



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 27, 2022 – 10:08 AM EDT

PDB ID : 7UUL  
Title : Crystal structure of aminoglycoside resistance enzyme ApmA, complex with kanamycin B and coenzyme A  
Authors : Stogios, P.J.; Evdokimova, E.; Di Leo, R.; Bordeleau, E.; Wright, G.D.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2022-04-28  
Resolution : 2.26 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

The following versions of software and data (see [references](#) ①) 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	:	2.31.2
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)	:	2.31.2

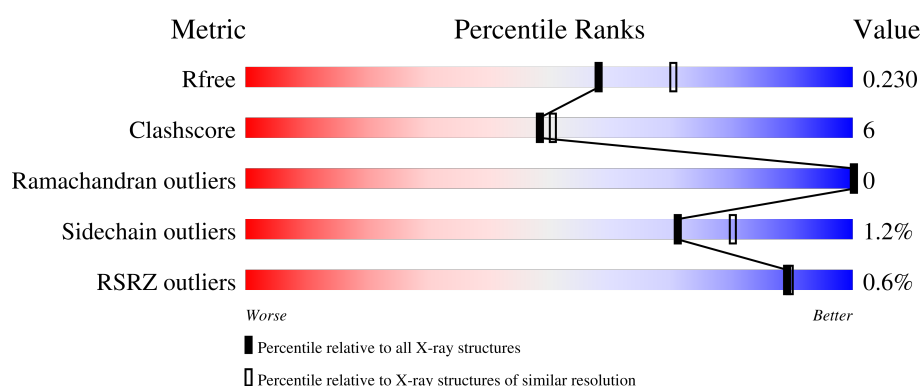
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\geq 3$ , 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	276	
1	B	276	
1	C	276	
1	D	276	
1	E	276	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	276	 <div>92%7%</div>

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
3	COA	A	302	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15641 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.

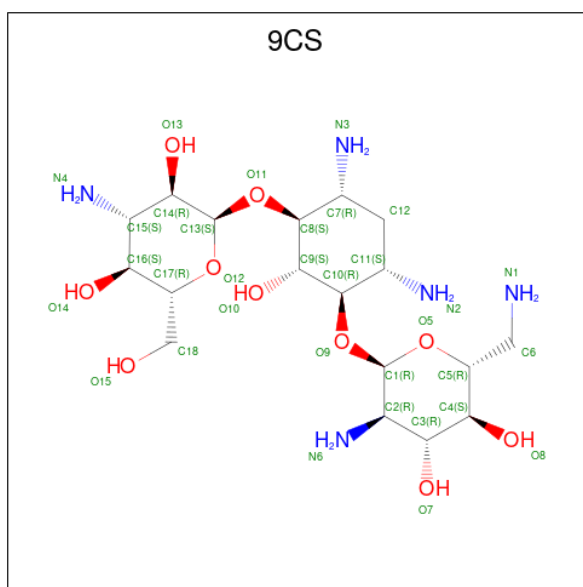
- Molecule 1 is a protein called Aminocyclitol acetyltransferase ApmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	2	0
			2201	1406	368	418	9			
1	B	275	Total	C	N	O	S	0	1	0
			2208	1410	373	416	9			
1	C	273	Total	C	N	O	S	0	1	0
			2194	1403	369	413	9			
1	D	275	Total	C	N	O	S	0	0	0
			2200	1406	369	416	9			
1	E	276	Total	C	N	O	S	0	1	0
			2214	1414	371	420	9			
1	F	275	Total	C	N	O	S	0	0	0
			2200	1405	370	416	9			

There are 12 discrepancies between the modelled and reference sequences:

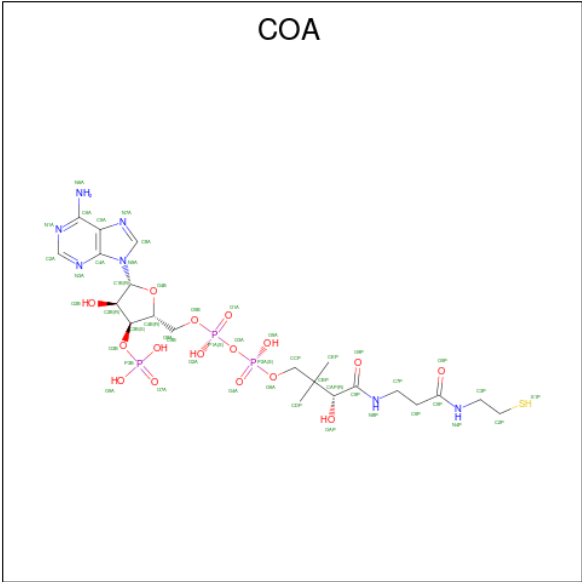
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLN	-	expression tag	UNP A0A1D0AST6
A	0	GLY	-	expression tag	UNP A0A1D0AST6
B	-1	GLN	-	expression tag	UNP A0A1D0AST6
B	0	GLY	-	expression tag	UNP A0A1D0AST6
C	-1	GLN	-	expression tag	UNP A0A1D0AST6
C	0	GLY	-	expression tag	UNP A0A1D0AST6
D	-1	GLN	-	expression tag	UNP A0A1D0AST6
D	0	GLY	-	expression tag	UNP A0A1D0AST6
E	-1	GLN	-	expression tag	UNP A0A1D0AST6
E	0	GLY	-	expression tag	UNP A0A1D0AST6
F	-1	GLN	-	expression tag	UNP A0A1D0AST6
F	0	GLY	-	expression tag	UNP A0A1D0AST6

- Molecule 2 is (1R,2S,3S,4R,6S)-4,6-DIAMINO-3-[(3-AMINO-3-DEOXY-ALPHA-D-GLUCOPYRANOSYL)OXY]-2-HYDROXYCYCLOHEXYL 2,6-DIAMINO-2,6-DIDEOXY-ALPHA-D-GLUCOPYRANOSIDE (three-letter code: 9CS) (formula: C<sub>18</sub>H<sub>37</sub>N<sub>5</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



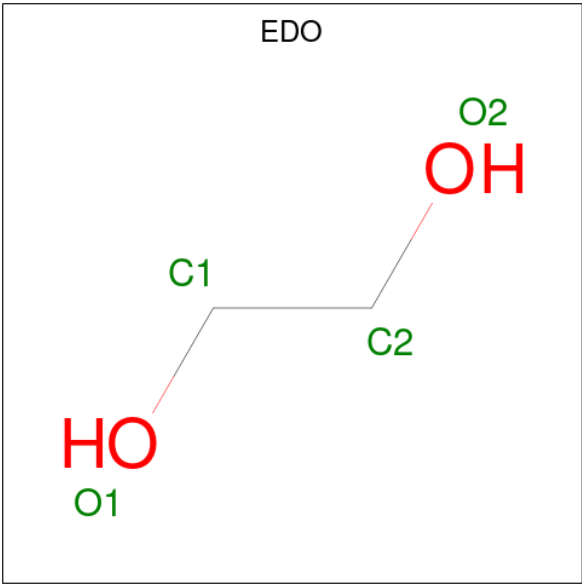
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	18	5	10		
2	B	1	Total	C	N	O	0	0
			33	18	5	10		
2	C	1	Total	C	N	O	0	0
			33	18	5	10		
2	C	1	Total	C	N	O	0	0
			33	18	5	10		
2	D	1	Total	C	N	O	0	0
			33	18	5	10		
2	E	1	Total	C	N	O	0	0
			33	18	5	10		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



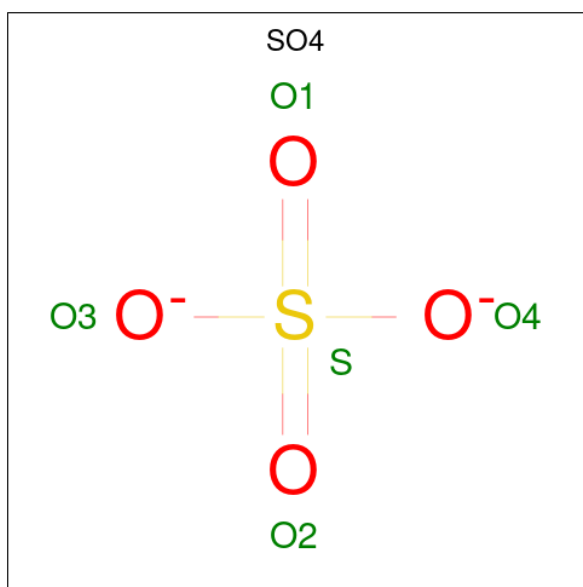
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

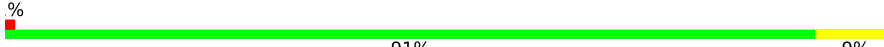
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	323	Total	O	0	14
			337	337		
7	B	307	Total	O	0	7
			314	314		
7	C	348	Total	O	0	13
			361	361		
7	D	281	Total	O	0	13
			294	294		
7	E	309	Total	O	0	12
			321	321		
7	F	261	Total	O	0	12
			273	273		

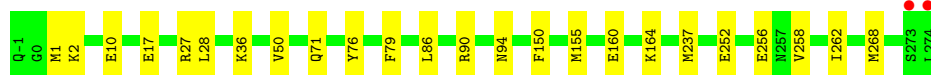


- Molecule 1: Aminocyclitol acetyltransferase ApmA



- Molecule 1: Aminocyclitol acetyltransferase ApmA

Chain E:  91% 9%



- Molecule 1: Aminocyclitol acetyltransferase ApmA

Chain F:  92% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.09Å 131.69Å 157.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.47 – 2.26 29.47 – 2.25	Depositor EDS
% Data completeness (in resolution range)	83.3 (29.47-2.26) 88.4 (29.47-2.25)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 2.26Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.172 , 0.232 0.172 , 0.230	Depositor DCC
$R_{free}$ test set	2000 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15641	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 9CS, EDO, COA, CL

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	0.43	0/2261	0.60	0/3065
1	B	0.44	0/2265	0.61	0/3069
1	C	0.43	0/2252	0.60	0/3053
1	D	0.43	0/2254	0.60	0/3054
1	E	0.41	0/2271	0.59	0/3077
1	F	0.40	0/2254	0.59	0/3055
All	All	0.42	0/13557	0.60	0/18373

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	2201	0	2132	33	0
1	B	2208	0	2145	39	0
1	C	2194	0	2128	20	0
1	D	2200	0	2135	37	0
1	E	2214	0	2147	14	0
1	F	2200	0	2132	15	0
2	A	33	0	37	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	33	0	37	3	0
2	C	66	0	74	2	0
2	D	33	0	37	2	0
2	E	33	0	37	1	0
3	A	48	0	32	24	0
3	B	48	0	32	15	0
3	C	48	0	32	3	0
3	D	48	0	32	11	0
3	E	48	0	32	1	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	16	0	24	1	0
4	D	4	0	6	0	0
4	E	4	0	6	0	0
4	F	8	0	12	0	0
5	A	10	0	0	1	0
5	B	15	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	0	0
6	D	1	0	0	0	0
7	A	337	0	0	4	0
7	B	314	0	0	2	0
7	C	361	0	0	4	0
7	D	294	0	0	4	0
7	E	321	0	0	2	0
7	F	273	0	0	2	0
All	All	15641	0	13261	161	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 6.

The worst 5 of 161 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)
3:A:302:COA:HN4	1:B:132:HIS:CB	1.69	1.06
1:B:126:ASN:HB2	3:B:302:COA:H22	1.38	1.01
3:A:302:COA:HN4	1:B:132:HIS:HB3	1.27	1.00
3:A:302:COA:N4P	1:B:132:HIS:CB	2.26	0.97
3:A:302:COA:H31	1:B:132:HIS:CG	2.04	0.92

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/276 (99%)	271 (99%)	3 (1%)	0	100	100
1	B	274/276 (99%)	266 (97%)	8 (3%)	0	100	100
1	C	272/276 (99%)	266 (98%)	6 (2%)	0	100	100
1	D	273/276 (99%)	267 (98%)	6 (2%)	0	100	100
1	E	275/276 (100%)	269 (98%)	6 (2%)	0	100	100
1	F	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
All	All	1641/1656 (99%)	1603 (98%)	38 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/238 (100%)	236 (99%)	2 (1%)	81	88
1	B	238/238 (100%)	233 (98%)	5 (2%)	53	62
1	C	237/238 (100%)	236 (100%)	1 (0%)	91	94
1	D	237/238 (100%)	233 (98%)	4 (2%)	60	71
1	E	239/238 (100%)	236 (99%)	3 (1%)	69	79
1	F	237/238 (100%)	234 (99%)	3 (1%)	69	79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1426/1428 (100%)	1408 (99%)	18 (1%)	71 79

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	256	GLU
1	F	227	ARG
1	F	207	SER
1	D	30	ARG
1	E	27	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	E	303	-	3,3,3	0.45	0	2,2,2	0.57	0
2	9CS	E	301	-	35,35,35	1.51	6 (17%)	46,52,52	1.33	6 (13%)
5	SO4	F	303	-	4,4,4	0.24	0	6,6,6	0.32	0
2	9CS	A	301	-	35,35,35	1.40	4 (11%)	46,52,52	1.22	6 (13%)
2	9CS	D	301	-	35,35,35	1.61	5 (14%)	46,52,52	1.25	6 (13%)
2	9CS	C	302	-	35,35,35	1.60	6 (17%)	46,52,52	1.30	6 (13%)
4	EDO	F	301	-	3,3,3	0.48	0	2,2,2	0.21	0
5	SO4	B	304	-	4,4,4	0.20	0	6,6,6	0.43	0
4	EDO	C	305	-	3,3,3	0.42	0	2,2,2	0.60	0
4	EDO	F	302	-	3,3,3	0.35	0	2,2,2	0.64	0
4	EDO	B	303	-	3,3,3	0.46	0	2,2,2	0.43	0
3	COA	D	302	-	41,50,50	1.07	4 (9%)	52,75,75	1.58	7 (13%)
4	EDO	A	303	-	3,3,3	0.46	0	2,2,2	0.58	0
5	SO4	C	308	-	4,4,4	0.22	0	6,6,6	0.11	0
4	EDO	C	307	-	3,3,3	0.48	0	2,2,2	0.34	0
5	SO4	A	305	-	4,4,4	0.19	0	6,6,6	0.26	0
5	SO4	E	304	-	4,4,4	0.25	0	6,6,6	0.44	0
2	9CS	B	301	-	35,35,35	1.43	4 (11%)	46,52,52	1.20	3 (6%)
4	EDO	C	306	-	3,3,3	0.47	0	2,2,2	0.14	0
5	SO4	B	306	-	4,4,4	0.18	0	6,6,6	0.36	0
5	SO4	D	304	-	4,4,4	0.18	0	6,6,6	0.45	0
4	EDO	C	304	-	3,3,3	0.40	0	2,2,2	0.14	0
3	COA	E	302	-	41,50,50	0.89	1 (2%)	52,75,75	1.25	6 (11%)
4	EDO	D	303	-	3,3,3	0.49	0	2,2,2	0.40	0
5	SO4	A	304	-	4,4,4	0.19	0	6,6,6	0.42	0
5	SO4	B	305	-	4,4,4	0.33	0	6,6,6	0.49	0
3	COA	B	302	-	41,50,50	1.17	3 (7%)	52,75,75	2.08	16 (30%)
2	9CS	C	301	-	35,35,35	1.44	5 (14%)	46,52,52	1.15	3 (6%)
3	COA	A	302	-	41,50,50	0.93	1 (2%)	52,75,75	1.45	6 (11%)
3	COA	C	303	-	41,50,50	1.08	3 (7%)	52,75,75	1.31	6 (11%)

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	EDO	E	303	-	-	0/1/1/1	-
2	9CS	E	301	-	-	2/12/72/72	0/3/3/3
2	9CS	A	301	-	-	2/12/72/72	0/3/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	9CS	D	301	-	-	3/12/72/72	0/3/3/3
2	9CS	C	302	-	-	3/12/72/72	0/3/3/3
4	EDO	F	301	-	-	0/1/1/1	-
4	EDO	C	305	-	-	1/1/1/1	-
4	EDO	F	302	-	-	0/1/1/1	-
4	EDO	B	303	-	-	1/1/1/1	-
3	COA	D	302	-	-	11/44/64/64	0/3/3/3
4	EDO	A	303	-	-	1/1/1/1	-
4	EDO	C	307	-	-	0/1/1/1	-
2	9CS	B	301	-	-	3/12/72/72	0/3/3/3
4	EDO	C	306	-	-	1/1/1/1	-
4	EDO	C	304	-	-	1/1/1/1	-
3	COA	E	302	-	-	16/44/64/64	0/3/3/3
4	EDO	D	303	-	-	0/1/1/1	-
3	COA	B	302	-	-	15/44/64/64	0/3/3/3
2	9CS	C	301	-	-	3/12/72/72	0/3/3/3
3	COA	A	302	-	-	15/44/64/64	0/3/3/3
3	COA	C	303	-	-	9/44/64/64	0/3/3/3

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	9CS	C15-N4	-3.75	1.41	1.47
2	D	301	9CS	C15-N4	-3.65	1.41	1.47
2	A	301	9CS	C2-N6	-3.57	1.41	1.47
2	B	301	9CS	C15-N4	-3.54	1.41	1.47
2	C	302	9CS	C2-N6	-3.31	1.42	1.47

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	COA	C3P-N4P-C5P	6.65	135.18	122.84
3	B	302	COA	C6P-C7P-N8P	6.04	124.08	111.90
3	A	302	COA	O6A-CCP-CBP	5.14	118.82	110.55
2	E	301	9CS	C4-C3-C2	-4.96	102.55	111.07
3	B	302	COA	O6A-CCP-CBP	4.91	118.44	110.55

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	COA	C5B-O5B-P1A-O2A
3	A	302	COA	CCP-O6A-P2A-O3A
3	A	302	COA	CCP-O6A-P2A-O4A
3	A	302	COA	CCP-O6A-P2A-O5A
3	A	302	COA	CDP-CBP-CCP-O6A

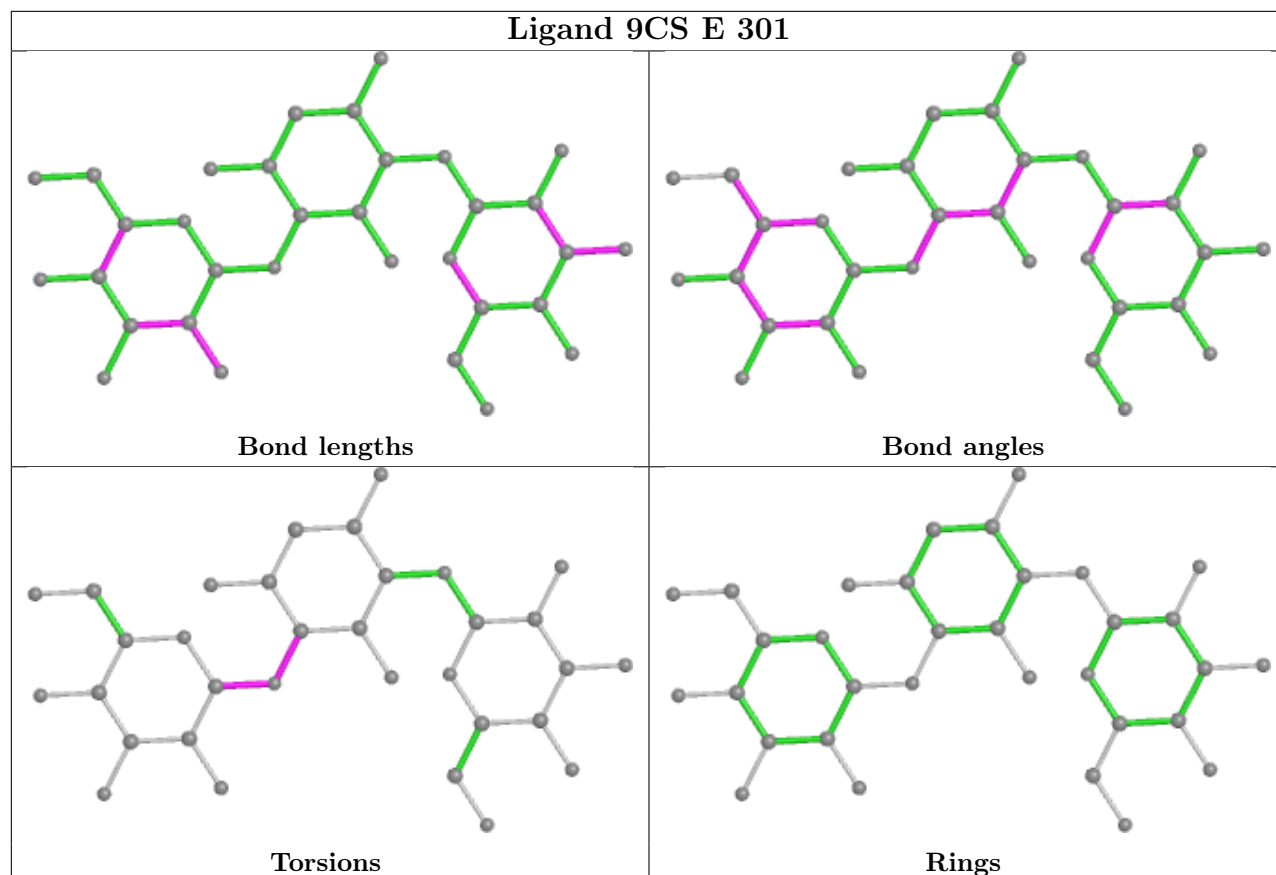
There are no ring outliers.

13 monomers are involved in 62 short contacts:

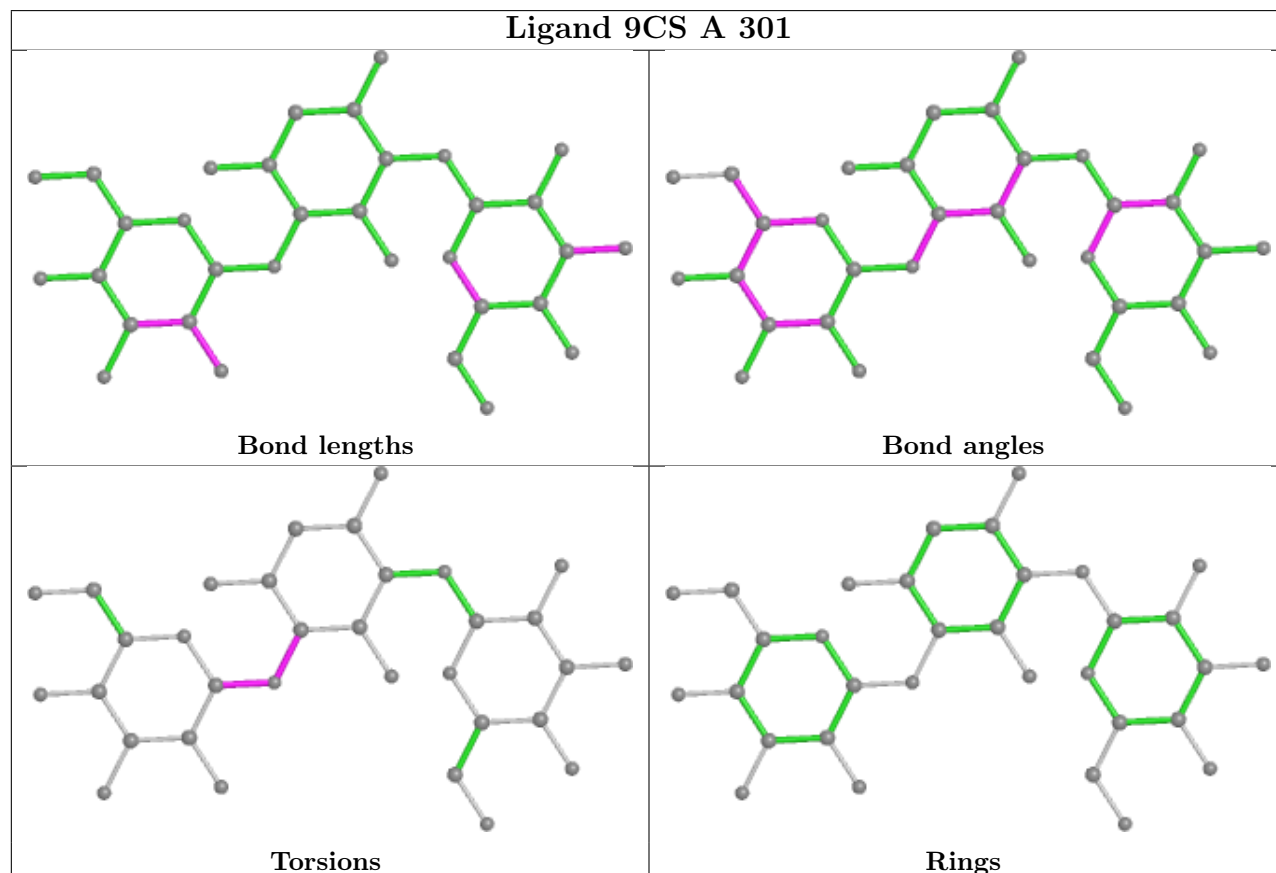
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	9CS	1	0
2	A	301	9CS	2	0
2	D	301	9CS	2	0
2	C	302	9CS	1	0
3	D	302	COA	11	0
4	C	307	EDO	1	0
2	B	301	9CS	3	0
3	E	302	COA	1	0
5	A	304	SO4	1	0
3	B	302	COA	15	0
2	C	301	9CS	1	0
3	A	302	COA	24	0
3	C	303	COA	3	0

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.

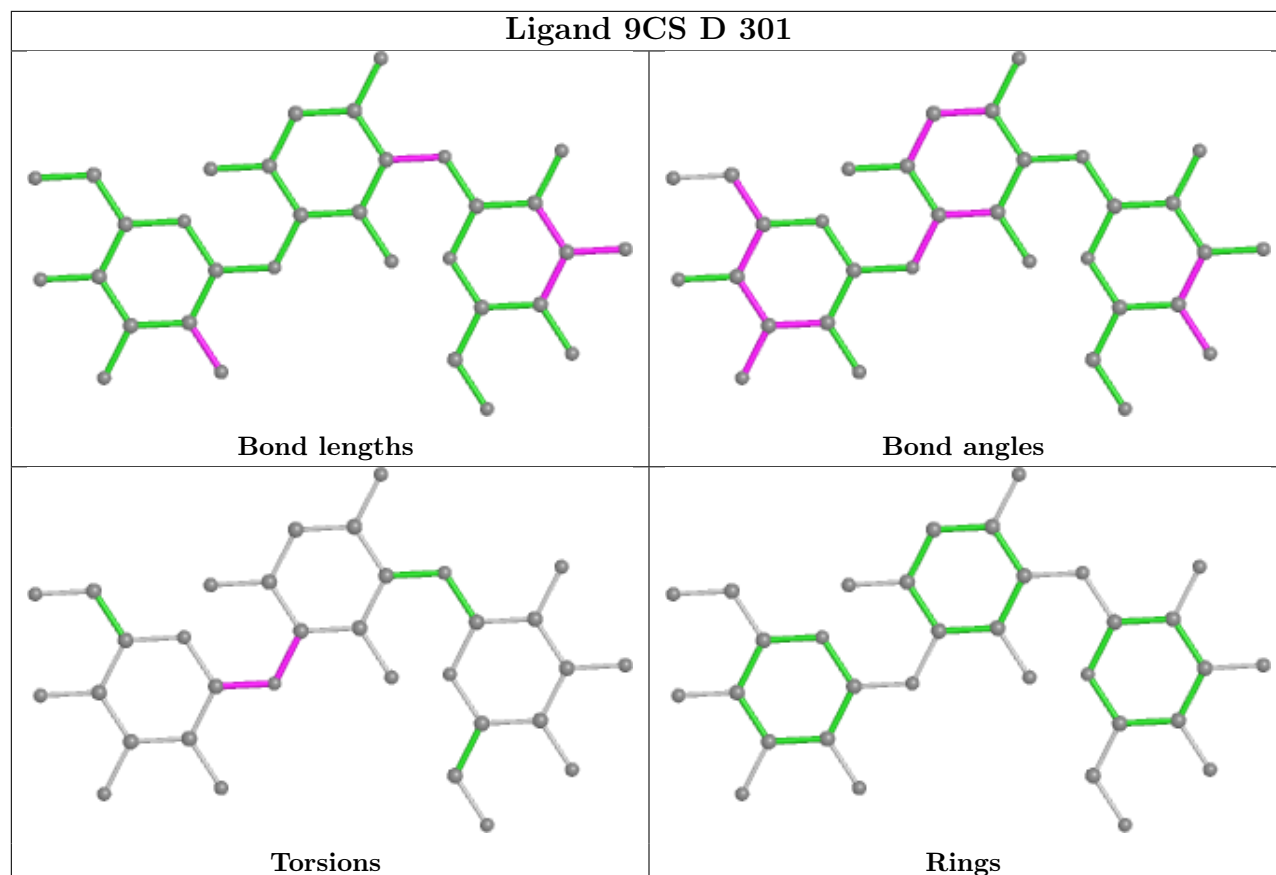
## Ligand 9CS E 301



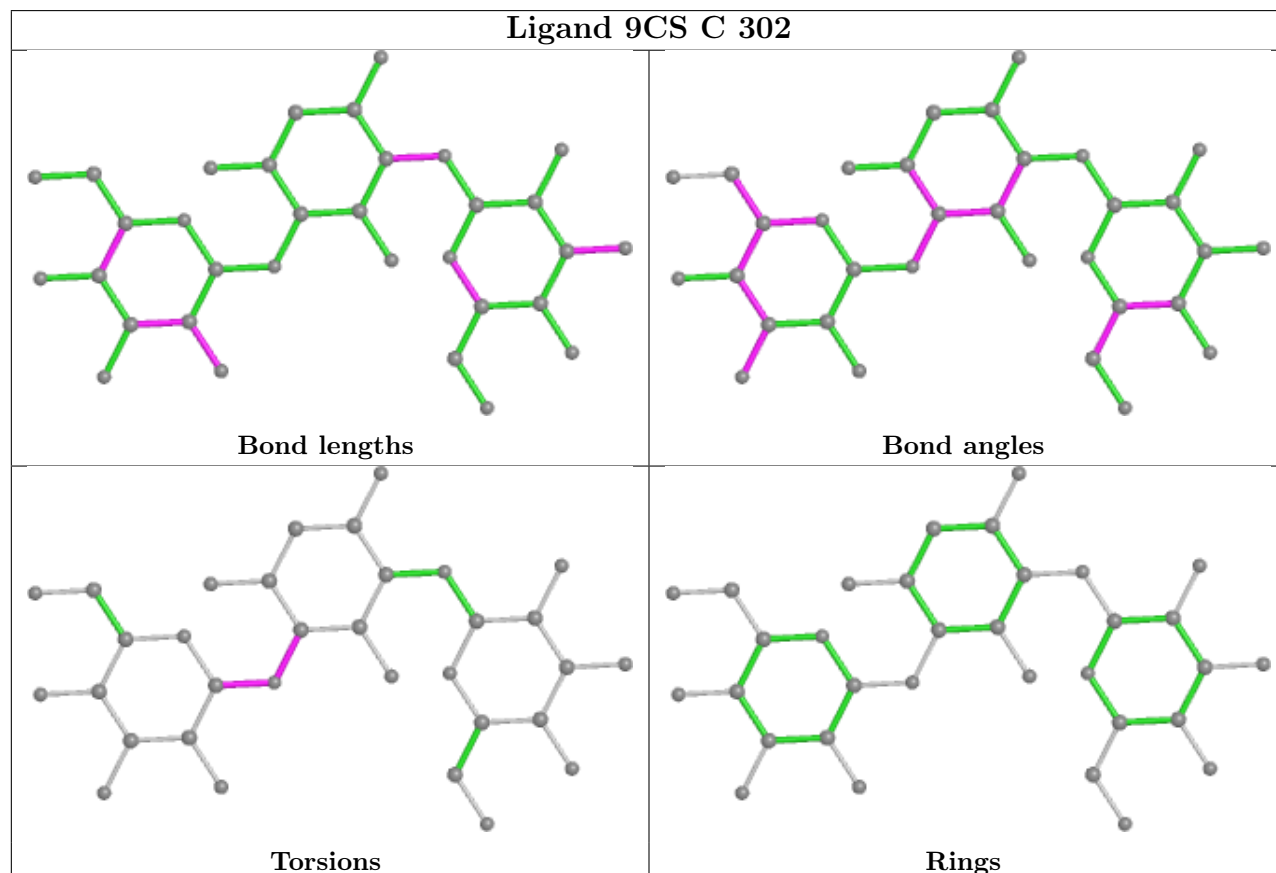
## Ligand 9CS A 301

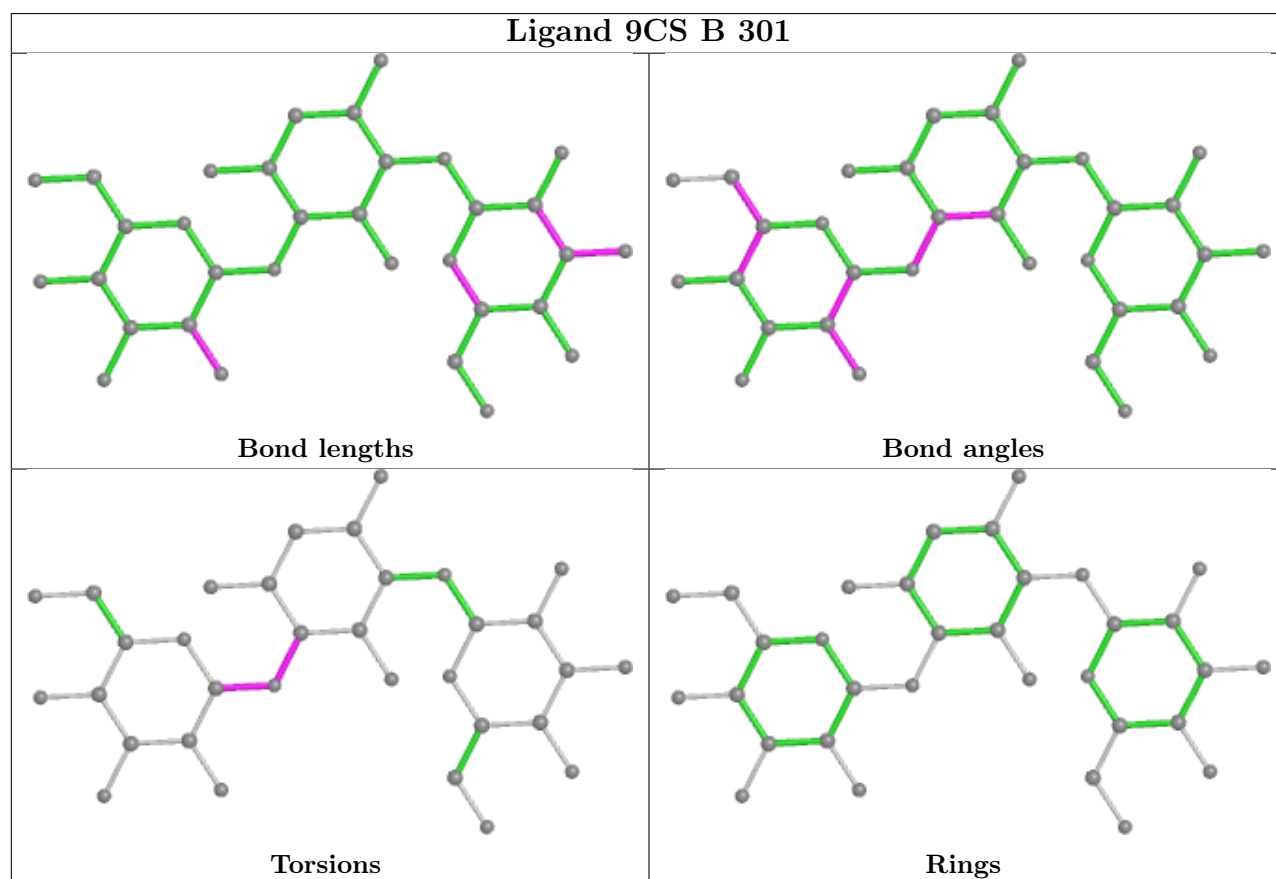
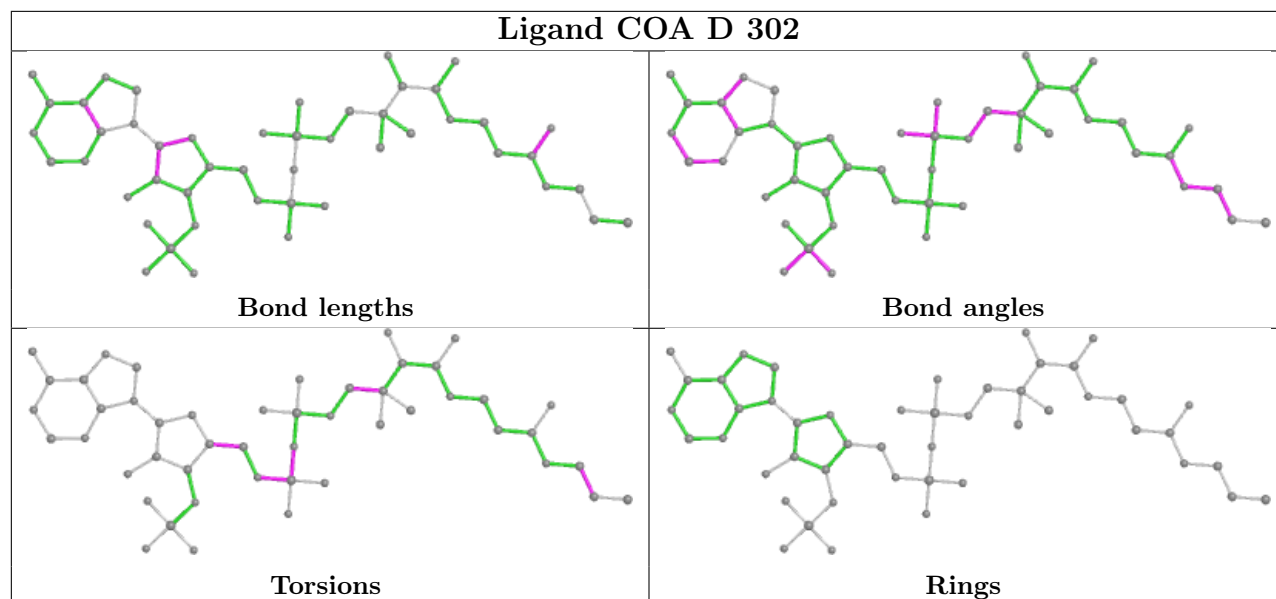


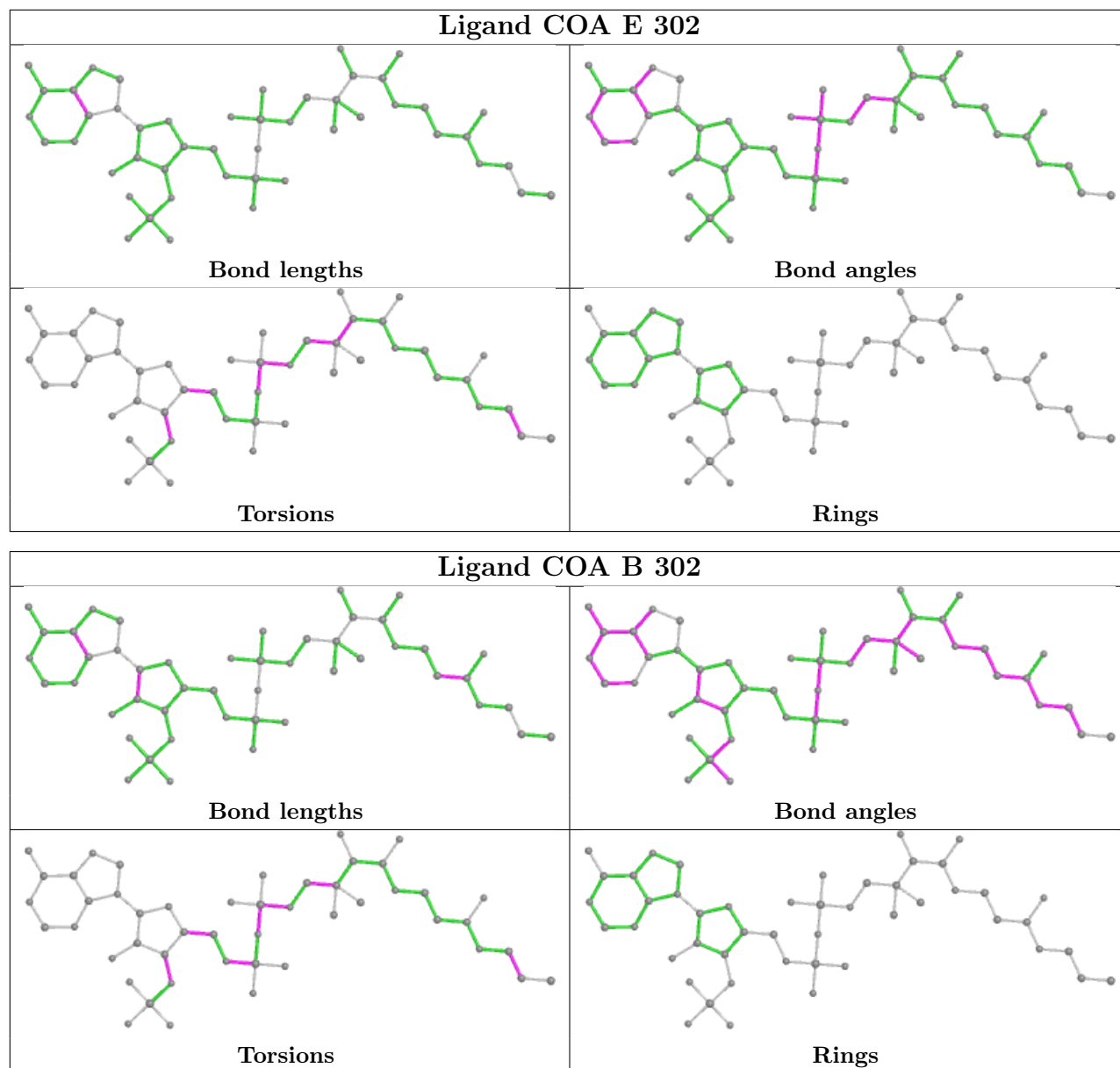
## Ligand 9CS D 301

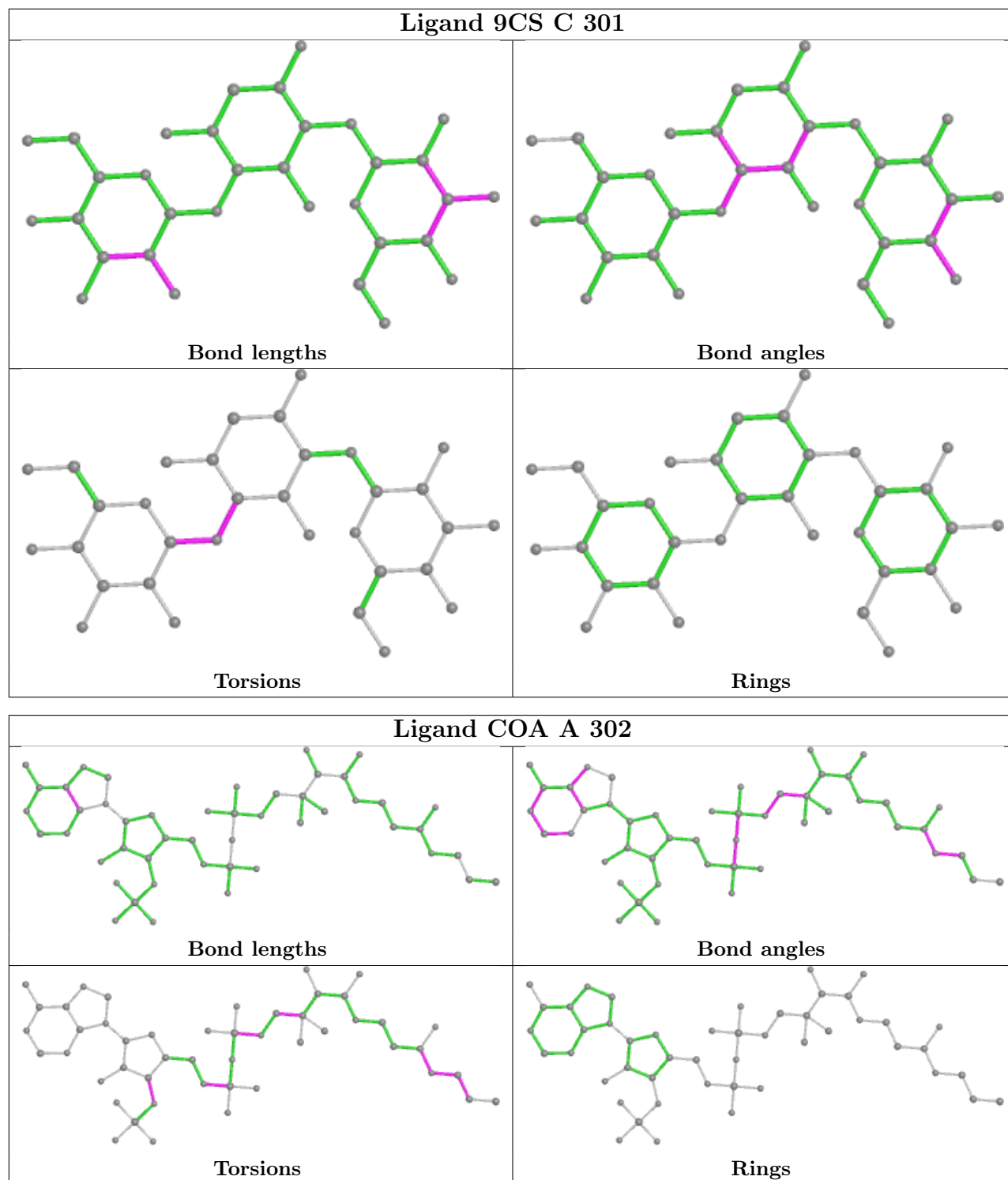


## Ligand 9CS C 302

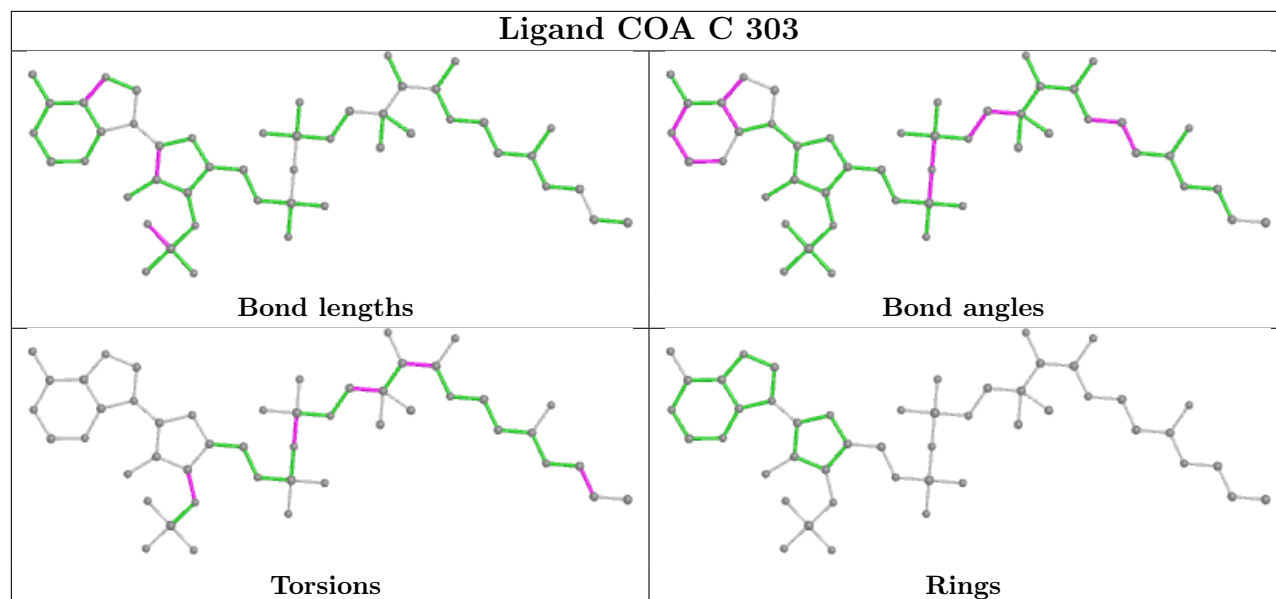












## 5.7 Other polymers [i](#)

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	274/276 (99%)	-0.46	0 <a href="#">100</a> <a href="#">100</a>	24, 34, 49, 65	0
1	B	275/276 (99%)	-0.32	3 (1%) <a href="#">80</a> <a href="#">82</a>	24, 34, 58, 86	0
1	C	273/276 (98%)	-0.52	2 (0%) <a href="#">87</a> <a href="#">88</a>	24, 32, 50, 77	0
1	D	275/276 (99%)	-0.35	2 (0%) <a href="#">87</a> <a href="#">88</a>	24, 36, 58, 94	0
1	E	276/276 (100%)	-0.32	2 (0%) <a href="#">87</a> <a href="#">88</a>	26, 37, 57, 90	0
1	F	275/276 (99%)	-0.40	1 (0%) <a href="#">92</a> <a href="#">93</a>	25, 36, 70, 103	0
All	All	1648/1656 (99%)	-0.39	10 (0%) <a href="#">89</a> <a href="#">89</a>	24, 35, 58, 103	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	GLY	4.3
1	E	274	LEU	4.1
1	E	273	SER	3.1
1	F	273	SER	3.1
1	B	273	SER	2.8

### 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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

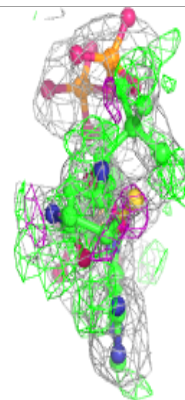
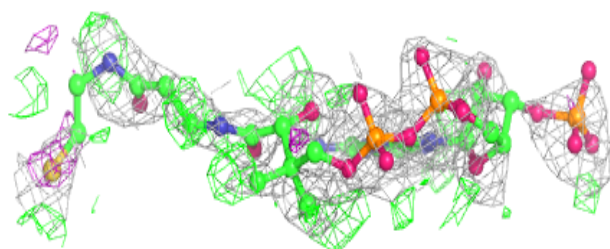
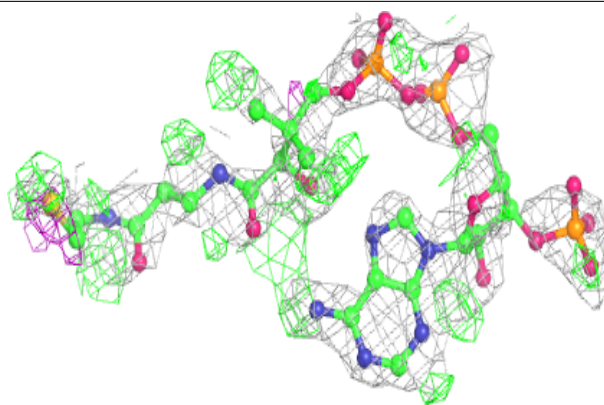
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	COA	A	302	48/48	0.72	0.29	30,39,50,56	48
3	COA	D	302	48/48	0.75	0.24	31,42,60,68	48
3	COA	E	302	48/48	0.80	0.23	35,43,53,58	48
4	EDO	C	304	4/4	0.82	0.19	40,48,48,53	0
4	EDO	C	306	4/4	0.85	0.25	51,53,53,54	0
6	CL	D	305	1/1	0.85	0.12	59,59,59,59	0
4	EDO	B	303	4/4	0.86	0.13	44,48,51,52	0
4	EDO	F	301	4/4	0.86	0.11	53,54,54,55	0
3	COA	B	302	48/48	0.86	0.19	27,38,47,51	48
5	SO4	B	306	5/5	0.87	0.37	47,48,62,66	0
3	COA	C	303	48/48	0.88	0.14	34,43,58,63	48
5	SO4	B	305	5/5	0.90	0.25	42,48,51,63	0
4	EDO	C	305	4/4	0.90	0.18	44,47,48,49	0
5	SO4	D	304	5/5	0.90	0.18	40,45,57,59	0
5	SO4	A	305	5/5	0.90	0.23	64,67,74,85	0
4	EDO	A	303	4/4	0.91	0.19	44,47,47,52	0
5	SO4	E	304	5/5	0.93	0.24	46,52,63,63	0
2	9CS	B	301	33/33	0.94	0.12	28,31,35,39	0
2	9CS	A	301	33/33	0.95	0.10	27,31,35,37	0
2	9CS	C	302	33/33	0.95	0.12	24,30,36,38	0
2	9CS	D	301	33/33	0.95	0.10	28,31,35,37	0
4	EDO	F	302	4/4	0.95	0.11	37,38,39,41	0
2	9CS	E	301	33/33	0.95	0.09	27,33,41,43	0
2	9CS	C	301	33/33	0.96	0.09	25,31,33,38	0
4	EDO	E	303	4/4	0.96	0.08	42,43,43,44	0
5	SO4	F	303	5/5	0.96	0.16	38,42,53,55	0
5	SO4	A	304	5/5	0.96	0.12	44,47,50,54	0
4	EDO	C	307	4/4	0.97	0.12	31,31,34,37	0
5	SO4	B	304	5/5	0.97	0.23	42,49,54,56	0
4	EDO	D	303	4/4	0.98	0.09	36,37,39,40	0
5	SO4	C	308	5/5	0.98	0.08	35,44,46,48	0

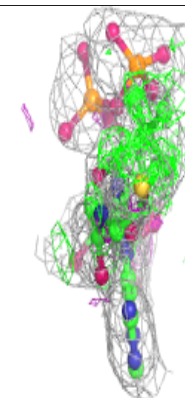
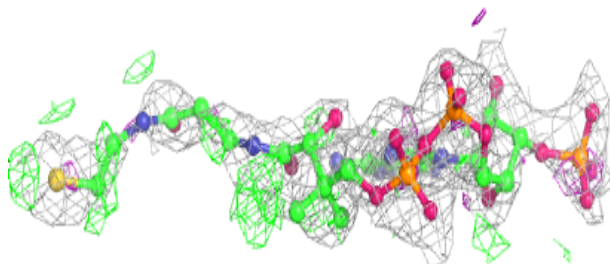
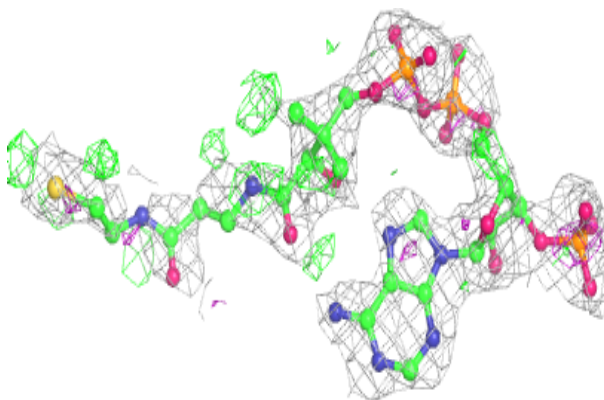
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around COA A 302:**

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

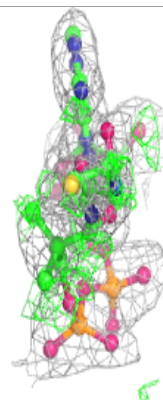
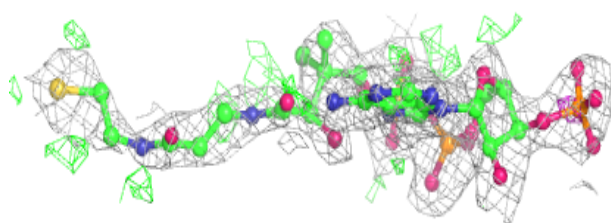
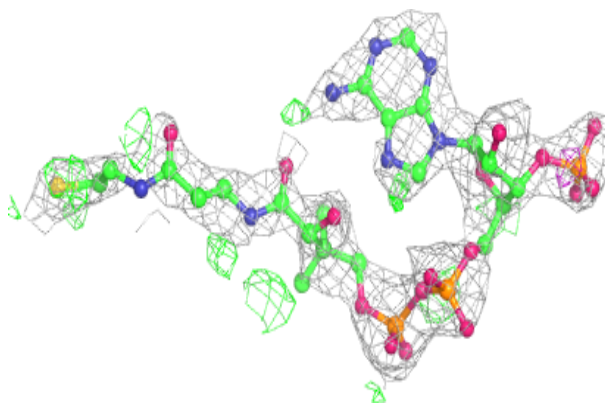
**Electron density around COA D 302:**

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

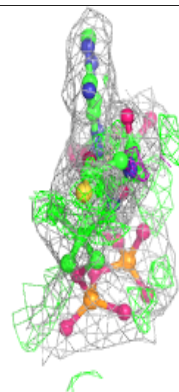
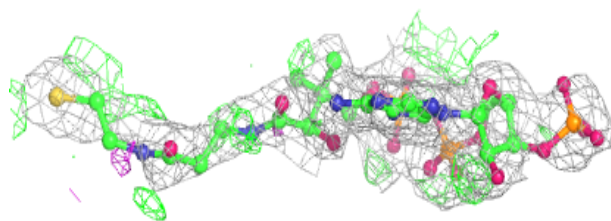
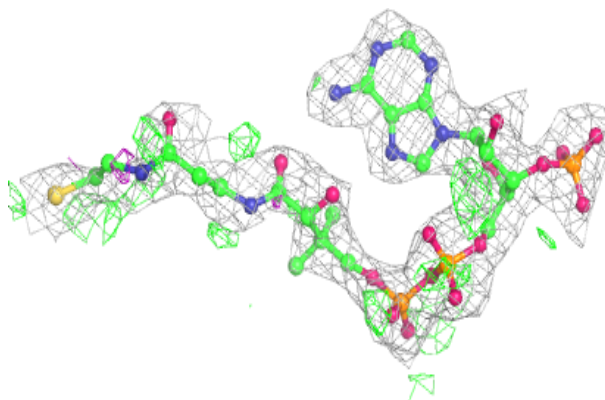


**Electron density around COA E 302:**

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

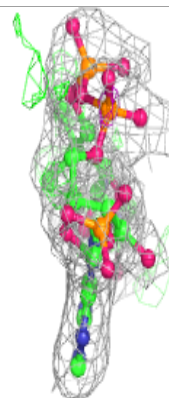
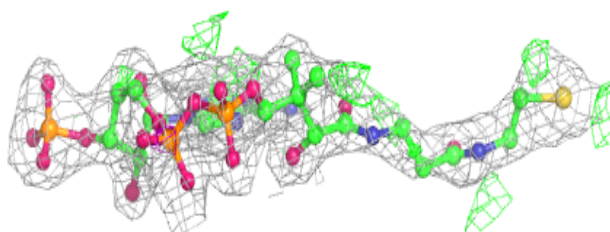
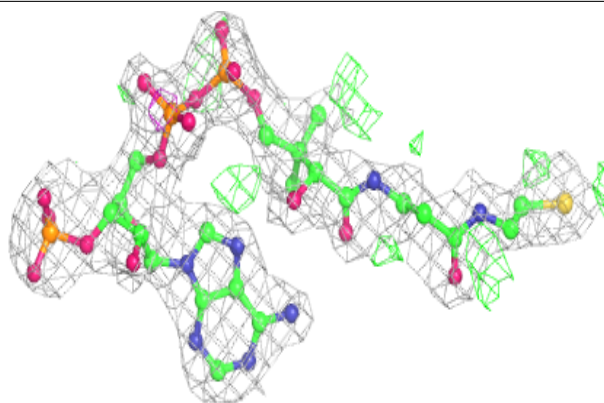
**Electron density around COA B 302:**

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

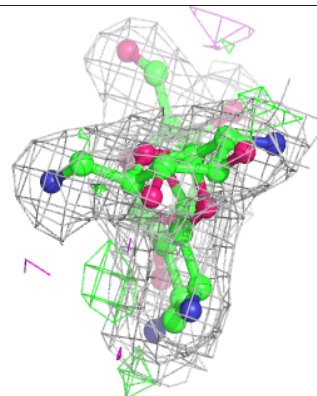
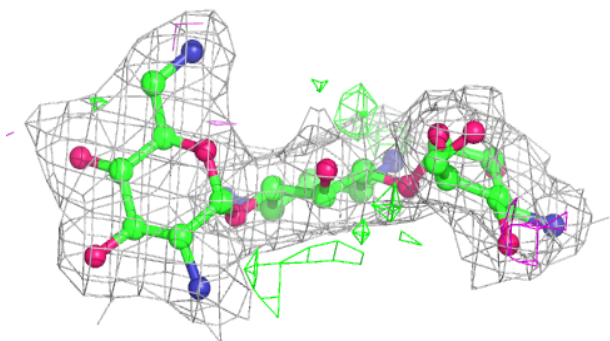
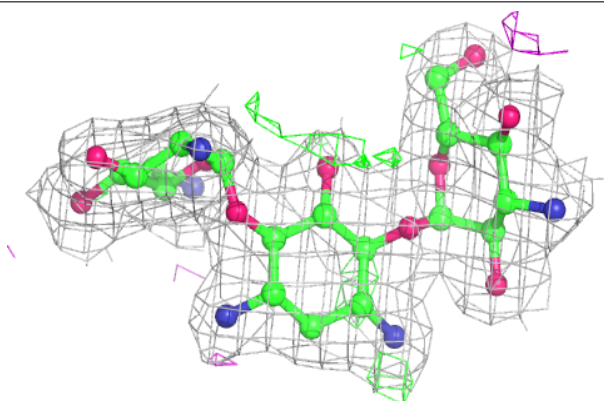


**Electron density around COA C 303:**

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

**Electron density around 9CS B 301:**

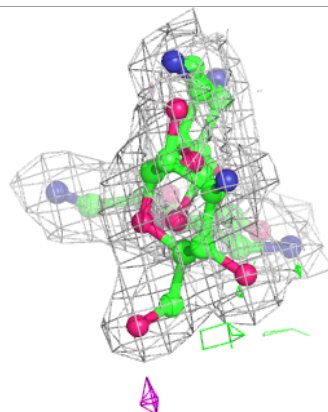
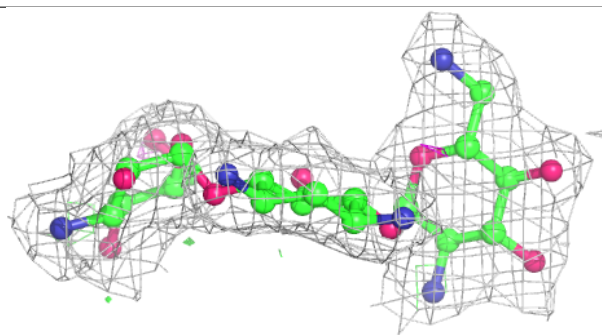
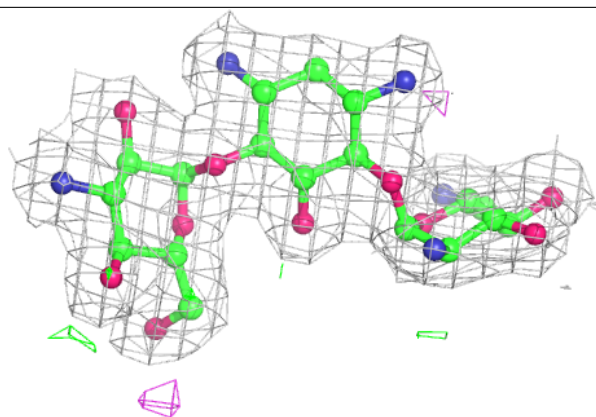
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



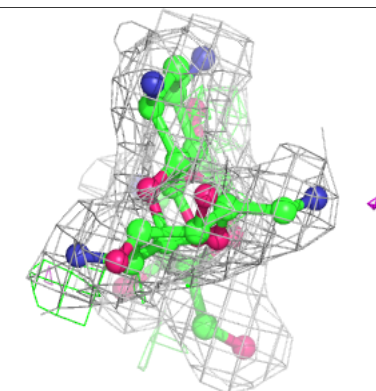
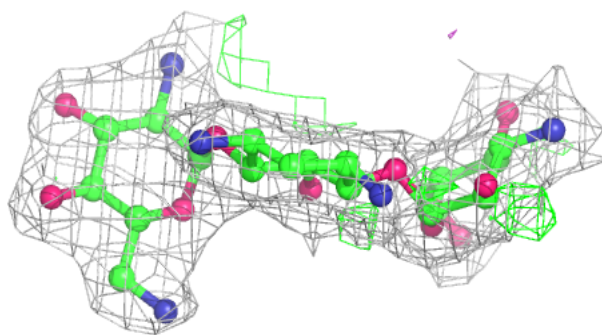
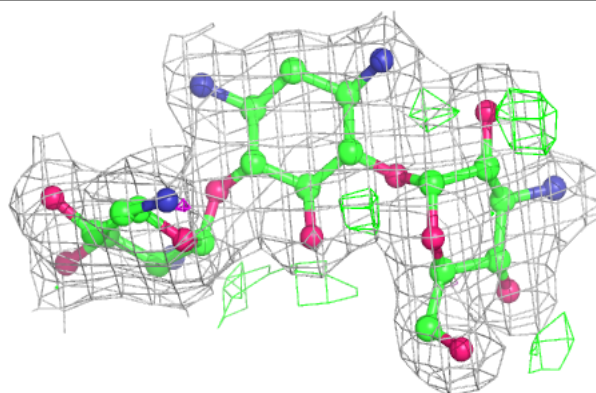


**Electron density around 9CS A 301:**

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

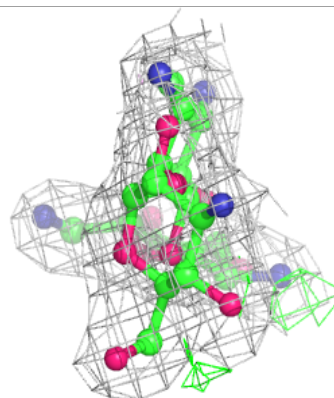
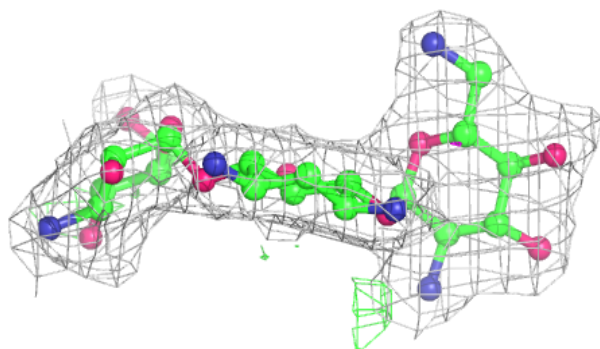
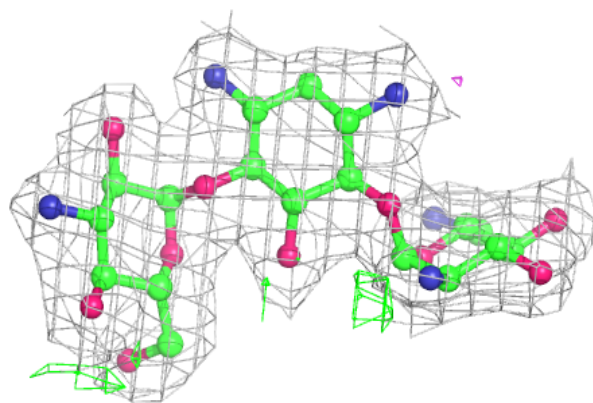
**Electron density around 9CS C 302:**

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

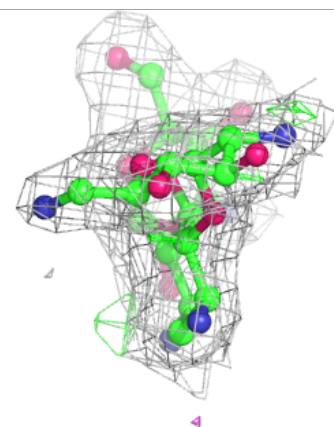
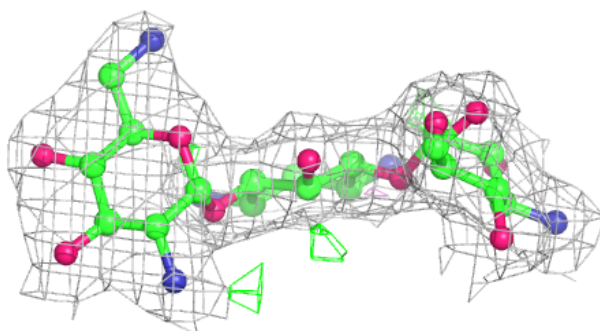
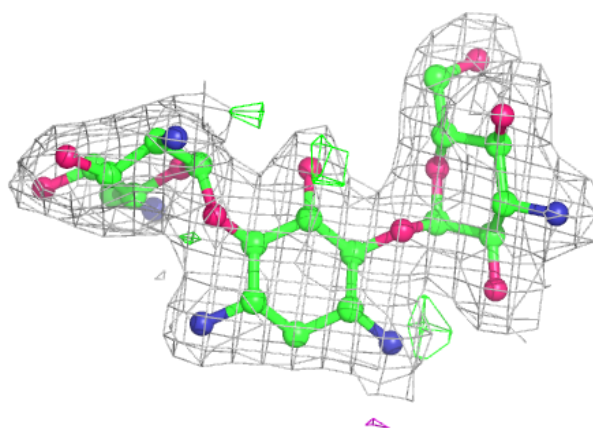


**Electron density around 9CS D 301:**

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

**Electron density around 9CS E 301:**

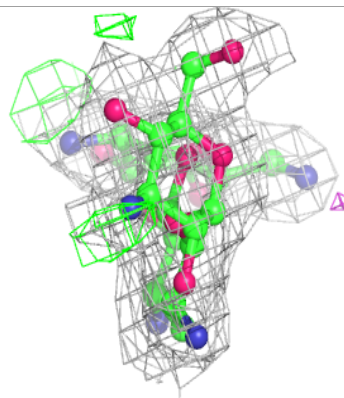
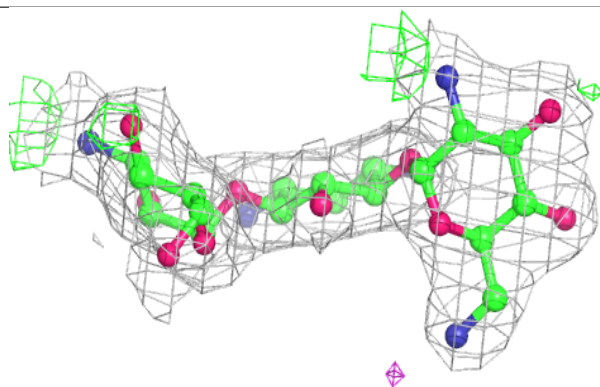
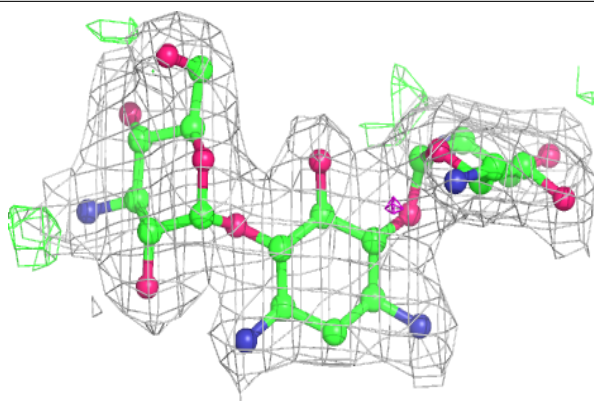
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 9CS C 301:**

$2mF_o-DF_c$  (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.