
1	A	157	GLU	CB-CG	-12.34	1.28	1.52
1	B	26	LYS	CB-CG	-11.61	1.21	1.52
1	C	30	GLU	CB-CG	-10.88	1.31	1.52
1	A	26	LYS	CB-CG	-10.13	1.25	1.52
1	C	91	LYS	CB-CG	-9.68	1.26	1.52
1	A	33	LYS	CB-CG	-9.52	1.26	1.52
1	B	160	LYS	CA-CB	-8.97	1.34	1.53
1	B	201	GLU	CA-CB	-8.36	1.35	1.53
1	C	60	LYS	CB-CG	-8.27	1.30	1.52
1	A	161	LYS	CB-CG	-7.92	1.31	1.52
1	C	157	GLU	CA-CB	-7.82	1.36	1.53
1	C	200	VAL	CA-CB	-7.10	1.39	1.54
1	B	183	LYS	CA-CB	-6.36	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	GLU	CB-CG	5.86	1.63	1.52
1	C	161	LYS	CB-CG	-5.82	1.36	1.52
1	C	150	GLU	CG-CD	5.77	1.60	1.51
1	B	141	TYR	CD1-CE1	5.44	1.47	1.39
1	C	116	LYS	CB-CG	-5.43	1.37	1.52
1	A	144	ASN	CB-CG	-5.41	1.38	1.51
1	A	5	LYS	CB-CG	-5.02	1.39	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	TYR	CB-CG-CD1	-12.32	113.61	121.00
1	B	43	TYR	CB-CG-CD2	11.94	128.16	121.00
1	B	182	ARG	CG-CD-NE	11.29	135.50	111.80
1	B	183	LYS	N-CA-CB	7.81	124.67	110.60
1	B	141	TYR	N-CA-CB	7.16	123.49	110.60
1	C	182	ARG	N-CA-CB	-6.58	98.76	110.60
1	A	193	LYS	CA-CB-CG	6.51	127.71	113.40
1	A	185	GLU	CA-CB-CG	-6.00	100.19	113.40
1	C	176	ILE	CB-CG1-CD1	-5.95	97.25	113.90
1	B	185	GLU	N-CA-CB	-5.84	100.09	110.60
1	B	157	GLU	N-CA-CB	-5.83	100.11	110.60
1	C	155	LYS	CD-CE-NZ	5.56	124.48	111.70
1	C	50	GLY	N-CA-C	-5.49	99.37	113.10
1	B	183	LYS	CB-CA-C	-5.31	99.79	110.40
1	C	171	HIS	N-CA-C	-5.18	97.02	111.00
1	A	157	GLU	CA-CB-CG	5.07	124.54	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ASN	Mainchain

## 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	1728	0	1696	41	0
1	B	1637	0	1604	55	1
1	C	1705	0	1665	47	2
2	A	23	0	12	3	0
2	B	23	0	12	1	0
2	C	23	0	12	1	0
3	A	27	0	12	1	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
4	A	14	0	0	2	0
4	B	7	0	0	0	0
4	C	3	0	0	0	0
All	All	5244	0	5037	139	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (139) 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:47:ARG:HH11	1:B:47:ARG:HG2	1.13	1.08
1:C:169:PHE:O	1:C:171:HIS:O	1.72	1.04
1:B:68:GLU:HG3	1:C:79:TRP:CE3	1.93	1.03
1:A:63:ASN:HD22	1:A:63:ASN:C	1.82	0.83
1:C:50:GLY:O	1:C:51:ILE:HG13	1.78	0.83
1:B:47:ARG:NH1	1:B:47:ARG:HG2	1.91	0.82
1:B:60:LYS:O	1:B:61:MET:HB2	1.80	0.81
1:A:163:TYR:CE2	4:A:2011:HOH:O	2.33	0.81
1:B:68:GLU:HG3	1:C:79:TRP:CZ3	2.21	0.76
1:A:200:VAL:O	1:A:201:GLU:HB2	1.84	0.76
1:A:40:LYS:HG3	1:A:88:LEU:HD22	1.69	0.75
1:B:60:LYS:O	1:B:61:MET:CB	2.38	0.72
1:B:136:ASN:C	1:B:136:ASN:HD22	1.96	0.69
1:C:136:ASN:C	1:C:136:ASN:HD22	1.96	0.69
1:C:105:VAL:HG21	1:C:120:MET:HG2	1.76	0.68
1:A:163:TYR:CD2	4:A:2011:HOH:O	2.46	0.67
1:B:155:LYS:O	1:B:157:GLU:N	2.28	0.67
1:C:138:PRO:HG2	1:C:141:TYR:HB2	1.77	0.67
1:A:105:VAL:HG21	1:A:120:MET:HG2	1.79	0.64
1:B:137:VAL:HG12	1:B:138:PRO:O	1.98	0.63
1:B:47:ARG:HH11	1:B:47:ARG:CG	1.99	0.63
1:C:144:ASN:H	1:C:144:ASN:HD22	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:CG2	1:A:176:ILE:HD12	2.28	0.62
1:B:68:GLU:CG	1:C:79:TRP:CE3	2.78	0.61
1:A:131:VAL:HG23	1:A:176:ILE:HD12	1.83	0.61
1:B:150:GLU:N	1:B:154:GLU:OE2	2.34	0.60
1:A:63:ASN:ND2	1:A:63:ASN:C	2.49	0.60
1:B:58:TYR:HA	1:B:63:ASN:OD1	2.02	0.59
1:C:144:ASN:H	1:C:144:ASN:ND2	2.00	0.59
1:C:55:ILE:HG21	1:C:74:PHE:CE1	2.37	0.59
1:C:21:LYS:NZ	3:C:212:ADP:O2B	2.36	0.59
1:C:171:HIS:C	1:C:172:GLU:HG2	2.23	0.58
1:A:4:ASP:O	1:A:90:LEU:HD21	2.03	0.58
1:C:77:ASN:O	1:C:80:GLU:HG2	2.03	0.58
1:C:66:SER:HB3	1:C:69:THR:OG1	2.03	0.57
1:B:156:VAL:HG23	1:B:157:GLU:N	2.19	0.57
1:A:121:ASN:N	1:A:122:PRO:HD2	2.18	0.57
1:B:188:HIS:O	1:B:192:VAL:HG23	2.05	0.57
1:A:167:LYS:HA	1:A:170:ALA:HB2	1.86	0.56
1:C:162:ILE:HA	1:C:165:THR:OG1	2.05	0.56
1:C:142:ALA:O	1:C:145:ARG:HG2	2.06	0.56
1:B:178:ILE:HG21	1:B:187:ILE:HG23	1.88	0.55
1:C:50:GLY:O	1:C:51:ILE:CG1	2.52	0.54
1:B:85:ILE:O	1:B:86:LYS:C	2.38	0.54
1:B:58:TYR:CD1	1:B:65:MET:HG3	2.43	0.54
1:A:156:VAL:O	1:A:160:LYS:HG2	2.08	0.53
1:B:107:TYR:CE2	2:B:211:ATM:H2'	2.44	0.53
1:B:25:SER:O	1:B:29:VAL:HG23	2.08	0.53
1:A:116:LYS:HD2	1:A:120:MET:CE	2.38	0.53
1:A:107:TYR:CE1	2:A:211:ATM:H2'	2.44	0.53
1:B:155:LYS:O	1:B:156:VAL:C	2.47	0.53
1:B:68:GLU:HG3	1:C:79:TRP:CD2	2.44	0.52
1:A:58:TYR:HA	1:A:63:ASN:ND2	2.25	0.52
1:A:176:ILE:HD13	1:A:194:GLU:HG2	1.92	0.52
1:A:145:ARG:HD2	3:A:212:ADP:O4'	2.09	0.52
1:A:109:SER:OG	1:A:165:THR:HG21	2.09	0.51
1:B:141:TYR:O	1:B:142:ALA:C	2.48	0.51
1:B:121:ASN:N	1:B:122:PRO:HD2	2.26	0.51
1:A:164:GLU:O	1:A:167:LYS:HG3	2.11	0.51
1:B:6:LYS:HZ1	1:B:130:ASP:CG	2.15	0.50
1:C:29:VAL:HA	1:C:32:LEU:CD1	2.42	0.49
1:C:144:ASN:N	1:C:144:ASN:HD22	2.10	0.49
1:A:14:GLU:OE2	1:A:102:TYR:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:PHE:O	1:C:171:HIS:N	2.45	0.49
1:C:3:ASP:OD1	1:C:4:ASP:N	2.46	0.49
1:B:14:GLU:OE1	1:B:103:SER:OG	2.27	0.49
1:A:156:VAL:O	1:A:160:LYS:CG	2.61	0.48
1:B:194:GLU:C	1:B:196:THR:N	2.67	0.48
1:B:63:ASN:OD1	1:B:63:ASN:C	2.52	0.48
1:C:188:HIS:O	1:C:192:VAL:HG23	2.15	0.47
1:C:171:HIS:O	1:C:172:GLU:HG2	2.14	0.47
1:A:43:TYR:CD1	1:A:43:TYR:N	2.83	0.47
1:C:107:TYR:CE1	2:C:211:ATM:H2'	2.49	0.47
1:C:60:LYS:HB2	1:C:62:GLU:HG3	1.97	0.47
1:A:121:ASN:N	1:A:122:PRO:CD	2.78	0.47
1:A:137:VAL:HG12	1:A:180:ALA:HB3	1.97	0.47
1:B:82:MET:HA	1:B:82:MET:CE	2.45	0.47
1:C:191:ILE:O	1:C:195:VAL:HG23	2.13	0.47
1:C:136:ASN:C	1:C:136:ASN:ND2	2.66	0.47
1:B:200:VAL:O	1:B:200:VAL:HG12	2.15	0.46
1:A:200:VAL:HG22	1:A:201:GLU:H	1.79	0.46
1:C:187:ILE:O	1:C:188:HIS:C	2.52	0.46
1:B:170:ALA:HA	1:B:175:TRP:CD1	2.51	0.46
1:B:47:ARG:NH1	1:B:47:ARG:CG	2.64	0.46
1:C:190:ASP:N	1:C:190:ASP:OD1	2.48	0.46
1:B:191:ILE:O	1:B:195:VAL:HG23	2.16	0.46
1:B:98:ASP:O	1:B:99:ARG:HB2	2.16	0.46
1:B:13:PHE:CD2	1:B:25:SER:HB3	2.51	0.45
1:B:98:ASP:OD1	1:B:98:ASP:C	2.55	0.45
1:C:75:SER:HA	1:C:78:ARG:HH21	1.81	0.45
1:A:35:ASN:N	1:A:35:ASN:HD22	2.14	0.45
1:C:11:ILE:HG12	1:C:131:VAL:HG12	1.98	0.45
1:C:28:LEU:O	1:C:32:LEU:CD1	2.65	0.45
1:B:6:LYS:HB2	1:B:205:PHE:CD2	2.52	0.45
1:C:144:ASN:N	1:C:144:ASN:ND2	2.64	0.45
1:C:60:LYS:O	1:C:61:MET:HB2	2.16	0.45
1:A:10:PHE:HB2	1:A:89:LEU:HD11	1.99	0.44
1:B:156:VAL:CG2	1:B:157:GLU:N	2.81	0.44
1:B:136:ASN:ND2	1:B:136:ASN:C	2.67	0.44
1:C:4:ASP:OD1	1:C:4:ASP:N	2.50	0.44
1:C:105:VAL:HG21	1:C:120:MET:CG	2.46	0.44
1:B:54:ILE:O	1:B:55:ILE:C	2.56	0.44
1:B:176:ILE:HD13	1:B:194:GLU:HG2	1.99	0.43
1:A:40:LYS:CG	1:A:93:ILE:HG21	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LYS:NZ	1:B:203:GLU:OE2	2.49	0.43
1:C:121:ASN:N	1:C:122:PRO:HD2	2.34	0.43
1:A:41:HIS:O	1:A:42:LEU:HD23	2.18	0.43
1:C:31:TYR:O	1:C:34:ASN:HB2	2.19	0.42
1:A:74:PHE:CD1	2:A:211:ATM:C4	3.03	0.42
1:B:208:LEU:HA	1:B:209:TRP:HA	1.80	0.42
1:B:6:LYS:HE2	1:B:8:GLY:O	2.19	0.42
1:C:162:ILE:C	1:C:164:GLU:N	2.72	0.42
1:C:45:PRO:HG3	1:C:74:PHE:HE1	1.85	0.42
1:A:40:LYS:HG3	1:A:88:LEU:CD2	2.44	0.42
1:B:20:GLY:HA2	3:B:212:ADP:O1A	2.20	0.42
1:B:16:LEU:HD11	1:B:163:TYR:HB2	2.02	0.41
1:A:107:TYR:CE1	1:A:162:ILE:HD13	2.55	0.41
1:B:156:VAL:HG23	1:B:157:GLU:H	1.84	0.41
1:B:192:VAL:O	1:B:193:LYS:C	2.59	0.41
1:C:74:PHE:O	1:C:77:ASN:HB3	2.21	0.41
1:A:6:LYS:NZ	1:A:130:ASP:OD2	2.46	0.41
1:A:107:TYR:CZ	2:A:211:ATM:H2'	2.55	0.41
1:B:13:PHE:CE2	1:B:25:SER:HB3	2.56	0.41
1:B:176:ILE:CD1	1:B:194:GLU:HG2	2.50	0.41
1:A:116:LYS:HD2	1:A:120:MET:HE2	2.01	0.41
1:A:140:ASN:O	1:A:143:GLN:HG2	2.21	0.41
1:A:134:TYR:HH	1:A:163:TYR:HE2	1.66	0.41
1:A:188:HIS:O	1:A:192:VAL:HG23	2.20	0.41
1:B:194:GLU:C	1:B:196:THR:H	2.22	0.41
1:B:41:HIS:CD2	1:B:41:HIS:C	2.93	0.41
1:B:58:TYR:HD1	1:B:65:MET:HG3	1.85	0.41
1:A:93:ILE:HD12	1:A:93:ILE:N	2.36	0.41
1:B:136:ASN:HD21	1:B:163:TYR:HE1	1.68	0.41
1:B:6:LYS:HB2	1:B:205:PHE:CE2	2.56	0.41
1:C:208:LEU:HA	1:C:209:TRP:HA	1.73	0.40
1:C:10:PHE:CD2	1:C:129:PRO:HA	2.57	0.40
1:A:88:LEU:HD22	1:A:93:ILE:HG21	2.02	0.40
1:C:156:VAL:O	1:C:157:GLU:C	2.59	0.40
1:C:67:ASN:O	1:C:70:ILE:HG22	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LYS:NZ	1:C:48:GLU:OE1[2_545]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:HIS:O	1:C:171:HIS:CE1[6_554]	1.99	0.21

## 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	206/212 (97%)	190 (92%)	13 (6%)	3 (2%)	10	42
1	B	191/212 (90%)	169 (88%)	19 (10%)	3 (2%)	9	40
1	C	199/212 (94%)	175 (88%)	17 (8%)	7 (4%)	3	20
All	All	596/636 (94%)	534 (90%)	49 (8%)	13 (2%)	6	31

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	SER
1	A	201	GLU
1	B	156	VAL
1	C	51	ILE
1	B	61	MET
1	C	170	ALA
1	A	113	ASN
1	C	143	GLN
1	B	202	PRO
1	C	182	ARG
1	C	172	GLU
1	C	200	VAL
1	C	99	ARG

### 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	191/195 (98%)	171 (90%)	20 (10%)	7	27
1	B	181/195 (93%)	160 (88%)	21 (12%)	5	23
1	C	188/195 (96%)	165 (88%)	23 (12%)	5	21
All	All	560/585 (96%)	496 (89%)	64 (11%)	5	24

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	18	ARG
1	A	53	GLN
1	A	61	MET
1	A	63	ASN
1	A	68	GLU
1	A	73	LEU
1	A	86	LYS
1	A	87	SER
1	A	98	ASP
1	A	103	SER
1	A	109	SER
1	A	140	ASN
1	A	145	ARG
1	A	147	ASP
1	A	150	GLU
1	A	156	VAL
1	A	165	THR
1	A	198	ILE
1	A	204	GLU
1	B	4	ASP
1	B	9	LYS
1	B	11	ILE
1	B	47	ARG
1	B	61	MET
1	B	65	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	87	SER
1	B	109	SER
1	B	124	GLN
1	B	131	VAL
1	B	136	ASN
1	B	150	GLU
1	B	152	ILE
1	B	155	LYS
1	B	157	GLU
1	B	161	LYS
1	B	166	TYR
1	B	183	LYS
1	B	185	GLU
1	B	193	LYS
1	B	196	THR
1	C	7	LYS
1	C	21	LYS
1	C	30	GLU
1	C	32	LEU
1	C	60	LYS
1	C	61	MET
1	C	83	ASN
1	C	87	SER
1	C	109	SER
1	C	116	LYS
1	C	121	ASN
1	C	131	VAL
1	C	136	ASN
1	C	144	ASN
1	C	145	ARG
1	C	147	ASP
1	C	173	ASP
1	C	190	ASP
1	C	194	GLU
1	C	196	THR
1	C	199	LYS
1	C	201	GLU
1	C	203	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	34	ASN
1	A	35	ASN
1	A	41	HIS
1	A	63	ASN
1	A	67	ASN
1	A	121	ASN
1	A	140	ASN
1	A	168	HIS
1	B	67	ASN
1	B	121	ASN
1	B	136	ASN
1	B	188	HIS
1	B	206	ASN
1	C	34	ASN
1	C	41	HIS
1	C	46	ASN
1	C	136	ASN
1	C	144	ASN
1	C	177	ASN
1	C	206	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands 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
3	ADP	B	212	-	24,29,29	1.13	2 (8%)	29,45,45	1.33	3 (10%)
2	ATM	C	211	-	20,24,24	2.98	3 (15%)	24,35,35	1.93	5 (20%)
2	ATM	B	211	-	20,24,24	1.51	3 (15%)	24,35,35	2.46	4 (16%)
2	ATM	A	211	-	20,24,24	1.45	2 (10%)	24,35,35	1.71	5 (20%)
3	ADP	C	212	-	24,29,29	1.05	1 (4%)	29,45,45	1.39	2 (6%)
3	ADP	A	212	-	24,29,29	1.10	1 (4%)	29,45,45	1.37	5 (17%)

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	ADP	B	212	-	-	1/12/32/32	0/3/3/3
2	ATM	C	211	-	-	9/10/25/25	0/2/2/2
2	ATM	B	211	-	-	6/10/25/25	0/2/2/2
2	ATM	A	211	-	-	5/10/25/25	0/2/2/2
3	ADP	C	212	-	-	3/12/32/32	0/3/3/3
3	ADP	A	212	-	-	1/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	211	ATM	N4'-N3'	11.85	1.54	1.23
2	C	211	ATM	O4-C4	4.57	1.36	1.24
2	A	211	ATM	O4-C4	4.53	1.35	1.24
2	B	211	ATM	O4-C4	4.22	1.35	1.24
3	B	212	ADP	C5-C4	3.21	1.49	1.40
2	B	211	ATM	N4'-N3'	-3.04	1.15	1.23
2	A	211	ATM	N4'-N3'	-3.01	1.15	1.23
3	C	212	ADP	C5-C4	2.94	1.48	1.40
3	A	212	ADP	C5-C4	2.45	1.47	1.40
2	B	211	ATM	P-OP3	2.27	1.63	1.54
2	C	211	ATM	P-OP2	2.22	1.63	1.54
3	B	212	ADP	C2-N3	2.13	1.35	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	211	ATM	C3'-N3'-N4'	7.57	139.93	115.78
2	B	211	ATM	C4-N3-C2	7.06	121.10	115.14
2	C	211	ATM	C4-N3-C2	6.22	120.39	115.14
2	A	211	ATM	C4-N3-C2	5.55	119.83	115.14
2	B	211	ATM	O5'-P-OP1	3.97	117.60	106.47
3	A	212	ADP	N3-C2-N1	-3.81	122.72	128.68
2	C	211	ATM	C5-C6-N1	-3.48	118.44	122.19
3	C	212	ADP	PA-O3A-PB	-3.32	121.44	132.83
2	A	211	ATM	C5-C6-N1	-3.29	118.65	122.19
3	C	212	ADP	N3-C2-N1	-3.19	123.69	128.68
3	B	212	ADP	N3-C2-N1	-3.09	123.85	128.68
2	C	211	ATM	C2'-C3'-C4'	2.99	105.73	103.01
2	C	211	ATM	C2'-C1'-N1	-2.98	107.40	114.27
3	B	212	ADP	C4-C5-N7	-2.94	106.34	109.40
2	B	211	ATM	C5-C6-N1	-2.80	119.18	122.19
2	C	211	ATM	C5'-C4'-C3'	-2.57	106.46	114.29
2	A	211	ATM	O4'-C4'-C5'	-2.54	101.02	109.37
2	A	211	ATM	O5'-P-OP1	2.52	113.54	106.47
3	A	212	ADP	PA-O3A-PB	-2.41	124.55	132.83
3	A	212	ADP	N6-C6-N1	2.29	123.33	118.57
3	B	212	ADP	C2-N1-C6	2.26	122.63	118.75
3	A	212	ADP	C4-C5-N7	-2.23	107.08	109.40
3	A	212	ADP	C2-N1-C6	2.12	122.38	118.75
2	A	211	ATM	C2'-C3'-C4'	2.09	104.91	103.01

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	212	ADP	PA-O3A-PB-O2B
2	C	211	ATM	C5'-O5'-P-OP1
2	C	211	ATM	C5'-O5'-P-OP3
2	B	211	ATM	C5'-O5'-P-OP1
2	B	211	ATM	C5'-O5'-P-OP2
2	B	211	ATM	C5'-O5'-P-OP3
2	A	211	ATM	C5'-O5'-P-OP3
2	C	211	ATM	C3'-C4'-C5'-O5'
2	B	211	ATM	C3'-C4'-C5'-O5'
2	A	211	ATM	C3'-C4'-C5'-O5'
2	C	211	ATM	O4'-C4'-C5'-O5'
2	B	211	ATM	O4'-C4'-C5'-O5'

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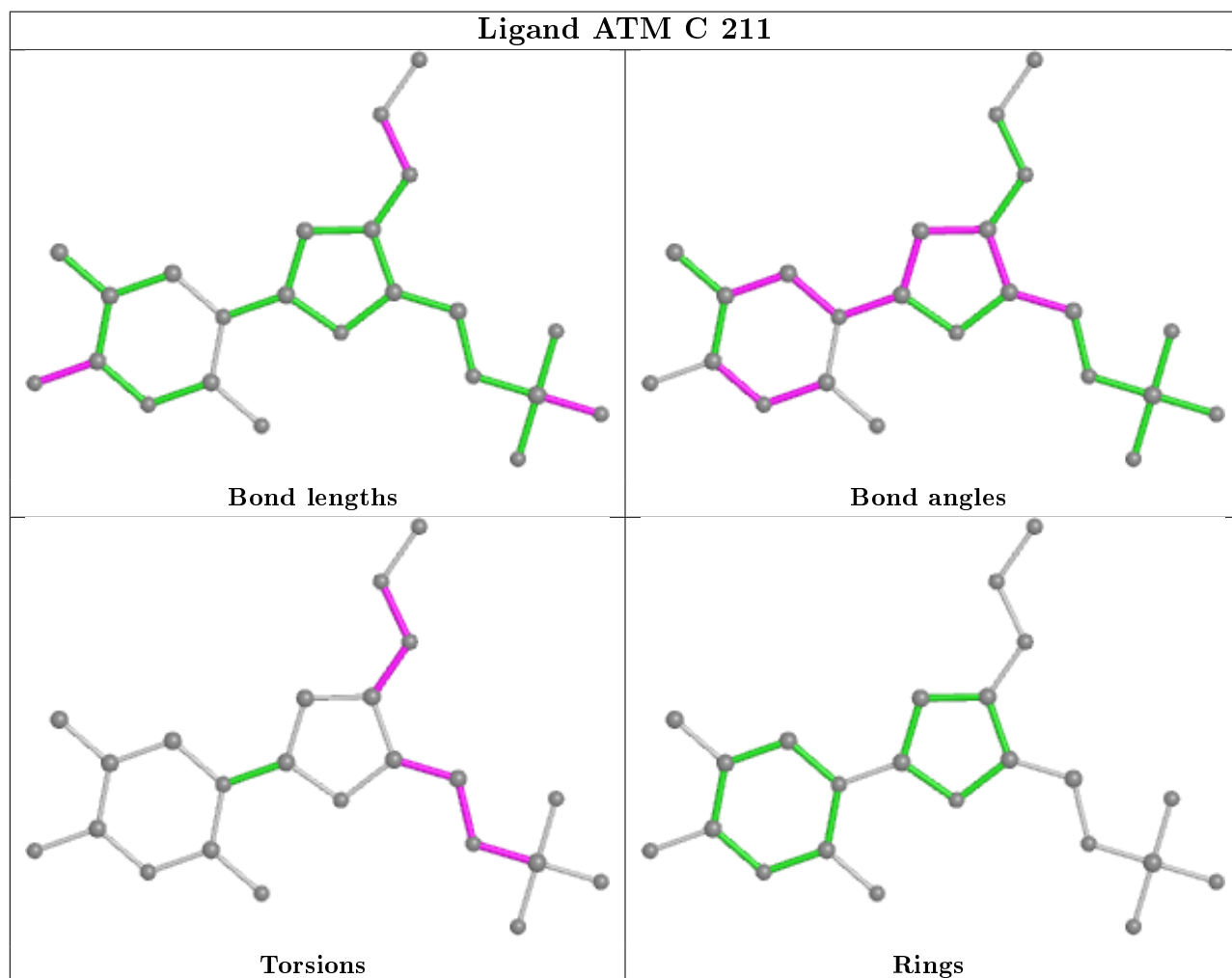
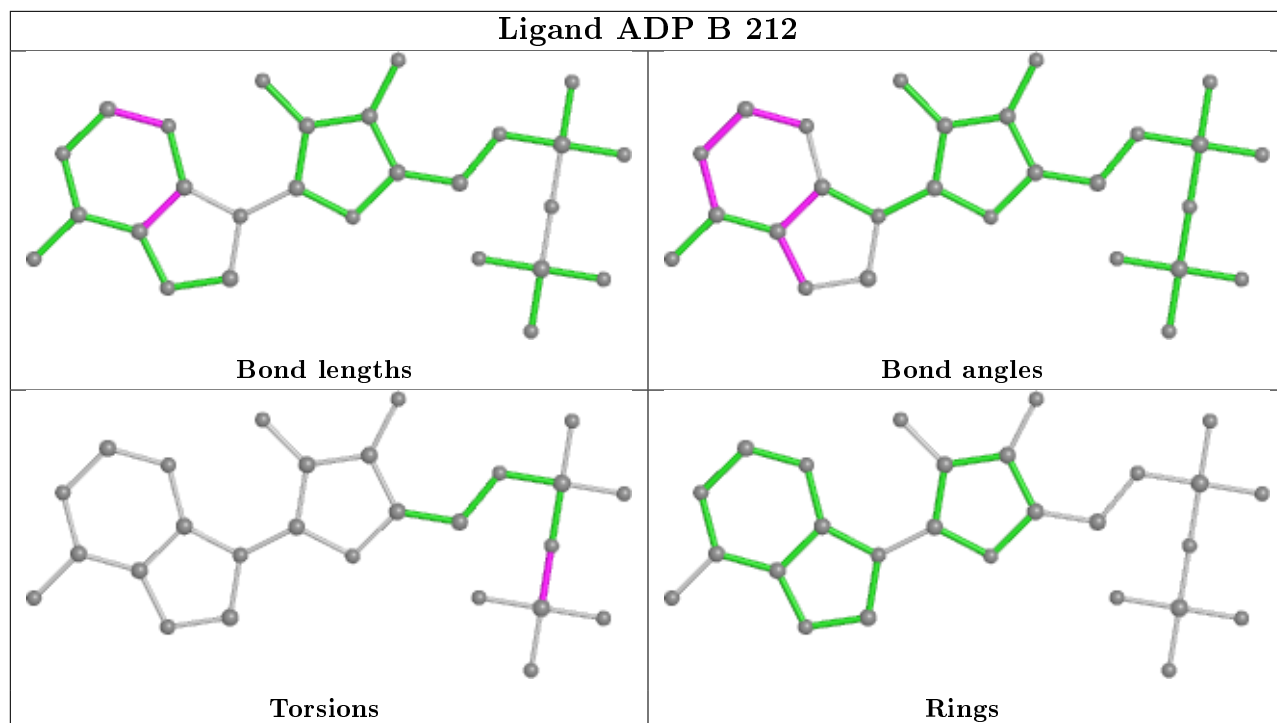
Mol	Chain	Res	Type	Atoms
2	A	211	ATM	O4'-C4'-C5'-O5'
2	A	211	ATM	C5'-O5'-P-OP1
2	C	211	ATM	C4'-C3'-N3'-N4'
2	B	211	ATM	C4'-C3'-N3'-N4'
2	C	211	ATM	C3'-N3'-N4'-N5'
2	A	211	ATM	C5'-O5'-P-OP2
3	C	212	ADP	PA-O3A-PB-O1B
3	A	212	ADP	PA-O3A-PB-O2B
2	C	211	ATM	C4'-C5'-O5'-P
2	C	211	ATM	C5'-O5'-P-OP2
2	C	211	ATM	C2'-C3'-N3'-N4'
3	C	212	ADP	PA-O3A-PB-O2B
3	C	212	ADP	PA-O3A-PB-O3B

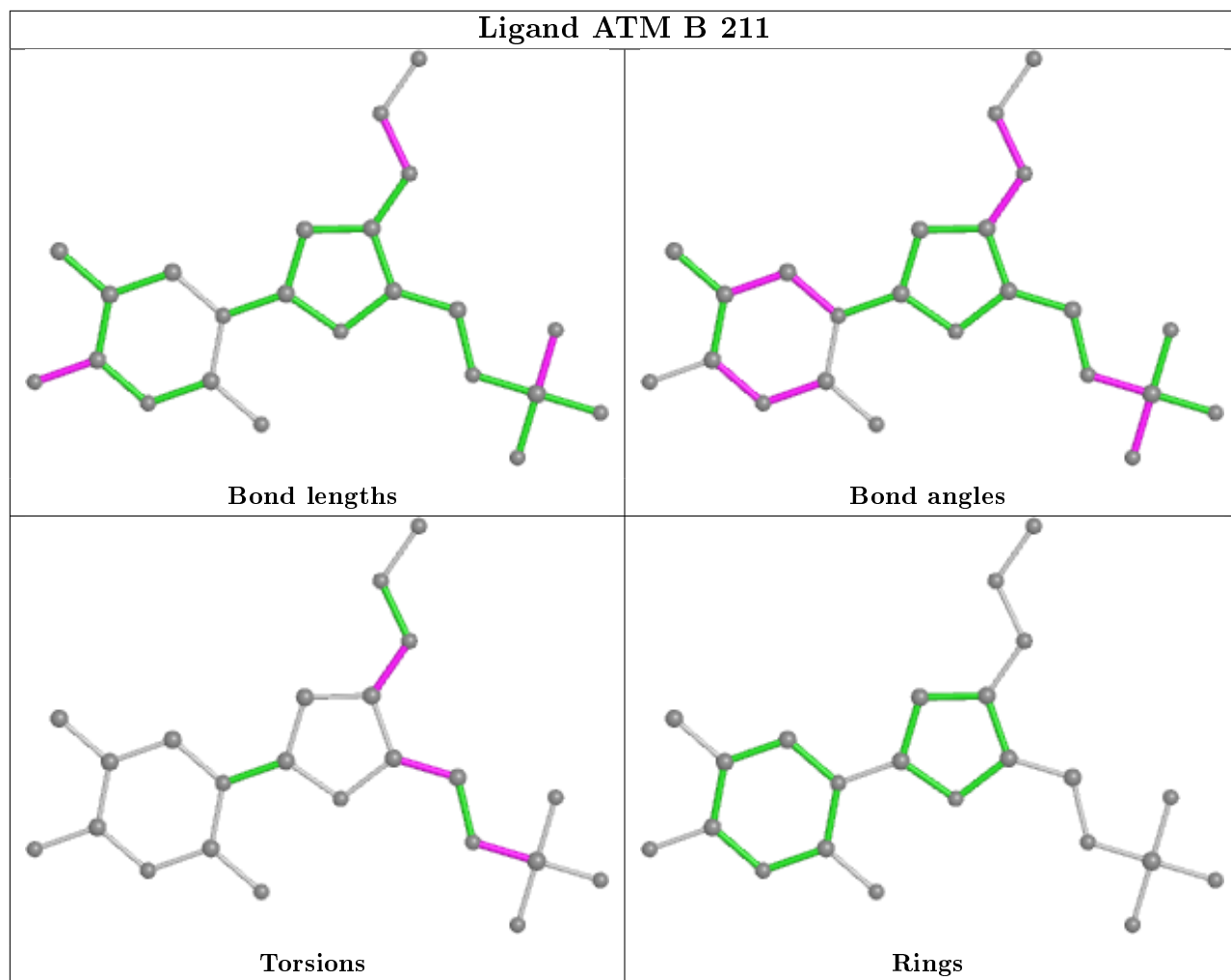
There are no ring outliers.

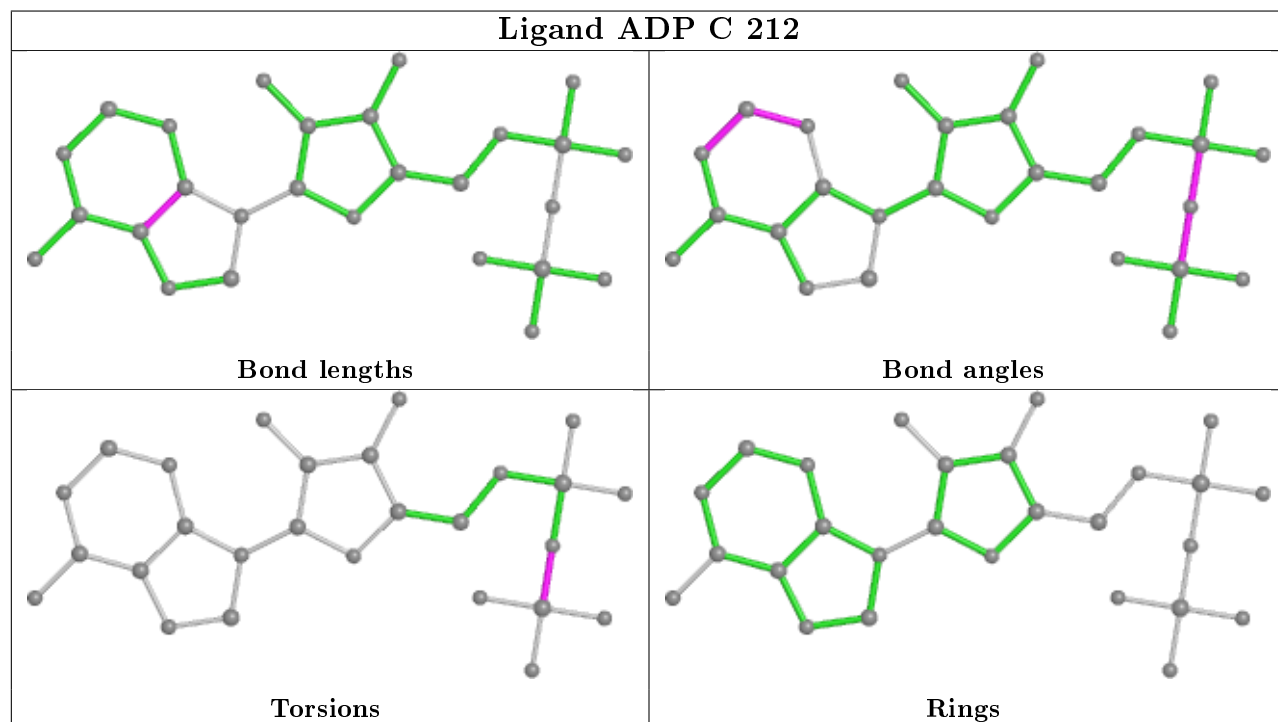
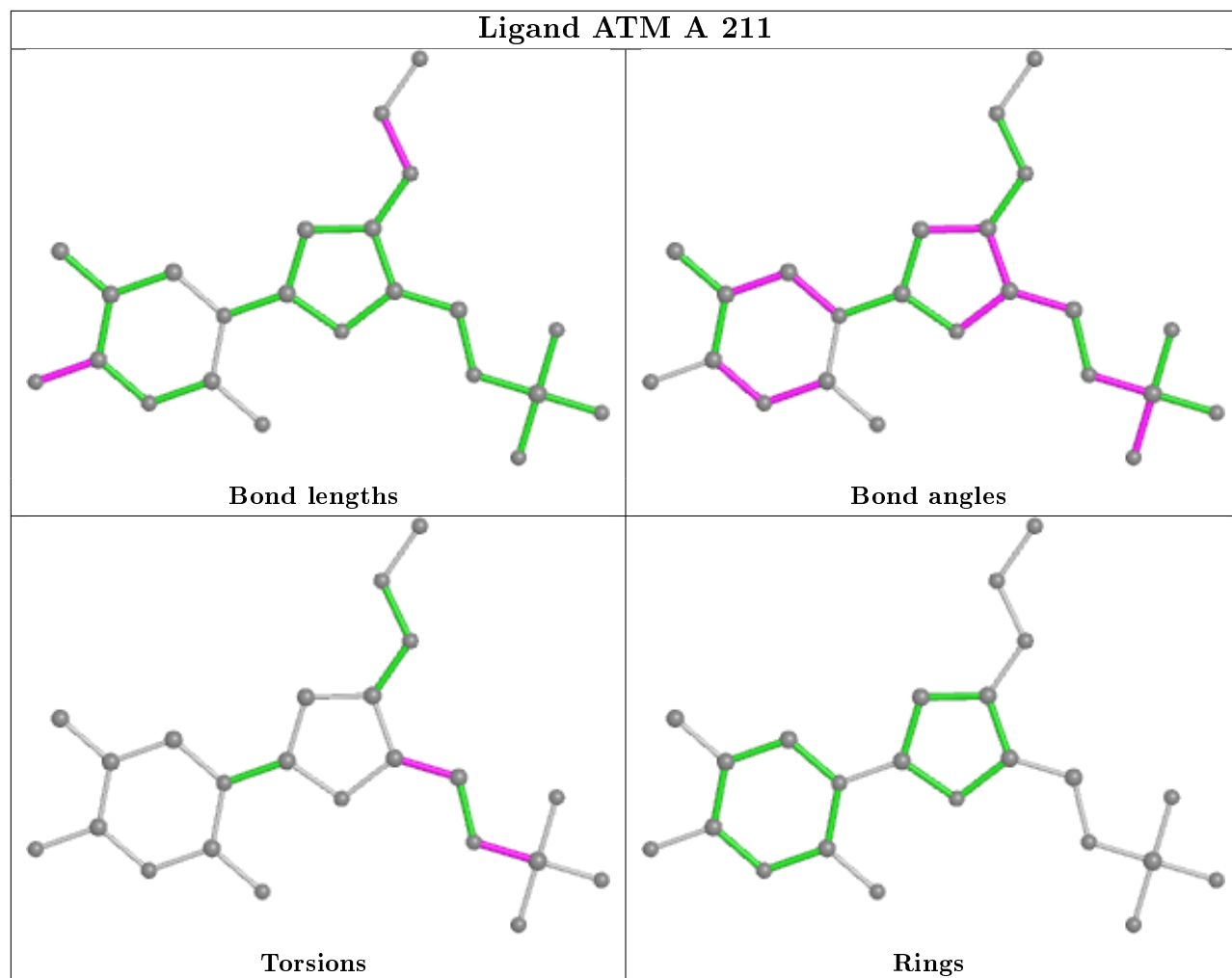
6 monomers are involved in 8 short contacts:

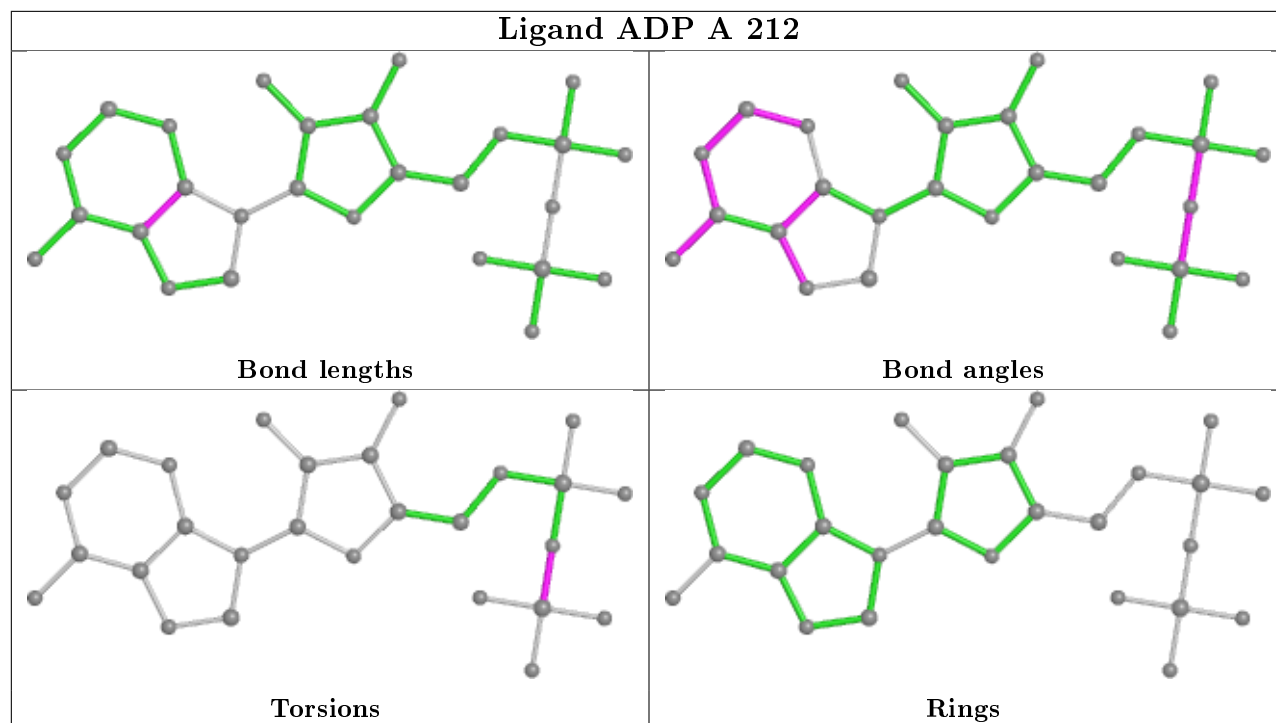
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	212	ADP	1	0
2	C	211	ATM	1	0
2	B	211	ATM	1	0
2	A	211	ATM	3	0
3	C	212	ADP	1	0
3	A	212	ADP	1	0

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	208/212 (98%)	-0.47	2 (0%) 82 59	8, 23, 41, 49	18 (8%)
1	B	197/212 (92%)	-0.27	0 100 100	22, 35, 50, 56	23 (11%)
1	C	205/212 (96%)	-0.15	0 100 100	24, 41, 58, 63	26 (12%)
All	All	610/636 (95%)	-0.30	2 (0%) 94 84	8, 34, 53, 63	67 (10%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	VAL	2.5
1	A	202	PRO	2.4

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

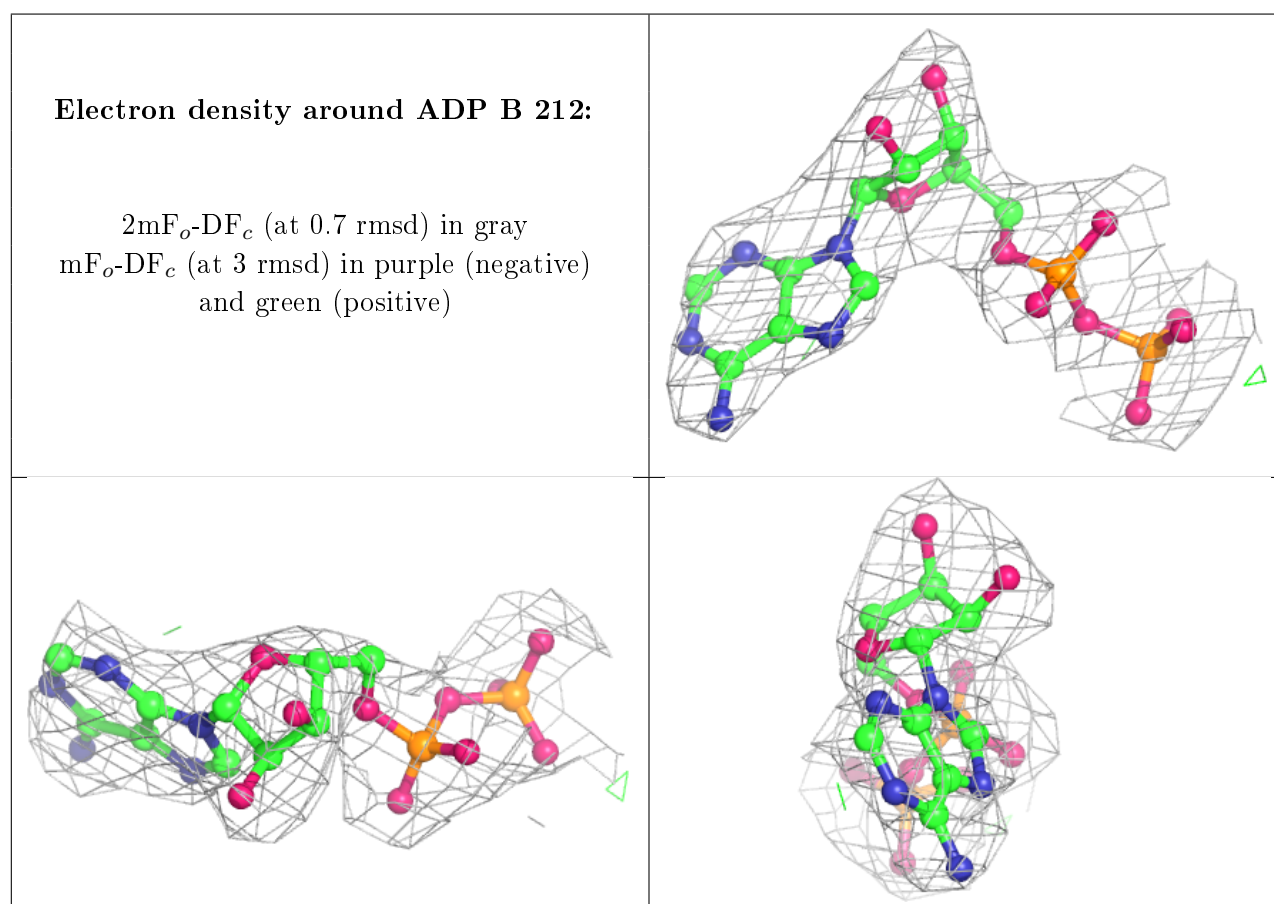
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ADP	B	212	27/27	0.92	0.19	50,54,58,58	0

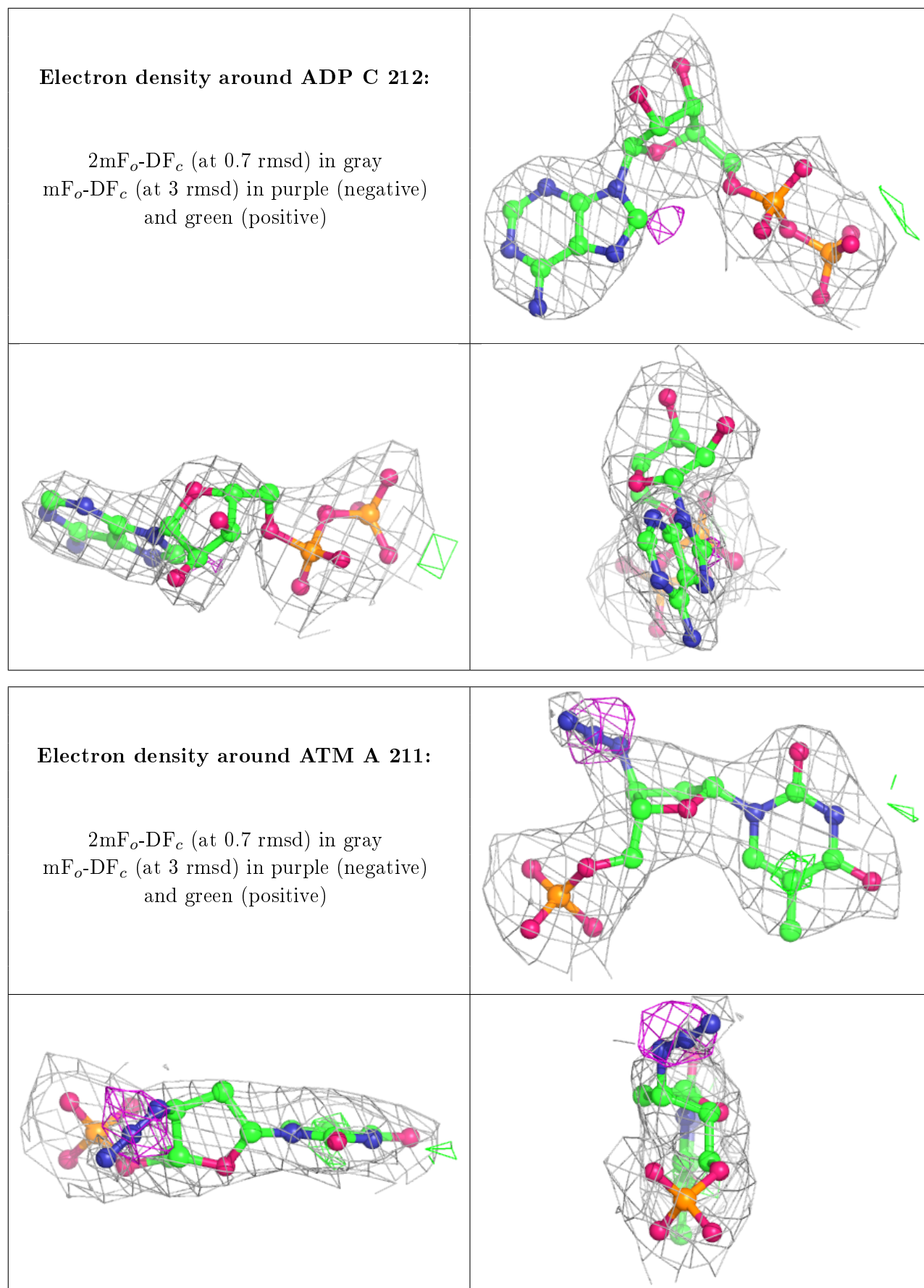
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	C	212	27/27	0.93	0.17	36,42,47,48	0
2	ATM	A	211	23/23	0.95	0.18	15,24,32,37	0
2	ATM	C	211	23/23	0.96	0.14	30,37,40,41	2
2	ATM	B	211	23/23	0.97	0.19	27,30,37,38	2
3	ADP	A	212	27/27	0.98	0.12	25,34,38,39	0

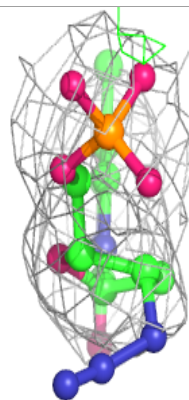
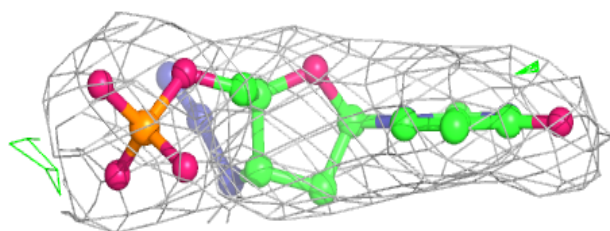
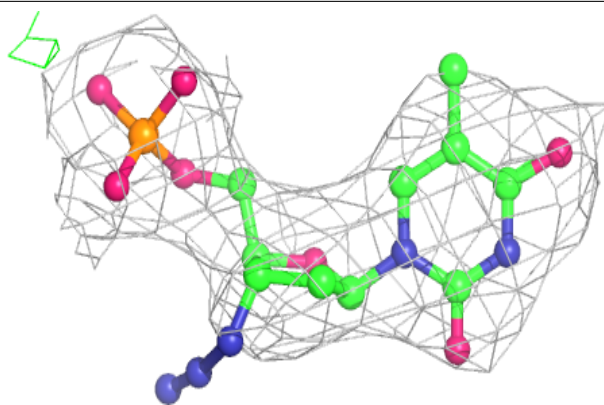
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



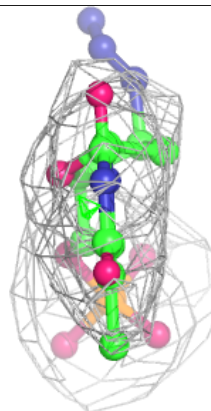
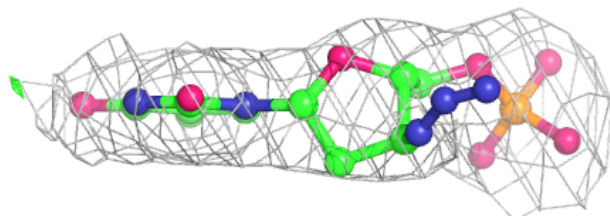
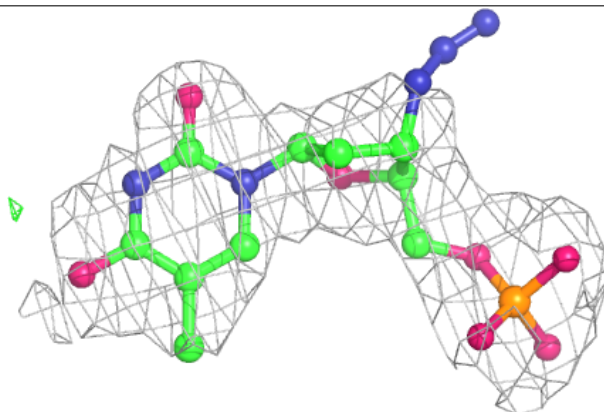


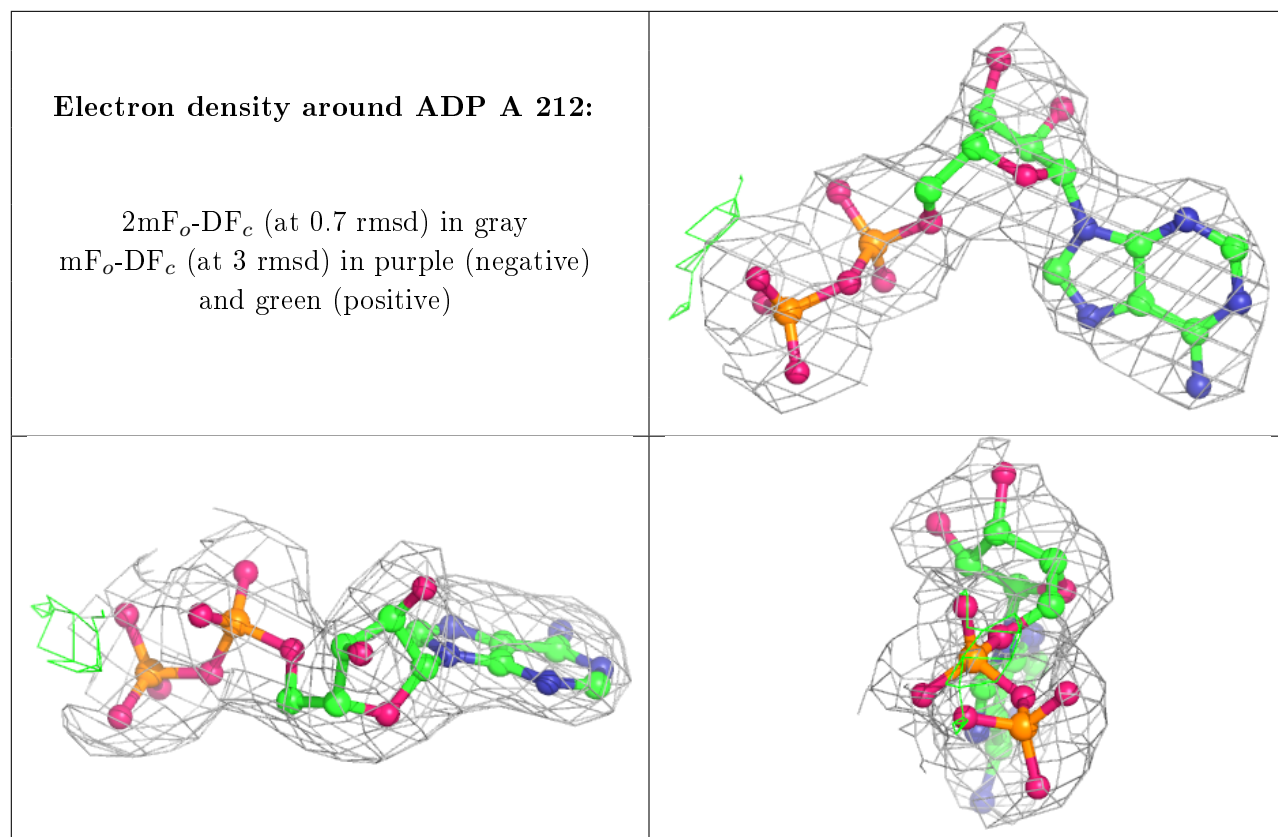
**Electron density around ATM C 211:**

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

**Electron density around ATM B 211:**

$2mF_o-DF_c$  (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.