



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 06:44 AM UTC

PDB ID : 7MQL / pdb_00007mql
Title : AAC(3)-IIIa in complex with CoA and neomycin
Authors : Zielinski, M.; Berghuis, A.M.
Deposited on : 2021-05-05
Resolution : 1.60 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

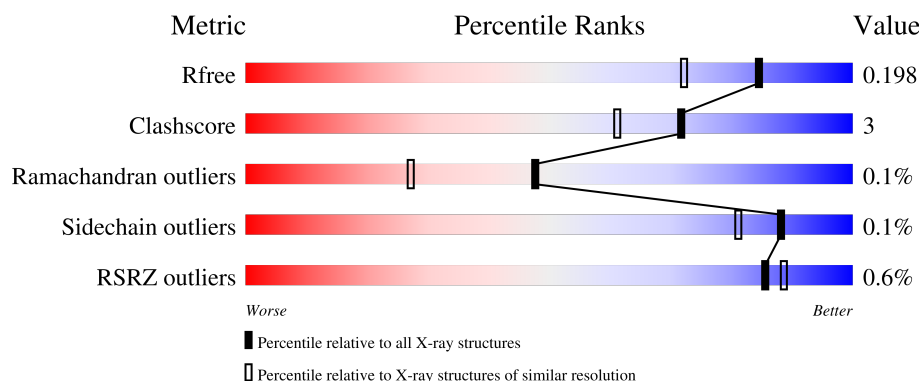
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	274	% 92% 5%
1	B	274	89% 6% 5%
1	C	274	88% 7% 5%
1	D	274	% 91% 5% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	FMT	D	505	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10178 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.

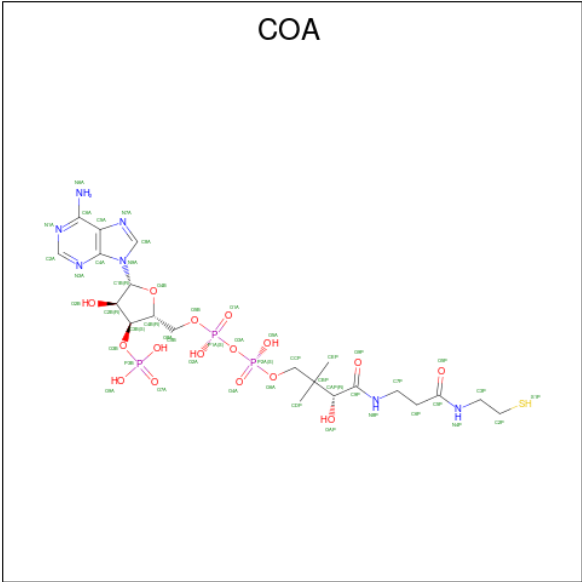
- Molecule 1 is a protein called Aminoglycoside N(3)-acetyltransferase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	10	0
			2079	1322	359	388	10			
1	B	261	Total	C	N	O	S	0	11	0
			2092	1333	366	382	11			
1	C	260	Total	C	N	O	S	0	11	0
			2088	1331	363	383	11			
1	D	261	Total	C	N	O	S	0	10	0
			2091	1329	368	383	11			

There are 12 discrepancies between the modelled and reference sequences:

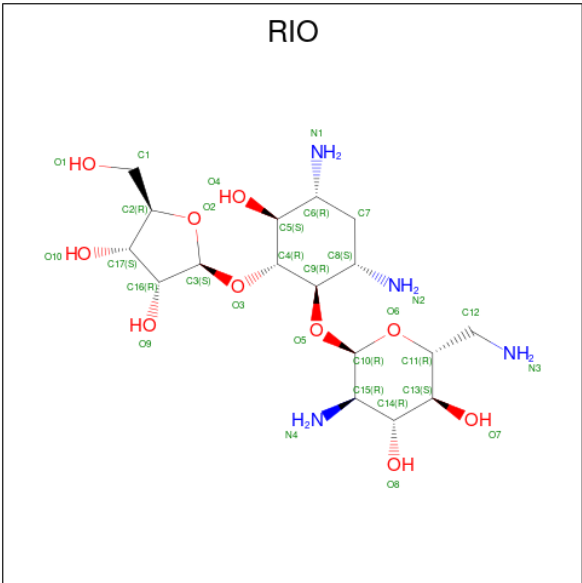
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P29808
A	-1	SER	-	expression tag	UNP P29808
A	0	HIS	-	expression tag	UNP P29808
B	-2	GLY	-	expression tag	UNP P29808
B	-1	SER	-	expression tag	UNP P29808
B	0	HIS	-	expression tag	UNP P29808
C	-2	GLY	-	expression tag	UNP P29808
C	-1	SER	-	expression tag	UNP P29808
C	0	HIS	-	expression tag	UNP P29808
D	-2	GLY	-	expression tag	UNP P29808
D	-1	SER	-	expression tag	UNP P29808
D	0	HIS	-	expression tag	UNP P29808

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



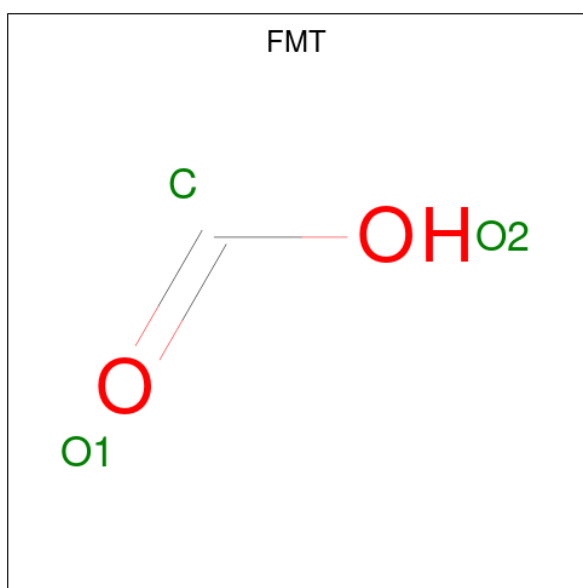
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	1
			96	42	14	32	6	2		
2	B	1	Total	C	N	O	P	S	0	1
			96	42	14	32	6	2		
2	C	1	Total	C	N	O	P	S	0	1
			96	42	14	32	6	2		
2	D	1	Total	C	N	O	P	S	0	1
			96	42	14	32	6	2		

- Molecule 3 is RIBOSTAMYCIN (CCD ID: RIO) (formula: C₁₇H₃₄N₄O₁₀) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	1
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		
4	C	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		
4	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is water.

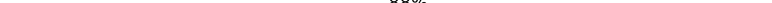
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	304	Total 304	O 304	0	4
5	B	317	Total 317	O 317	0	4
5	C	348	Total 348	O 348	0	5
5	D	327	Total 327	O 327	0	4

- Molecule 1: Aminoglycoside N(3)-acetyltransferase III

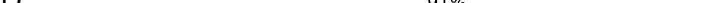


- Chain B:  89% 6% 5%



- Chain C:  88% 7% 5%



- Chain D:  91% 5% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	130.58Å 90.88Å 100.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.05 – 1.60 31.05 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.05-1.60) 99.9 (31.05-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.176 , 0.199 0.176 , 0.198	Depositor DCC
R_{free} test set	1646 reflections (0.86%)	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.835	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10178	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 43.79 % 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 1.6760e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, COA, FMT, 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	0.34	0/2124	0.50	0/2897
1	B	0.35	0/2137	0.53	0/2911
1	C	0.35	0/2133	0.50	0/2906
1	D	0.34	0/2135	0.51	0/2908
All	All	0.34	0/8529	0.51	0/11622

There are no bond length outliers.

There are no bond angle outliers.

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	A	2079	0	1995	7	0
1	B	2092	0	2031	9	0
1	C	2088	0	2023	19	0
1	D	2091	0	2028	14	0
2	A	96	0	64	0	0
2	B	96	0	64	2	0
2	C	96	0	64	0	0
2	D	96	0	64	0	0
3	A	31	0	34	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	34	2	0
3	C	31	0	34	4	0
3	D	31	0	34	3	0
4	A	6	0	2	0	0
4	B	6	0	2	0	0
4	C	3	0	1	0	0
4	D	9	0	3	2	0
5	A	304	0	0	3	0
5	B	317	0	0	4	1
5	C	348	0	0	8	1
5	D	327	0	0	4	1
All	All	10178	0	8477	57	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 3.

All (57) 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:D:198[B]:ARG:HG3	1:D:198[B]:ARG:HH11	1.52	0.75
1:C:176:HIS:NE2	5:C:404[B]:HOH:O	2.28	0.65
1:D:123:GLU:OE2	3:D:504[A]:RIO:N1	2.33	0.61
1:D:198[B]:ARG:HG3	1:D:198[B]:ARG:NH1	2.18	0.59
3:A:302[A]:RIO:H11	3:A:302[A]:RIO:HN2A	1.68	0.57
1:C:123:GLU:OE2	3:C:303[A]:RIO:N1	2.37	0.57
1:D:201[B]:ARG:HH11	1:D:201[B]:ARG:HG2	1.72	0.55
1:D:236[B]:ARG:NH1	1:D:245:TYR:OH	2.40	0.55
1:D:201[B]:ARG:HG2	1:D:201[B]:ARG:NH1	2.22	0.54
1:C:148:VAL:HG13	1:C:149[A]:GLU:HG2	1.90	0.54
1:D:222[A]:GLU:OE1	5:D:601:HOH:O	2.19	0.53
1:B:131[B]:ARG:NH2	1:C:157:ALA:O	2.42	0.52
1:C:63:MET:HG3	1:C:110:LEU:CD2	2.39	0.52
3:C:303[A]:RIO:N3	5:C:405:HOH:O	2.34	0.52
1:B:28:LEU:HD11	1:B:163:LEU:HB2	1.92	0.51
1:D:126:MET:HG3	1:D:151:PRO:HG2	1.92	0.50
1:D:148[A]:VAL:HG22	5:D:634:HOH:O	2.11	0.50
1:B:52[A]:MET:HE1	1:B:113:TRP:NE1	2.27	0.49
1:C:149[B]:GLU:OE2	5:C:401:HOH:O	2.20	0.49
3:D:504[A]:RIO:H11	3:D:504[A]:RIO:HN2A	1.77	0.49
1:C:126:MET:HG3	1:C:151:PRO:HG2	1.94	0.49
1:B:10:HIS:NE2	1:B:53:ASP:OD2	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:TRP:CD1	1:C:114:PRO:HD2	2.48	0.47
1:C:12[A]:HIS:HD2	5:C:623:HOH:O	1.95	0.47
1:D:113:TRP:CD1	1:D:114:PRO:HD2	2.49	0.47
1:D:52[B]:MET:HE3	5:D:899:HOH:O	2.13	0.47
1:D:81:LEU:HD21	4:D:505:FMT:H	1.94	0.47
1:A:170[B]:ASP:HB3	1:A:222:GLU:HB2	1.96	0.47
3:D:504[A]:RIO:H17	5:D:858:HOH:O	2.15	0.46
2:B:301[A]:COA:H8A	5:B:633:HOH:O	2.16	0.46
1:C:222[B]:GLU:OE1	1:C:226[B]:ARG:NH2	2.49	0.46
2:B:301[B]:COA:H8A	5:B:633:HOH:O	2.16	0.45
1:A:258[A]:GLN:HG3	5:A:579:HOH:O	2.17	0.45
1:A:117:HIS:NE2	5:A:406:HOH:O	2.31	0.45
1:A:123:GLU:OE2	3:A:302[A]:RIO:N1	2.49	0.45
1:A:183[B]:LYS:HE3	5:A:613:HOH:O	2.17	0.44
3:C:303[A]:RIO:O2	3:C:303[A]:RIO:N4	2.46	0.44
1:C:63:MET:HG3	1:C:110:LEU:HD23	1.98	0.44
1:C:12[B]:HIS:CD2	5:C:433:HOH:O	2.70	0.44
1:B:170[B]:ASP:HB3	1:B:222:GLU:HB2	1.99	0.44
1:C:169:LEU:HB2	1:C:222[B]:GLU:CD	2.42	0.44
1:C:131:ARG:NH2	5:C:406:HOH:O	2.35	0.44
3:B:302[A]:RIO:H11	3:B:302[A]:RIO:HN2A	1.82	0.43
1:B:123:GLU:OE2	3:B:302[A]:RIO:N1	2.51	0.43
1:B:12[A]:HIS:HD2	5:B:600:HOH:O	2.00	0.43
1:C:148:VAL:HG23	5:C:621:HOH:O	2.19	0.42
1:C:6:ILE:N	5:C:420:HOH:O	2.51	0.42
1:C:222[B]:GLU:O	1:C:226[B]:ARG:HG3	2.19	0.42
1:A:67:TRP:CD1	1:A:97:ALA:HB1	2.54	0.42
1:A:111:ARG:O	1:A:116:VAL:HG11	2.20	0.42
1:B:243:ASP:HB3	5:B:420:HOH:O	2.20	0.41
1:C:28:LEU:HD11	1:C:163:LEU:HB2	2.02	0.41
1:D:81:LEU:HD21	4:D:505:FMT:C	2.51	0.41
3:C:303[A]:RIO:HN2A	3:C:303[A]:RIO:H11	1.86	0.41
1:C:63:MET:HG3	1:C:110:LEU:HD22	2.02	0.41
1:D:236[A]:ARG:HG2	1:D:245:TYR:CD2	2.55	0.41
1:B:126:MET:HG3	1:B:151:PRO:HB2	2.04	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)
5:C:427:HOH:O	5:D:760:HOH:O[1_554]	2.07	0.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:516:HOH:O	5:B:626:HOH:O[2_555]	2.16	0.04

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	268/274 (98%)	260 (97%)	8 (3%)	0	100	100
1	B	269/274 (98%)	262 (97%)	6 (2%)	1 (0%)	30	14
1	C	268/274 (98%)	260 (97%)	8 (3%)	0	100	100
1	D	268/274 (98%)	263 (98%)	5 (2%)	0	100	100
All	All	1073/1096 (98%)	1045 (97%)	27 (2%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104	SER

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	209/214 (98%)	209 (100%)	0	100	100
1	B	210/214 (98%)	208 (99%)	2 (1%)	68	50
1	C	210/214 (98%)	210 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	210/214 (98%)	210 (100%)	0	100	100
All	All	839/856 (98%)	837 (100%)	2 (0%)	88	81

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

Mol	Chain	Res	Type
1	B	238[A]	LYS
1	B	238[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	HIS
1	C	132	GLN
1	D	250	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	A	115	1	3,6,7	0.78	0	1,6,8	0.51	0
1	CSO	D	115	1	3,6,7	0.59	0	1,6,8	0.51	0
1	CSO	C	115	1	3,6,7	0.57	0	1,6,8	0.88	0
1	CSO	B	115	1	3,6,7	0.48	0	1,6,8	0.90	0

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
1	CSO	A	115	1	-	0/1/5/7	-
1	CSO	D	115	1	-	0/1/5/7	-
1	CSO	C	115	1	-	0/1/5/7	-
1	CSO	B	115	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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
2	COA	A	301[B]	-	47,50,50	2.83	18 (38%)	69,75,75	1.97	17 (24%)
3	RIO	A	302[A]	-	32,33,33	3.68	9 (28%)	46,49,49	1.28	8 (17%)
2	COA	C	301[B]	-	47,50,50	2.82	18 (38%)	69,75,75	1.95	17 (24%)
4	FMT	B	304	-	2,2,2	0.67	0	1,1,1	0.16	0
4	FMT	A	303[A]	-	2,2,2	0.60	0	1,1,1	0.21	0
2	COA	D	503[B]	-	47,50,50	2.83	19 (40%)	69,75,75	1.99	17 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	B	301[B]	-	47,50,50	2.82	18 (38%)	69,75,75	1.99	17 (24%)
3	RIO	D	504[A]	-	32,33,33	3.63	9 (28%)	46,49,49	1.18	5 (10%)
4	FMT	D	502	-	2,2,2	0.59	0	1,1,1	0.21	0
3	RIO	C	303[A]	-	32,33,33	3.63	9 (28%)	46,49,49	1.28	7 (15%)
4	FMT	A	304	-	2,2,2	0.63	0	1,1,1	0.24	0
2	COA	A	301[A]	-	47,50,50	2.76	15 (31%)	69,75,75	2.07	20 (28%)
2	COA	C	301[A]	-	47,50,50	2.65	16 (34%)	69,75,75	2.11	20 (28%)
4	FMT	C	302	-	2,2,2	0.63	0	1,1,1	0.24	0
2	COA	D	503[A]	-	47,50,50	2.72	17 (36%)	69,75,75	2.10	18 (26%)
4	FMT	D	501	-	2,2,2	0.42	0	1,1,1	0.00	0
2	COA	B	301[A]	-	47,50,50	2.67	15 (31%)	69,75,75	2.14	19 (27%)
4	FMT	D	505	-	2,2,2	0.61	0	1,1,1	0.18	0
3	RIO	B	302[A]	-	32,33,33	3.65	9 (28%)	46,49,49	1.21	5 (10%)
4	FMT	B	303[A]	-	2,2,2	0.57	0	1,1,1	0.23	0

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
2	COA	D	503[A]	-	-	2/48/64/64	0/3/3/3
3	RIO	C	303[A]	-	-	2/12/68/68	0/3/3/3
2	COA	D	503[B]	-	-	3/48/64/64	0/3/3/3
2	COA	B	301[B]	-	-	1/48/64/64	0/3/3/3
2	COA	A	301[B]	-	-	4/48/64/64	0/3/3/3
2	COA	B	301[A]	-	-	1/48/64/64	0/3/3/3
2	COA	A	301[A]	-	-	2/48/64/64	0/3/3/3
3	RIO	B	302[A]	-	-	7/12/68/68	0/3/3/3
3	RIO	D	504[A]	-	-	6/12/68/68	0/3/3/3
2	COA	C	301[A]	-	-	3/48/64/64	0/3/3/3
3	RIO	A	302[A]	-	-	3/12/68/68	0/3/3/3
2	COA	C	301[B]	-	-	4/48/64/64	0/3/3/3

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302[A]	RIO	C3-C16	13.11	1.69	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[A]	RIO	C3-C16	13.10	1.69	1.52
3	D	504[A]	RIO	C3-C16	12.60	1.69	1.52
3	C	303[A]	RIO	C3-C16	12.45	1.68	1.52
3	D	504[A]	RIO	C17-C16	-10.32	1.25	1.53
3	A	302[A]	RIO	C17-C16	-10.26	1.25	1.53
3	C	303[A]	RIO	C17-C16	-10.23	1.25	1.53
3	B	302[A]	RIO	C17-C16	-10.16	1.25	1.53
2	A	301[B]	COA	O4B-C1B	8.90	1.62	1.42
2	C	301[B]	COA	O4B-C1B	8.90	1.62	1.42
2	A	301[A]	COA	O4B-C1B	8.74	1.62	1.42
2	D	503[B]	COA	O4B-C1B	8.69	1.62	1.42
2	B	301[B]	COA	O4B-C1B	8.67	1.62	1.42
2	C	301[A]	COA	O4B-C1B	8.51	1.61	1.42
2	D	503[A]	COA	O4B-C1B	8.21	1.61	1.42
2	B	301[A]	COA	O4B-C1B	8.18	1.60	1.42
3	D	504[A]	RIO	O2-C3	-7.33	1.28	1.41
3	C	303[A]	RIO	O2-C3	-7.21	1.28	1.41
3	A	302[A]	RIO	O2-C3	-6.98	1.29	1.41
3	B	302[A]	RIO	O2-C3	-6.90	1.29	1.41
2	D	503[A]	COA	O4B-C4B	-6.29	1.31	1.45
2	B	301[B]	COA	O4B-C4B	-6.27	1.31	1.45
2	A	301[B]	COA	O4B-C4B	-6.25	1.31	1.45
2	D	503[B]	COA	O4B-C4B	-6.24	1.31	1.45
2	C	301[B]	COA	O4B-C4B	-6.21	1.31	1.45
2	A	301[A]	COA	O4B-C4B	-6.17	1.31	1.45
2	B	301[A]	COA	O4B-C4B	-6.14	1.31	1.45
2	C	301[A]	COA	O4B-C4B	-6.03	1.31	1.45
2	B	301[B]	COA	C5P-N4P	5.95	1.47	1.33
2	C	301[B]	COA	C5P-N4P	5.92	1.47	1.33
2	A	301[B]	COA	C5P-N4P	5.92	1.47	1.33
2	D	503[B]	COA	C5P-N4P	5.91	1.47	1.33
2	A	301[A]	COA	C5P-N4P	5.83	1.47	1.33
2	B	301[A]	COA	C5P-N4P	5.60	1.46	1.33
2	A	301[B]	COA	C6A-N6A	5.59	1.48	1.34
2	C	301[B]	COA	C2B-C1B	-5.59	1.35	1.53
2	D	503[A]	COA	C5P-N4P	5.58	1.46	1.33
2	B	301[A]	COA	C6A-N6A	5.57	1.48	1.34
2	B	301[B]	COA	C2B-C1B	-5.57	1.36	1.53
2	B	301[B]	COA	C6A-N6A	5.57	1.48	1.34
2	D	503[B]	COA	C2B-C1B	-5.56	1.36	1.53
2	D	503[B]	COA	C6A-N6A	5.54	1.48	1.34
2	D	503[A]	COA	C6A-N6A	5.53	1.48	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301[B]	COA	C2B-C1B	-5.52	1.36	1.53
2	C	301[B]	COA	C6A-N6A	5.51	1.48	1.34
2	A	301[A]	COA	C6A-N6A	5.49	1.48	1.34
2	D	503[A]	COA	C2B-C1B	-5.46	1.36	1.53
2	A	301[A]	COA	C2B-C1B	-5.41	1.36	1.53
2	C	301[A]	COA	C5P-N4P	5.40	1.46	1.33
2	B	301[A]	COA	C2B-C1B	-5.37	1.36	1.53
2	C	301[A]	COA	C2B-C1B	-5.35	1.36	1.53
2	C	301[A]	COA	C6A-N6A	5.35	1.47	1.34
2	A	301[B]	COA	C9P-N8P	5.22	1.45	1.33
2	C	301[B]	COA	C9P-N8P	5.18	1.45	1.33
2	A	301[A]	COA	C9P-N8P	5.09	1.45	1.33
2	B	301[B]	COA	P2A-O3A	5.09	1.65	1.59
2	A	301[B]	COA	P2A-O3A	5.02	1.64	1.59
2	C	301[A]	COA	C9P-N8P	5.00	1.45	1.33
2	D	503[B]	COA	C9P-N8P	5.00	1.45	1.33
2	B	301[B]	COA	C9P-N8P	4.99	1.45	1.33
2	D	503[B]	COA	P2A-O3A	4.83	1.64	1.59
2	D	503[A]	COA	C9P-N8P	4.75	1.44	1.33
2	B	301[A]	COA	C9P-N8P	4.65	1.44	1.33
2	C	301[B]	COA	P2A-O3A	4.61	1.64	1.59
3	A	302[A]	RIO	C14-C15	-4.55	1.47	1.53
2	C	301[A]	COA	P3B-O3B	4.48	1.67	1.59
3	C	303[A]	RIO	C1-C2	-4.48	1.36	1.51
3	D	504[A]	RIO	C1-C2	-4.45	1.36	1.51
3	B	302[A]	RIO	C1-C2	-4.45	1.36	1.51
2	A	301[A]	COA	P2A-O3A	4.45	1.64	1.59
3	C	303[A]	RIO	C14-C15	-4.44	1.48	1.53
3	D	504[A]	RIO	O2-C2	4.40	1.54	1.45
3	C	303[A]	RIO	O2-C2	4.38	1.54	1.45
3	B	302[A]	RIO	O2-C2	4.37	1.54	1.45
3	A	302[A]	RIO	C1-C2	-4.36	1.37	1.51
3	A	302[A]	RIO	O2-C2	4.32	1.54	1.45
2	B	301[A]	COA	P2A-O3A	4.17	1.64	1.59
2	C	301[B]	COA	P3B-O3B	4.11	1.66	1.59
2	D	503[A]	COA	P3B-O3B	4.09	1.66	1.59
2	D	503[A]	COA	P2A-O3A	3.99	1.63	1.59
2	D	503[B]	COA	P3B-O3B	3.94	1.66	1.59
2	D	503[A]	COA	C2A-N3A	3.88	1.40	1.33
3	D	504[A]	RIO	C14-C15	-3.86	1.48	1.53
2	A	301[A]	COA	P3B-O3B	3.79	1.66	1.59
2	A	301[A]	COA	C2A-N3A	3.77	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[A]	COA	C2A-N3A	3.75	1.40	1.33
2	A	301[B]	COA	P3B-O3B	3.74	1.66	1.59
2	B	301[B]	COA	P3B-O3B	3.67	1.66	1.59
3	B	302[A]	RIO	C14-C15	-3.66	1.49	1.53
2	D	503[B]	COA	C2A-N3A	3.63	1.40	1.33
2	C	301[B]	COA	C2A-N3A	3.58	1.40	1.33
2	A	301[B]	COA	C2A-N3A	3.57	1.40	1.33
2	B	301[A]	COA	C2A-N3A	3.54	1.40	1.33
2	B	301[A]	COA	P3B-O3B	3.50	1.65	1.59
2	B	301[B]	COA	C2A-N3A	3.47	1.40	1.33
3	A	302[A]	RIO	O6-C10	3.26	1.50	1.41
3	C	303[A]	RIO	O6-C10	3.22	1.50	1.41
2	B	301[B]	COA	P1A-O3A	3.20	1.63	1.59
2	A	301[A]	COA	C5A-N7A	-3.15	1.33	1.39
3	B	302[A]	RIO	O6-C10	3.14	1.49	1.41
2	A	301[B]	COA	C5A-N7A	-3.09	1.33	1.39
3	C	303[A]	RIO	C17-C2	3.09	1.60	1.53
2	C	301[B]	COA	P1A-O3A	3.06	1.62	1.59
3	D	504[A]	RIO	O6-C10	3.05	1.49	1.41
2	D	503[B]	COA	O5P-C5P	-2.99	1.17	1.23
3	D	504[A]	RIO	C17-C2	2.93	1.60	1.53
2	D	503[A]	COA	O5P-C5P	-2.93	1.17	1.23
2	C	301[A]	COA	P2A-O3A	2.92	1.62	1.59
2	D	503[A]	COA	C5A-N7A	-2.90	1.33	1.39
2	D	503[B]	COA	C5A-N7A	-2.88	1.33	1.39
3	A	302[A]	RIO	C17-C2	2.86	1.60	1.53
2	C	301[B]	COA	C5A-N7A	-2.85	1.33	1.39
3	B	302[A]	RIO	C17-C2	2.81	1.60	1.53
2	A	301[B]	COA	O5P-C5P	-2.77	1.17	1.23
2	D	503[B]	COA	P1A-O3A	2.75	1.62	1.59
2	A	301[A]	COA	C5A-C4A	-2.74	1.34	1.39
2	C	301[A]	COA	C5A-N7A	-2.72	1.34	1.39
2	B	301[B]	COA	C5A-N7A	-2.71	1.34	1.39
2	B	301[B]	COA	O5P-C5P	-2.71	1.17	1.23
2	B	301[A]	COA	C5A-C4A	-2.68	1.34	1.39
2	A	301[B]	COA	C5A-C4A	-2.66	1.34	1.39
2	C	301[B]	COA	O5P-C5P	-2.66	1.18	1.23
2	B	301[B]	COA	C6P-C5P	2.64	1.56	1.51
2	D	503[B]	COA	C6P-C5P	2.60	1.56	1.51
2	A	301[A]	COA	O5P-C5P	-2.59	1.18	1.23
2	B	301[B]	COA	C5A-C4A	-2.59	1.34	1.39
2	D	503[A]	COA	C5A-C4A	-2.55	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503[B]	COA	C5A-C4A	-2.52	1.34	1.39
2	B	301[A]	COA	P1A-O3A	2.52	1.62	1.59
2	B	301[A]	COA	O5P-C5P	-2.51	1.18	1.23
2	B	301[A]	COA	C5A-N7A	-2.51	1.34	1.39
2	A	301[B]	COA	P1A-O3A	2.46	1.62	1.59
2	D	503[B]	COA	O3B-C3B	-2.45	1.35	1.44
2	D	503[A]	COA	O3B-C3B	-2.45	1.35	1.44
2	D	503[B]	COA	O9P-C9P	-2.45	1.18	1.23
2	A	301[B]	COA	C6P-C5P	2.45	1.56	1.51
2	C	301[B]	COA	C6P-C5P	2.45	1.56	1.51
2	C	301[A]	COA	O5P-C5P	-2.41	1.18	1.23
2	C	301[B]	COA	O3B-C3B	-2.40	1.35	1.44
2	D	503[A]	COA	O9P-C9P	-2.38	1.18	1.23
2	B	301[B]	COA	O3B-C3B	-2.36	1.36	1.44
2	D	503[B]	COA	P1A-O5B	2.34	1.68	1.59
2	A	301[B]	COA	O3B-C3B	-2.33	1.36	1.44
2	B	301[A]	COA	C6P-C5P	2.33	1.56	1.51
2	C	301[A]	COA	O3B-C3B	-2.32	1.36	1.44
2	C	301[B]	COA	P1A-O5B	2.30	1.68	1.59
2	A	301[A]	COA	O3B-C3B	-2.29	1.36	1.44
2	A	301[A]	COA	C6P-C5P	2.28	1.55	1.51
2	D	503[A]	COA	C8A-N9A	-2.28	1.33	1.37
2	C	301[B]	COA	C5A-C4A	-2.28	1.35	1.39
3	A	302[A]	RIO	O10-C17	2.26	1.48	1.43
3	B	302[A]	RIO	O10-C17	2.26	1.48	1.43
2	C	301[B]	COA	O9P-C9P	-2.24	1.19	1.23
2	B	301[A]	COA	O3B-C3B	-2.23	1.36	1.44
2	A	301[B]	COA	P1A-O5B	2.23	1.68	1.59
3	C	303[A]	RIO	O10-C17	2.22	1.48	1.43
2	D	503[A]	COA	P1A-O5B	2.20	1.68	1.59
2	B	301[B]	COA	O9P-C9P	-2.20	1.19	1.23
2	C	301[A]	COA	C6P-C5P	2.20	1.55	1.51
2	D	503[B]	COA	C8A-N9A	-2.15	1.33	1.37
2	B	301[B]	COA	P1A-O5B	2.15	1.67	1.59
2	A	301[A]	COA	P1A-O5B	2.14	1.67	1.59
2	C	301[A]	COA	P1A-O3A	2.14	1.61	1.59
2	B	301[B]	COA	P2A-O6A	2.12	1.67	1.59
2	D	503[A]	COA	C6P-C5P	2.09	1.55	1.51
3	D	504[A]	RIO	O10-C17	2.08	1.48	1.43
2	C	301[A]	COA	P1A-O5B	2.07	1.67	1.59
2	A	301[B]	COA	P2A-O6A	2.05	1.67	1.59
2	A	301[B]	COA	O9P-C9P	-2.04	1.19	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301[B]	COA	P2A-O6A	2.04	1.67	1.59
2	C	301[A]	COA	C5A-C4A	-2.03	1.35	1.39
2	D	503[B]	COA	P2A-O6A	2.03	1.67	1.59

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301[A]	COA	C5A-C4A-N3A	-6.32	118.02	126.72
2	A	301[B]	COA	C5A-C4A-N3A	-6.08	118.34	126.72
2	D	503[A]	COA	C5A-C4A-N3A	-6.06	118.37	126.72
2	B	301[A]	COA	C5A-C4A-N3A	-6.01	118.45	126.72
2	C	301[A]	COA	C5A-C4A-N3A	-5.93	118.55	126.72
2	D	503[B]	COA	C5A-C4A-N3A	-5.92	118.57	126.72
2	B	301[B]	COA	C5A-C4A-N3A	-5.83	118.69	126.72
2	C	301[B]	COA	C5A-C4A-N3A	-5.81	118.71	126.72
2	B	301[B]	COA	N6A-C6A-N1A	-5.57	105.97	118.38
2	C	301[B]	COA	N3A-C2A-N1A	-5.53	120.21	128.58
2	D	503[B]	COA	N3A-C2A-N1A	-5.51	120.23	128.58
2	B	301[B]	COA	N3A-C2A-N1A	-5.51	120.24	128.58
2	D	503[A]	COA	N3A-C2A-N1A	-5.44	120.35	128.58
2	D	503[B]	COA	N6A-C6A-N1A	-5.43	106.28	118.38
2	C	301[A]	COA	N3A-C2A-N1A	-5.40	120.41	128.58
2	B	301[A]	COA	N3A-C2A-N1A	-5.39	120.43	128.58
2	C	301[B]	COA	N6A-C6A-N1A	-5.37	106.41	118.38
2	A	301[B]	COA	N3A-C2A-N1A	-5.35	120.49	128.58
2	A	301[A]	COA	N3A-C2A-N1A	-5.27	120.60	128.58
2	A	301[A]	COA	N3A-C4A-N9A	5.14	135.90	127.17
2	A	301[B]	COA	N6A-C6A-N1A	-5.05	107.13	118.38
2	B	301[A]	COA	C6P-C7P-N8P	-5.05	101.25	112.00
2	B	301[A]	COA	N6A-C6A-N1A	-5.03	107.17	118.38
2	C	301[A]	COA	N3A-C4A-N9A	4.91	135.51	127.17
2	D	503[A]	COA	N3A-C4A-N9A	4.90	135.49	127.17
2	B	301[A]	COA	N3A-C4A-N9A	4.77	135.29	127.17
2	A	301[B]	COA	N3A-C4A-N9A	4.69	135.14	127.17
2	D	503[A]	COA	N6A-C6A-N1A	-4.66	107.99	118.38
2	A	301[A]	COA	C6P-C7P-N8P	-4.54	102.34	112.00
2	C	301[A]	COA	N6A-C6A-N1A	-4.46	108.44	118.38
2	A	301[A]	COA	N6A-C6A-N1A	-4.45	108.45	118.38
2	D	503[B]	COA	N3A-C4A-N9A	4.39	134.64	127.17
2	D	503[A]	COA	C6P-C7P-N8P	-4.33	102.78	112.00
2	C	301[B]	COA	N3A-C4A-N9A	4.32	134.52	127.17
2	B	301[B]	COA	N3A-C4A-N9A	4.27	134.43	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[A]	COA	C6P-C7P-N8P	-4.27	102.92	112.00
2	D	503[A]	COA	N9A-C8A-N7A	-4.22	107.95	113.94
2	B	301[A]	COA	N9A-C8A-N7A	-4.15	108.05	113.94
2	D	503[B]	COA	C5A-C6A-N6A	4.06	133.33	123.29
2	D	503[B]	COA	N9A-C8A-N7A	-4.05	108.19	113.94
2	B	301[B]	COA	N9A-C8A-N7A	-4.02	108.23	113.94
2	B	301[B]	COA	C5A-C6A-N6A	4.02	133.24	123.29
2	C	301[A]	COA	O4B-C1B-N9A	4.01	115.79	108.09
2	C	301[B]	COA	C5A-C6A-N6A	3.98	133.15	123.29
2	A	301[B]	COA	N9A-C8A-N7A	-3.89	108.41	113.94
2	A	301[A]	COA	N9A-C8A-N7A	-3.88	108.43	113.94
2	A	301[B]	COA	C6P-C7P-N8P	-3.88	103.74	112.00
2	B	301[B]	COA	C6P-C7P-N8P	-3.86	103.79	112.00
2	C	301[A]	COA	CDP-CBP-CAP	3.68	115.03	108.77
2	C	301[B]	COA	N9A-C8A-N7A	-3.67	108.73	113.94
2	B	301[A]	COA	C2A-N3A-C4A	3.67	120.79	111.83
2	B	301[B]	COA	C2A-N3A-C4A	3.65	120.75	111.83
2	A	301[B]	COA	C2A-N3A-C4A	3.60	120.63	111.83
2	D	503[B]	COA	C2A-N3A-C4A	3.59	120.61	111.83
2	A	301[A]	COA	C2A-N3A-C4A	3.58	120.57	111.83
2	A	301[B]	COA	C5A-C6A-N6A	3.55	132.08	123.29
2	C	301[B]	COA	C2A-N3A-C4A	3.54	120.48	111.83
2	D	503[A]	COA	C2A-N3A-C4A	3.51	120.40	111.83
2	D	503[A]	COA	O6A-CCP-CBP	-3.42	105.05	110.55
2	B	301[A]	COA	C5A-C6A-N6A	3.40	131.71	123.29
2	D	503[B]	COA	C6P-C7P-N8P	-3.39	104.78	112.00
2	D	503[A]	COA	C5A-C6A-N6A	3.39	131.68	123.29
2	C	301[A]	COA	C2A-N3A-C4A	3.38	120.09	111.83
2	B	301[A]	COA	CDP-CBP-CAP	3.37	114.51	108.77
2	D	503[A]	COA	C4B-O4B-C1B	-3.34	102.08	109.47
2	C	301[B]	COA	C6P-C7P-N8P	-3.34	104.89	112.00
3	B	302[A]	RIO	C3-C16-C17	3.33	106.43	102.29
2	C	301[A]	COA	N9A-C8A-N7A	-3.32	109.22	113.94
2	A	301[A]	COA	C4B-O4B-C1B	-3.27	102.24	109.47
2	C	301[A]	COA	C3B-C2B-C1B	3.27	107.09	99.89
2	D	503[A]	COA	C6A-C5A-C4A	3.21	121.56	117.18
3	A	302[A]	RIO	C7-C6-C5	3.18	114.85	110.08
2	A	301[A]	COA	C6A-C5A-C4A	3.18	121.52	117.18
2	D	503[B]	COA	C4B-O4B-C1B	-3.17	102.47	109.47
2	C	301[A]	COA	C5A-C6A-N6A	3.16	131.11	123.29
2	B	301[A]	COA	C4B-O4B-C1B	-3.15	102.52	109.47
2	A	301[B]	COA	C4B-O4B-C1B	-3.14	102.53	109.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301[A]	COA	O4B-C1B-N9A	3.10	114.05	108.09
2	C	301[A]	COA	C4B-O4B-C1B	-3.09	102.65	109.47
2	C	301[A]	COA	O6A-CCP-CBP	-3.06	105.62	110.55
2	B	301[A]	COA	C3B-C2B-C1B	3.06	106.61	99.89
2	C	301[B]	COA	C4B-O4B-C1B	-3.04	102.75	109.47
2	D	503[A]	COA	C5A-N7A-C8A	3.00	108.17	103.45
2	B	301[B]	COA	C4B-O4B-C1B	-2.99	102.87	109.47
2	D	503[A]	COA	C4A-N9A-C8A	2.99	108.88	105.74
2	A	301[A]	COA	C5A-C6A-N6A	2.98	130.66	123.29
3	C	303[A]	RIO	C10-O5-C9	-2.98	110.92	117.98
2	B	301[A]	COA	C4A-N9A-C8A	2.96	108.84	105.74
2	C	301[B]	COA	C3B-C2B-C1B	2.95	106.38	99.89
2	D	503[B]	COA	C5A-N7A-C8A	2.95	108.08	103.45
3	D	504[A]	RIO	C3-O3-C4	-2.93	111.03	117.98
2	B	301[A]	COA	O6A-CCP-CBP	-2.92	105.85	110.55
3	D	504[A]	RIO	C3-C16-C17	2.91	105.91	102.29
3	D	504[A]	RIO	C10-O5-C9	-2.91	111.09	117.98
2	A	301[A]	COA	C3B-C2B-C1B	2.88	106.23	99.89
2	B	301[B]	COA	C3B-C2B-C1B	2.87	106.21	99.89
2	C	301[A]	COA	C6A-C5A-C4A	2.87	121.10	117.18
3	C	303[A]	RIO	C3-O3-C4	-2.84	111.24	117.98
3	B	302[A]	RIO	O2-C3-C16	2.82	108.57	104.98
2	A	301[B]	COA	C3B-C2B-C1B	2.82	106.10	99.89
2	B	301[B]	COA	C5A-N7A-C8A	2.82	107.88	103.45
2	C	301[B]	COA	O4B-C1B-N9A	2.81	113.49	108.09
2	C	301[A]	COA	C7P-C6P-C5P	-2.79	107.75	112.39
2	A	301[B]	COA	C6A-C5A-C4A	2.77	120.97	117.18
3	B	302[A]	RIO	C10-O5-C9	-2.77	111.41	117.98
3	A	302[A]	RIO	C10-O5-C9	-2.75	111.46	117.98
2	D	503[B]	COA	C6A-C5A-C4A	2.73	120.90	117.18
2	D	503[A]	COA	O4B-C1B-N9A	2.72	113.32	108.09
2	A	301[A]	COA	O6A-CCP-CBP	-2.72	106.17	110.55
2	B	301[A]	COA	C5A-N7A-C8A	2.71	107.72	103.45
3	C	303[A]	RIO	C7-C6-C5	2.69	114.10	110.08
2	A	301[B]	COA	C5A-N7A-C8A	2.68	107.66	103.45
3	A	302[A]	RIO	C3-C16-C17	2.67	105.62	102.29
3	C	303[A]	RIO	O6-C11-C13	2.66	114.49	109.70
2	D	503[B]	COA	C3B-C2B-C1B	2.66	105.74	99.89
2	A	301[A]	COA	O5A-P2A-O3A	2.65	114.44	107.27
2	A	301[A]	COA	C7P-C6P-C5P	-2.65	107.98	112.39
2	B	301[A]	COA	C6A-C5A-C4A	2.65	120.79	117.18
2	B	301[A]	COA	C2B-C3B-C4B	-2.63	98.63	103.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[A]	COA	C7P-N8P-C9P	-2.62	117.84	122.55
3	C	303[A]	RIO	C3-C16-C17	2.61	105.54	102.29
2	D	503[A]	COA	C3B-C2B-C1B	2.61	105.63	99.89
2	A	301[A]	COA	C5A-N7A-C8A	2.60	107.53	103.45
2	D	503[A]	COA	CEP-CBP-CAP	2.59	113.18	108.77
2	C	301[A]	COA	O3A-P2A-O4A	-2.57	102.98	110.70
2	C	301[B]	COA	C5A-N7A-C8A	2.55	107.46	103.45
2	A	301[A]	COA	O4B-C1B-N9A	2.55	112.98	108.09
3	A	302[A]	RIO	C3-O3-C4	-2.51	112.02	117.98
2	C	301[B]	COA	C6A-C5A-C4A	2.51	120.60	117.18
2	D	503[B]	COA	C4A-N9A-C8A	2.50	108.37	105.74
2	A	301[A]	COA	C4A-N9A-C8A	2.50	108.36	105.74
2	B	301[A]	COA	C7P-N8P-C9P	-2.48	118.10	122.55
2	B	301[B]	COA	C4A-N9A-C8A	2.45	108.31	105.74
3	A	302[A]	RIO	O2-C3-C16	2.41	108.05	104.98
2	B	301[B]	COA	C4A-N9A-C1B	-2.41	121.00	126.63
2	B	301[B]	COA	C6A-C5A-C4A	2.39	120.44	117.18
2	C	301[B]	COA	CDP-CBP-CAP	2.39	112.84	108.77
2	B	301[B]	COA	CDP-CBP-CAP	2.38	112.82	108.77
2	D	503[B]	COA	C4A-N9A-C1B	-2.36	121.12	126.63
2	A	301[B]	COA	C4A-N9A-C8A	2.35	108.20	105.74
2	C	301[A]	COA	C4A-N9A-C8A	2.29	108.14	105.74
3	C	303[A]	RIO	C12-C11-C13	-2.28	107.46	112.80
2	D	503[B]	COA	O4B-C1B-N9A	2.27	112.46	108.09
3	A	302[A]	RIO	O6-C11-C13	2.27	113.78	109.70
2	B	301[B]	COA	O4B-C1B-N9A	2.26	112.43	108.09
2	B	301[A]	COA	C3P-N4P-C5P	-2.26	118.62	122.82
3	D	504[A]	RIO	O6-C11-C12	2.20	110.30	106.07
2	A	301[A]	COA	CDP-CBP-CAP	2.20	112.52	108.77
2	C	301[B]	COA	C4A-N9A-C1B	-2.20	121.48	126.63
3	A	302[A]	RIO	C5-C6-N1	-2.18	106.63	110.94
2	C	301[A]	COA	O5A-P2A-O3A	2.17	113.13	107.27
2	A	301[B]	COA	O4B-C1B-N9A	2.17	112.25	108.09
2	B	301[B]	COA	C7P-N8P-C9P	-2.15	118.69	122.55
2	C	301[B]	COA	C4A-N9A-C8A	2.14	107.98	105.74
2	A	301[B]	COA	C4A-N9A-C1B	-2.14	121.63	126.63
2	A	301[B]	COA	O5A-P2A-O3A	2.14	113.05	107.27
3	B	302[A]	RIO	C3-O3-C4	-2.13	112.93	117.98
3	B	302[A]	RIO	C1-C2-C17	-2.12	110.09	115.10
2	D	503[A]	COA	C2P-C3P-N4P	-2.11	107.52	112.31
2	C	301[A]	COA	C5A-N7A-C8A	2.11	106.76	103.45
2	A	301[A]	COA	C7P-N8P-C9P	-2.10	118.78	122.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301[B]	COA	C7P-N8P-C9P	-2.09	118.79	122.55
3	C	303[A]	RIO	C14-C13-C11	2.08	114.00	110.23
2	A	301[A]	COA	O3A-P2A-O4A	-2.06	104.50	110.70
2	D	503[A]	COA	C2B-C3B-C4B	-2.05	99.66	103.24
3	D	504[A]	RIO	C1-C2-C17	-2.04	110.28	115.10
3	A	302[A]	RIO	C12-C11-C13	-2.04	108.04	112.80
2	D	503[B]	COA	CEP-CBP-CAP	2.03	112.23	108.77
2	A	301[B]	COA	CDP-CBP-CAP	2.03	112.22	108.77
2	D	503[B]	COA	O6A-CCP-CBP	-2.02	107.31	110.55

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302[A]	RIO	C16-C3-O3-C4
3	B	302[A]	RIO	C16-C3-O3-C4
3	D	504[A]	RIO	C16-C3-O3-C4
3	D	504[A]	RIO	O6-C11-C12-N3
3	D	504[A]	RIO	C13-C11-C12-N3
3	C	303[A]	RIO	O1-C1-C2-O2
3	C	303[A]	RIO	O1-C1-C2-C17
3	B	302[A]	RIO	O1-C1-C2-O2
3	D	504[A]	RIO	O1-C1-C2-C17
3	D	504[A]	RIO	O1-C1-C2-O2
3	D	504[A]	RIO	O2-C3-O3-C4
3	B	302[A]	RIO	O1-C1-C2-C17
2	C	301[B]	COA	P1A-O3A-P2A-O4A
3	A	302[A]	RIO	O2-C3-O3-C4
3	B	302[A]	RIO	O2-C3-O3-C4
3	A	302[A]	RIO	O6-C11-C12-N3
2	A	301[B]	COA	P1A-O3A-P2A-O4A
2	C	301[A]	COA	P1A-O3A-P2A-O4A
2	D	503[B]	COA	P1A-O3A-P2A-O4A
2	C	301[B]	COA	C3B-O3B-P3B-O8A
2	C	301[B]	COA	P1A-O3A-P2A-O5A
2	B	301[A]	COA	C2P-C3P-N4P-C5P
2	D	503[A]	COA	C2P-C3P-N4P-C5P
2	A	301[A]	COA	C3B-O3B-P3B-O8A
2	A	301[B]	COA	C3B-O3B-P3B-O8A
2	C	301[A]	COA	C3B-O3B-P3B-O8A
3	B	302[A]	RIO	C9-C4-O3-C3
3	B	302[A]	RIO	C5-C4-O3-C3

Continued on next page...

Continued from previous page...

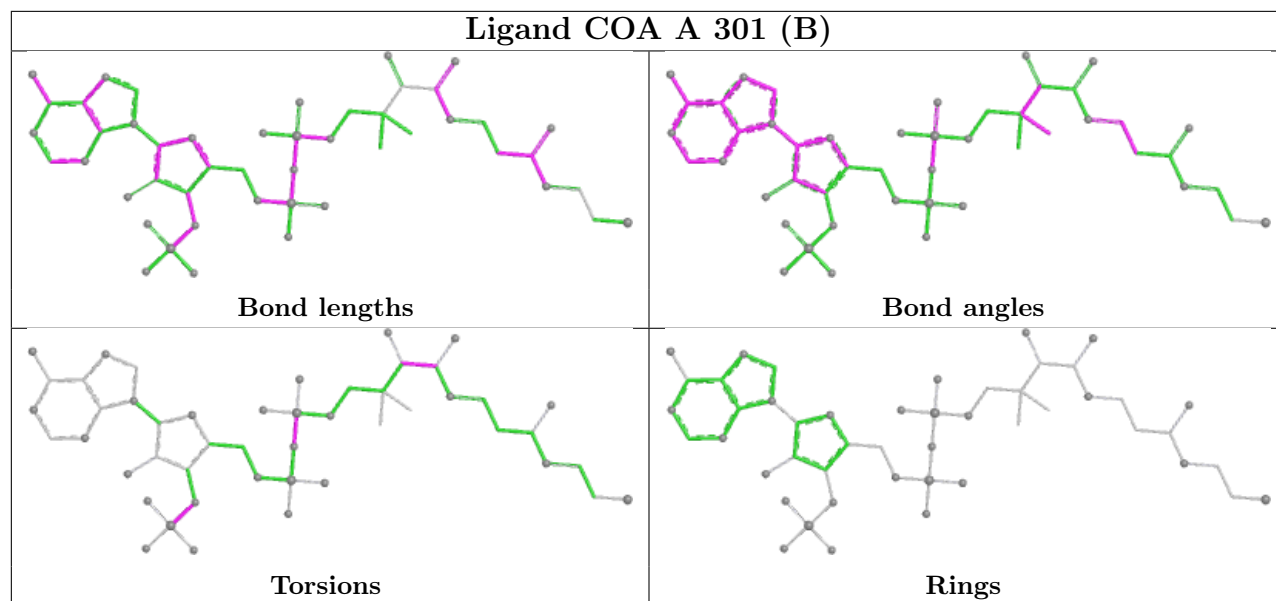
Mol	Chain	Res	Type	Atoms
2	A	301[A]	COA	N8P-C9P-CAP-OAP
2	A	301[B]	COA	N8P-C9P-CAP-OAP
2	B	301[B]	COA	N8P-C9P-CAP-OAP
2	C	301[A]	COA	N8P-C9P-CAP-OAP
2	C	301[B]	COA	N8P-C9P-CAP-OAP
2	D	503[A]	COA	N8P-C9P-CAP-OAP
2	D	503[B]	COA	N8P-C9P-CAP-OAP
3	B	302[A]	RIO	O6-C10-O5-C9
2	A	301[B]	COA	P1A-O3A-P2A-O5A
2	D	503[B]	COA	P1A-O3A-P2A-O5A

There are no ring outliers.

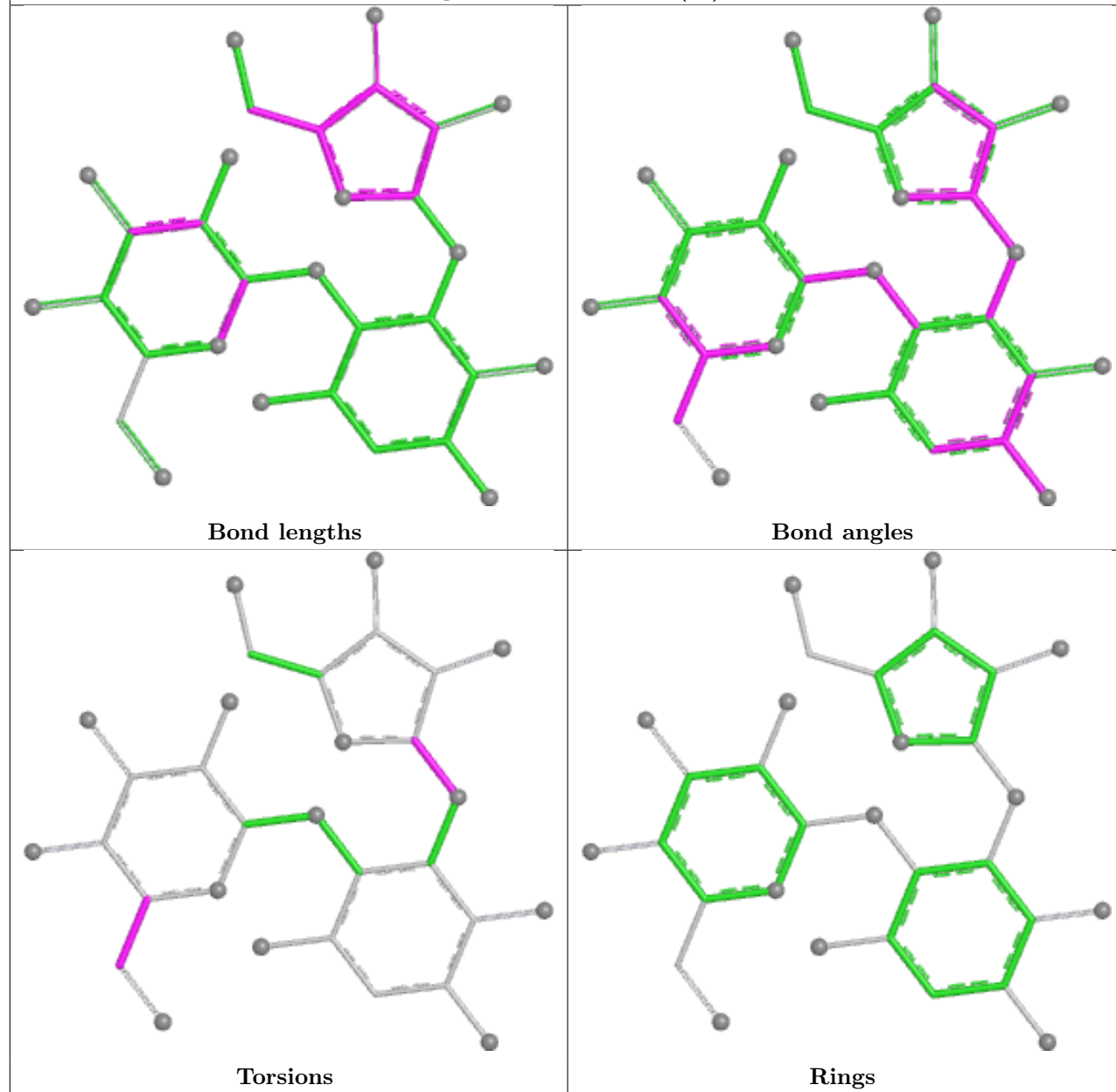
7 monomers are involved in 15 short contacts:

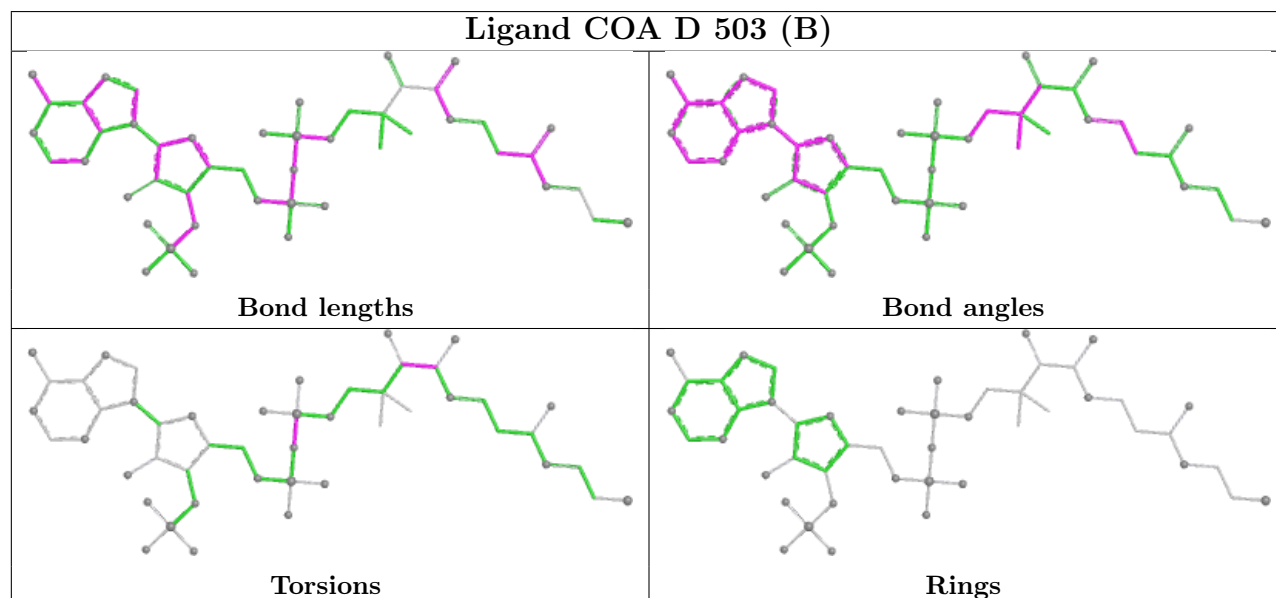
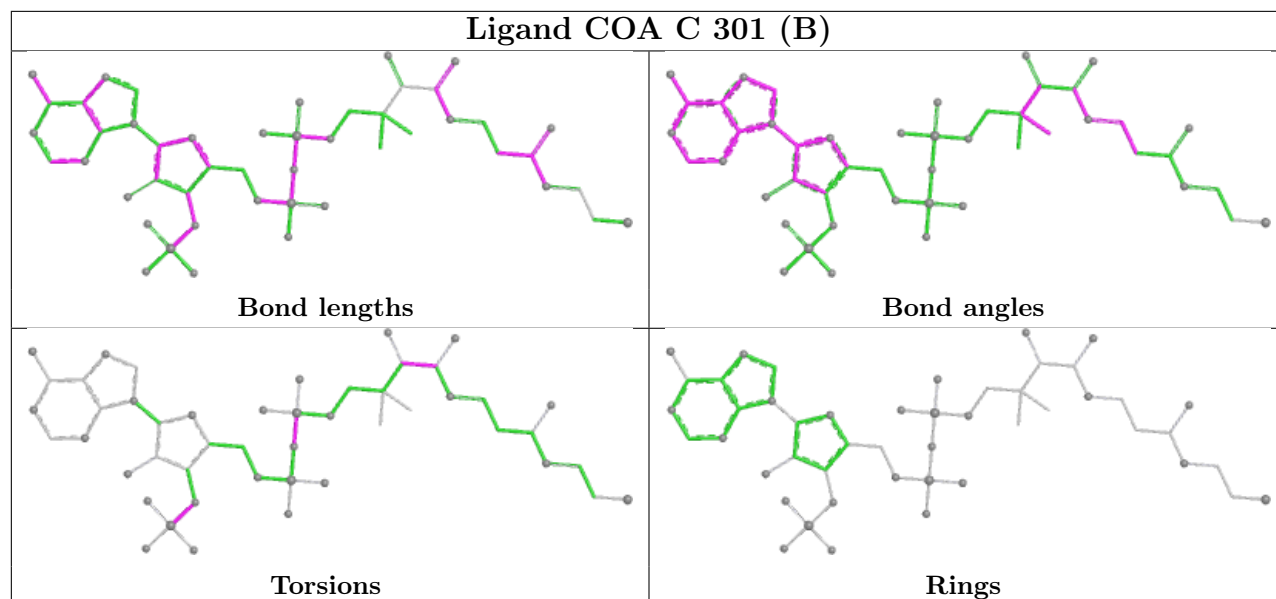
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302[A]	RIO	2	0
2	B	301[B]	COA	1	0
3	D	504[A]	RIO	3	0
3	C	303[A]	RIO	4	0
2	B	301[A]	COA	1	0
4	D	505	FMT	2	0
3	B	302[A]	RIO	2	0

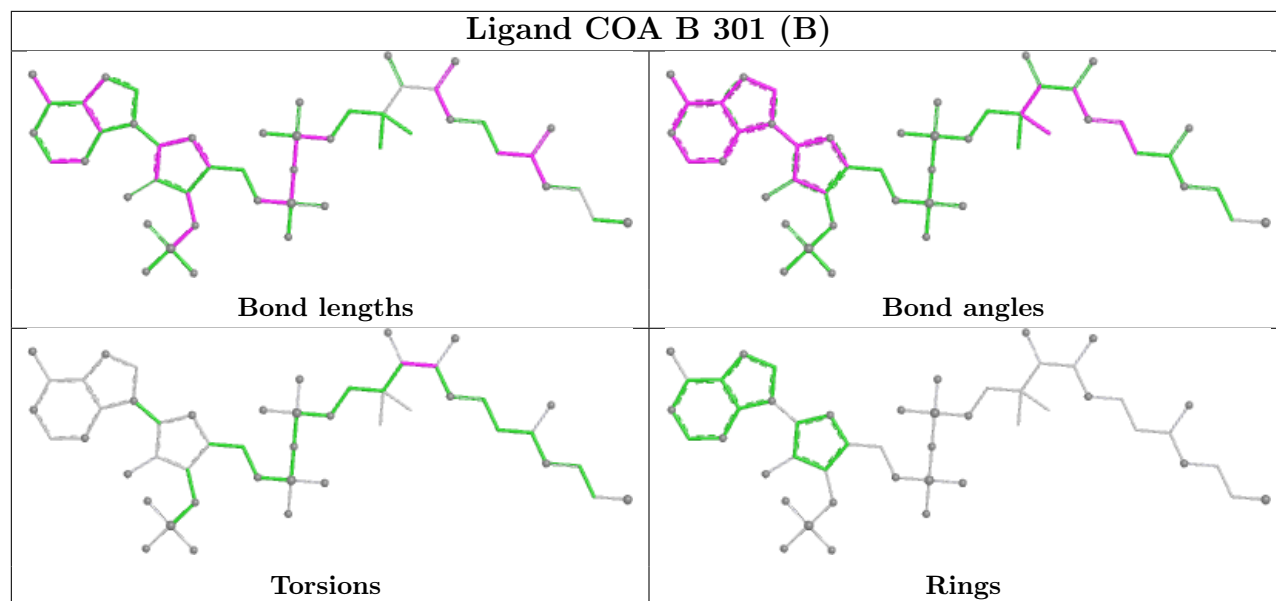
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



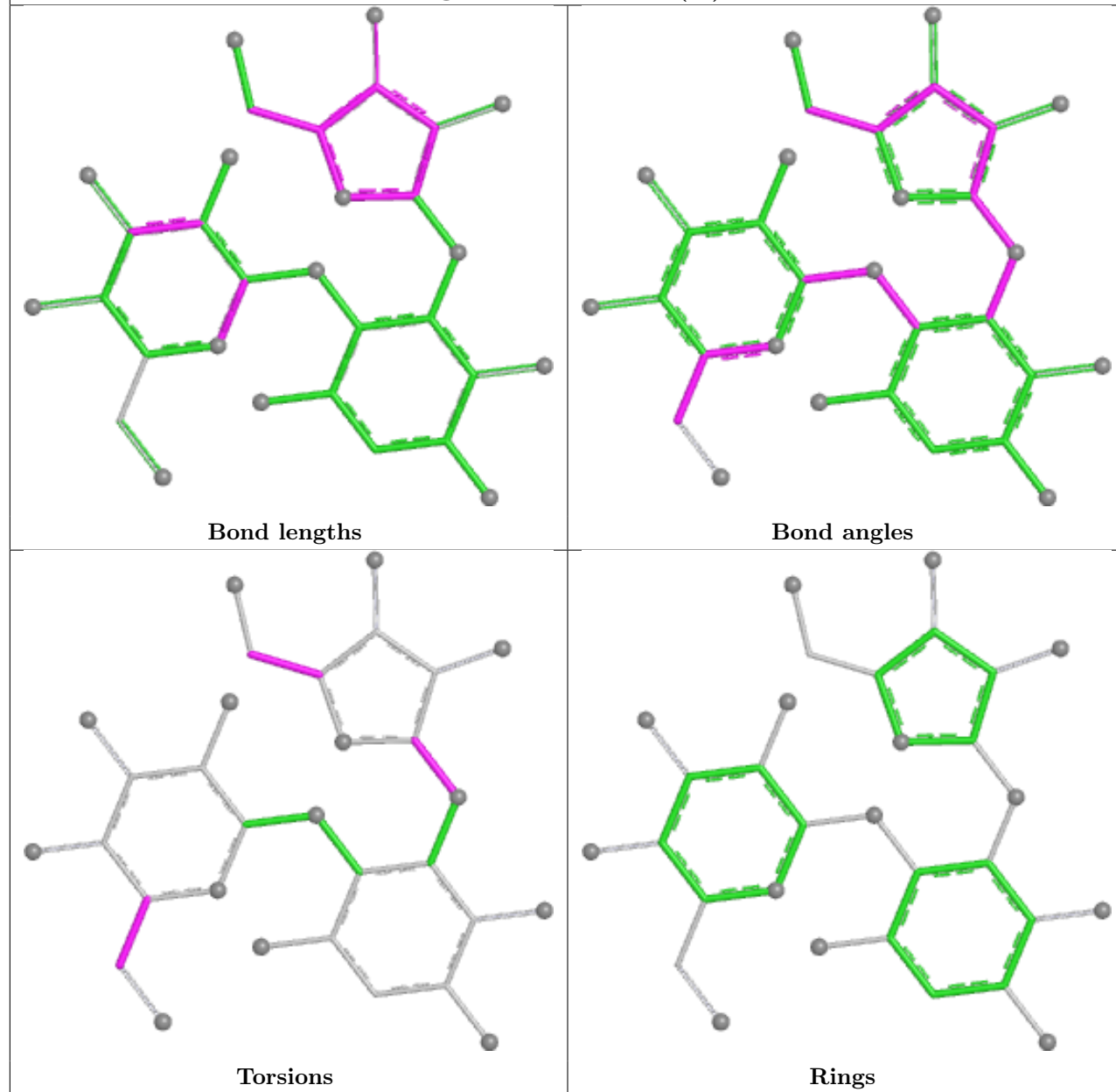
Ligand RIO A 302 (A)



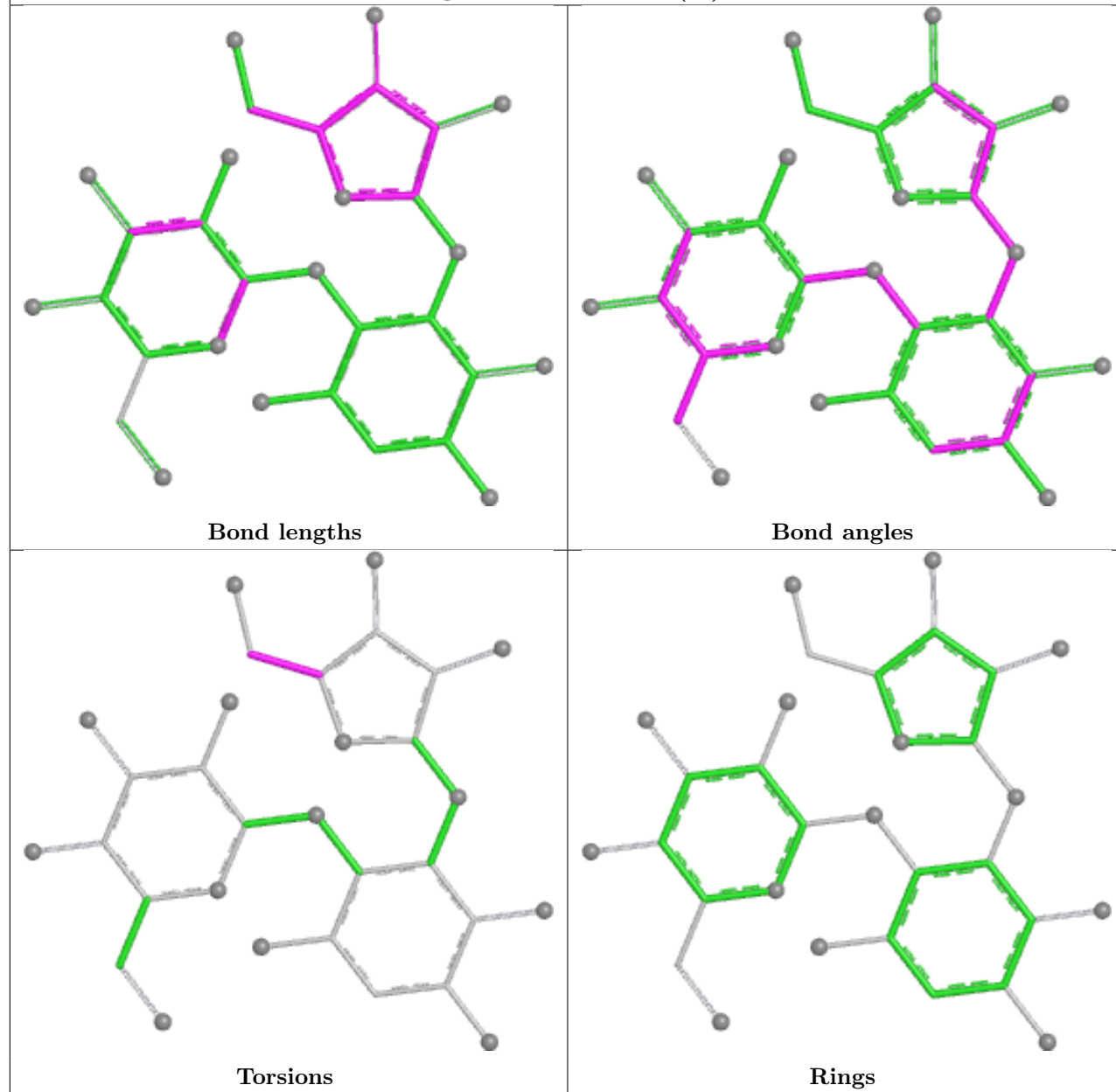


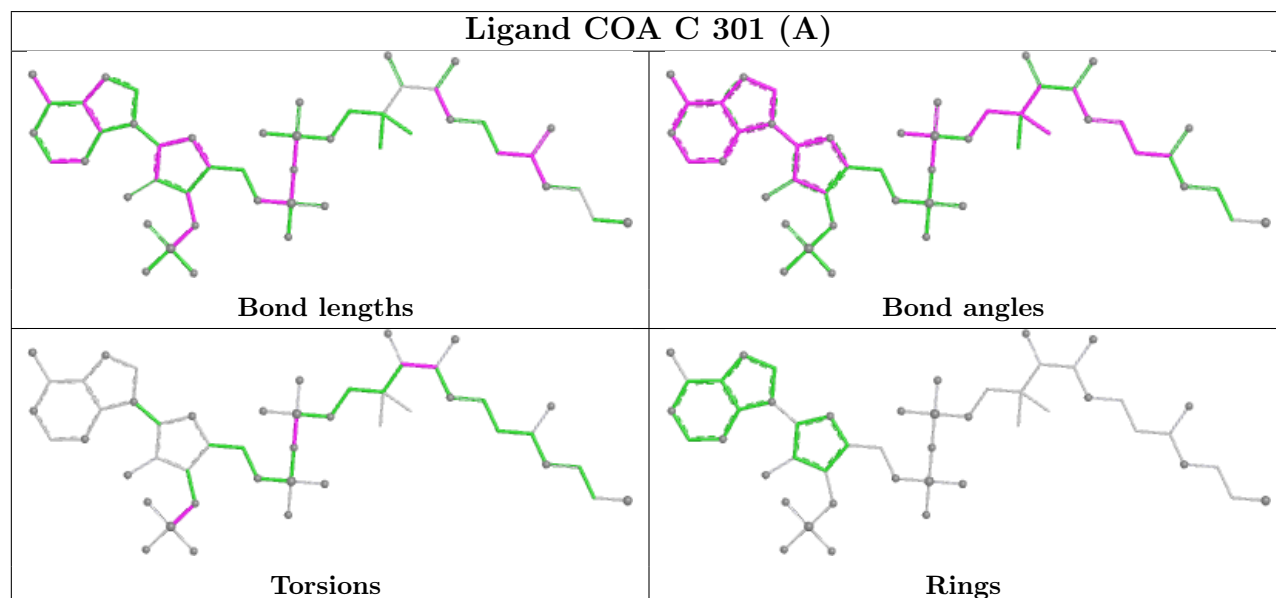
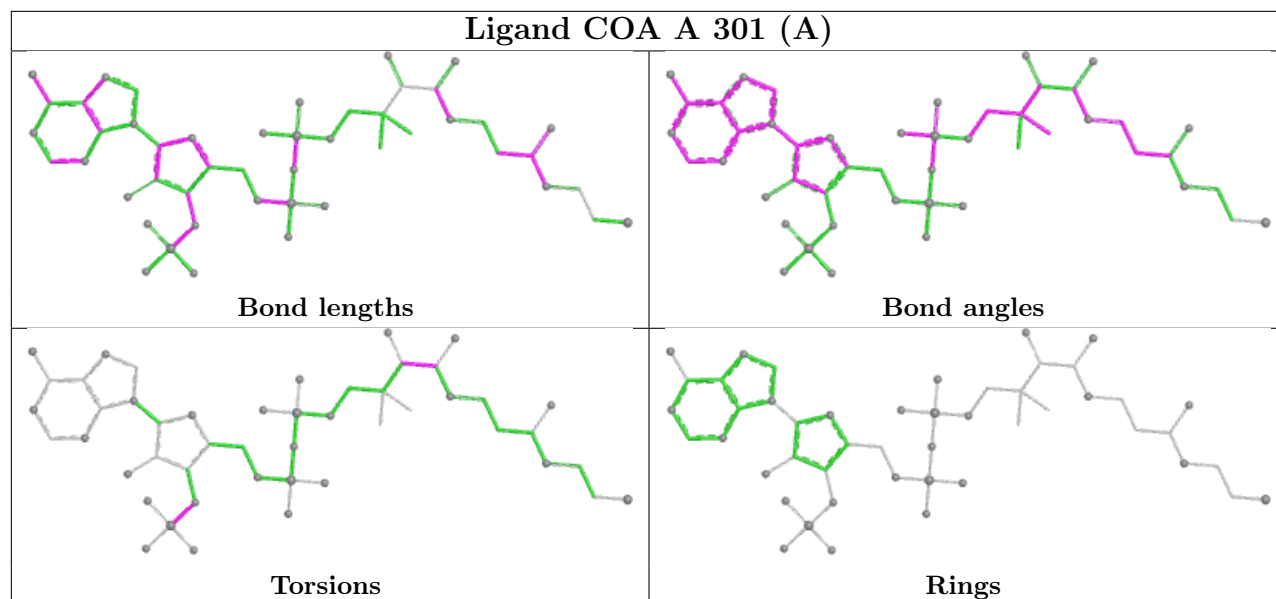


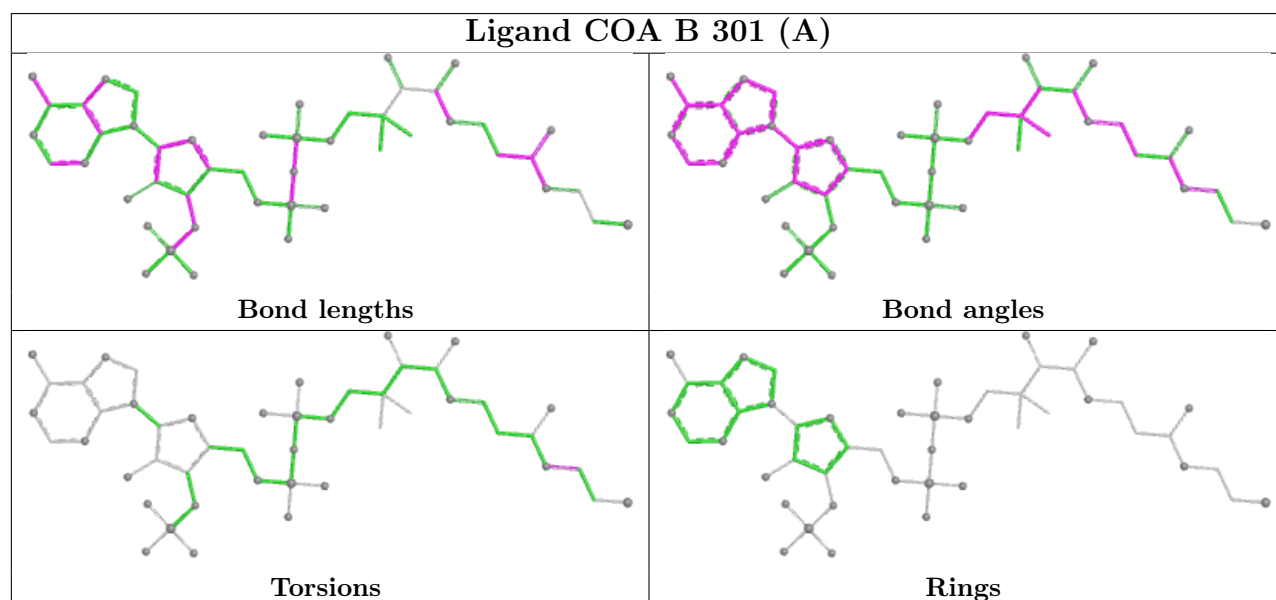
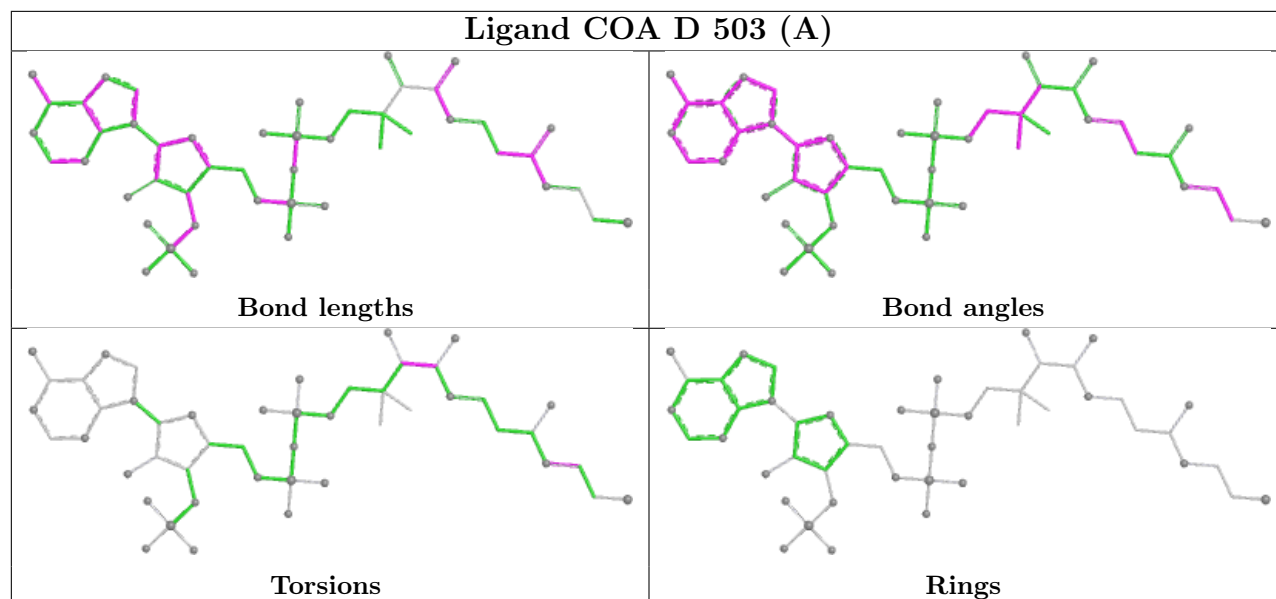
Ligand RIO D 504 (A)

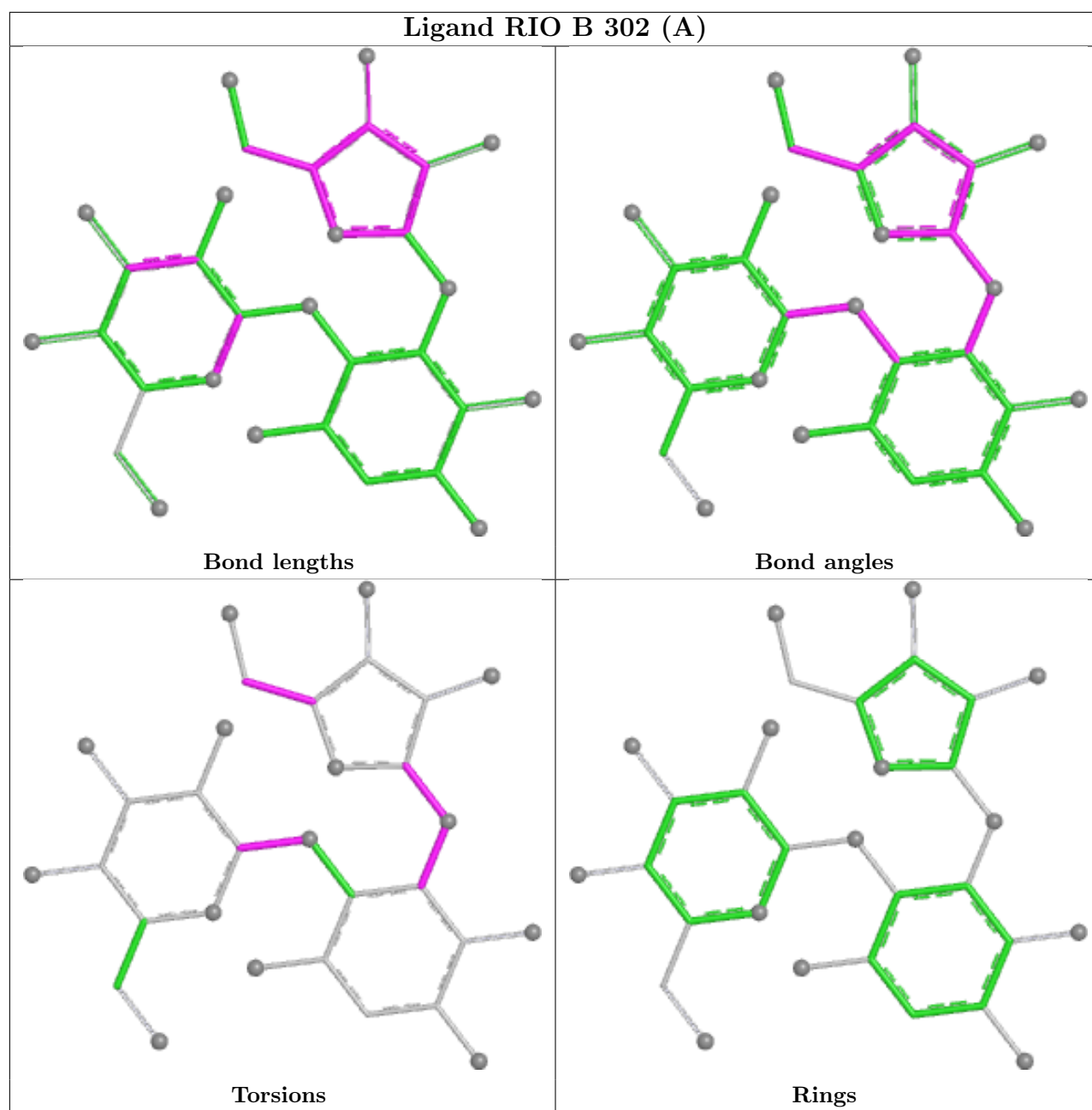


Ligand RIO C 303 (A)









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, 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	260/274 (94%)	-0.33	2 (0%) 82 86	9, 17, 37, 55	10 (3%)
1	B	260/274 (94%)	-0.42	1 (0%) 88 91	7, 15, 36, 54	11 (4%)
1	C	259/274 (94%)	-0.40	1 (0%) 88 91	7, 16, 32, 47	11 (4%)
1	D	260/274 (94%)	-0.39	2 (0%) 82 86	8, 17, 30, 43	10 (3%)
All	All	1039/1096 (94%)	-0.39	6 (0%) 85 88	7, 16, 34, 55	42 (4%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ILE	4.3
1	A	6	ILE	4.0
1	D	6	ILE	3.7
1	C	6	ILE	3.2
1	A	76	SER	2.6
1	D	201[A]	ARG	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSO	A	115	7/8	0.96	0.06	13,15,25,29	0
1	CSO	B	115	7/8	0.97	0.05	12,14,23,25	0
1	CSO	D	115	7/8	0.97	0.05	16,17,23,24	0
1	CSO	C	115	7/8	0.98	0.04	11,12,23,25	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

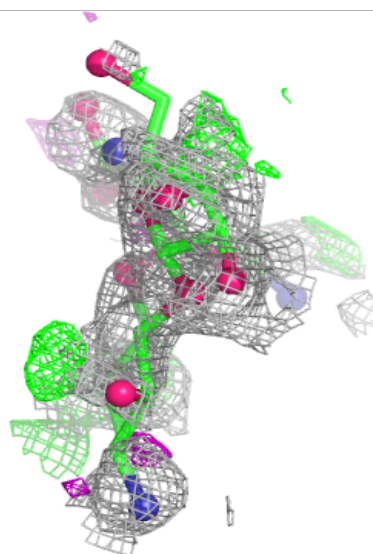
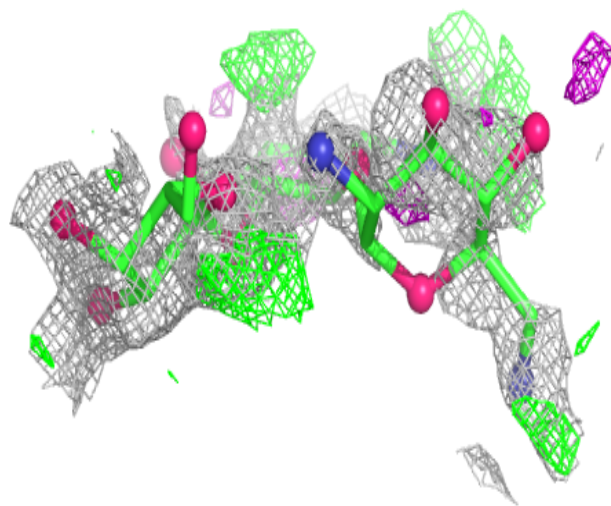
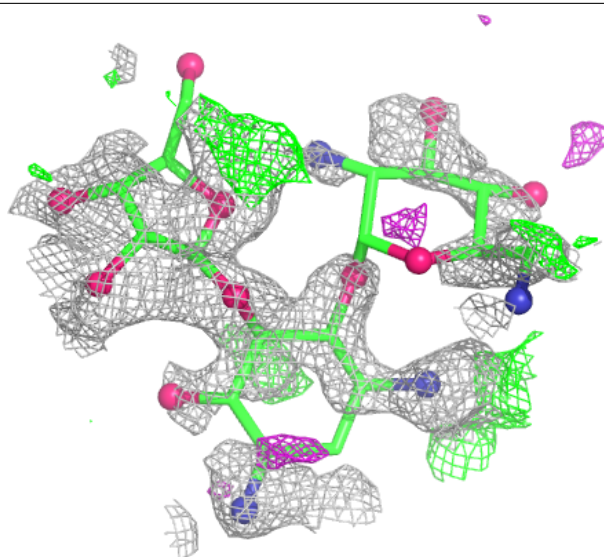
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	RIO	C	303[A]	31/31	0.55	0.22	35,56,70,75	31
3	RIO	B	302[A]	31/31	0.61	0.21	25,44,62,63	31
3	RIO	D	504[A]	31/31	0.63	0.20	25,48,62,66	31
4	FMT	A	304	3/3	0.67	0.16	38,38,43,46	0
3	RIO	A	302[A]	31/31	0.69	0.20	28,48,58,62	31
4	FMT	A	303[A]	3/3	0.81	0.16	30,30,31,35	3
4	FMT	D	505	3/3	0.81	0.13	41,41,46,53	0
4	FMT	C	302	3/3	0.85	0.41	32,32,34,35	0
4	FMT	D	502	3/3	0.86	0.24	37,37,42,45	0
4	FMT	B	303[A]	3/3	0.89	0.10	24,24,27,30	3
4	FMT	B	304	3/3	0.96	0.07	13,13,23,28	0
4	FMT	D	501	3/3	0.96	0.08	16,16,17,27	0
2	COA	C	301[A]	48/48	0.97	0.06	12,15,27,28	48
2	COA	C	301[B]	48/48	0.97	0.06	12,16,26,28	48
2	COA	D	503[A]	48/48	0.97	0.06	12,17,27,29	48
2	COA	D	503[B]	48/48	0.97	0.06	12,17,27,29	48
2	COA	A	301[A]	48/48	0.97	0.06	13,18,28,31	48
2	COA	A	301[B]	48/48	0.97	0.06	13,18,27,31	48
2	COA	B	301[A]	48/48	0.97	0.06	11,15,25,29	48
2	COA	B	301[B]	48/48	0.97	0.06	11,15,25,28	48

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.

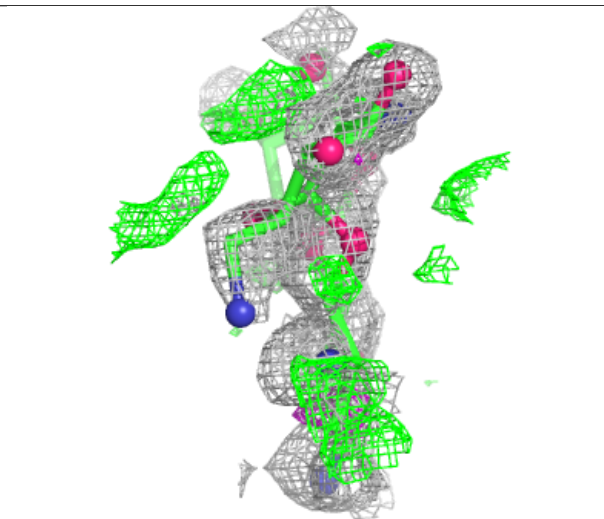
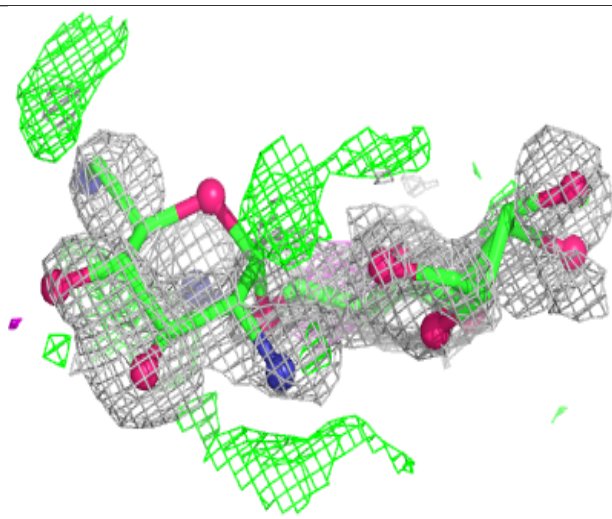
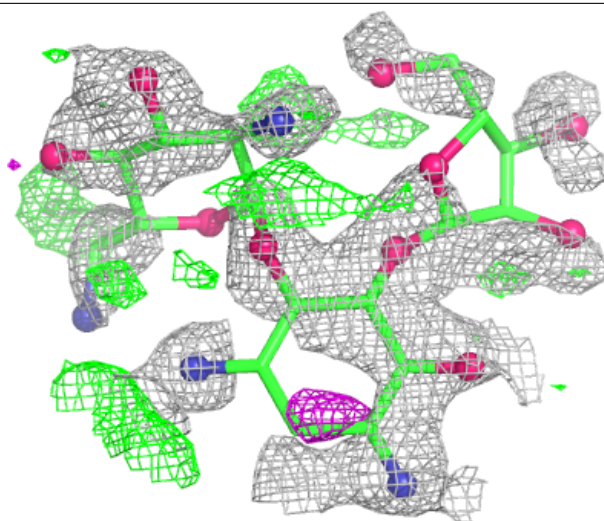
Electron density around RIO C 303 (A):

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



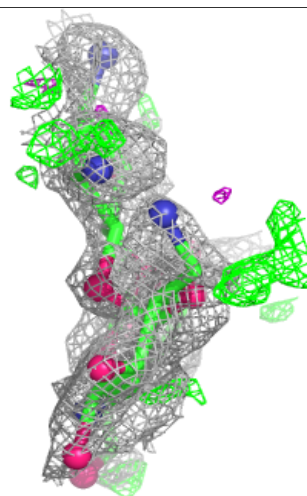
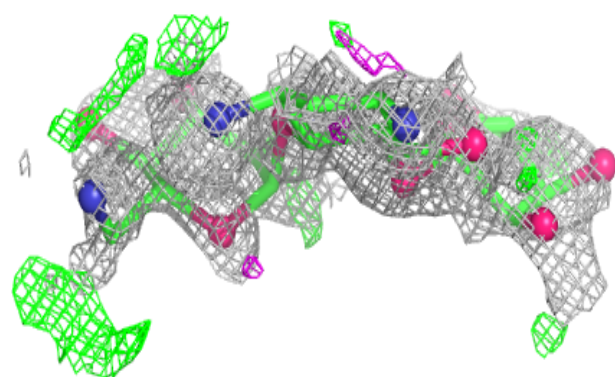
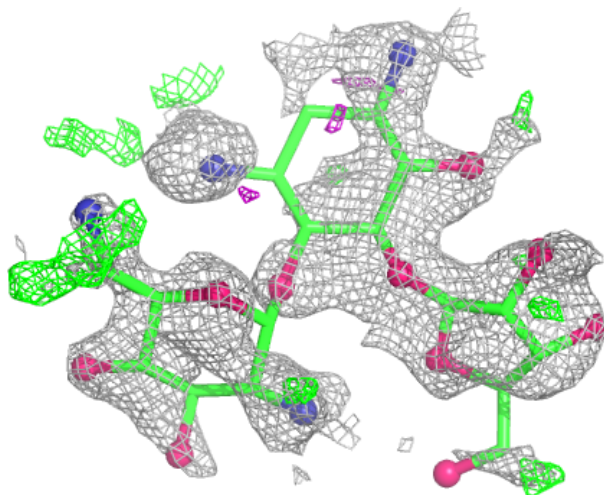
Electron density around RIO B 302 (A):

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



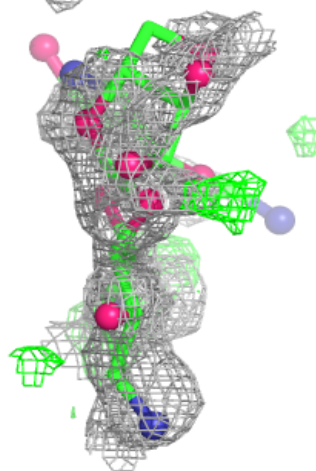
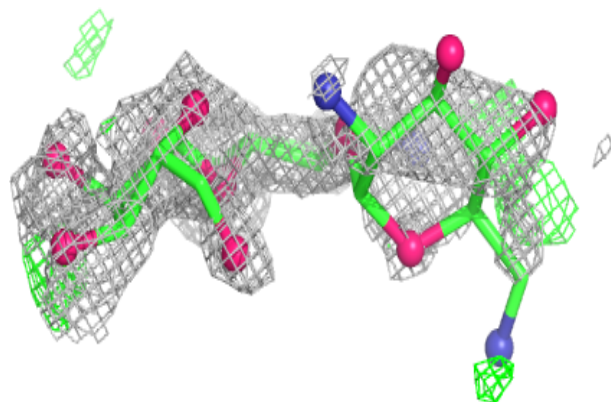
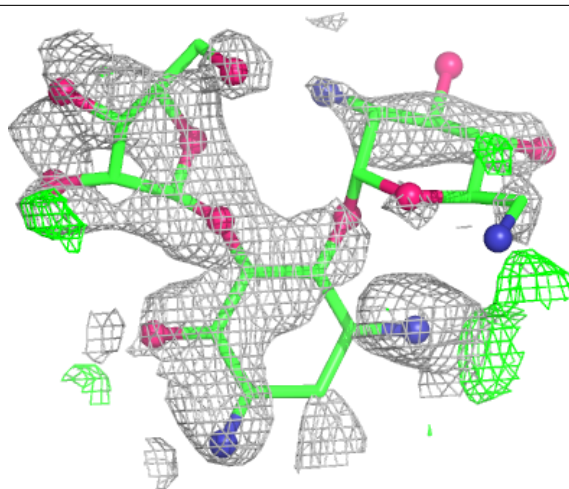
Electron density around RIO D 504 (A):

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



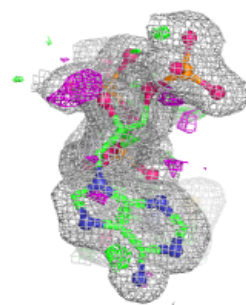
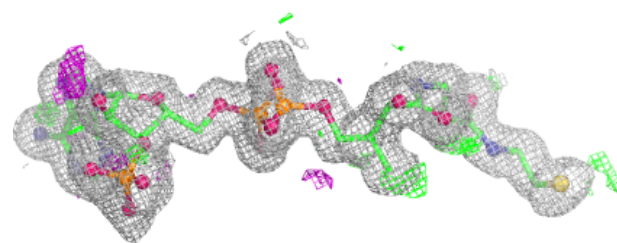
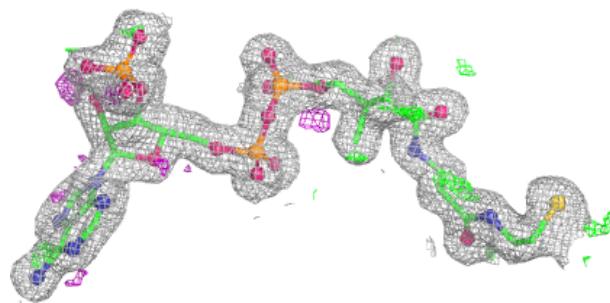
Electron density around RIO A 302 (A):

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

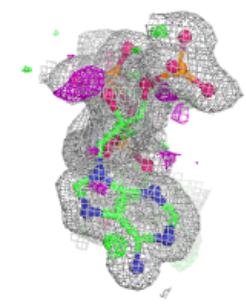
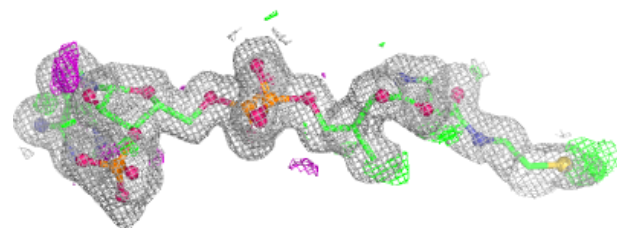
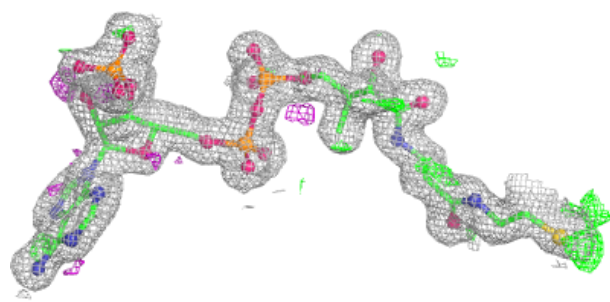


Electron density around COA C 301 (A):

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

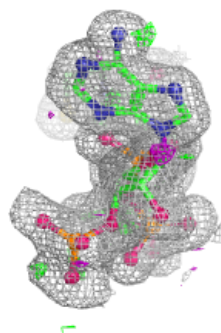
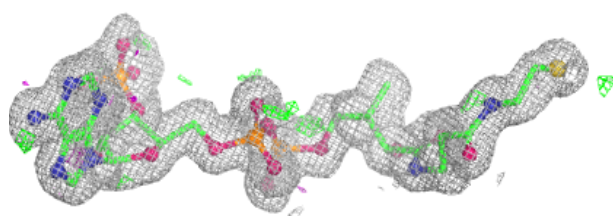
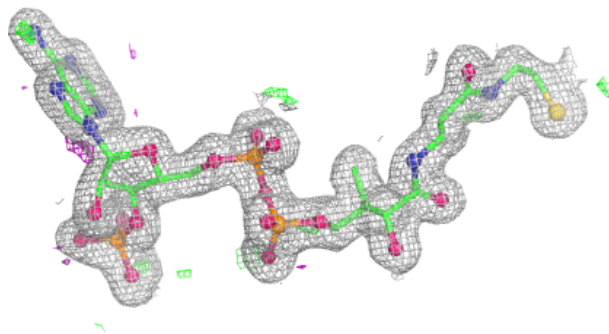
**Electron density around COA C 301 (B):**

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

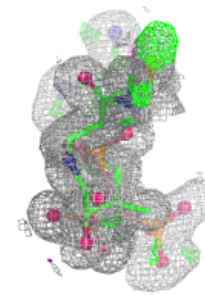
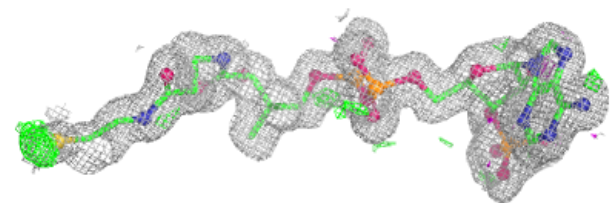
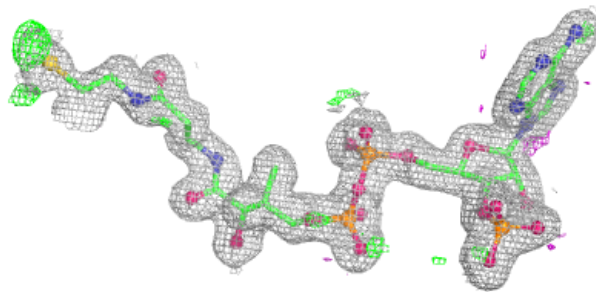


Electron density around COA D 503 (A):

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

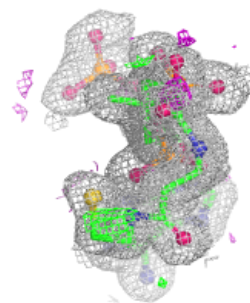
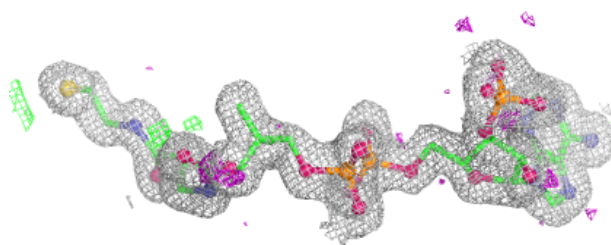
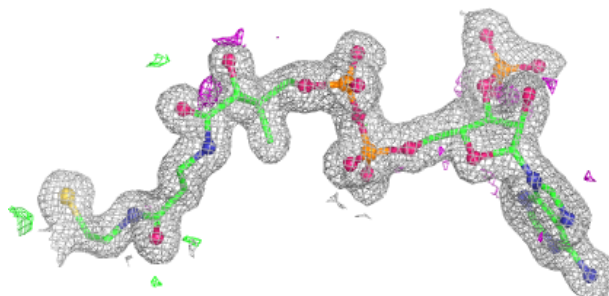
**Electron density around COA D 503 (B):**

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

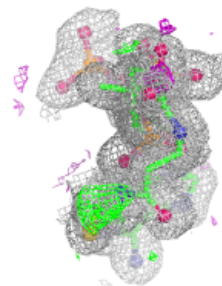
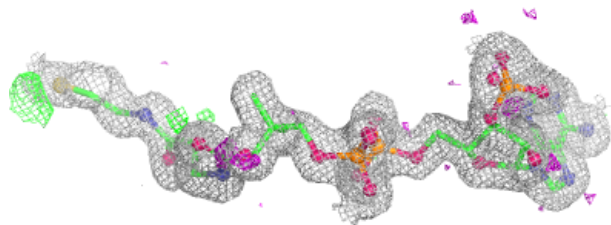
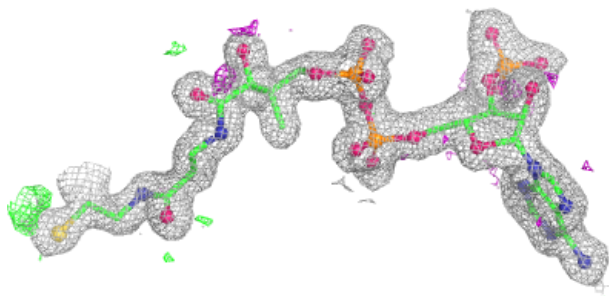


Electron density around COA A 301 (A):

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

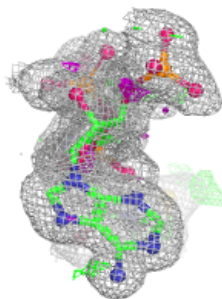
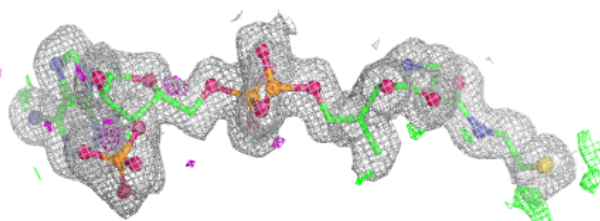
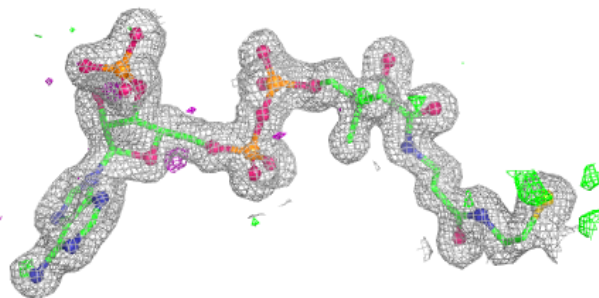
**Electron density around COA A 301 (B):**

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

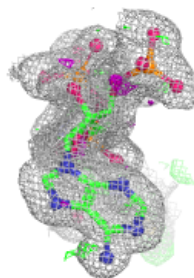
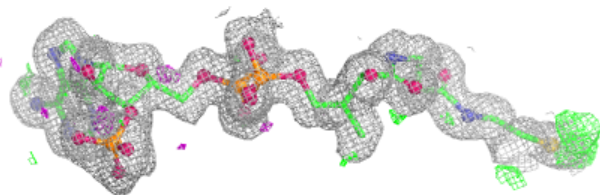
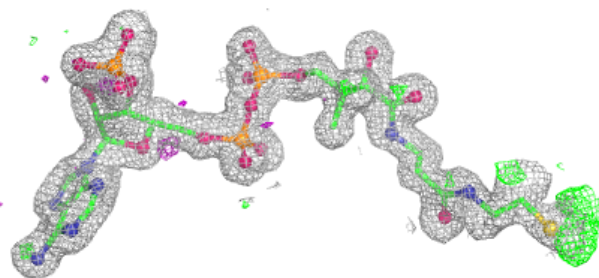


Electron density around COA B 301 (A):

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

**Electron density around COA B 301 (B):**

$2mF_o-DF_c$ (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.