



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:01 am BST

PDB ID : 1M4G  
Title : Aminoglycoside 2'-N-acetyltransferase from Mycobacterium tuberculosis-  
Complex with Coenzyme A and Ribostamycin  
Authors : Vetting, M.W.; Hegde, S.S.; Javid-Majd, F.; Blanchard, J.S.; Roderick, S.L.  
Deposited on : 2002-07-02  
Resolution : 1.80 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.

---

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

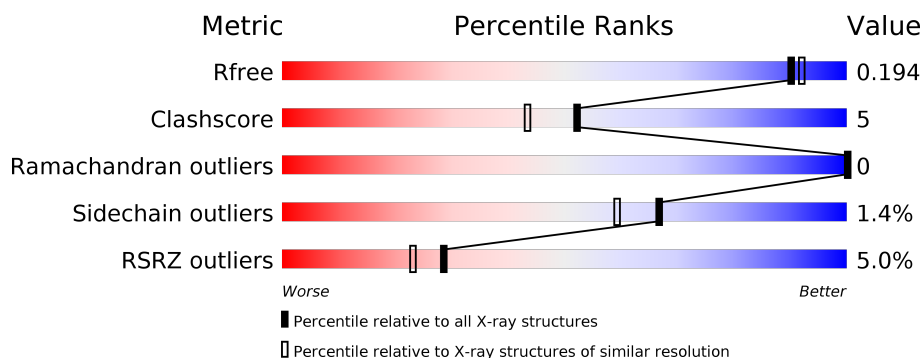
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	181	<div> <div>3%</div> <div>94%</div> <div>5%</div> </div>
1	B	181	<div> <div>7%</div> <div>90%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

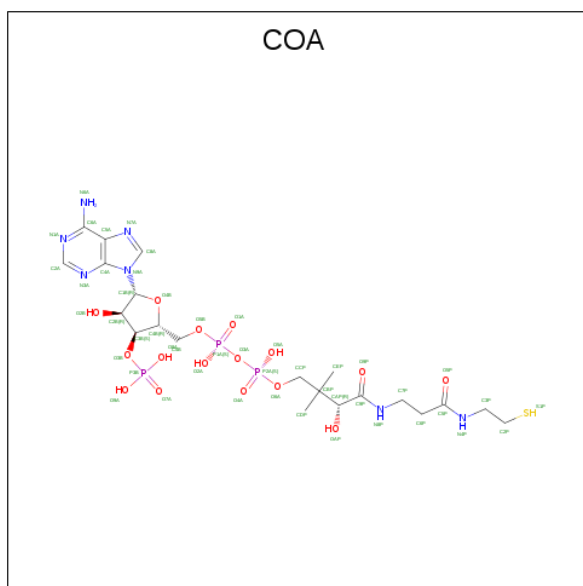
There are 5 unique types of molecules in this entry. The entry contains 3314 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aminoglycoside 2'-N-acetyltransferase.

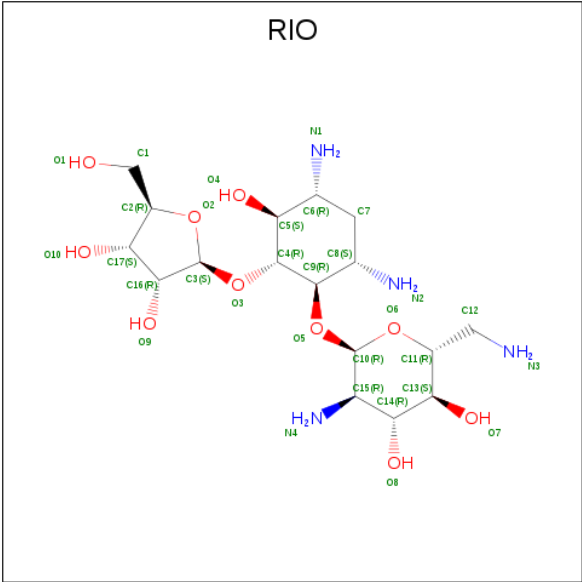
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1412	884	265	256	7			
1	B	176	Total	C	N	O	S	0	0	0
			1371	859	257	249	6			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



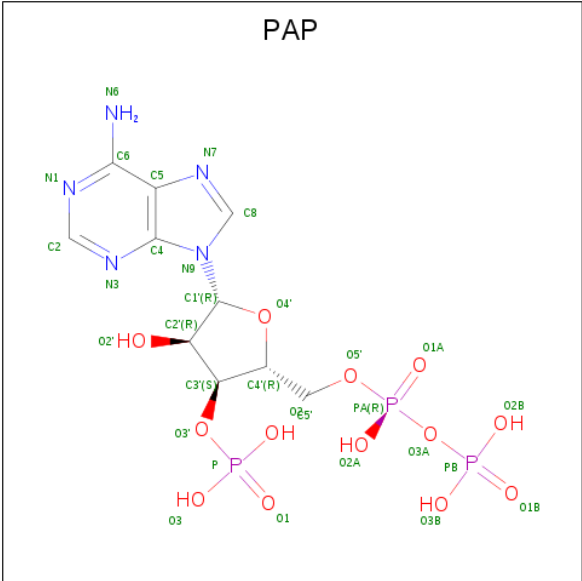
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		
2	B	1	Total	C	N	O	P S	0	0
			48	21	7	16	3 1		

- Molecule 3 is RIBOSTAMYCIN (three-letter code: RIO) (formula:  $C_{17}H_{34}N_4O_{10}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	17	4	10		
3	B	1	Total	C	N	O	0	0
			31	17	4	10		

- Molecule 4 is 3'-PHOSPHATE-ADENOSINE-5'-DIPHOSPHATE (three-letter code: PAP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

Continued on next page...

*Continued from previous page...*

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

- Molecule 5 is water.

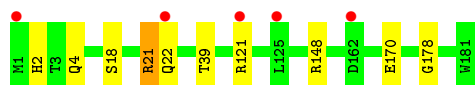
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	159	Total	O	0	0
			159	159		
5	B	152	Total	O	0	0
			152	152		

### 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.

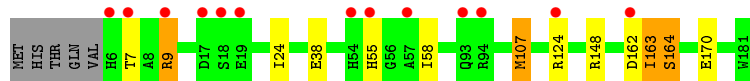
- Molecule 1: Aminoglycoside 2'-N-acetyltransferase

Chain A: 



- Molecule 1: Aminoglycoside 2'-N-acetyltransferase

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.70 Å 86.40 Å 98.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 24.04 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-1.80) 98.0 (24.04-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.60 (at 1.80 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.165 , 0.202 0.155 , 0.194	Depositor DCC
$R_{free}$ test set	1922 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3314	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PAP, COA, RIO

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	1.02	2/1447 (0.1%)	1.02	3/1971 (0.2%)
1	B	0.98	1/1405 (0.1%)	1.04	5/1914 (0.3%)
All	All	1.00	3/2852 (0.1%)	1.03	8/3885 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	MET	CB-CG	8.14	1.77	1.51
1	A	170	GLU	CD-OE1	6.59	1.32	1.25
1	A	170	GLU	CG-CD	5.83	1.60	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	MET	CB-CG-SD	-11.41	78.17	112.40
1	A	148	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	148	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	B	148	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	148	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	B	107	MET	CG-SD-CE	-6.56	89.70	100.20
1	B	7	THR	N-CA-C	-6.13	94.45	111.00
1	A	21	ARG	NE-CZ-NH2	-5.97	117.32	120.30

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	1412	0	1374	8	0
1	B	1371	0	1331	24	0
2	A	48	0	32	1	1
2	B	48	0	32	0	0
3	A	31	0	34	0	0
3	B	31	0	34	0	0
4	B	62	0	22	0	0
5	A	159	0	0	2	0
5	B	152	0	0	8	1
All	All	3314	0	2859	32	1

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 5.

All (32) 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:107:MET:CG	1:B:107:MET:CB	1.77	1.57
1:B:107:MET:SD	1:B:107:MET:CB	2.31	1.18
1:B:9:ARG:HG2	1:B:9:ARG:HH11	1.01	1.07
1:B:9:ARG:HG2	1:B:9:ARG:NH1	1.77	0.96
1:B:163:ILE:HD13	1:B:163:ILE:O	1.67	0.94
1:B:107:MET:SD	1:B:107:MET:HB2	2.04	0.93
1:B:163:ILE:HD12	1:B:163:ILE:H	1.31	0.93
1:A:2:HIS:HD2	1:A:4:GLN:H	1.14	0.92
1:B:9:ARG:CG	1:B:9:ARG:HH11	1.85	0.90
1:B:163:ILE:N	1:B:163:ILE:HD12	1.90	0.85
1:A:2:HIS:CD2	1:A:4:GLN:H	1.97	0.83
1:B:163:ILE:O	5:B:718:HOH:O	2.11	0.69
1:B:163:ILE:H	1:B:163:ILE:CD1	2.04	0.67
1:B:38:GLU:OE2	5:B:700:HOH:O	2.11	0.67
1:B:163:ILE:N	1:B:163:ILE:CD1	2.55	0.67
1:B:170:GLU:HG3	5:B:714:HOH:O	1.95	0.66
1:B:164:SER:HA	5:B:718:HOH:O	1.99	0.63
1:B:124:ARG:HG3	5:B:635:HOH:O	2.01	0.61

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:HG21	1:A:178:GLY:HA3	1.89	0.55
1:A:18:SER:O	1:A:22:GLN:HG3	2.09	0.53
1:B:124:ARG:NH2	5:B:753:HOH:O	2.30	0.49
1:B:162:ASP:OD2	5:B:734:HOH:O	2.20	0.48
1:B:163:ILE:O	1:B:163:ILE:CD1	2.52	0.47
1:B:124:ARG:NE	5:B:753:HOH:O	2.41	0.47
1:A:21:ARG:NH1	5:A:619:HOH:O	2.40	0.47
1:B:107:MET:CG	1:B:107:MET:CA	2.82	0.45
1:A:121:ARG:NH2	5:A:655:HOH:O	2.51	0.43
1:A:2:HIS:CD2	1:A:4:GLN:N	2.78	0.42
1:B:24:ILE:CG1	1:B:58:ILE:HD13	2.50	0.41
1:A:121:ARG:HH22	2:A:502:COA:H71	1.86	0.41
1:B:24:ILE:HG12	1:B:58:ILE:HD13	2.01	0.41
1:B:9:ARG:CG	1:B:9:ARG:NH1	2.55	0.41

All (1) 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)
2:A:502:COA:N6A	5:B:725:HOH:O[2_564]	2.12	0.08

## 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	179/181 (99%)	178 (99%)	1 (1%)	0	100	100
1	B	174/181 (96%)	172 (99%)	2 (1%)	0	100	100
All	All	353/362 (98%)	350 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	143/143 (100%)	143 (100%)	0	100	100
1	B	138/143 (96%)	134 (97%)	4 (3%)	42	29
All	All	281/286 (98%)	277 (99%)	4 (1%)	67	59

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	ARG
1	B	55	HIS
1	B	163	ILE
1	B	164	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	22	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 carbohydrates in this entry.

## 5.6 Ligand geometry

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
4	PAP	B	601	-	28,33,33	1.61	5 (17%)	35,52,52	1.10	3 (8%)
2	COA	A	502	-	41,50,50	1.51	6 (14%)	52,75,75	1.13	5 (9%)
4	PAP	B	600	-	28,33,33	1.53	4 (14%)	35,52,52	1.31	4 (11%)
3	RIO	A	500	-	33,33,33	1.13	4 (12%)	47,49,49	1.35	7 (14%)
2	COA	B	503	-	41,50,50	1.50	7 (17%)	52,75,75	1.09	5 (9%)
3	RIO	B	501	-	33,33,33	1.19	3 (9%)	47,49,49	1.34	6 (12%)

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	PAP	B	601	-	-	5/17/37/37	0/3/3/3
2	COA	A	502	-	-	4/44/64/64	0/3/3/3
4	PAP	B	600	-	-	2/17/37/37	0/3/3/3
3	RIO	A	500	-	-	5/12/68/68	0/3/3/3
2	COA	B	503	-	-	6/44/64/64	0/3/3/3
3	RIO	B	501	-	-	5/12/68/68	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	PAP	P-O3'	5.47	1.69	1.59
2	B	503	COA	C4A-N3A	4.88	1.42	1.35
4	B	601	PAP	P-O3'	4.62	1.68	1.59
2	A	502	COA	C9P-N8P	3.94	1.42	1.33
2	B	503	COA	P3B-O3B	3.87	1.66	1.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	COA	O4B-C1B	3.52	1.46	1.41
2	A	502	COA	CEP-CBP	3.29	1.61	1.53
4	B	601	PAP	O4'-C1'	3.10	1.45	1.41
2	A	502	COA	C7P-C6P	3.03	1.61	1.51
2	B	503	COA	C2A-N1A	3.01	1.39	1.33
4	B	601	PAP	C2-N1	3.01	1.39	1.33
4	B	600	PAP	PB-O3B	2.91	1.66	1.54
4	B	601	PAP	C4-N3	2.74	1.39	1.35
3	B	501	RIO	C15-N4	2.54	1.51	1.47
2	A	502	COA	C4A-N3A	2.52	1.39	1.35
4	B	601	PAP	PB-O3B	2.52	1.64	1.54
3	A	500	RIO	C7-C8	2.52	1.59	1.53
4	B	600	PAP	C2-N1	2.46	1.38	1.33
2	B	503	COA	CEP-CBP	2.43	1.59	1.53
2	A	502	COA	C2A-N3A	2.37	1.35	1.32
3	A	500	RIO	C9-C4	2.32	1.57	1.52
3	A	500	RIO	C15-N4	2.26	1.50	1.47
3	B	501	RIO	C3-C16	-2.25	1.50	1.52
4	B	600	PAP	O4'-C1'	2.16	1.44	1.41
3	B	501	RIO	C14-C15	2.14	1.56	1.53
2	B	503	COA	C2A-N3A	2.08	1.35	1.32
3	A	500	RIO	O2-C3	2.05	1.45	1.41
2	B	503	COA	P1A-O2A	-2.04	1.45	1.55
2	B	503	COA	OAP-CAP	2.03	1.46	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	RIO	O3-C3-O2	-4.61	106.44	111.43
4	B	600	PAP	C1'-N9-C4	-3.71	120.11	126.64
4	B	600	PAP	O2B-PB-O3A	3.55	116.53	104.64
3	B	501	RIO	O3-C3-O2	-3.44	107.70	111.43
2	A	502	COA	C1B-N9A-C4A	-3.28	120.88	126.64
3	B	501	RIO	O5-C9-C4	3.13	115.42	107.48
3	A	500	RIO	C10-O6-C11	2.95	119.48	113.69
3	B	501	RIO	C10-O5-C9	2.79	124.87	117.96
2	B	503	COA	C1B-N9A-C4A	-2.71	121.88	126.64
2	B	503	COA	CAP-C9P-N8P	-2.63	111.35	116.58
3	B	501	RIO	C10-O6-C11	2.60	118.79	113.69
4	B	600	PAP	C2'-C3'-C4'	-2.51	98.78	103.22
3	A	500	RIO	O5-C9-C8	-2.50	103.21	109.18
2	B	503	COA	C4A-C5A-N7A	2.47	111.97	109.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	PAP	C4-C5-N7	2.46	111.97	109.40
2	B	503	COA	N6A-C6A-N1A	2.46	123.68	118.57
3	A	500	RIO	O3-C4-C9	2.41	113.59	107.48
4	B	601	PAP	N6-C6-N1	2.40	123.56	118.57
2	A	502	COA	C4A-C5A-N7A	2.38	111.88	109.40
2	A	502	COA	N6A-C6A-N1A	2.37	123.49	118.57
3	A	500	RIO	O5-C9-C4	2.32	113.38	107.48
2	B	503	COA	C6P-C5P-N4P	-2.30	112.55	116.42
2	A	502	COA	O3B-P3B-O7A	-2.25	100.69	109.39
3	A	500	RIO	C10-O5-C9	2.22	123.47	117.96
3	B	501	RIO	C12-C11-C13	-2.20	108.77	113.10
3	B	501	RIO	O3-C4-C5	2.14	112.97	107.28
3	A	500	RIO	C5-C6-N1	-2.12	106.77	110.97
2	A	502	COA	C5A-C6A-N6A	-2.10	117.17	120.35
4	B	601	PAP	C5-C6-N6	-2.06	117.22	120.35
4	B	600	PAP	N6-C6-N1	2.04	122.82	118.57

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	601	PAP	O4'-C4'-C5'-O5'
4	B	601	PAP	C3'-C4'-C5'-O5'
2	A	502	COA	CCP-O6A-P2A-O3A
2	B	503	COA	C3B-O3B-P3B-O7A
2	B	503	COA	CCP-O6A-P2A-O3A
3	B	501	RIO	C4-C9-O5-C10
3	A	500	RIO	C9-C4-O3-C3
3	A	500	RIO	C4-C9-O5-C10
3	B	501	RIO	C5-C4-O3-C3
3	B	501	RIO	C9-C4-O3-C3
3	A	500	RIO	C5-C4-O3-C3
3	A	500	RIO	O6-C10-O5-C9
2	A	502	COA	O5P-C5P-N4P-C3P
2	B	503	COA	C6P-C7P-N8P-C9P
4	B	601	PAP	C3'-O3'-P-O2
4	B	601	PAP	C3'-O3'-P-O3
2	B	503	COA	C3B-O3B-P3B-O8A
2	B	503	COA	P2A-O3A-P1A-O1A
3	A	500	RIO	C8-C9-O5-C10
3	B	501	RIO	C8-C9-O5-C10
2	A	502	COA	CCP-O6A-P2A-O4A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	502	COA	CCP-O6A-P2A-O5A
2	B	503	COA	CCP-O6A-P2A-O5A
3	B	501	RIO	O6-C10-O5-C9
4	B	601	PAP	C5'-O5'-PA-O3A
4	B	600	PAP	C3'-O3'-P-O3
4	B	600	PAP	O4'-C4'-C5'-O5'

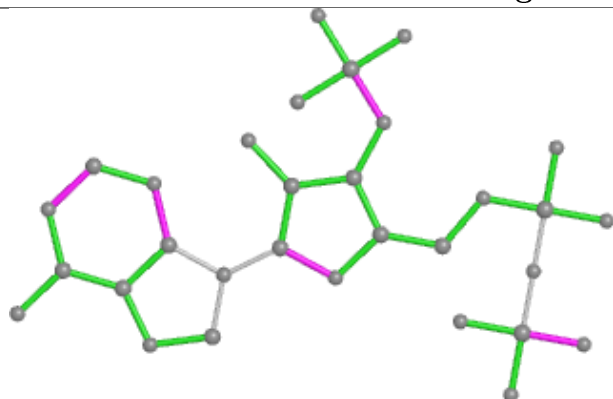
There are no ring outliers.

1 monomer is involved in 2 short contacts:

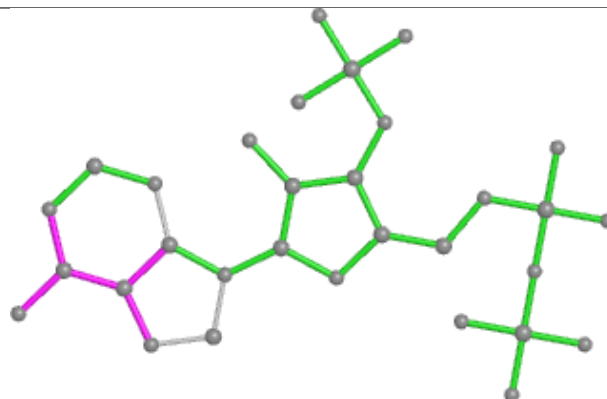
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	COA	1	1

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.

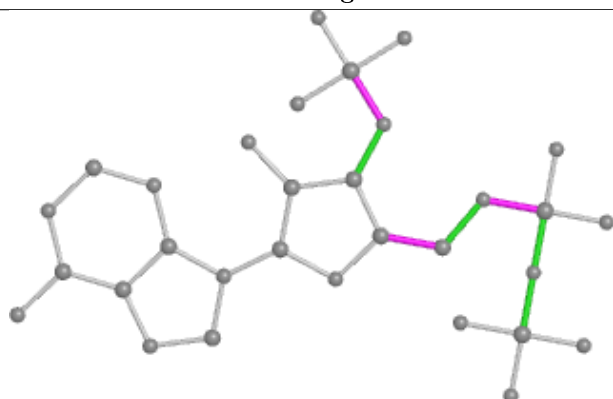
## Ligand PAP B 601



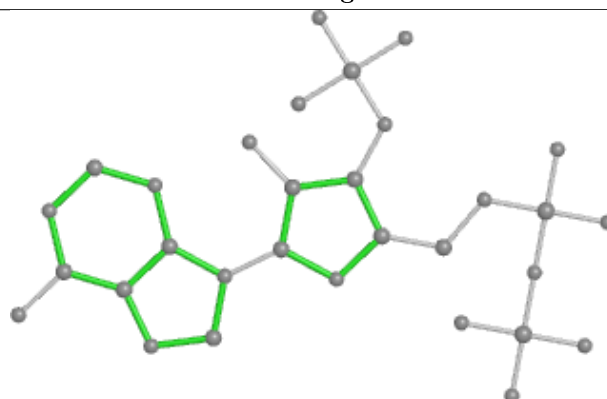
Bond lengths



Bond angles

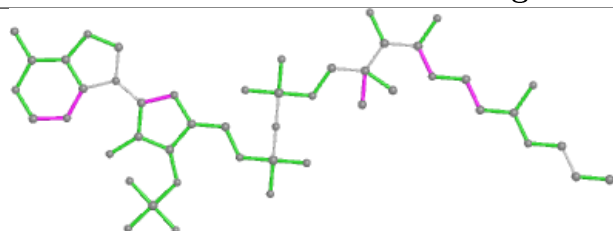


Torsions

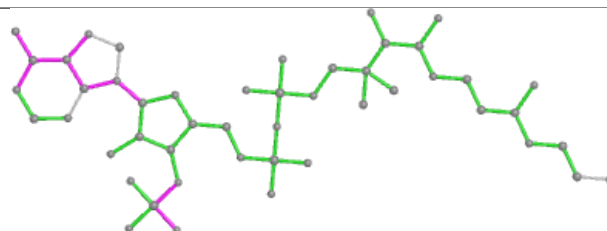


Rings

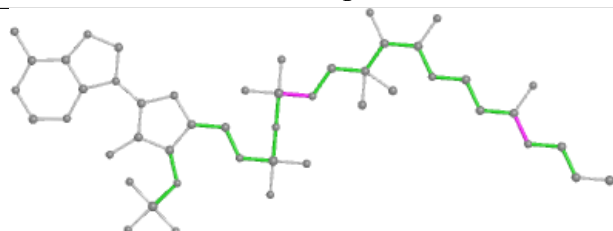
## Ligand COA A 502



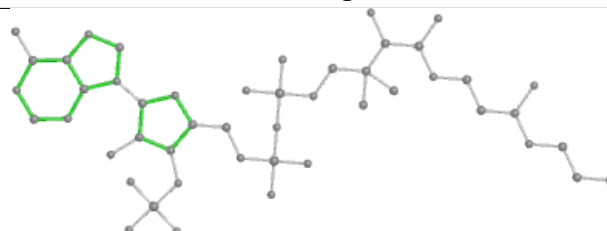
Bond lengths



Bond angles

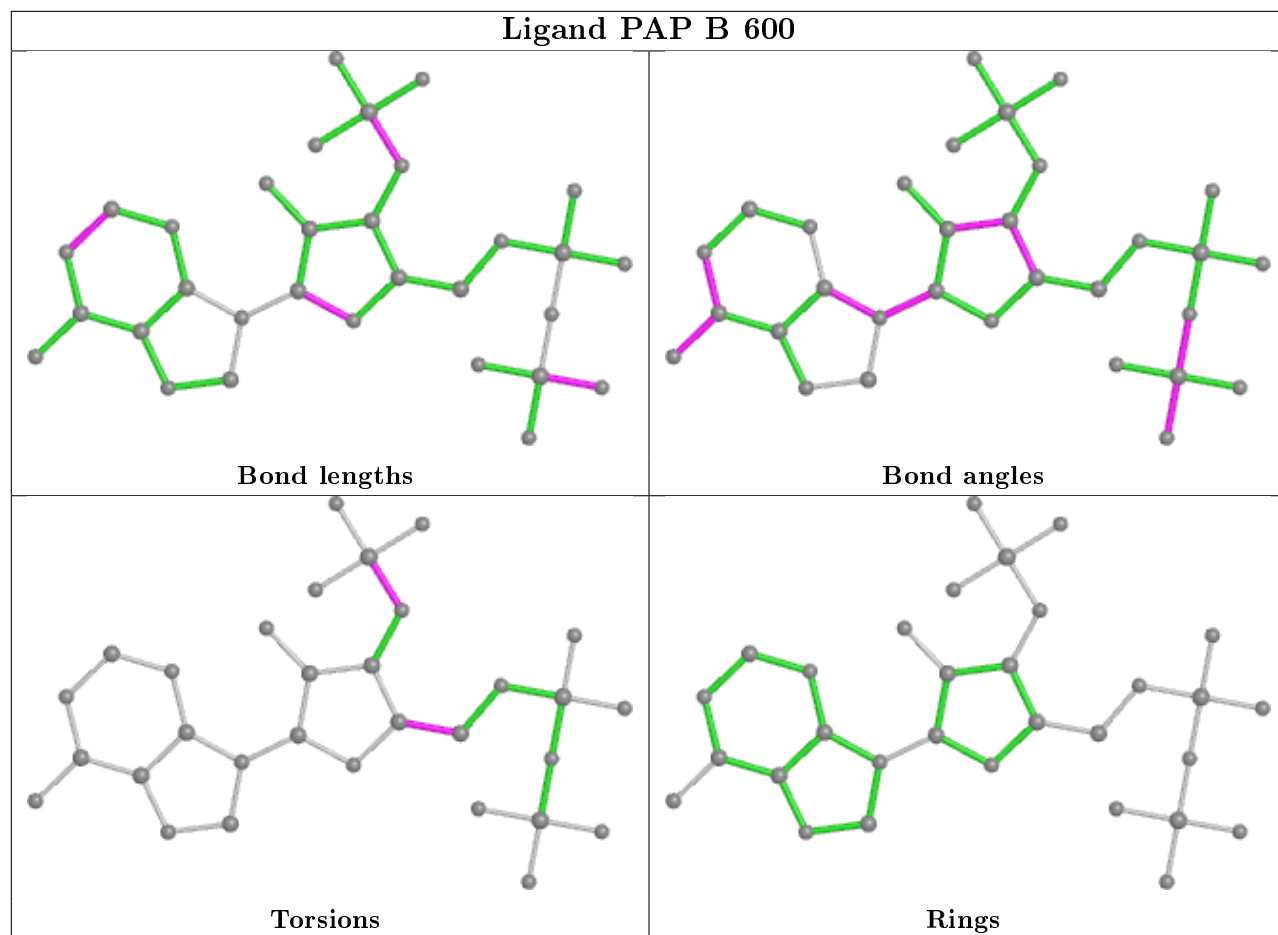


Torsions

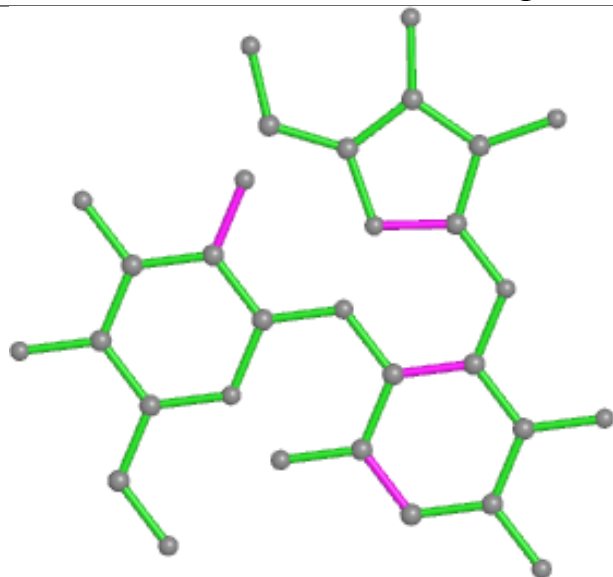


Rings

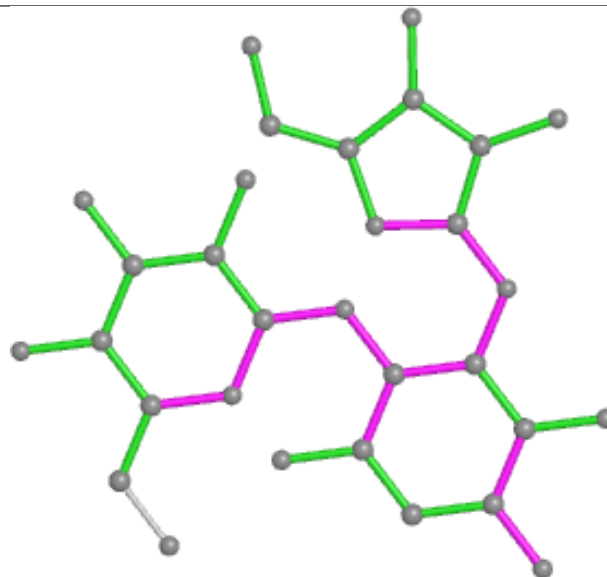
## Ligand PAP B 600



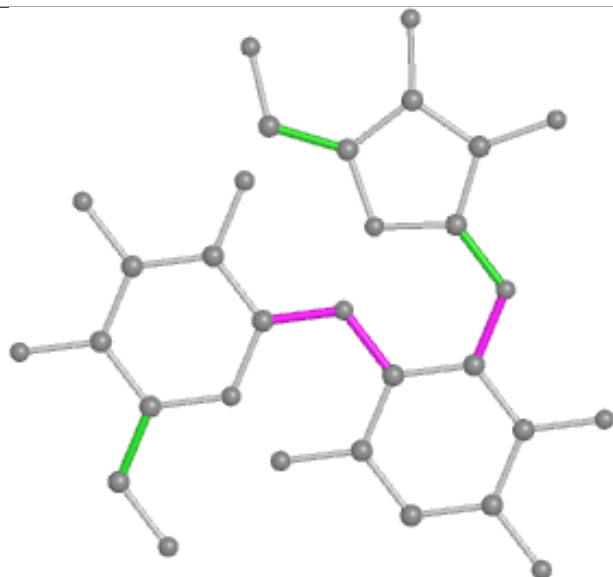
## Ligand RIO A 500



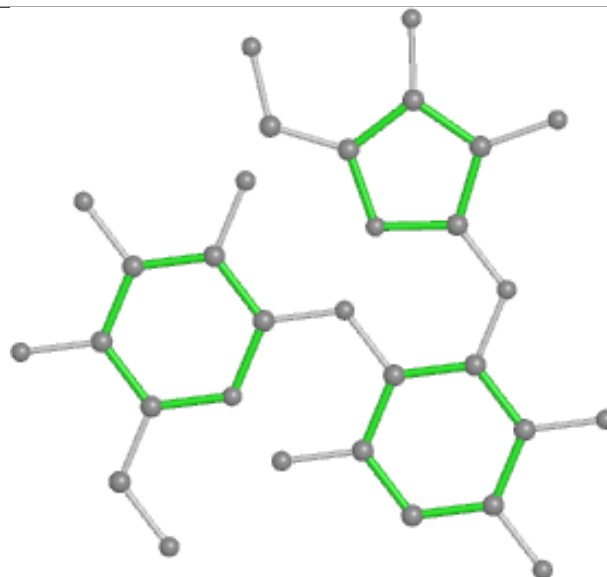
Bond lengths



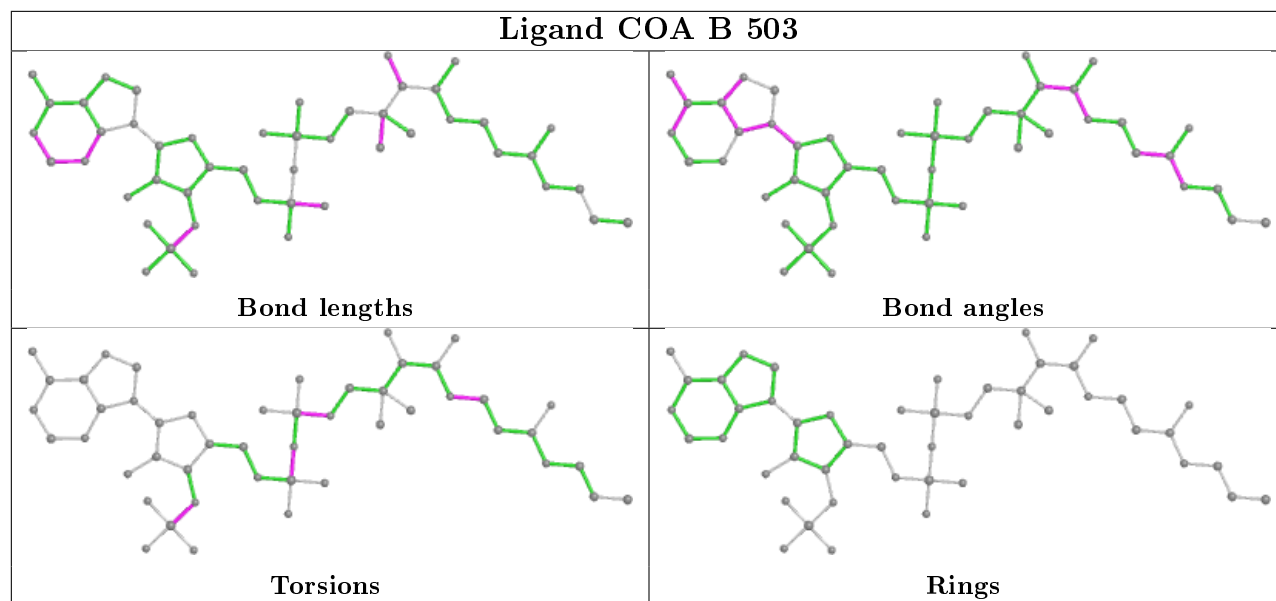
Bond angles

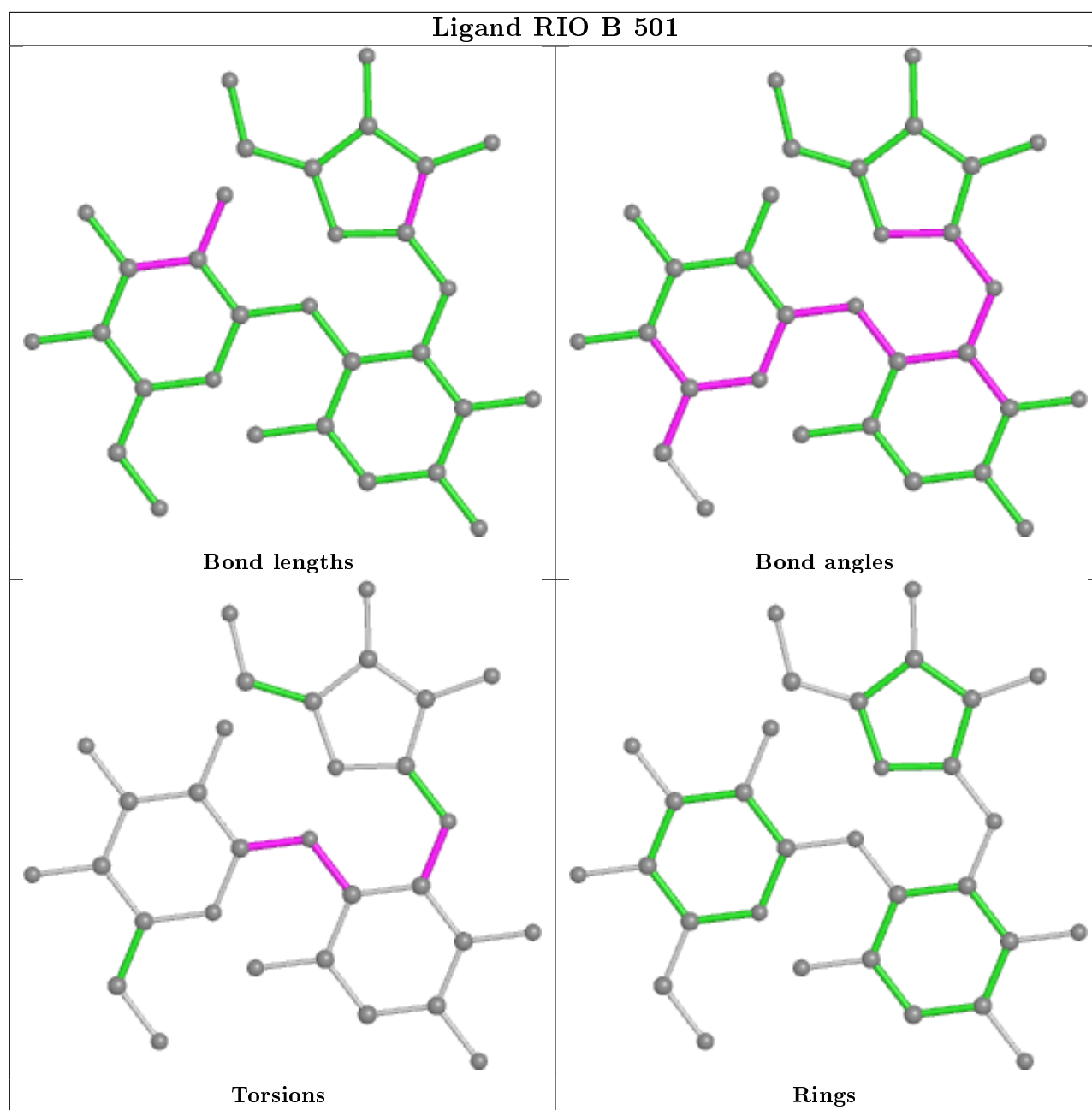


Torsions



Rings





## 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	181/181 (100%)	-0.10	5 (2%)	53	47	9, 13, 27, 37	0
1	B	176/181 (97%)	0.06	13 (7%)	14	11	8, 14, 33, 45	0
All	All	357/362 (98%)	-0.02	18 (5%)	28	23	8, 13, 30, 45	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	HIS	5.4
1	B	6	HIS	4.5
1	A	1	MET	4.4
1	B	124	ARG	3.6
1	B	54	HIS	3.4
1	A	162	ASP	3.4
1	B	162	ASP	3.4
1	A	121	ARG	3.1
1	B	9	ARG	2.9
1	B	94	ARG	2.7
1	B	19	GLU	2.6
1	B	57	ALA	2.3
1	B	18	SER	2.2
1	B	93	GLN	2.1
1	B	7	THR	2.1
1	A	125	LEU	2.1
1	B	17	ASP	2.1
1	A	22	GLN	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

There are no carbohydrates in this entry.

## 6.4 Ligands

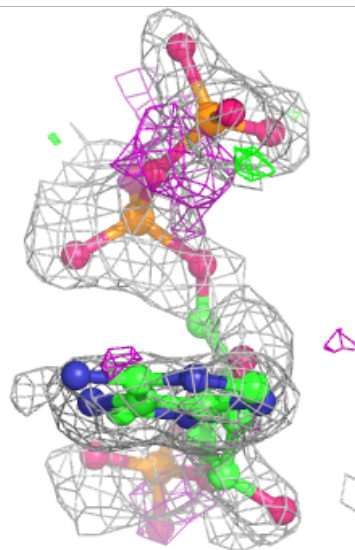
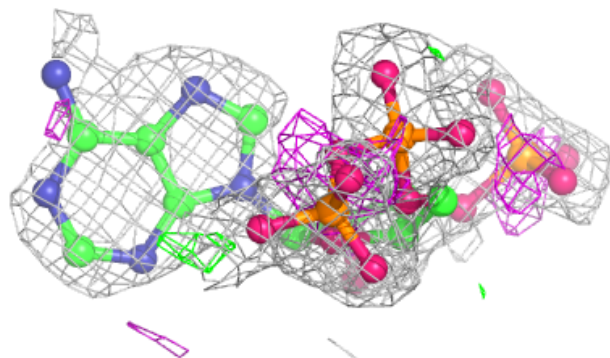
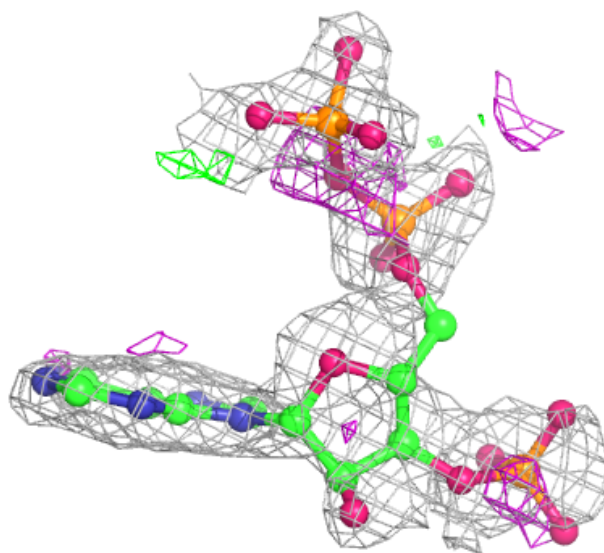
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PAP	B	601	31/31	0.78	0.33	39,46,54,55	0
2	COA	B	503	48/48	0.88	0.18	15,21,55,56	0
4	PAP	B	600	31/31	0.90	0.22	22,32,38,40	0
2	COA	A	502	48/48	0.92	0.12	12,21,30,31	0
3	RIO	A	500	31/31	0.93	0.10	11,14,27,29	0
3	RIO	B	501	31/31	0.94	0.10	8,12,19,22	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.

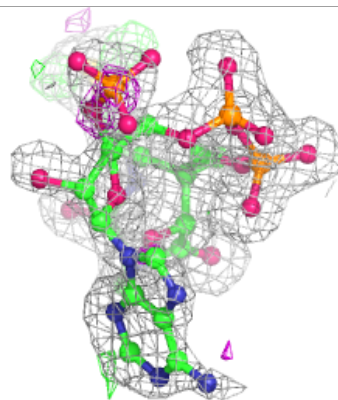
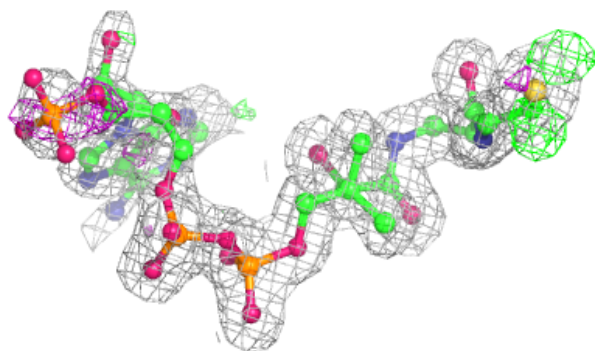
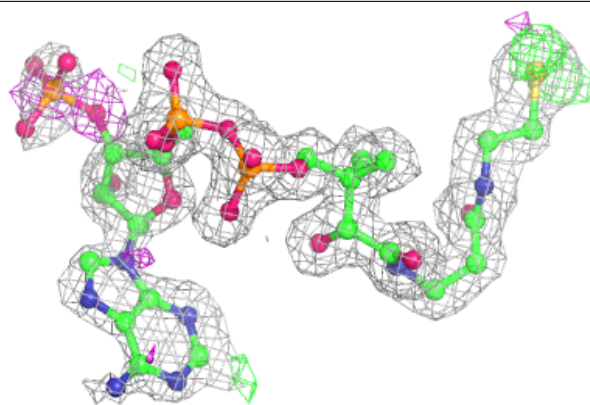
**Electron density around PAP B 601:**

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

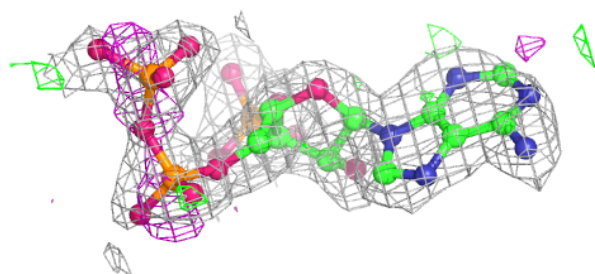
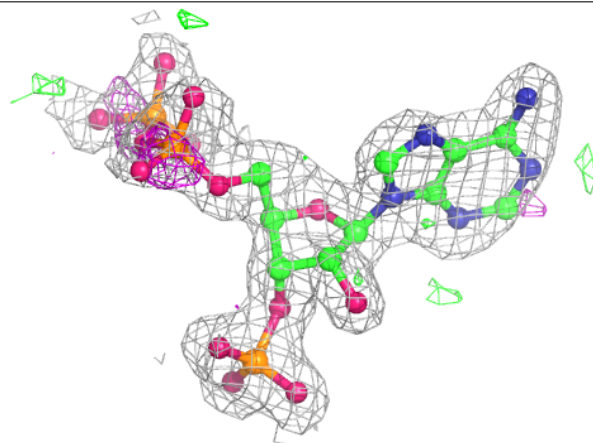


**Electron density around COA B 503:**

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

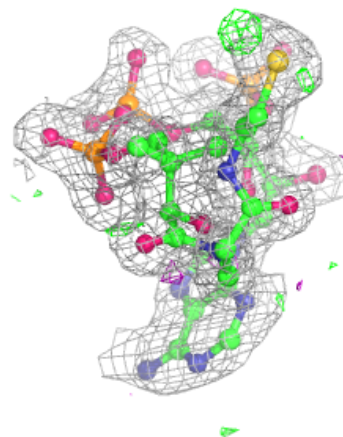
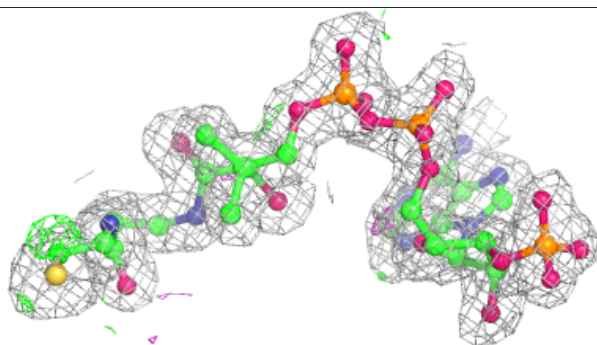
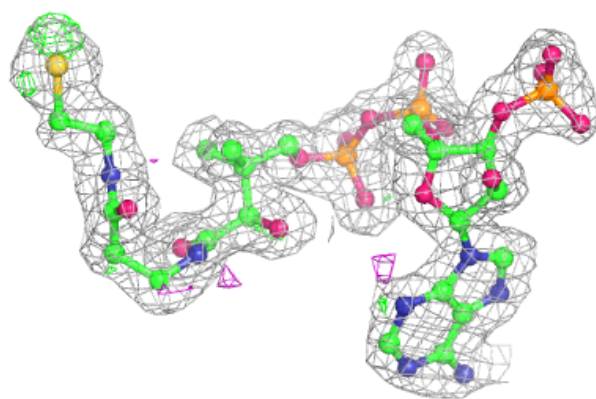
**Electron density around PAP B 600:**

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



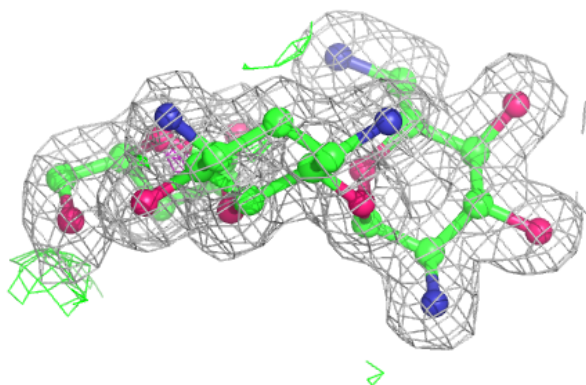
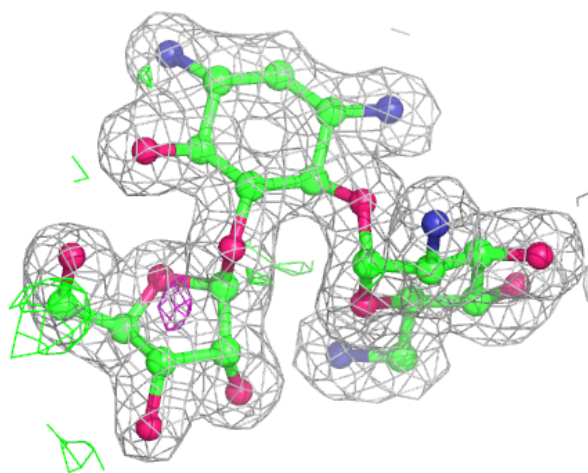
**Electron density around COA A 502:**

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



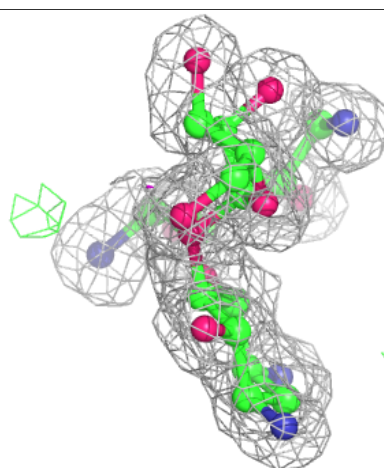
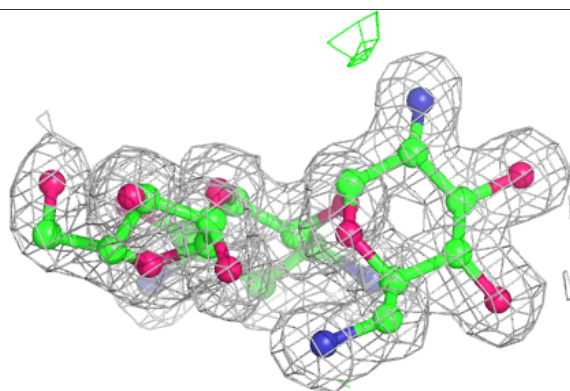
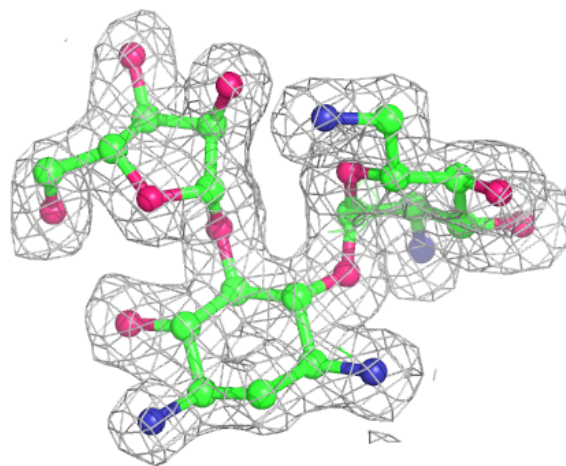
**Electron density around RIO A 500:**

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



**Electron density around RIO B 501:**

$2mF_o-DF_c$  (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.