

# Full wwPDB X-ray Structure Validation Report (i)

#### May 24, 2020 – 12:43 pm BST

PDB ID	:	1M4D
Title	:	Aminoglycoside 2'-N-acetyltransferase from Mycobacterium tuberculosis-
		Complex with Coenzyme A and Tobramycin
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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

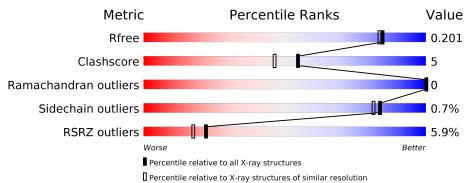
MolProbity		4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{Refmac}$	:	5.8.0158
$\operatorname{CCP4}$	:	$7.0.044 (\mathrm{Gargrove})$
Ideal 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 (i)

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
$R_{free}$	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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain						
1	А	181	92%	7% •					
1	В	181	90%	7% • •					



# 2 Entry composition (i)

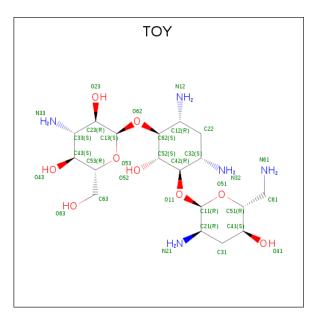
There are 5 unique types of molecules in this entry. The entry contains 3210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	Δ	181	Total	С	Ν	Ο	$\mathbf{S}$	0	0	Ο
T	11	101	1412	884	265	256	7	0	0	0
1	В	176	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
L	D	170	1371	859	257	249	6	0	0	0

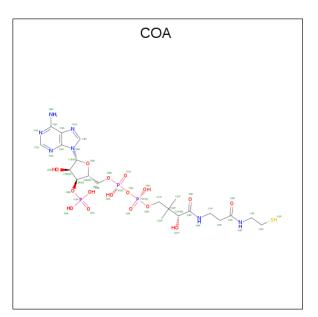
• Molecule 2 is TOBRAMYCIN (three-letter code: TOY) (formula: C<sub>18</sub>H<sub>37</sub>N<sub>5</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total         C         N         O           32         18         5         9	0	0
2	В	1	Total         C         N         O           32         18         5         9	0	0

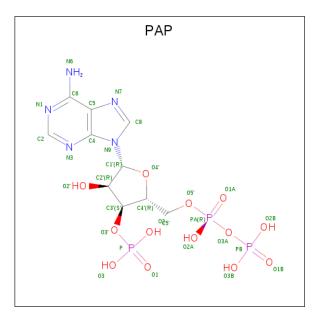
• Molecule 3 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	Δ	1	Total	С	Ν	Ο	Р	S	0	0
0	A	T	48	21	7	16	3	1	0	0
3	В	1	Total	С	Ν	Ο	Р	S	0	0
	D	L	48	21	7	16	3	1	0	0

• 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	А	1	Total 31		N 5		P 3	0	0



• Molecule 5 is water.

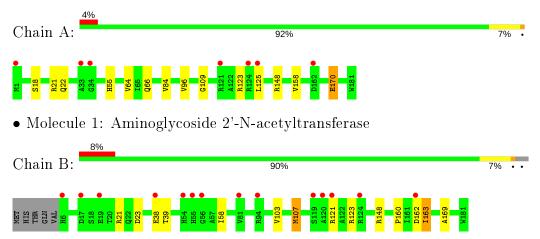
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	136	Total O 136 136	0	0
5	В	100	Total O 100 100	0	0



# 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





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	48.70Å 86.60Å 98.40Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	50.00 - 1.80	Depositor
Resolution (A)	25.95 - 1.80	EDS
% Data completeness	97.7 (50.00-1.80)	Depositor
(in resolution range)	97.5(25.95 - 1.80)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	0.04	Depositor
$< I/\sigma(I) > 1$	$4.38 (at 1.80 \text{\AA})$	Xtriage
Refinement program	CNS 1.0	Depositor
D D.	0.174 , $0.211$	Depositor
$R, R_{free}$	0.165 , $0.201$	DCC
$R_{free}$ test set	1922 reflections $(5.00\%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.39 , $55.7$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.46, \langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3210	wwPDB-VP
Average B, all atoms $(Å^2)$	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: PAP, COA, TOY

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).

Mal	Chain	Bo	nd lengths	Bond angles		
Mol Chain		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.12	4/1447~(0.3%)	1.06	2/1971~(0.1%)	
1	В	1.03	3/1405~(0.2%)	1.13	3/1914~(0.2%)	
All	All	1.08	7/2852~(0.2%)	1.09	5/3885~(0.1%)	

All (7) bond length outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	170	$\operatorname{GLU}$	CD-OE1	8.04	1.34	1.25
1	А	170	GLU	CG-CD	6.61	1.61	1.51
1	В	107	MET	CG-SD	-6.25	1.65	1.81
1	В	148	ARG	CZ-NH1	5.59	1.40	1.33
1	А	158	VAL	CB-CG1	5.53	1.64	1.52
1	В	169	ALA	CA-CB	5.30	1.63	1.52
1	А	64	VAL	CB-CG1	5.07	1.63	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	107	MET	CG-SD-CE	-21.53	65.75	100.20
1	А	21	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	В	107	MET	CA-CB-CG	-9.92	96.44	113.30
1	А	148	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	В	148	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.



#### 5.2 Too-close contacts (i)

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	А	1412	0	1374	10	0
1	В	1371	0	1331	21	0
2	А	32	0	37	0	0
2	В	32	0	37	0	0
3	А	48	0	32	1	0
3	В	48	0	32	1	0
4	А	31	0	11	2	0
5	А	136	0	0	4	0
5	В	100	0	0	1	0
All	All	3210	0	2854	30	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 5.

All (30) 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:CE	1:B:107:MET:SD	2.03	1.46
1:B:107:MET:CE	1:B:107:MET:CG	2.02	1.34
1:B:107:MET:CE	1:B:107:MET:HG3	1.58	1.27
1:A:170:GLU:HG2	5:A:727:HOH:O	1.52	1.09
1:B:107:MET:HE2	1:B:107:MET:HG3	1.02	1.00
1:B:163:ILE:HD13	1:B:163:ILE:O	1.81	0.80
1:B:163:ILE:N	1:B:163:ILE:HD12	2.00	0.77
1:B:163:ILE:HD12	1:B:163:ILE:H	1.55	0.71
1:A:84:VAL:HB	3:A:600:COA:H22	1.74	0.70
1:B:162:ASP:OD2	5:B:669:HOH:O	2.12	0.67
1:B:121:ARG:HH22	3:B:601:COA:HN8	1.42	0.66
1:B:163:ILE:N	1:B:163:ILE:CD1	2.59	0.65
1:B:107:MET:CE	1:B:107:MET:CB	2.74	0.65
1:A:18:SER:O	1:A:22:GLN:HG3	1.99	0.62
1:B:123:ARG:HH11	1:B:123:ARG:HG2	1.65	0.62
1:A:55:HIS:HD2	4:A:602:PAP:O2	1.84	0.61
1:B:58:ILE:HD12	1:B:58:ILE:N	2.18	0.58
1:B:38:GLU:HG3	1:B:39:THR:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:NH1	1:B:123:ARG:HG2	2.19	0.56
1:A:66:GLN:OE1	5:A:653:HOH:O	2.19	0.51
1:B:23:ASP:HB3	1:B:58:ILE:HD13	1.93	0.51
1:B:163:ILE:H	1:B:163:ILE:CD1	2.20	0.50
1:A:96:VAL:HG11	1:A:125:LEU:HD22	1.94	0.49
1:A:123:ARG:CD	5:A:704:HOH:O	2.61	0.48
1:B:160:PRO:HB3	1:B:163:ILE:HD13	1.97	0.47
1:A:123:ARG:HD2	5:A:704:HOH:O	2.15	0.47
1:B:123:ARG:CG	1:B:123:ARG:HH11	2.30	0.45
1:B:163:ILE:C	1:B:163:ILE:HD13	2.37	0.45
1:A:55:HIS:CD2	4:A:602:PAP:O2	2.67	0.44
1:A:109:GLY:O	1:B:21:ARG:NH2	2.50	0.42

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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	Perce	$\mathbf{ntiles}$
1	А	179/181~(99%)	177~(99%)	2(1%)	0	100	100
1	В	174/181~(96%)	170~(98%)	4 (2%)	0	100	100
All	All	353/362~(98%)	347~(98%)	6 (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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	143/143~(100%)	143~(100%)	0	100 100
1	В	138/143~(96%)	136~(99%)	2 (1%)	67 59
All	All	281/286~(98%)	279~(99%)	2 (1%)	84 81

analysed, and the total number of residues.

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	103	VAL
1	В	163	ILE

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

Mol	Chain	Res	Type
1	А	55	HIS
1	В	6	HIS

#### 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)

5 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



Mol	Туре	Chain	n Res Link		Bo	ond leng	ths	В	ond ang	les
	туре	Chain	Ites		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	COA	В	601	-	41,50,50	2.24	7 (17%)	$52,\!75,\!75$	1.07	4 (7%)
2	TOY	В	501	-	34,34,34	1.54	4 (11%)	$41,\!50,\!50$	1.44	<mark>6 (14%)</mark>
4	PAP	А	602	-	$28,\!33,\!33$	2.15	5 (17%)	$35,\!52,\!52$	1.28	4 (11%)
2	TOY	А	500	-	34,34,34	1.31	4 (11%)	$41,\!50,\!50$	1.15	4 (9%)
3	COA	А	600	-	41,50,50	2.00	8 (19%)	$52,\!75,\!75$	1.08	<mark>3 (5%)</mark>

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).

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	$\mathbf{Link}$	Chirals	Torsions	Rings
3	COA	В	601	-	-	5/44/64/64	0/3/3/3
2	TOY	В	501	-	-	3/12/68/68	0/3/3/3
4	PAP	А	602	-	-	3/17/37/37	0/3/3/3
2	TOY	А	500	-	-	3/12/68/68	0/3/3/3
3	COA	А	600	-	-	6/44/64/64	0/3/3/3

All (28) bond length outliers are listed below:
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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
3	В	601	COA	C2A-N3A	10.45	1.49	1.32
4	А	602	PAP	C2-N3	8.95	1.46	1.32
3	А	600	COA	C2A-N3A	8.50	1.45	1.32
3	В	601	COA	P3B-O3B	5.44	1.69	1.59
3	А	600	COA	C9P-N8P	4.91	1.44	1.33
2	В	501	TOY	C43-C33	4.40	1.59	1.53
4	А	602	PAP	P-O3'	3.77	1.66	1.59
3	В	601	COA	O4B-C1B	3.54	1.46	1.41
3	В	601	COA	C4A-N3A	3.31	1.40	1.35
3	А	600	COA	O4B-C1B	3.04	1.45	1.41
2	В	501	TOY	C31-C21	3.02	1.60	1.53
2	В	501	TOY	C61-C51	2.70	1.55	1.52
2	А	500	TOY	C43-C33	2.68	1.56	1.53
3	А	600	COA	P3B-O3B	2.65	1.64	1.59
3	В	601	COA	C5P-N4P	2.64	1.39	1.33
3	В	601	COA	C2A-N1A	2.49	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
4	А	602	PAP	PB-O3B	2.40	1.64	1.54
4	А	602	PAP	C2-N1	2.38	1.38	1.33
2	А	500	TOY	C31-C41	-2.37	1.48	1.52
3	А	600	COA	OAP-CAP	2.28	1.46	1.42
2	А	500	TOY	C61-C51	2.20	1.55	1.52
3	В	601	COA	OAP-CAP	2.20	1.46	1.42
3	А	600	COA	C5P-N4P	2.18	1.38	1.33
2	А	500	TOY	O53-C13	2.17	1.47	1.41
3	А	600	COA	CEP-CBP	2.14	1.58	1.53
2	В	501	TOY	O23-C23	2.13	1.48	1.43
4	А	602	PAP	C2'-C1'	-2.08	1.50	1.53
3	А	600	COA	C7P-C6P	2.05	1.57	1.51

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All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	600	COA	C1B-N9A-C4A	-4.24	119.20	126.64
2	В	501	TOY	O51-C51-C41	4.05	115.64	110.06
2	В	501	TOY	C63-C53-C43	3.47	121.12	113.00
4	А	602	PAP	C1'-N9-C4	-3.44	120.59	126.64
2	В	501	TOY	C31-C41-C51	3.17	114.88	110.77
2	А	500	TOY	O51-C51-C41	3.11	114.35	110.06
2	В	501	TOY	O41-C41-C51	-2.77	104.14	110.01
2	В	501	TOY	O62-C62-C52	2.68	114.40	107.28
2	А	500	TOY	O62-C62-C52	2.67	114.38	107.28
2	А	500	TOY	C13-O53-C53	2.55	118.70	113.69
3	А	600	COA	N3A-C2A-N1A	-2.52	124.74	128.68
2	А	500	TOY	O51-C51-C61	2.49	110.65	106.01
3	А	600	COA	O3B-P3B-O7A	-2.40	100.11	109.39
2	В	501	TOY	O51-C51-C61	2.38	110.44	106.01
4	А	602	PAP	C2'-C3'-C4'	-2.36	99.05	103.22
4	А	602	PAP	C5-C6-N6	-2.36	116.77	120.35
3	В	601	COA	C2B-C3B-C4B	-2.23	99.28	103.22
3	В	601	COA	C6P-C5P-N4P	-2.19	112.73	116.42
3	В	601	COA	CEP-CBP-CAP	2.17	112.58	108.82
4	А	602	PAP	N3-C2-N1	-2.15	125.32	128.68
3	В	601	COA	CAP-C9P-N8P	-2.02	112.55	116.58

There are no chirality outliers.

All (20) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	В	601	COA	CCP-O6A-P2A-O3A
3	А	600	COA	CCP-O6A-P2A-O3A
4	А	602	PAP	C3'-O3'-P-O2
2	А	500	TOY	O51-C11-O11-C42
2	В	501	TOY	O51-C11-O11-C42
2	В	501	TOY	C52-C42-O11-C11
2	А	500	TOY	C52-C42-O11-C11
2	А	500	TOY	C43-C53-C63-O63
3	В	601	COA	CCP-O6A-P2A-O5A
3	А	600	COA	CCP-O6A-P2A-O5A
3	В	601	COA	P2A-O3A-P1A-O1A
3	В	601	COA	P2A-O3A-P1A-O2A
2	В	501	TOY	C43-C53-C63-O63
3	А	600	COA	P2A-O3A-P1A-O1A
3	А	600	COA	C6P-C7P-N8P-C9P
3	А	600	COA	P2A-O3A-P1A-O2A
4	А	602	PAP	C4'-C5'-O5'-PA
3	В	601	COA	CCP-O6A-P2A-O4A
3	А	600	COA	CCP-O6A-P2A-O4A
4	А	602	PAP	C5'-O5'-PA-O1A

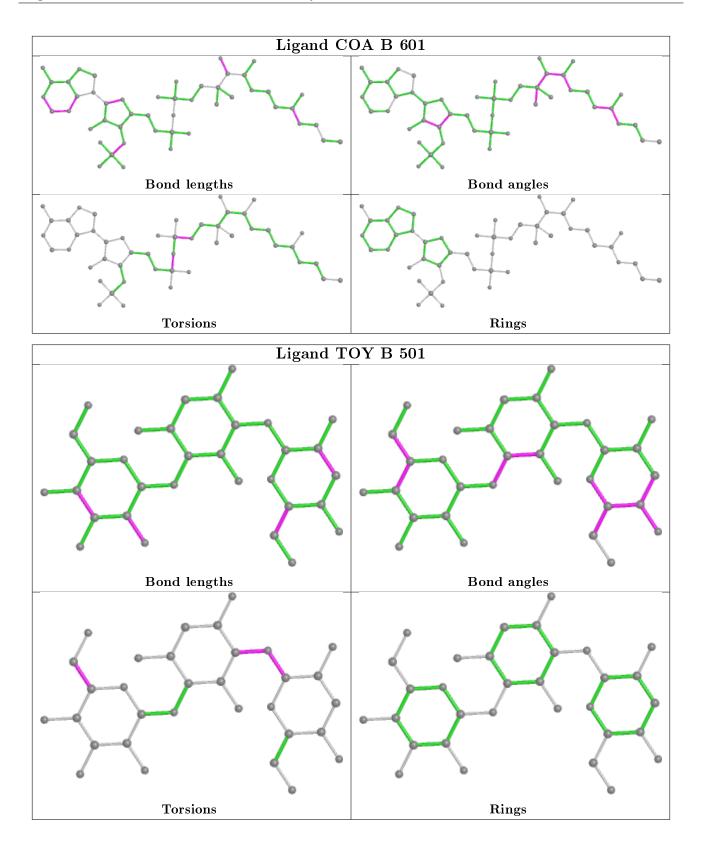
There are no ring outliers.

3 monomers are involved in 4 short contacts:

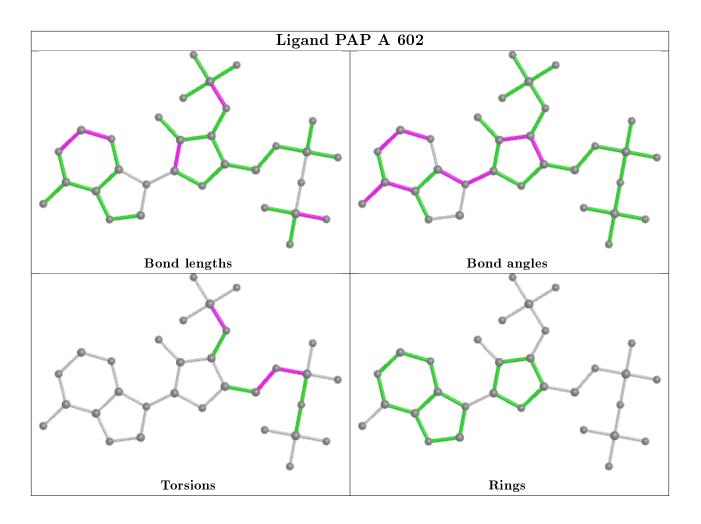
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	601	COA	1	0
4	А	602	PAP	2	0
3	А	600	COA	1	0

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

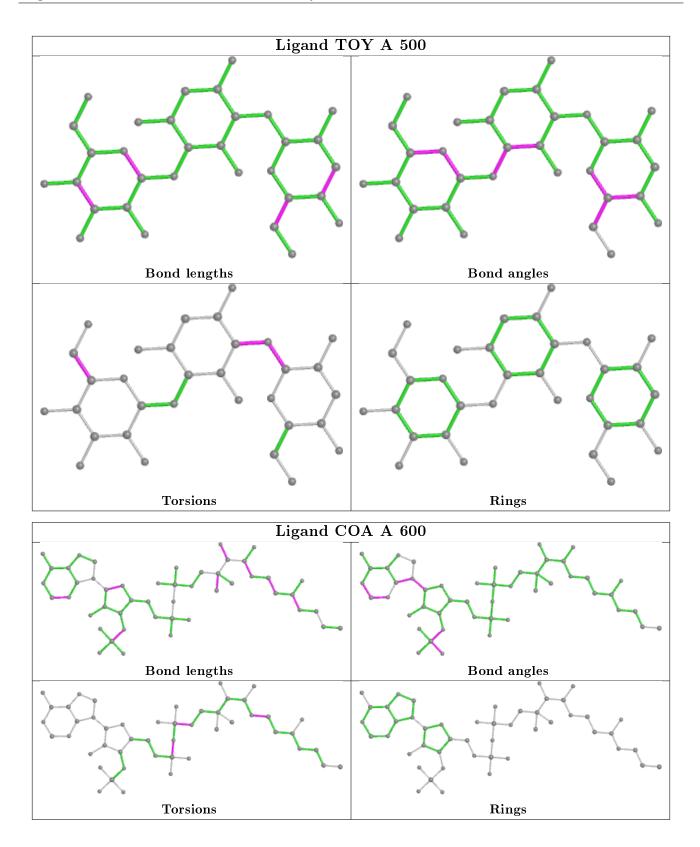












### 5.7 Other polymers (i)

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,  $95^{th}$  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	А	181/181~(100%)	-0.06	7 (3%) 39 33	12, 16, 35, 54	0
1	В	176/181~(97%)	0.21	14 (7%) 12 9	12, 18, 38, 50	0
All	All	357/362~(98%)	0.07	21 (5%) 22 17	12, 17, 39, 54	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	120	ALA	5.3
1	В	55	HIS	4.8
1	В	6	HIS	4.1
1	В	121	ARG	4.0
1	А	121	ARG	4.0
1	В	162	ASP	3.5
1	В	94	ARG	3.5
1	А	162	ASP	3.4
1	В	17	ASP	3.3
1	А	34	GLY	3.0
1	А	125	LEU	2.8
1	В	54	HIS	2.8
1	В	19	GLU	2.6
1	В	124	ARG	2.4
1	В	119	SER	2.3
1	В	38	GLU	2.3
1	А	1	MET	2.2
1	А	33	ALA	2.2
1	В	81	VAL	2.1
1	В	56	GLY	2.1
1	А	124	ARG	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 carbohydrates in this entry.

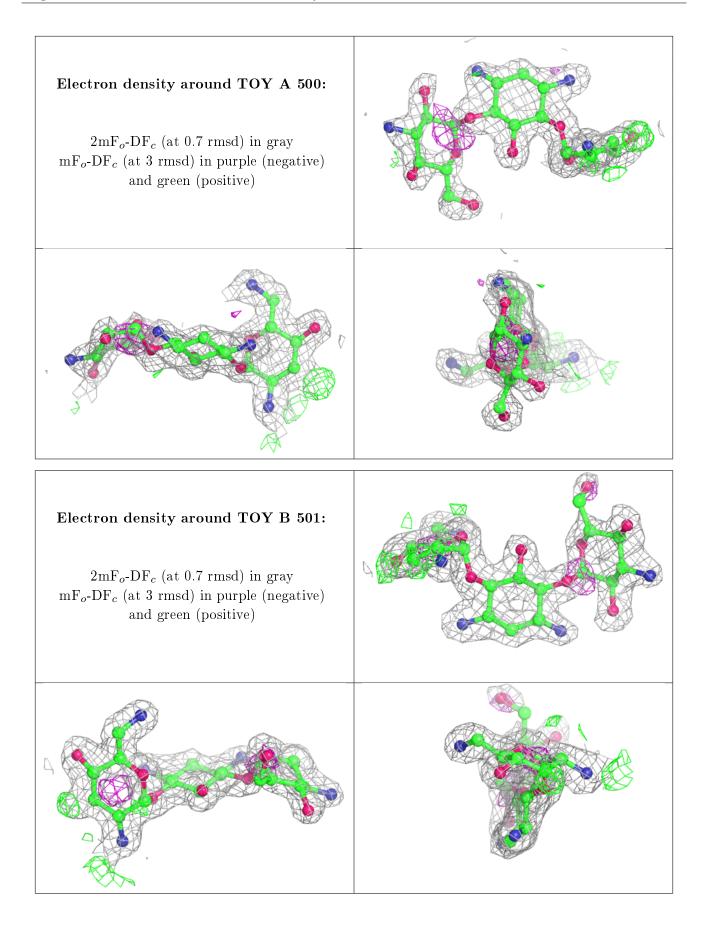
#### 6.4 Ligands (i)

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,  $95^{th}$  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.

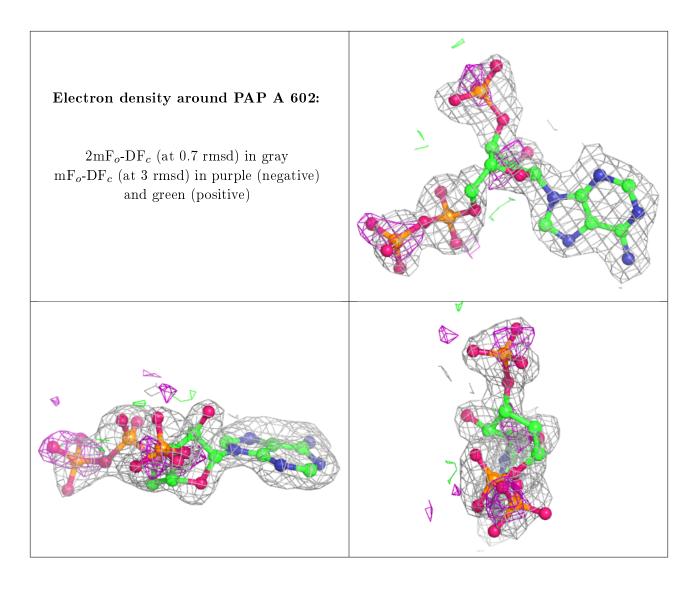
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	$Q{<}0.9$
2	TOY	А	500	32/32	0.72	0.21	$24,\!34,\!48,\!50$	0
2	TOY	В	501	32/32	0.74	0.24	$24,\!30,\!43,\!46$	0
4	PAP	А	602	31/31	0.77	0.27	39,47,64,64	0
3	COA	В	601	48/48	0.78	0.28	23,35,71,71	0
3	COA	А	600	48/48	0.92	0.12	$16,\!25,\!39,\!41$	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.

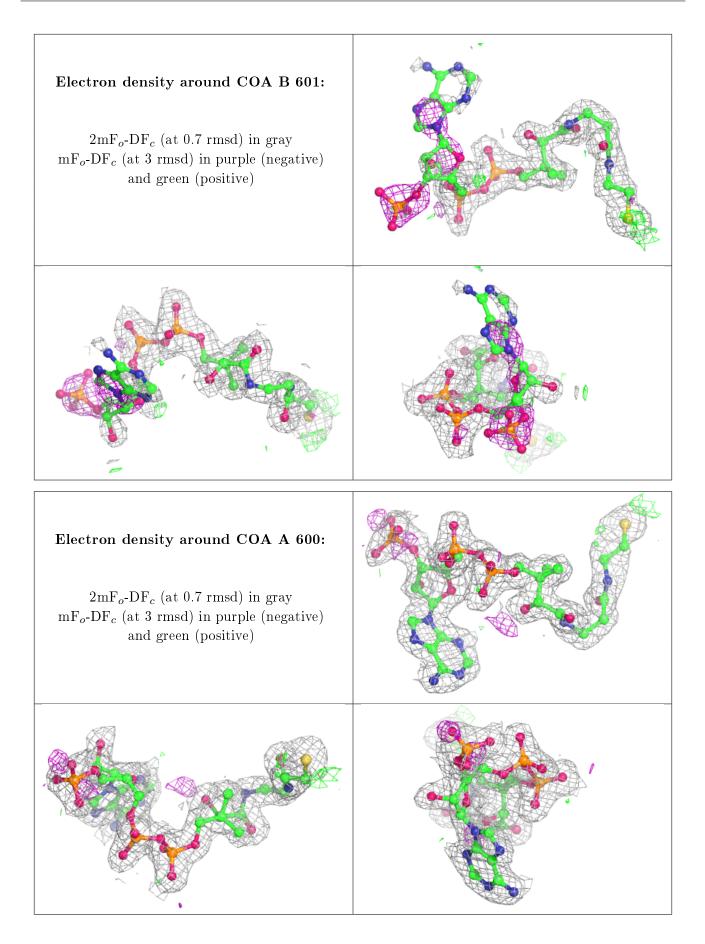














## 6.5 Other polymers (i)

There are no such residues in this entry.

