



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:24 AM UTC

PDB ID : 5US1 / pdb_00005us1
Title : Crystal structure of aminoglycoside acetyltransferase AAC(2')-Ia in complex with N2'-acetylgentamicin C1A and coenzyme A
Authors : Stogios, P.J.; Evdokimova, E.; Xu, Z.; Wawrzak, Z.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2017-02-13
Resolution : 2.48 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

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

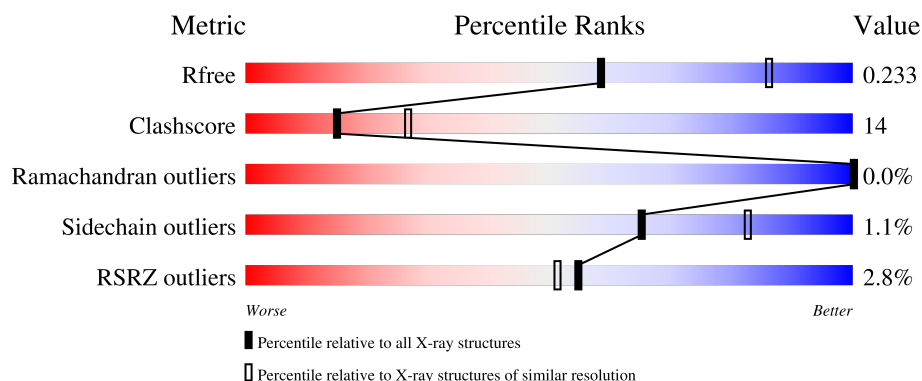
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	189	3% 77% 22% .
1	B	189	2% 78% 15% 6%
1	C	189	3% 70% 26% ..
1	D	189	6% 71% 22% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	189	3% 71% 26%
1	F	189	3% 62% 31% 7%
1	G	189	% 68% 25% 6%
1	H	189	2% 63% 30% 6%
1	I	189	2% 77% 17% 6%
1	J	189	3% 77% 18% 5%
1	K	189	3% 71% 26%
1	L	189	% 68% 25% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18350 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aminoglycoside 2'-N-acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1488	940	256	282	10			
1	B	178	Total	C	N	O	S	0	1	0
			1419	899	241	270	9			
1	C	185	Total	C	N	O	S	0	0	0
			1462	922	252	278	10			
1	D	177	Total	C	N	O	S	0	1	0
			1411	894	240	269	8			
1	E	184	Total	C	N	O	S	0	2	0
			1463	924	249	280	10			
1	F	176	Total	C	N	O	S	0	0	0
			1401	888	238	267	8			
1	G	177	Total	C	N	O	S	0	1	0
			1412	895	241	268	8			
1	H	178	Total	C	N	O	S	0	1	0
			1421	900	243	269	9			
1	I	178	Total	C	N	O	S	0	0	0
			1413	895	240	269	9			
1	J	179	Total	C	N	O	S	0	0	0
			1412	892	241	269	10			
1	K	184	Total	C	N	O	S	0	0	0
			1451	916	248	277	10			
1	L	178	Total	C	N	O	S	0	0	0
			1413	895	240	269	9			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP Q52424
A	-9	LEU	-	expression tag	UNP Q52424
A	-8	VAL	-	expression tag	UNP Q52424
A	-7	PRO	-	expression tag	UNP Q52424
A	-6	ARG	-	expression tag	UNP Q52424

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q52424
A	-4	SER	-	expression tag	UNP Q52424
A	-3	HIS	-	expression tag	UNP Q52424
A	-2	MET	-	expression tag	UNP Q52424
A	-1	GLY	-	expression tag	UNP Q52424
A	0	SER	-	expression tag	UNP Q52424
C	-10	GLY	-	expression tag	UNP Q52424
C	-9	LEU	-	expression tag	UNP Q52424
C	-8	VAL	-	expression tag	UNP Q52424
C	-7	PRO	-	expression tag	UNP Q52424
C	-6	ARG	-	expression tag	UNP Q52424
C	-5	GLY	-	expression tag	UNP Q52424
C	-4	SER	-	expression tag	UNP Q52424
C	-3	HIS	-	expression tag	UNP Q52424
C	-2	MET	-	expression tag	UNP Q52424
C	-1	GLY	-	expression tag	UNP Q52424
C	0	SER	-	expression tag	UNP Q52424
E	-10	GLY	-	expression tag	UNP Q52424
E	-9	LEU	-	expression tag	UNP Q52424
E	-8	VAL	-	expression tag	UNP Q52424
E	-7	PRO	-	expression tag	UNP Q52424
E	-6	ARG	-	expression tag	UNP Q52424
E	-5	GLY	-	expression tag	UNP Q52424
E	-4	SER	-	expression tag	UNP Q52424
E	-3	HIS	-	expression tag	UNP Q52424
E	-2	MET	-	expression tag	UNP Q52424
E	-1	GLY	-	expression tag	UNP Q52424
E	0	SER	-	expression tag	UNP Q52424
I	-10	GLY	-	expression tag	UNP Q52424
I	-9	LEU	-	expression tag	UNP Q52424
I	-8	VAL	-	expression tag	UNP Q52424
I	-7	PRO	-	expression tag	UNP Q52424
I	-6	ARG	-	expression tag	UNP Q52424
I	-5	GLY	-	expression tag	UNP Q52424
I	-4	SER	-	expression tag	UNP Q52424
I	-3	HIS	-	expression tag	UNP Q52424
I	-2	MET	-	expression tag	UNP Q52424
I	-1	GLY	-	expression tag	UNP Q52424
I	0	SER	-	expression tag	UNP Q52424
K	-10	GLY	-	expression tag	UNP Q52424
K	-9	LEU	-	expression tag	UNP Q52424
K	-8	VAL	-	expression tag	UNP Q52424

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	-7	PRO	-	expression tag	UNP Q52424
K	-6	ARG	-	expression tag	UNP Q52424
K	-5	GLY	-	expression tag	UNP Q52424
K	-4	SER	-	expression tag	UNP Q52424
K	-3	HIS	-	expression tag	UNP Q52424
K	-2	MET	-	expression tag	UNP Q52424
K	-1	GLY	-	expression tag	UNP Q52424
K	0	SER	-	expression tag	UNP Q52424
F	-10	GLY	-	expression tag	UNP Q52424
F	-9	LEU	-	expression tag	UNP Q52424
F	-8	VAL	-	expression tag	UNP Q52424
F	-7	PRO	-	expression tag	UNP Q52424
F	-6	ARG	-	expression tag	UNP Q52424
F	-5	GLY	-	expression tag	UNP Q52424
F	-4	SER	-	expression tag	UNP Q52424
F	-3	HIS	-	expression tag	UNP Q52424
F	-2	MET	-	expression tag	UNP Q52424
F	-1	GLY	-	expression tag	UNP Q52424
F	0	SER	-	expression tag	UNP Q52424
J	-10	GLY	-	expression tag	UNP Q52424
J	-9	LEU	-	expression tag	UNP Q52424
J	-8	VAL	-	expression tag	UNP Q52424
J	-7	PRO	-	expression tag	UNP Q52424
J	-6	ARG	-	expression tag	UNP Q52424
J	-5	GLY	-	expression tag	UNP Q52424
J	-4	SER	-	expression tag	UNP Q52424
J	-3	HIS	-	expression tag	UNP Q52424
J	-2	MET	-	expression tag	UNP Q52424
J	-1	GLY	-	expression tag	UNP Q52424
J	0	SER	-	expression tag	UNP Q52424
H	-10	GLY	-	expression tag	UNP Q52424
H	-9	LEU	-	expression tag	UNP Q52424
H	-8	VAL	-	expression tag	UNP Q52424
H	-7	PRO	-	expression tag	UNP Q52424
H	-6	ARG	-	expression tag	UNP Q52424
H	-5	GLY	-	expression tag	UNP Q52424
H	-4	SER	-	expression tag	UNP Q52424
H	-3	HIS	-	expression tag	UNP Q52424
H	-2	MET	-	expression tag	UNP Q52424
H	-1	GLY	-	expression tag	UNP Q52424
H	0	SER	-	expression tag	UNP Q52424
G	-10	GLY	-	expression tag	UNP Q52424

Continued on next page...

Continued from previous page...

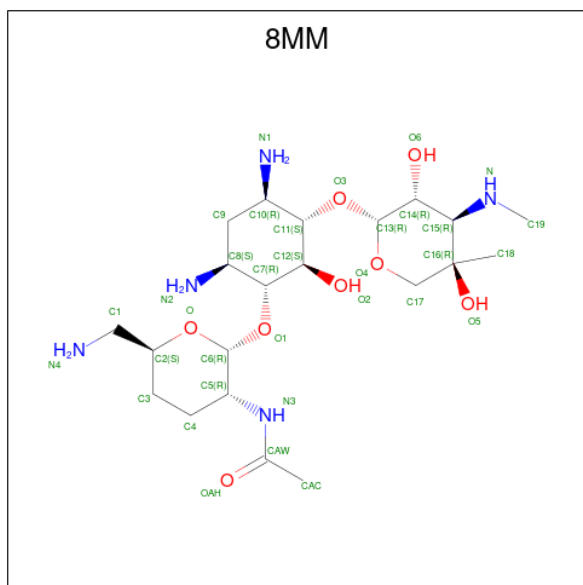
Chain	Residue	Modelled	Actual	Comment	Reference
G	-9	LEU	-	expression tag	UNP Q52424
G	-8	VAL	-	expression tag	UNP Q52424
G	-7	PRO	-	expression tag	UNP Q52424
G	-6	ARG	-	expression tag	UNP Q52424
G	-5	GLY	-	expression tag	UNP Q52424
G	-4	SER	-	expression tag	UNP Q52424
G	-3	HIS	-	expression tag	UNP Q52424
G	-2	MET	-	expression tag	UNP Q52424
G	-1	GLY	-	expression tag	UNP Q52424
G	0	SER	-	expression tag	UNP Q52424
B	-10	GLY	-	expression tag	UNP Q52424
B	-9	LEU	-	expression tag	UNP Q52424
B	-8	VAL	-	expression tag	UNP Q52424
B	-7	PRO	-	expression tag	UNP Q52424
B	-6	ARG	-	expression tag	UNP Q52424
B	-5	GLY	-	expression tag	UNP Q52424
B	-4	SER	-	expression tag	UNP Q52424
B	-3	HIS	-	expression tag	UNP Q52424
B	-2	MET	-	expression tag	UNP Q52424
B	-1	GLY	-	expression tag	UNP Q52424
B	0	SER	-	expression tag	UNP Q52424
D	-10	GLY	-	expression tag	UNP Q52424
D	-9	LEU	-	expression tag	UNP Q52424
D	-8	VAL	-	expression tag	UNP Q52424
D	-7	PRO	-	expression tag	UNP Q52424
D	-6	ARG	-	expression tag	UNP Q52424
D	-5	GLY	-	expression tag	UNP Q52424
D	-4	SER	-	expression tag	UNP Q52424
D	-3	HIS	-	expression tag	UNP Q52424
D	-2	MET	-	expression tag	UNP Q52424
D	-1	GLY	-	expression tag	UNP Q52424
D	0	SER	-	expression tag	UNP Q52424
L	-10	GLY	-	expression tag	UNP Q52424
L	-9	LEU	-	expression tag	UNP Q52424
L	-8	VAL	-	expression tag	UNP Q52424
L	-7	PRO	-	expression tag	UNP Q52424
L	-6	ARG	-	expression tag	UNP Q52424
L	-5	GLY	-	expression tag	UNP Q52424
L	-4	SER	-	expression tag	UNP Q52424
L	-3	HIS	-	expression tag	UNP Q52424
L	-2	MET	-	expression tag	UNP Q52424
L	-1	GLY	-	expression tag	UNP Q52424

Continued on next page...

Continued from previous page...

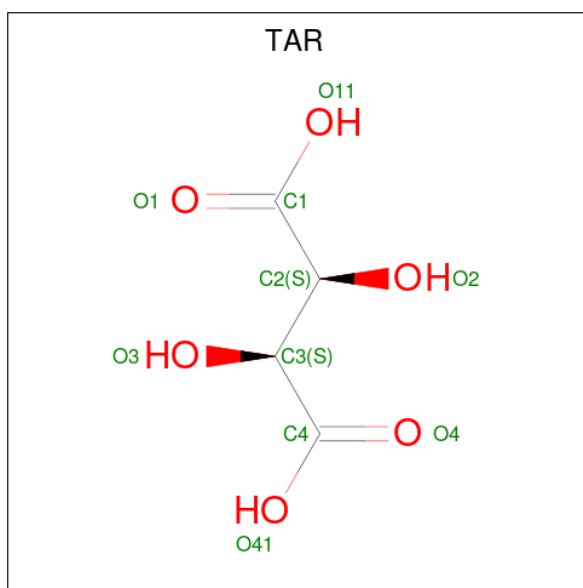
Chain	Residue	Modelled	Actual	Comment	Reference
L	0	SER	-	expression tag	UNP Q52424

- Molecule 2 is (1R,2S,3S,4R,6S)-4,6-diamino-3-[[3-deoxy-4-C-methyl-3-(methylamino)-beta-L-arabinopyranosyl]oxy]-2-hydroxycyclohexyl 2-(acetylamino)-6-amino-2,3,4,6-tetradeoxy-alpha-D-erythro-hexopyranoside (CCD ID: 8MM) (formula: C₂₁H₄₁N₅O₈).



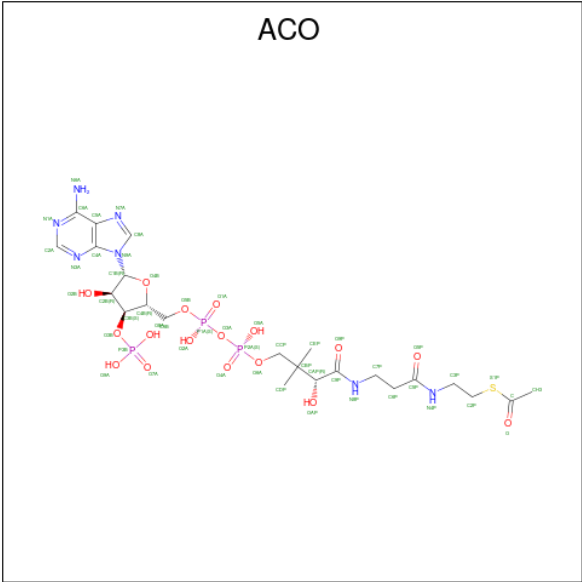
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	21	5	8		
2	B	1	Total	C	N	O	0	0
			34	21	5	8		
2	D	1	Total	C	N	O	0	0
			34	21	5	8		
2	E	1	Total	C	N	O	0	0
			34	21	5	8		
2	F	1	Total	C	N	O	0	0
			34	21	5	8		
2	G	1	Total	C	N	O	0	0
			34	21	5	8		
2	H	1	Total	C	N	O	0	0
			34	21	5	8		
2	I	1	Total	C	N	O	0	0
			34	21	5	8		
2	K	1	Total	C	N	O	0	0
			34	21	5	8		
2	L	1	Total	C	N	O	0	0
			34	21	5	8		

- Molecule 3 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



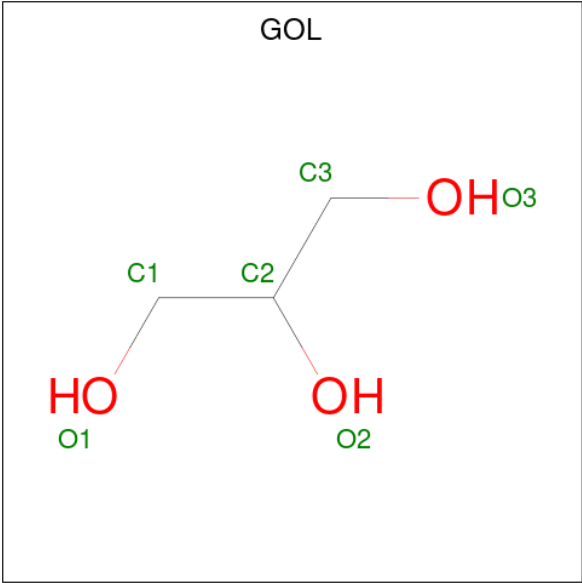
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	F	1	Total	C	O	0	0
			10	4	6		
3	H	1	Total	C	O	0	0
			10	4	6		
3	J	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



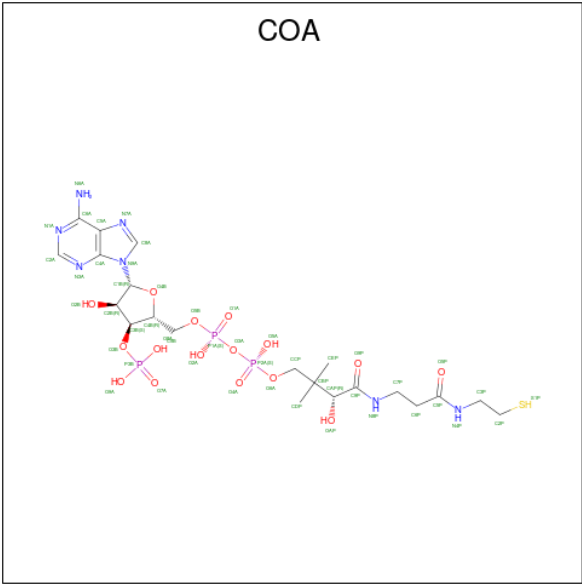
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
6	I	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
6	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total	O	0	0
			60	60		
7	B	54	Total	O	0	0
			54	54		
7	C	51	Total	O	0	1
			52	52		
7	D	42	Total	O	0	0
			42	42		
7	E	52	Total	O	0	0
			52	52		
7	F	20	Total	O	0	0
			20	20		
7	G	54	Total	O	0	0
			54	54		
7	H	37	Total	O	0	1
			38	38		

Continued on next page...

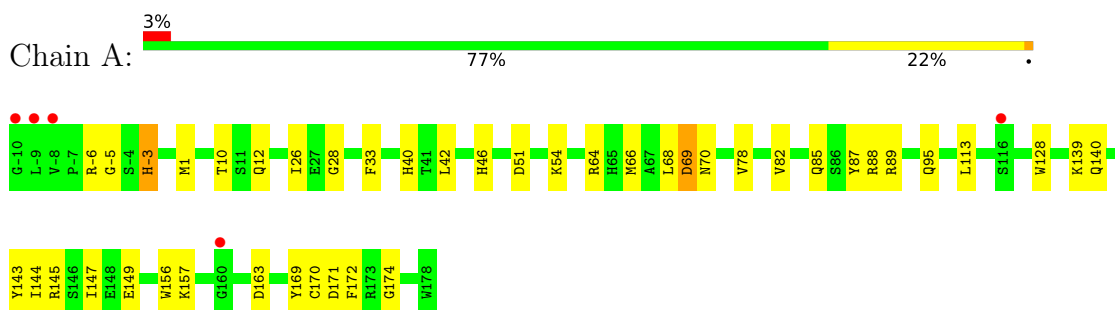
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	72	Total 72	O 72	0	0
7	J	53	Total 53	O 53	0	0
7	K	57	Total 57	O 57	0	0
7	L	27	Total 27	O 27	0	0

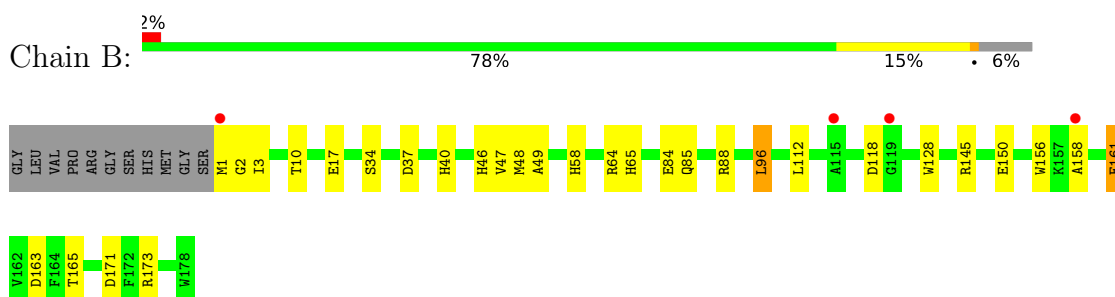
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

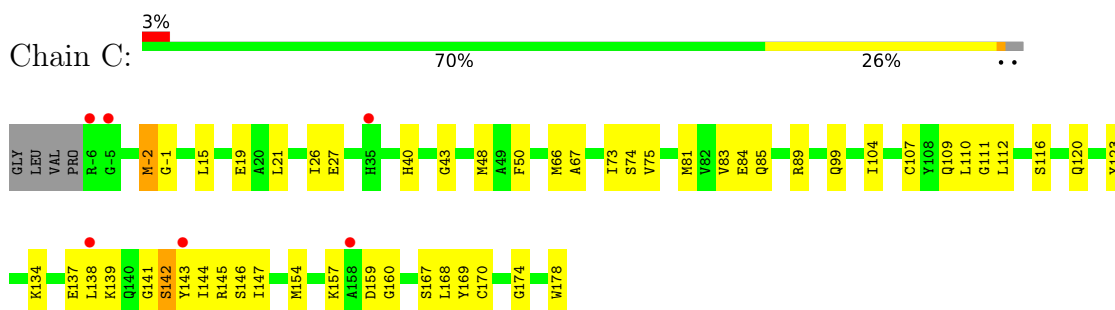
- Molecule 1: Aminoglycoside 2'-N-acetyltransferase



- Molecule 1: Aminoglycoside 2'-N-acetyltransferase

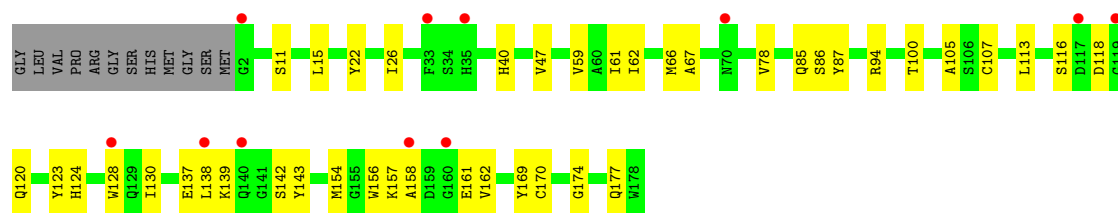


- Molecule 1: Aminoglycoside 2'-N-acetyltransferase

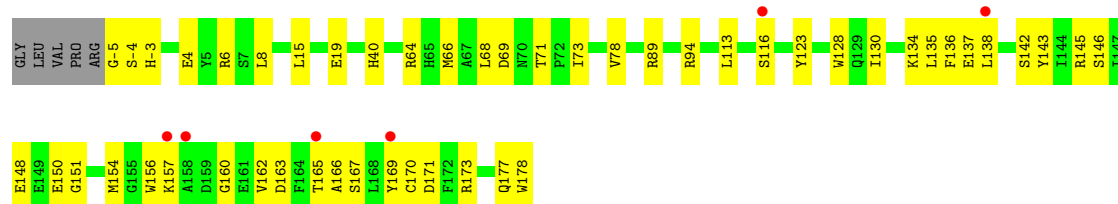


- Molecule 1: Aminoglycoside 2'-N-acetyltransferase

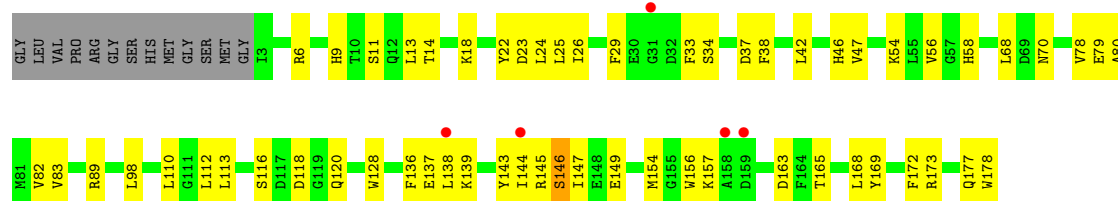




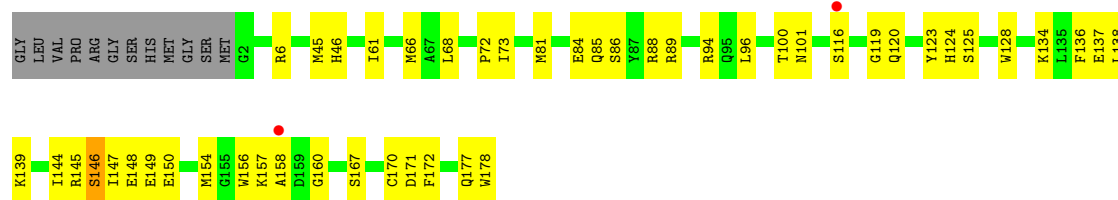
• Molecule 1: Aminoglycoside 2'-N-acetyltransferase



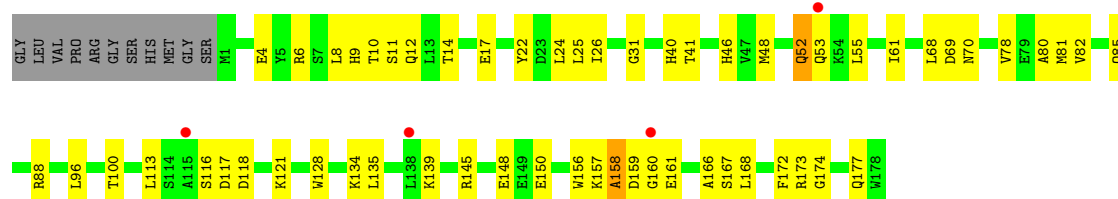
• Molecule 1: Aminoglycoside 2'-N-acetyltransferase



• Molecule 1: Aminoglycoside 2'-N-acetyltransferase

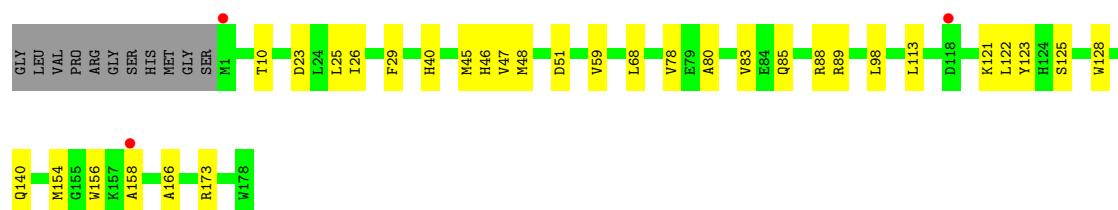


• Molecule 1: Aminoglycoside 2'-N-acetyltransferase



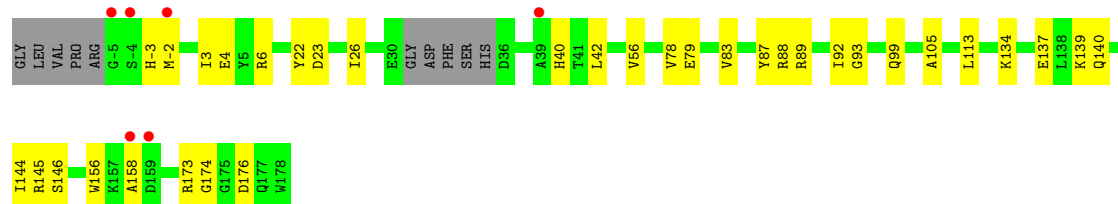
- Molecule 1: Aminoglycoside 2'-N-acetyltransferase

Chain I: 



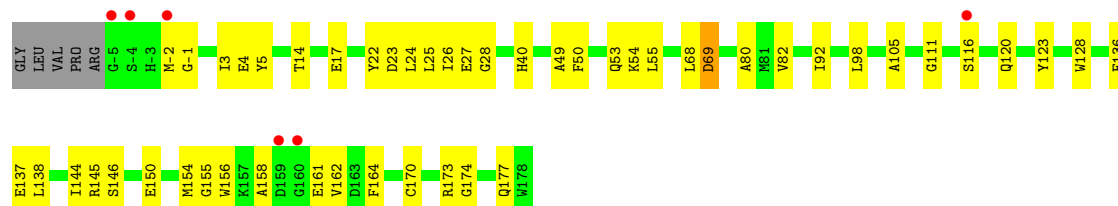
- Molecule 1: Aminoglycoside 2'-N-acetyltransferase

Chain J: 



- Molecule 1: Aminoglycoside 2'-N-acetyltransferase

Chain K: 



- Molecule 1: Aminoglycoside 2'-N-acetyltransferase

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	340.17Å 340.17Å 62.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.70 – 2.48 56.70 – 2.48	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.70-2.48) 100.0 (56.70-2.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.48Å)	Xtriage
Refinement program	PHENIX (DEV_2481: ???)	Depositor
R, R_{free}	0.187 , 0.230 0.190 , 0.233	Depositor DCC
R_{free} test set	4690 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18350	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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: COA, 8MM, TAR, GOL, ACO

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	0.24	0/1520	0.59	3/2044 (0.1%)
1	B	0.28	0/1452	0.48	0/1953
1	C	0.28	0/1493	0.51	2/2006 (0.1%)
1	D	0.21	0/1444	0.44	0/1943
1	E	0.26	0/1500	0.48	1/2016 (0.0%)
1	F	0.27	0/1431	0.54	0/1926
1	G	0.20	0/1446	0.44	0/1946
1	H	0.26	0/1454	0.53	2/1955 (0.1%)
1	I	0.21	0/1443	0.40	0/1941
1	J	0.19	0/1440	0.40	0/1934
1	K	0.29	0/1482	0.49	1/1992 (0.1%)
1	L	0.24	0/1443	0.57	2/1941 (0.1%)
All	All	0.25	0/17548	0.49	11/23597 (0.0%)

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

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

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ASP	N-CA-C	-11.24	89.08	108.08
1	L	159	ASP	N-CA-C	9.05	124.20	111.52
1	A	70	ASN	N-CA-C	-8.47	102.25	112.59
1	C	143	TYR	N-CA-C	6.34	118.78	108.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	69	ASP	N-CA-C	-5.74	98.57	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	88	ARG	Sidechain

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	1488	0	1438	31	0
1	B	1419	0	1371	21	0
1	C	1462	0	1408	68	0
1	D	1411	0	1359	38	0
1	E	1463	0	1409	39	0
1	F	1401	0	1348	53	0
1	G	1412	0	1358	49	0
1	H	1421	0	1376	52	0
1	I	1413	0	1363	24	0
1	J	1412	0	1366	28	0
1	K	1451	0	1395	38	0
1	L	1413	0	1363	42	0
2	A	34	0	0	1	0
2	B	34	0	0	0	0
2	D	34	0	0	0	0
2	E	34	0	0	1	0
2	F	34	0	0	2	0
2	G	34	0	0	0	0
2	H	34	0	0	1	0
2	I	34	0	0	0	0
2	K	34	0	0	0	0
2	L	34	0	0	1	0
3	A	10	0	4	0	0
3	D	10	0	4	0	0
3	F	10	0	4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	10	0	4	0	0
3	J	10	0	4	2	0
4	C	51	0	34	13	0
5	C	6	0	8	1	0
5	I	6	0	8	0	0
5	K	6	0	8	1	0
6	E	48	0	32	7	0
6	I	48	0	32	5	0
6	L	48	0	32	7	0
7	A	60	0	0	2	0
7	B	54	0	0	0	0
7	C	52	0	0	0	0
7	D	42	0	0	1	0
7	E	52	0	0	1	0
7	F	20	0	0	2	0
7	G	54	0	0	2	0
7	H	38	0	0	0	0
7	I	72	0	0	0	0
7	J	53	0	0	2	0
7	K	57	0	0	1	0
7	L	27	0	0	1	0
All	All	18350	0	16728	473	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 14.

The worst 5 of 473 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)
6:L:202:COA:O4B	6:L:202:COA:C1B	1.67	1.23
6:E:202:COA:O4B	6:E:202:COA:C1B	1.66	1.20
6:I:202:COA:O4B	6:I:202:COA:C1B	1.66	1.11
1:G:66:MET:HE3	1:G:170:CYS:CA	1.80	1.11
1:C:89:ARG:HH11	4:C:201:ACO:H4B	0.97	1.10

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	187/189 (99%)	182 (97%)	4 (2%)	1 (0%)	24	40
1	B	177/189 (94%)	167 (94%)	10 (6%)	0	100	100
1	C	183/189 (97%)	177 (97%)	6 (3%)	0	100	100
1	D	176/189 (93%)	167 (95%)	9 (5%)	0	100	100
1	E	184/189 (97%)	173 (94%)	11 (6%)	0	100	100
1	F	174/189 (92%)	169 (97%)	5 (3%)	0	100	100
1	G	176/189 (93%)	167 (95%)	9 (5%)	0	100	100
1	H	177/189 (94%)	168 (95%)	9 (5%)	0	100	100
1	I	176/189 (93%)	171 (97%)	5 (3%)	0	100	100
1	J	175/189 (93%)	167 (95%)	8 (5%)	0	100	100
1	K	182/189 (96%)	177 (97%)	5 (3%)	0	100	100
1	L	176/189 (93%)	168 (96%)	8 (4%)	0	100	100
All	All	2143/2268 (94%)	2053 (96%)	89 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-5	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/156 (100%)	154 (99%)	2 (1%)	61	80
1	B	149/156 (96%)	146 (98%)	3 (2%)	48	72
1	C	153/156 (98%)	151 (99%)	2 (1%)	61	80
1	D	148/156 (95%)	148 (100%)	0	100	100
1	E	154/156 (99%)	151 (98%)	3 (2%)	50	73
1	F	147/156 (94%)	144 (98%)	3 (2%)	48	72
1	G	148/156 (95%)	145 (98%)	3 (2%)	48	72
1	H	149/156 (96%)	148 (99%)	1 (1%)	76	88
1	I	148/156 (95%)	148 (100%)	0	100	100
1	J	148/156 (95%)	147 (99%)	1 (1%)	76	88
1	K	152/156 (97%)	152 (100%)	0	100	100
1	L	148/156 (95%)	147 (99%)	1 (1%)	76	88
All	All	1800/1872 (96%)	1781 (99%)	19 (1%)	65	83

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	116	SER
1	J	42	LEU
1	L	70	ASN
1	H	52	GLN
1	E	116	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	85	GLN
1	L	140	GLN
1	L	63	GLN
1	F	9	HIS
1	I	46	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

22 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	8MM	F	201	-	34,36,36	2.04	6 (17%)	39,53,53	2.95	11 (28%)
3	TAR	J	201	-	9,9,9	1.05	0	12,12,12	1.22	1 (8%)
2	8MM	H	201	-	34,36,36	2.19	5 (14%)	39,53,53	2.59	11 (28%)
2	8MM	B	400	-	34,36,36	1.99	4 (11%)	39,53,53	2.90	11 (28%)
2	8MM	K	201	-	34,36,36	2.10	6 (17%)	39,53,53	3.15	13 (33%)
5	GOL	C	202	-	5,5,5	0.35	0	5,5,5	0.36	0
3	TAR	D	202	-	9,9,9	1.04	0	12,12,12	1.13	0
4	ACO	C	201	-	51,53,53	3.75	15 (29%)	73,79,79	2.51	22 (30%)
6	COA	L	202	-	47,50,50	3.71	16 (34%)	69,75,75	2.02	19 (27%)
2	8MM	L	201	-	34,36,36	1.94	3 (8%)	39,53,53	2.58	12 (30%)
2	8MM	G	400	-	34,36,36	1.98	4 (11%)	39,53,53	2.68	11 (28%)
3	TAR	H	202	-	9,9,9	1.09	0	12,12,12	0.98	0
2	8MM	D	201	-	34,36,36	2.02	3 (8%)	39,53,53	2.68	11 (28%)
2	8MM	I	201	-	34,36,36	2.05	5 (14%)	39,53,53	2.84	11 (28%)
2	8MM	E	201	-	34,36,36	2.12	4 (11%)	39,53,53	2.53	12 (30%)
2	8MM	A	201	-	34,36,36	2.09	5 (14%)	39,53,53	3.60	12 (30%)
3	TAR	F	202	-	9,9,9	1.16	0	12,12,12	1.04	0
6	COA	E	202	-	47,50,50	3.73	15 (31%)	69,75,75	2.11	18 (26%)
6	COA	I	202	-	47,50,50	3.72	18 (38%)	69,75,75	1.90	17 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	I	203	-	5,5,5	0.36	0	5,5,5	0.35	0
5	GOL	K	202	-	5,5,5	0.33	0	5,5,5	0.33	0
3	TAR	A	202	-	9,9,9	1.03	0	12,12,12	1.00	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	8MM	F	201	-	-	4/15/69/69	0/3/3/3
3	TAR	J	201	-	-	3/12/12/12	-
2	8MM	H	201	-	-	5/15/69/69	0/3/3/3
2	8MM	B	400	-	-	6/15/69/69	0/3/3/3
2	8MM	K	201	-	-	5/15/69/69	0/3/3/3
5	GOL	C	202	-	-	0/4/4/4	-
3	TAR	D	202	-	-	4/12/12/12	-
4	ACO	C	201	-	-	9/51/67/67	0/3/3/3
6	COA	L	202	-	-	17/48/64/64	0/3/3/3
2	8MM	L	201	-	-	5/15/69/69	0/3/3/3
2	8MM	G	400	-	-	5/15/69/69	0/3/3/3
3	TAR	H	202	-	-	11/12/12/12	-
2	8MM	D	201	-	-	5/15/69/69	0/3/3/3
2	8MM	I	201	-	-	4/15/69/69	0/3/3/3
2	8MM	E	201	-	-	6/15/69/69	0/3/3/3
2	8MM	A	201	-	-	6/15/69/69	0/3/3/3
3	TAR	F	202	-	-	9/12/12/12	-
6	COA	E	202	-	-	5/48/64/64	0/3/3/3
6	COA	I	202	-	-	4/48/64/64	0/3/3/3
5	GOL	I	203	-	-	1/4/4/4	-
5	GOL	K	202	-	-	0/4/4/4	-
3	TAR	A	202	-	-	9/12/12/12	-

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	ACO	P2A-O3A	21.95	1.83	1.59
6	E	202	COA	P2A-O3A	11.96	1.72	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	202	COA	P2A-O3A	11.65	1.72	1.59
6	L	202	COA	P2A-O3A	11.22	1.71	1.59
6	L	202	COA	O4B-C1B	11.16	1.67	1.42

The worst 5 of 192 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	8MM	C5-N3-CAW	-16.49	100.80	122.90
2	K	201	8MM	C5-N3-CAW	-12.84	105.69	122.90
2	F	201	8MM	C5-N3-CAW	-12.17	106.59	122.90
2	I	201	8MM	C5-N3-CAW	-11.56	107.41	122.90
2	G	400	8MM	C5-N3-CAW	-10.83	108.39	122.90

There are no chirality outliers.

5 of 123 torsion outliers are listed below:

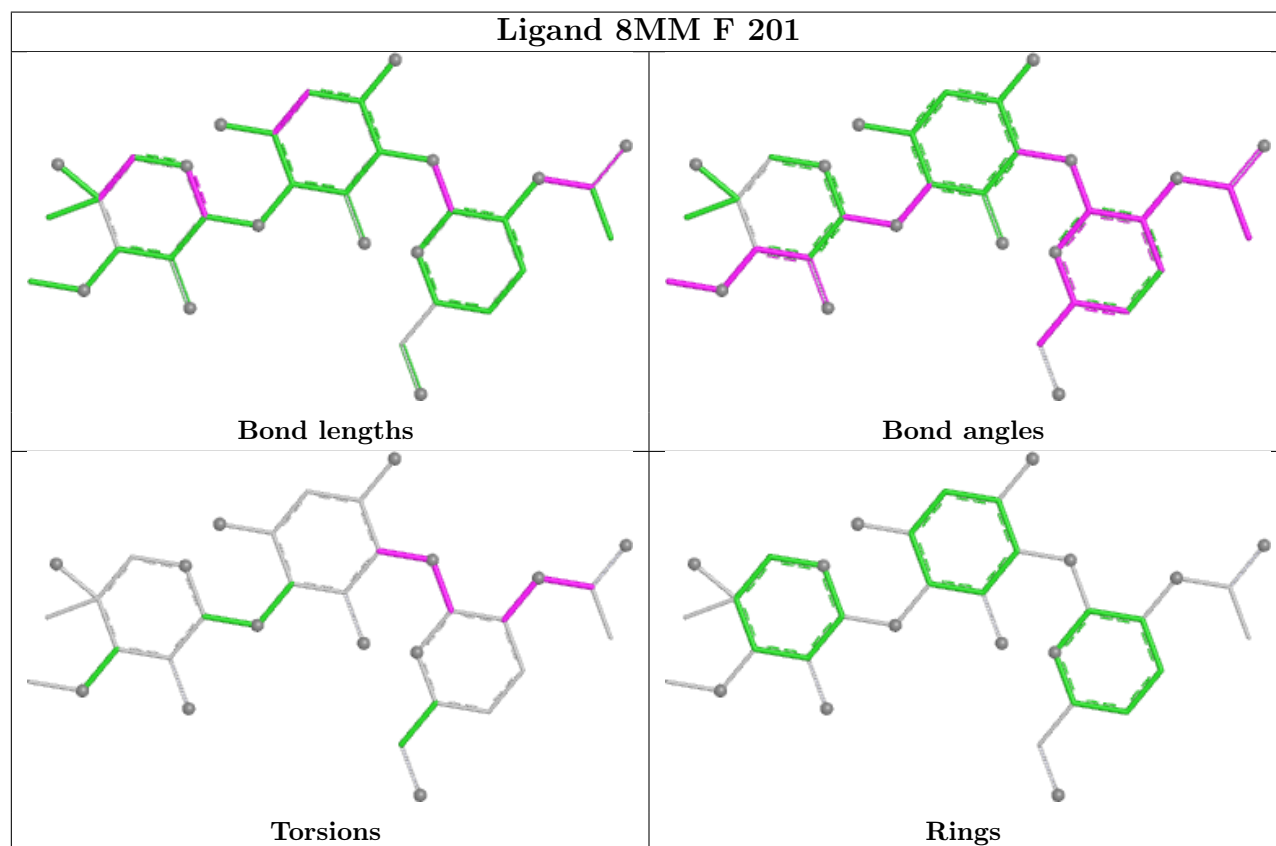
Mol	Chain	Res	Type	Atoms
2	A	201	8MM	OAH-CAW-N3-C5
2	A	201	8MM	N4-C1-C2-C3
2	A	201	8MM	N4-C1-C2-O
2	B	400	8MM	OAH-CAW-N3-C5
2	B	400	8MM	N4-C1-C2-C3

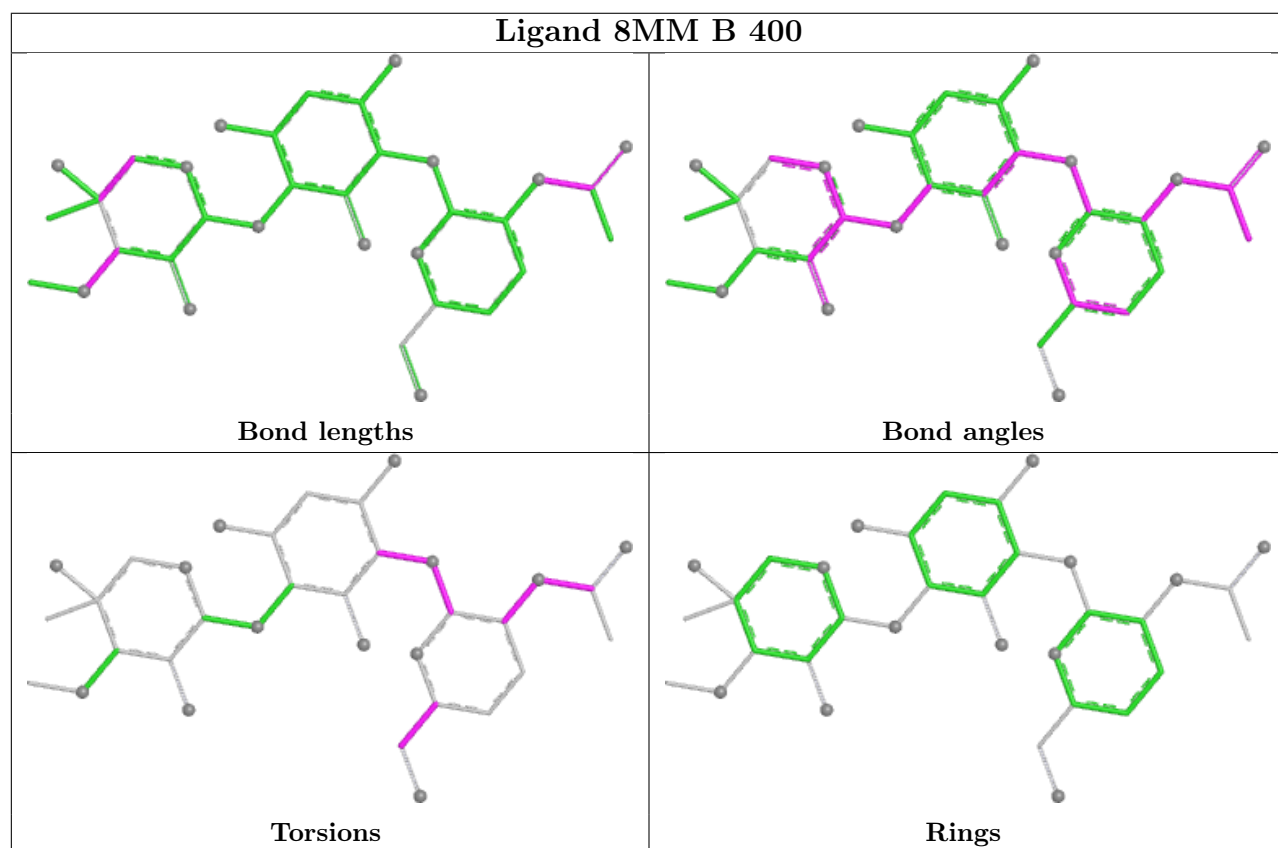
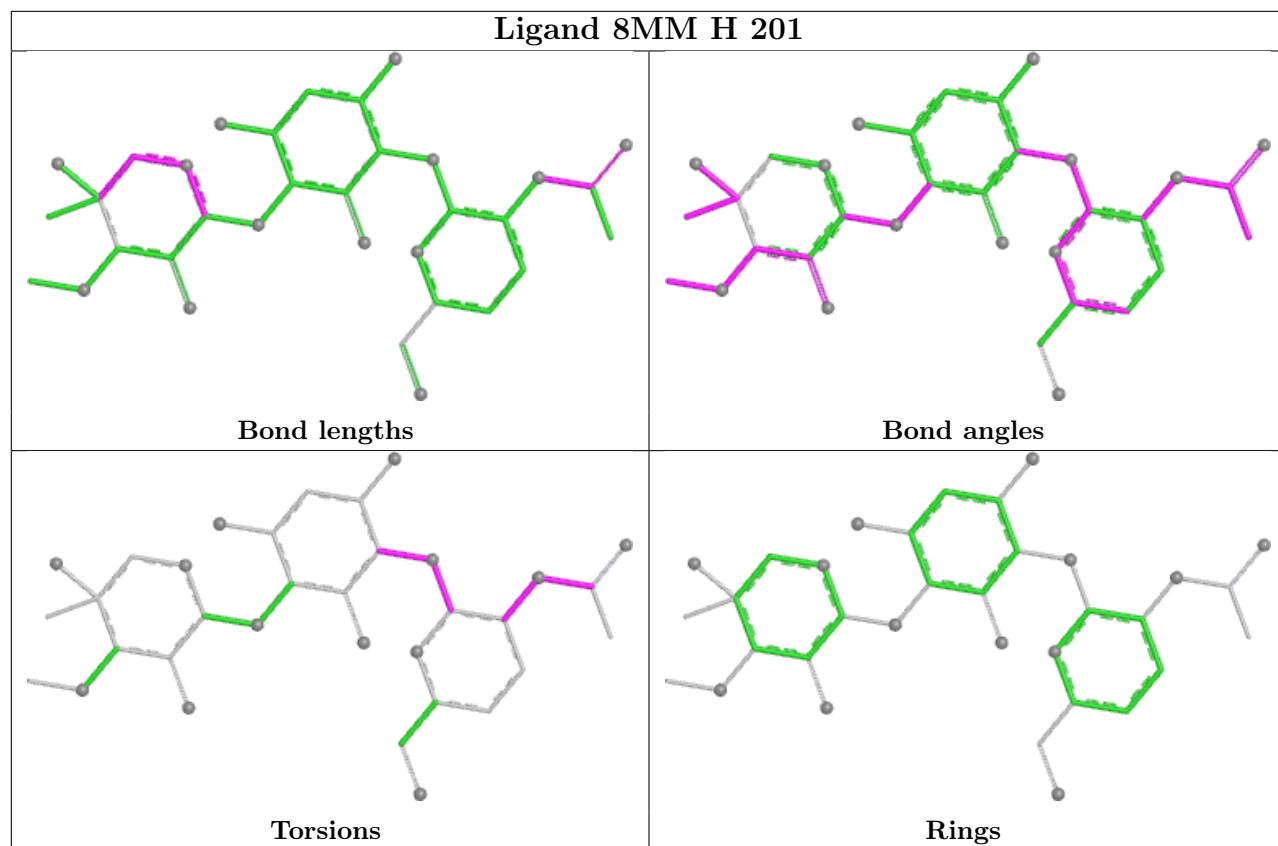
There are no ring outliers.

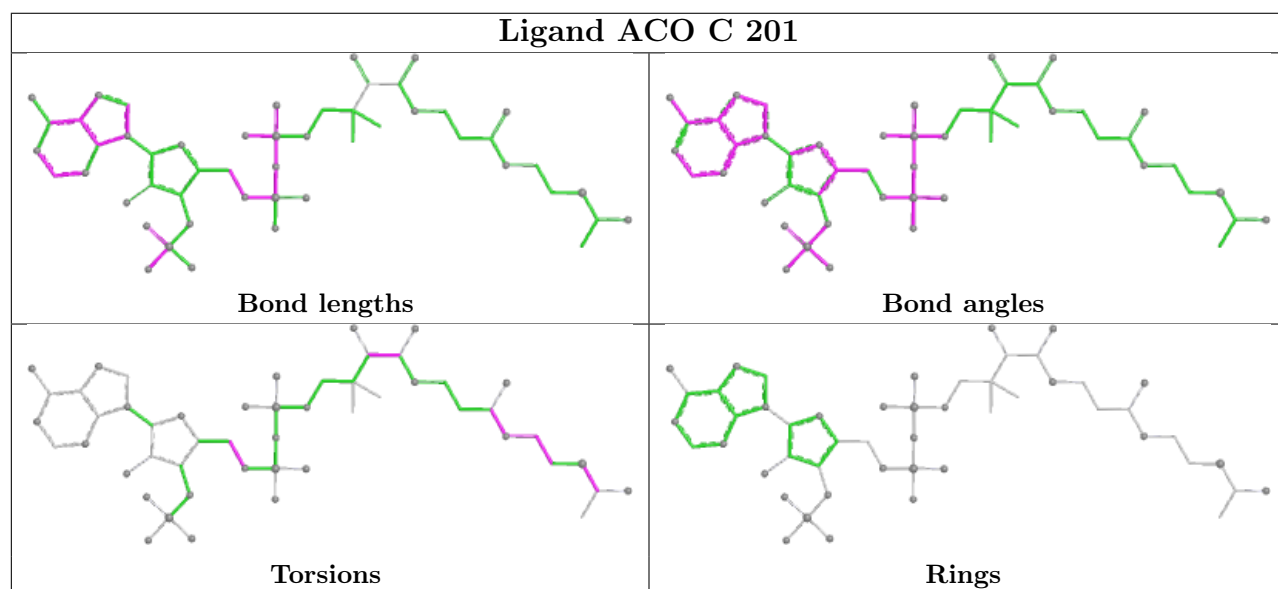
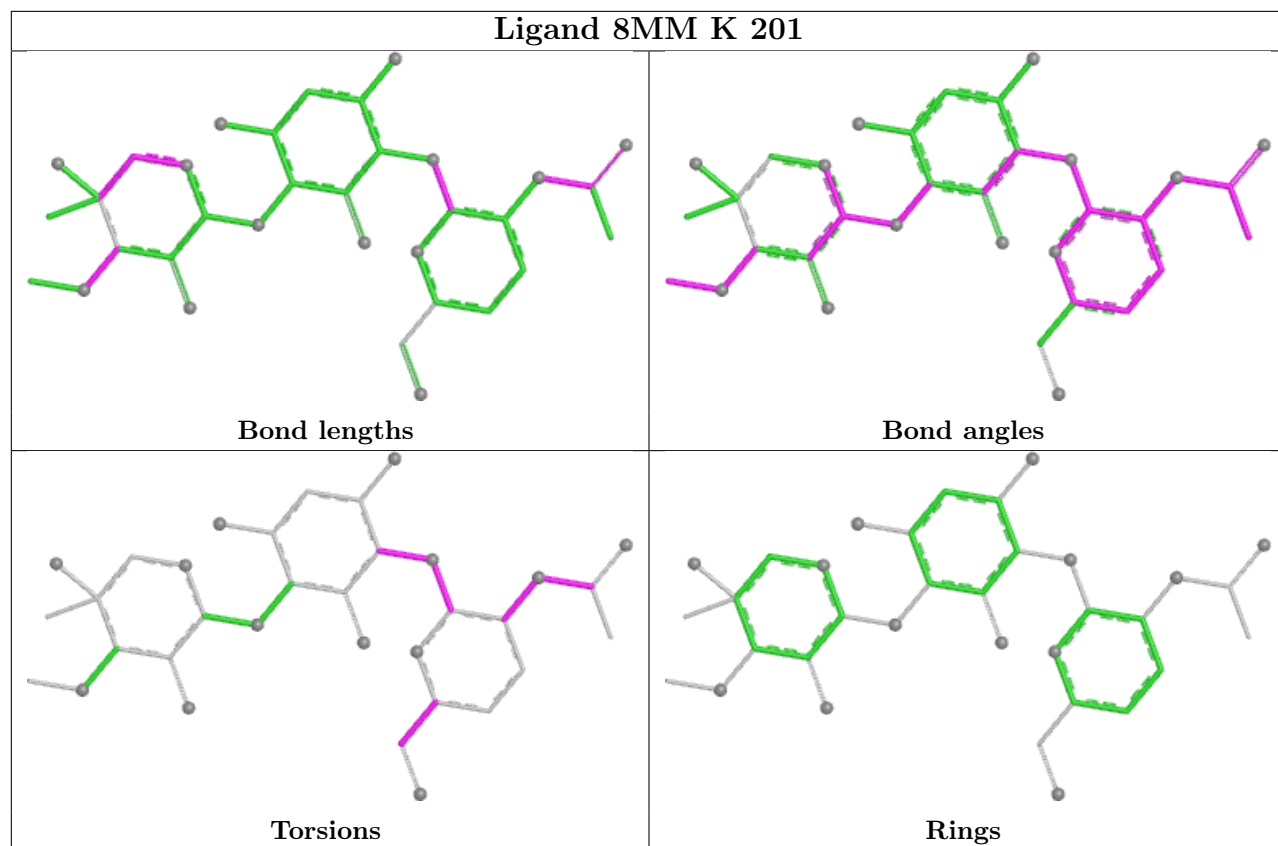
13 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	201	8MM	2	0
3	J	201	TAR	2	0
2	H	201	8MM	1	0
5	C	202	GOL	1	0
4	C	201	ACO	13	0
6	L	202	COA	7	0
2	L	201	8MM	1	0
2	E	201	8MM	1	0
2	A	201	8MM	1	0
3	F	202	TAR	1	0
6	E	202	COA	7	0
6	I	202	COA	5	0
5	K	202	GOL	1	0

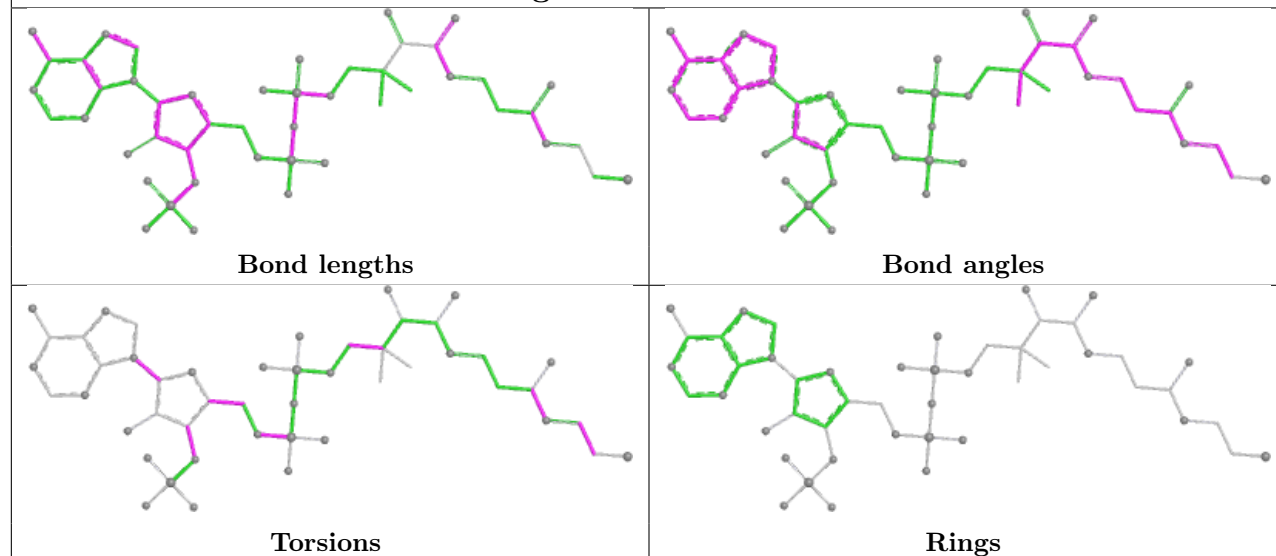
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



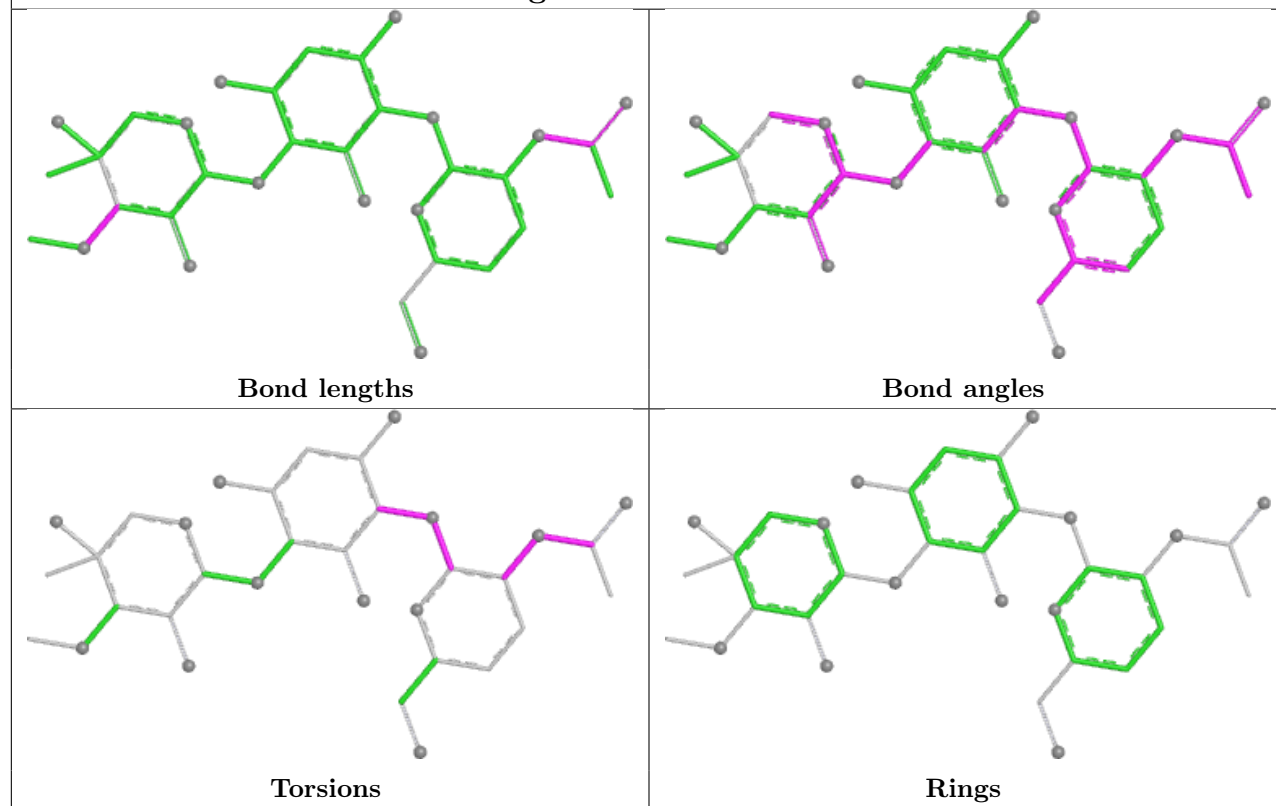


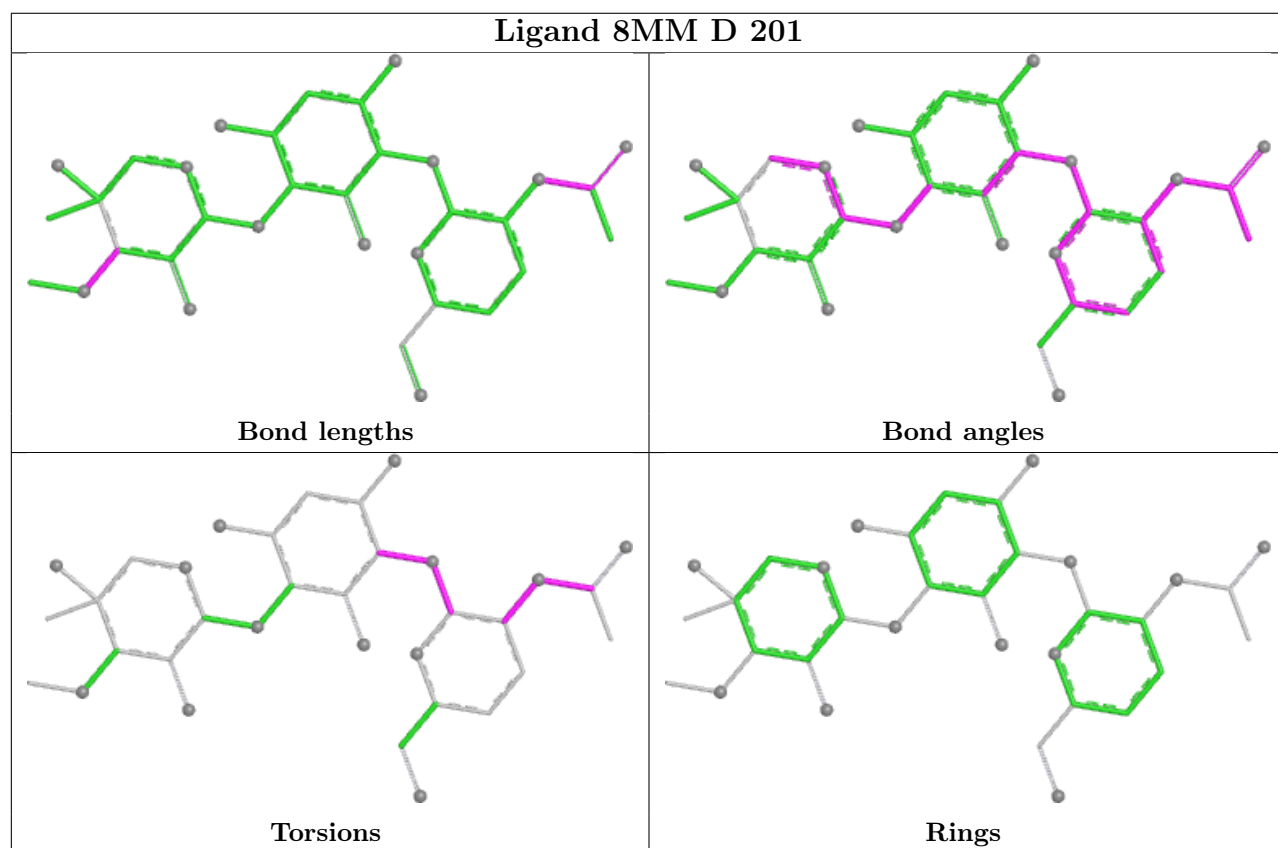
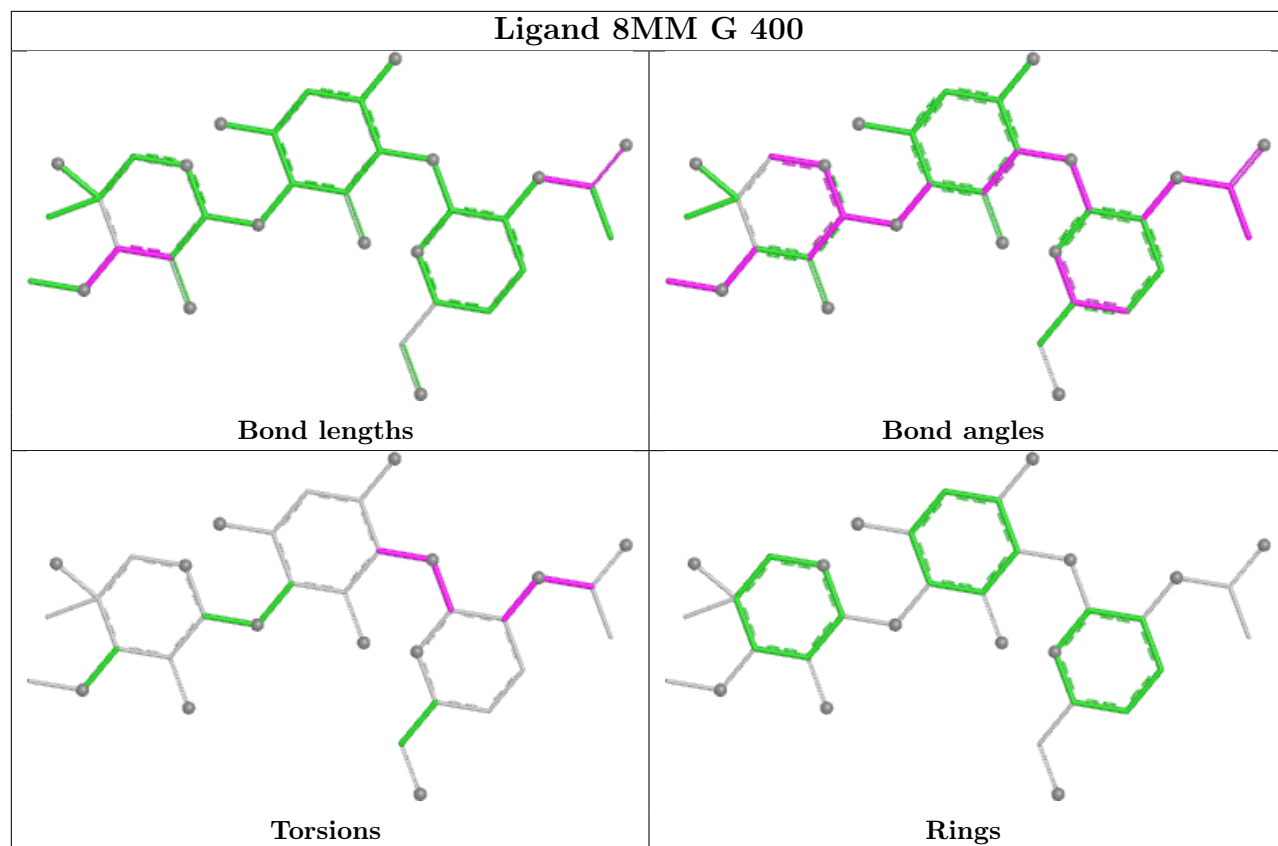


Ligand COA L 202

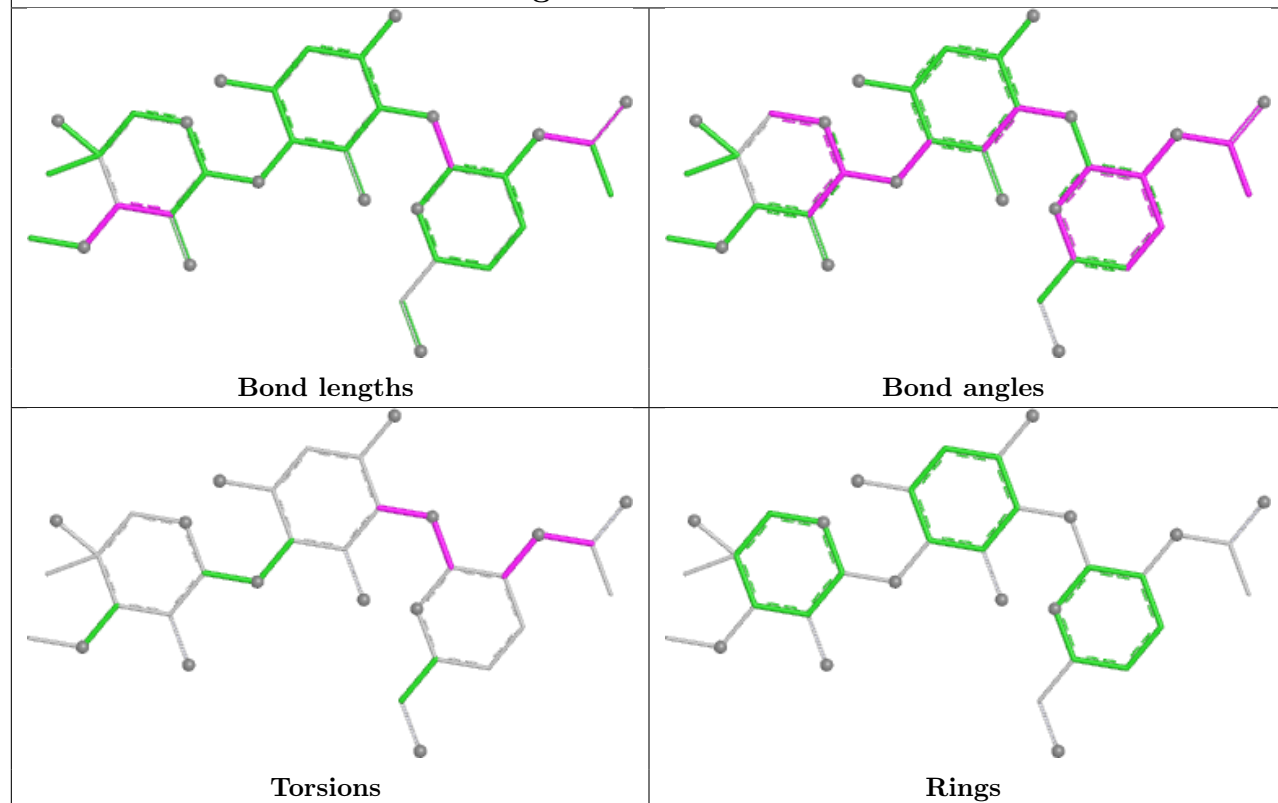


Ligand 8MM L 201

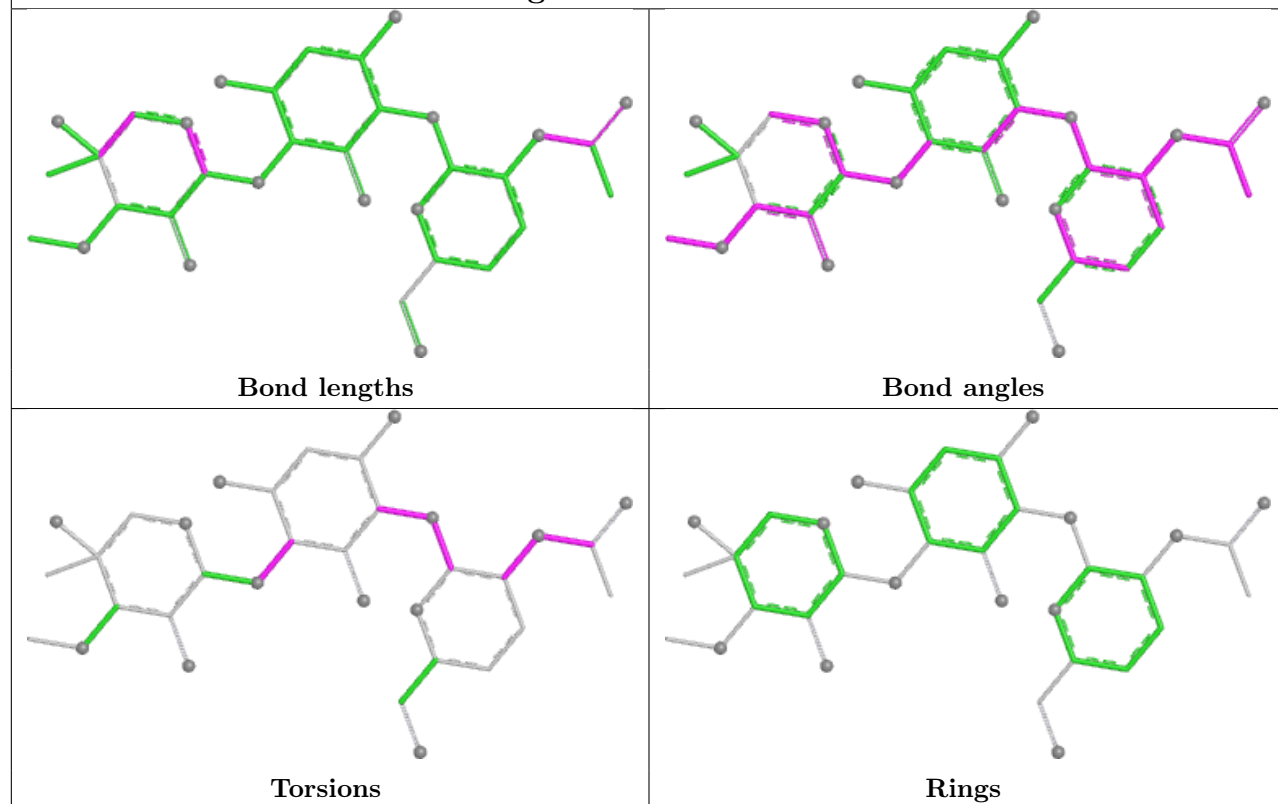


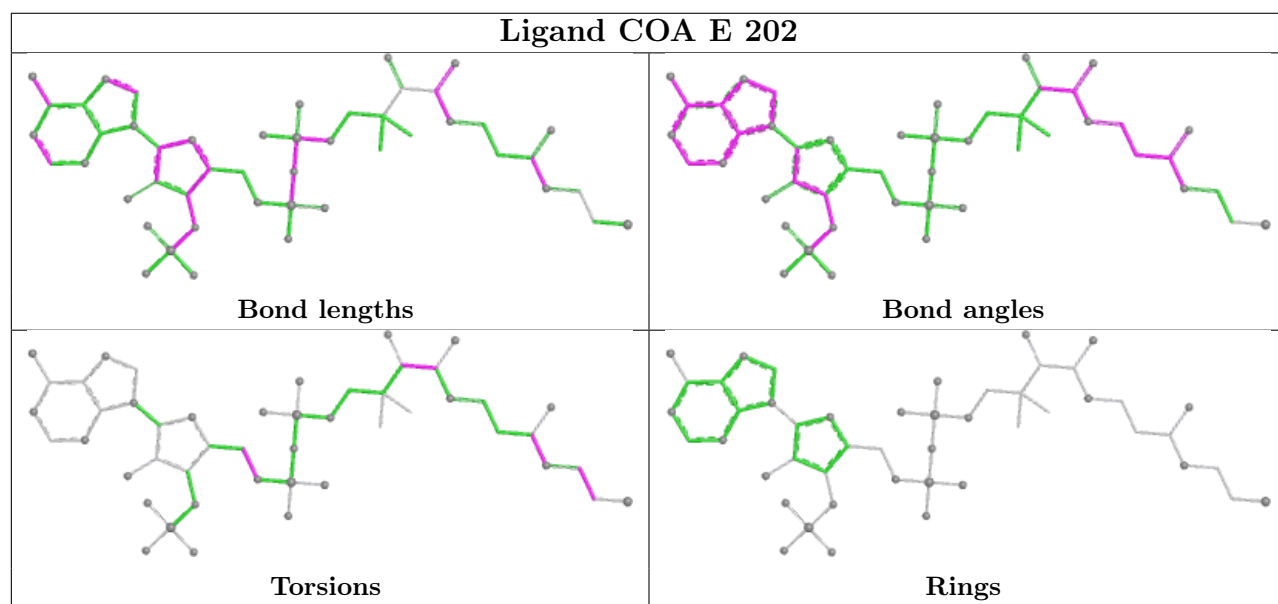
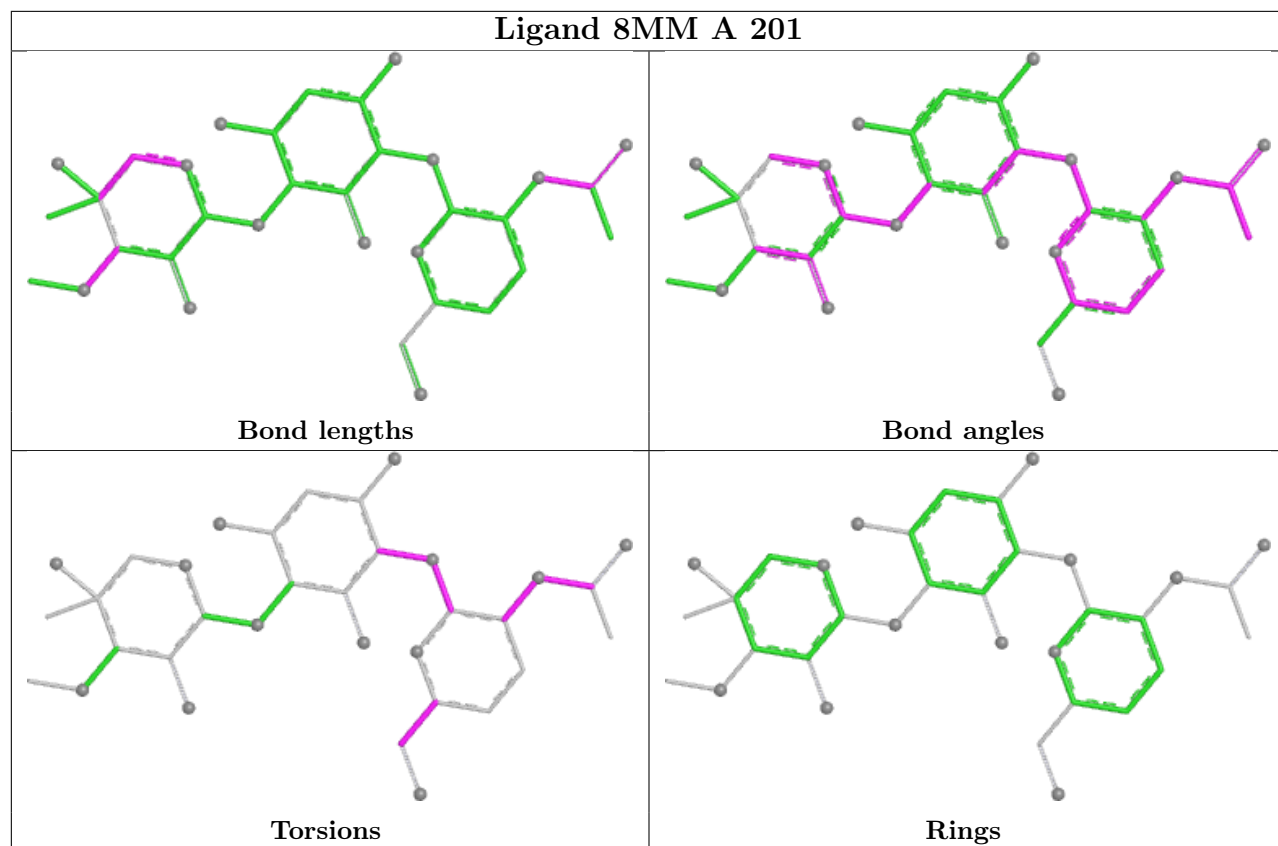


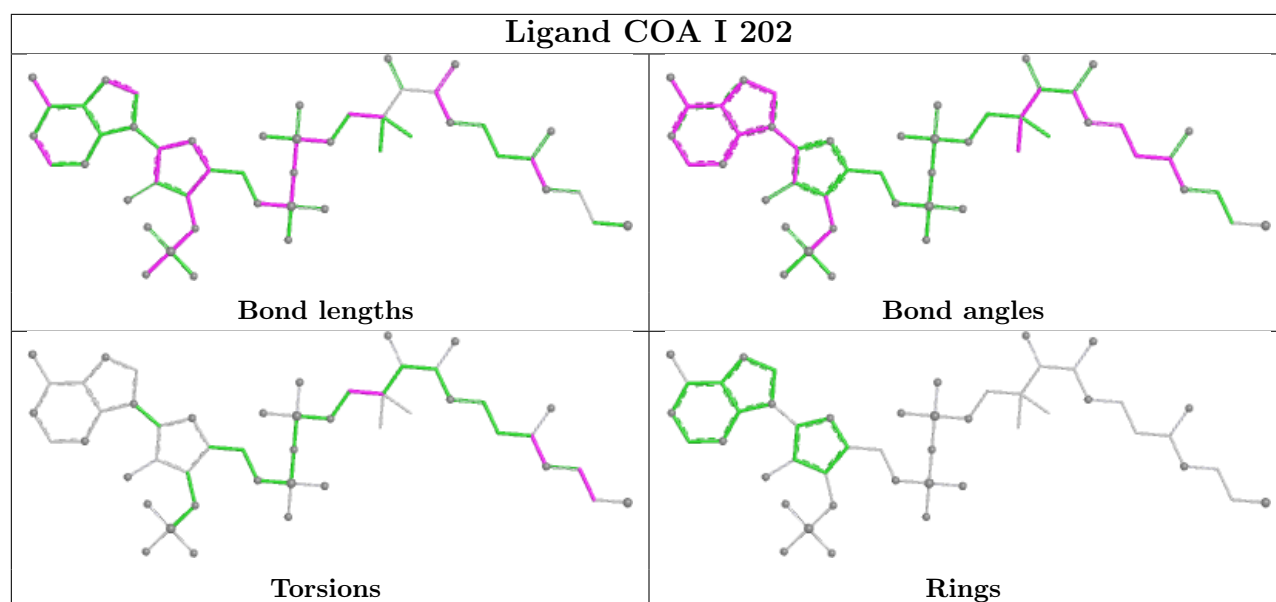
Ligand 8MM I 201



Ligand 8MM E 201







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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	189/189 (100%)	-0.04	5 (2%) 57 53	34, 52, 98, 146	0
1	B	178/189 (94%)	-0.03	4 (2%) 62 59	28, 59, 100, 171	1 (0%)
1	C	185/189 (97%)	0.07	6 (3%) 50 47	31, 61, 112, 162	0
1	D	177/189 (93%)	0.53	11 (6%) 26 23	42, 74, 128, 162	1 (0%)
1	E	184/189 (97%)	0.13	6 (3%) 49 45	29, 60, 116, 197	2 (1%)
1	F	176/189 (93%)	0.18	5 (2%) 55 51	32, 70, 117, 151	0
1	G	177/189 (93%)	-0.02	2 (1%) 78 76	34, 57, 105, 162	1 (0%)
1	H	178/189 (94%)	0.14	4 (2%) 62 59	32, 63, 112, 159	1 (0%)
1	I	178/189 (94%)	-0.17	3 (1%) 69 66	33, 49, 106, 158	0
1	J	179/189 (94%)	-0.03	6 (3%) 48 44	31, 54, 109, 130	0
1	K	184/189 (97%)	0.10	6 (3%) 49 45	32, 55, 112, 168	0
1	L	178/189 (94%)	0.05	2 (1%) 78 76	39, 62, 121, 159	0
All	All	2163/2268 (95%)	0.07	60 (2%) 55 51	28, 60, 116, 197	6 (0%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	138	LEU	4.7
1	J	158	ALA	4.4
1	B	158	ALA	3.3
1	E	138	LEU	3.3
1	A	116	SER	3.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

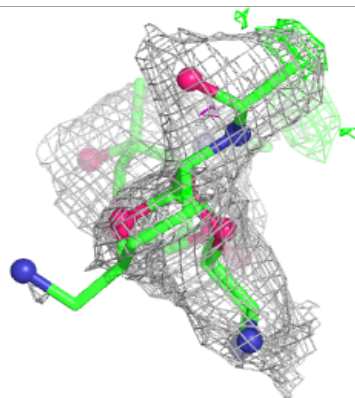
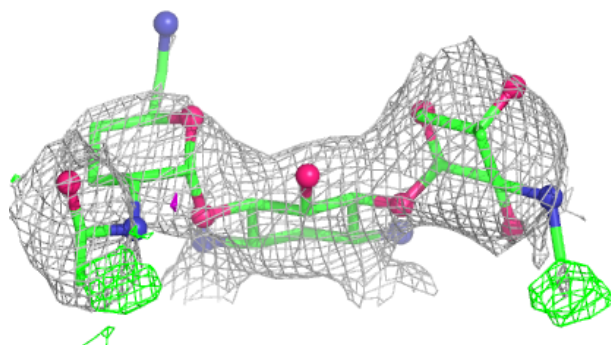
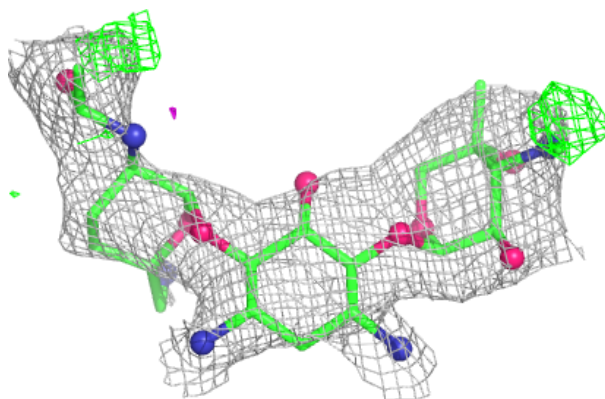
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8MM	F	201	34/34	0.69	0.15	82,121,128,130	0
5	GOL	K	202	6/6	0.72	0.18	71,80,82,82	0
2	8MM	D	201	34/34	0.76	0.14	78,95,109,110	0
3	TAR	H	202	10/10	0.77	0.15	90,96,98,100	0
6	COA	L	202	48/48	0.77	0.14	108,128,176,182	0
2	8MM	H	201	34/34	0.79	0.14	76,104,124,126	0
6	COA	I	202	48/48	0.80	0.14	113,126,164,165	0
2	8MM	A	201	34/34	0.80	0.15	58,76,95,103	0
2	8MM	E	201	34/34	0.82	0.14	64,106,111,114	0
2	8MM	L	201	34/34	0.82	0.13	68,78,101,102	0
3	TAR	D	202	10/10	0.83	0.15	112,116,123,123	0
4	ACO	C	201	51/51	0.83	0.16	75,105,137,140	0
5	GOL	I	203	6/6	0.83	0.16	87,93,96,99	0
3	TAR	A	202	10/10	0.85	0.14	61,83,88,93	0
3	TAR	J	201	10/10	0.86	0.14	92,99,103,104	0
2	8MM	K	201	34/34	0.86	0.11	51,73,114,119	0
3	TAR	F	202	10/10	0.87	0.13	70,85,97,102	0
2	8MM	I	201	34/34	0.88	0.12	46,60,95,97	0
6	COA	E	202	48/48	0.88	0.14	68,120,143,145	0
5	GOL	C	202	6/6	0.88	0.15	90,92,94,95	0
2	8MM	B	400	34/34	0.88	0.11	52,64,86,90	0
2	8MM	G	400	34/34	0.90	0.10	44,56,78,78	0

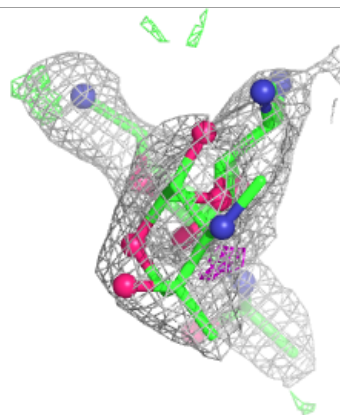
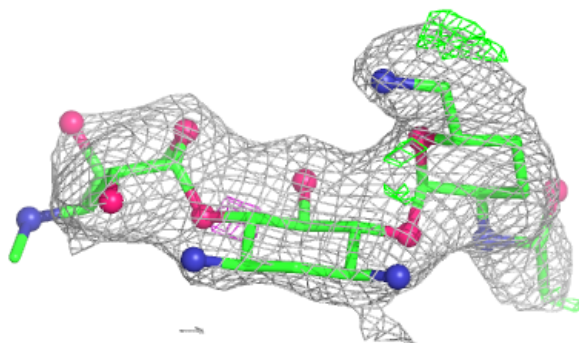
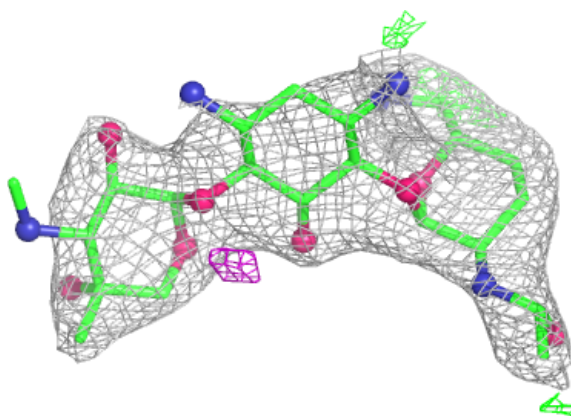
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8MM F 201:

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

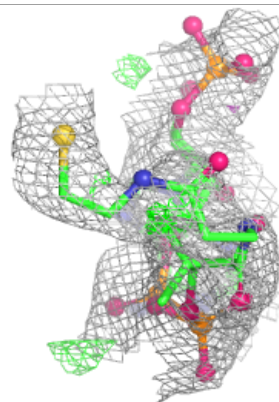
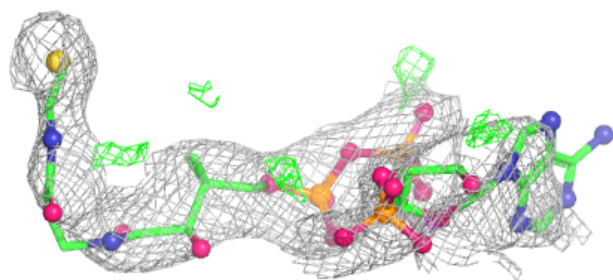
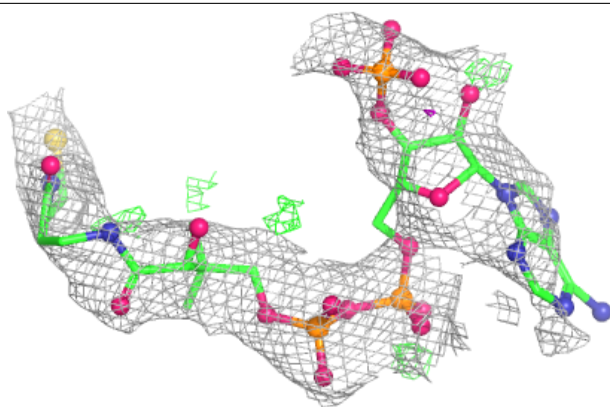
**Electron density around 8MM D 201:**

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

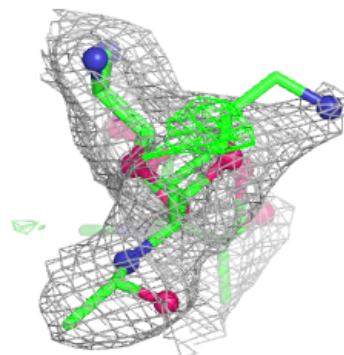
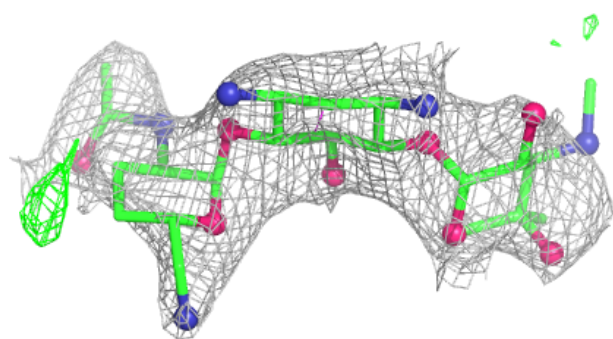
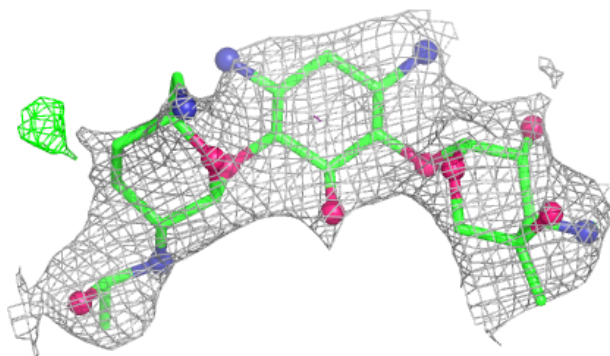


Electron density around COA L 202:

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

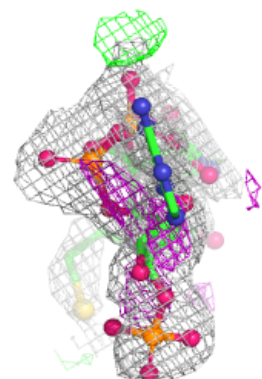
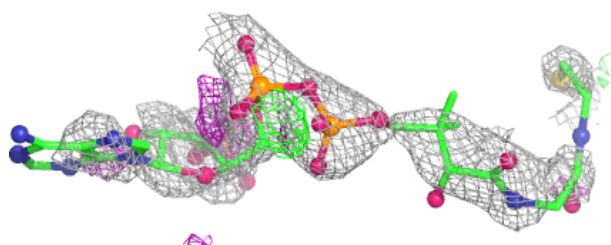
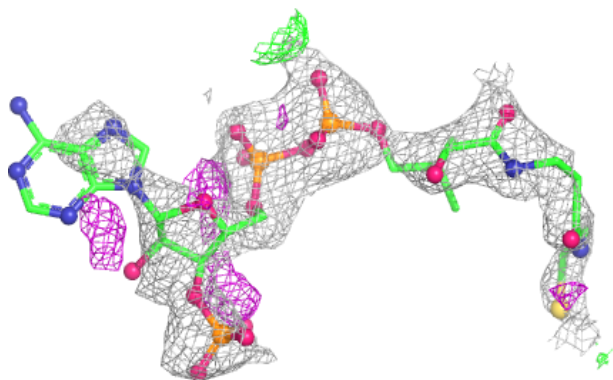
**Electron density around 8MM H 201:**

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

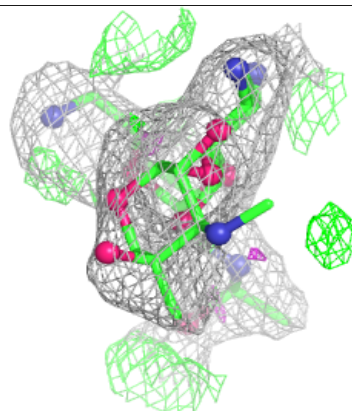
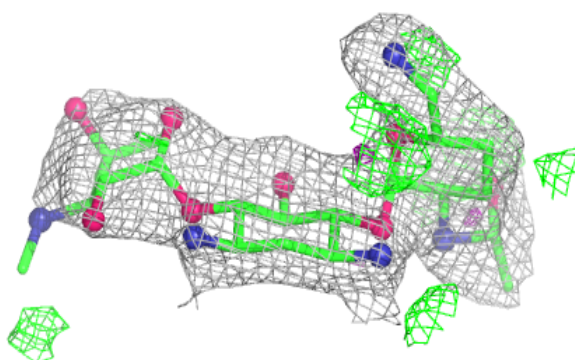
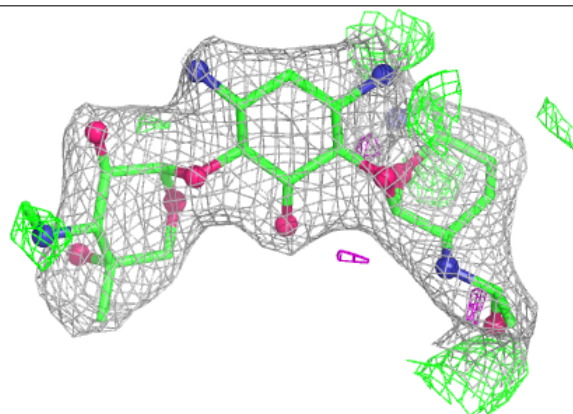


Electron density around COA I 202:

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

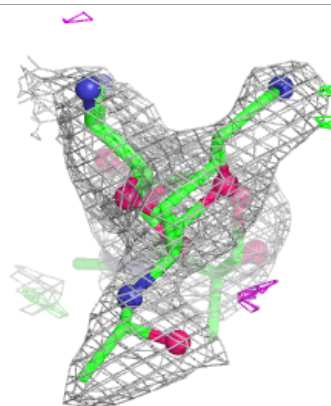
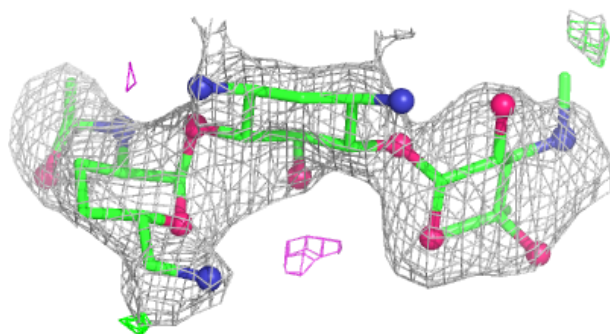
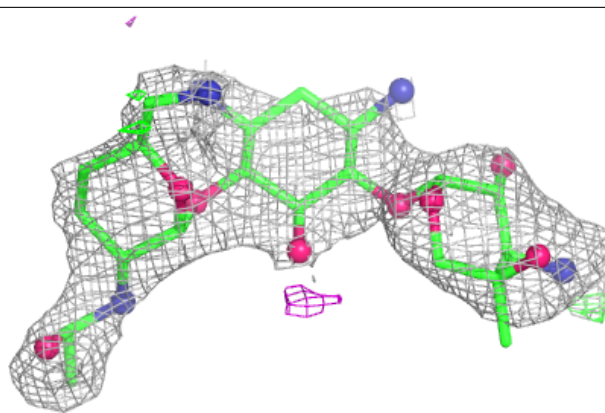
**Electron density around 8MM A 201:**

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

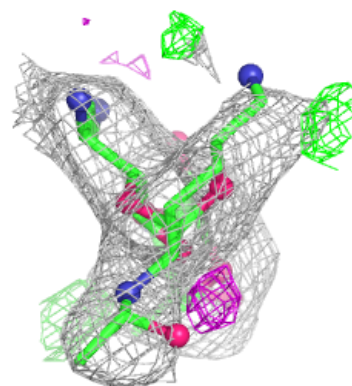
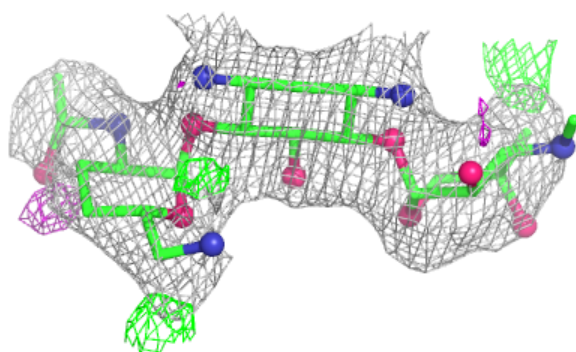
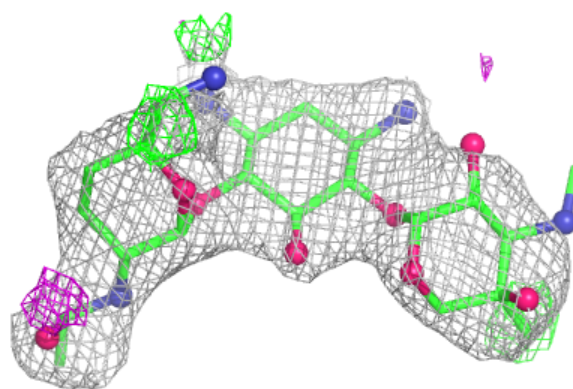


Electron density around 8MM E 201:

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

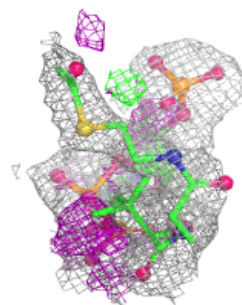
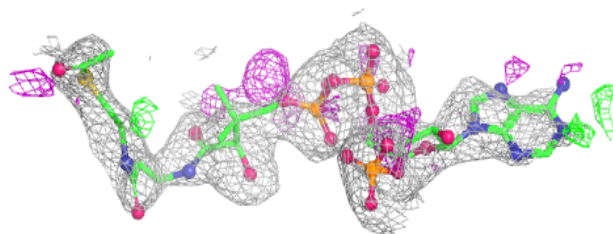
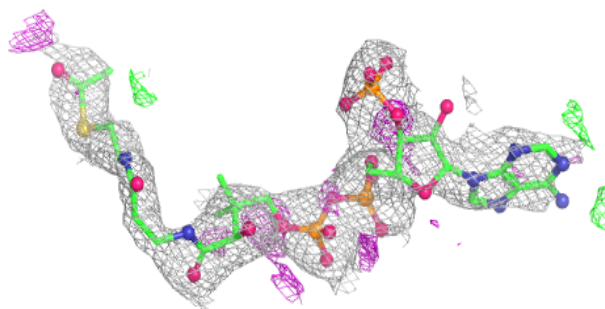
**Electron density around 8MM L 201:**

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

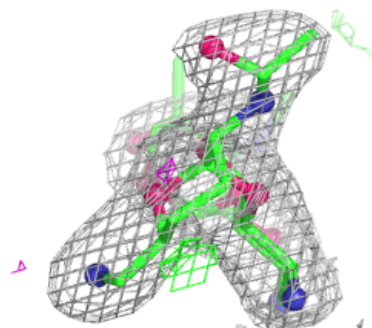
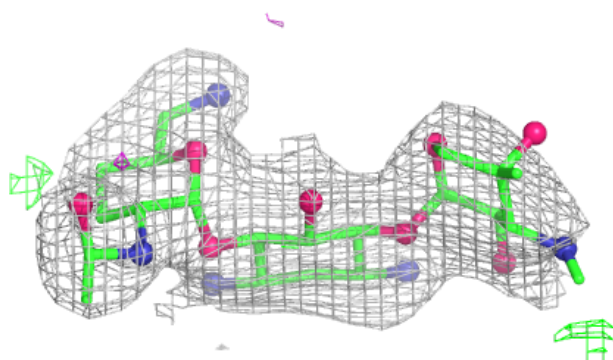
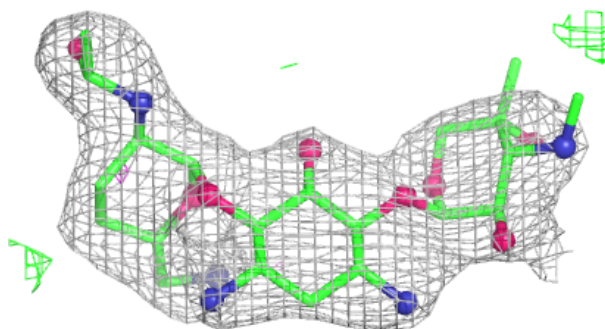


Electron density around ACO C 201:

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

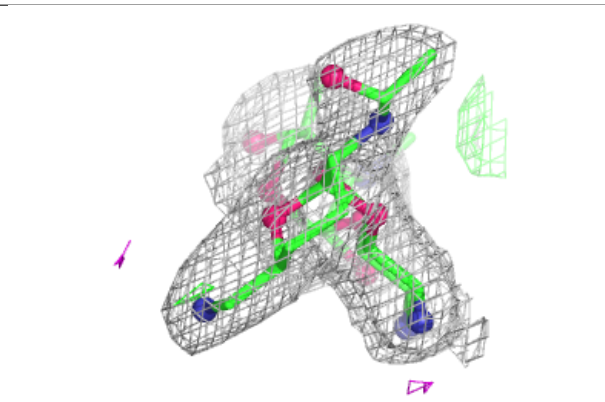
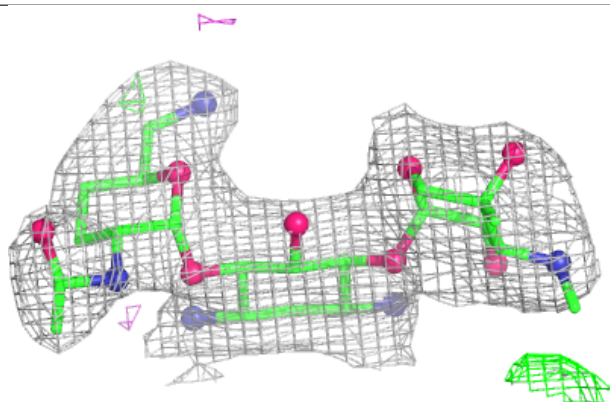
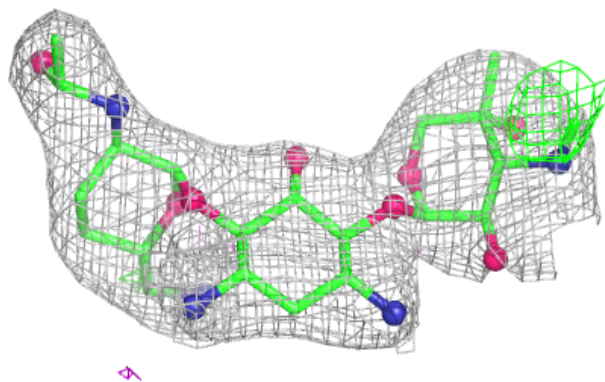
**Electron density around 8MM K 201:**

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

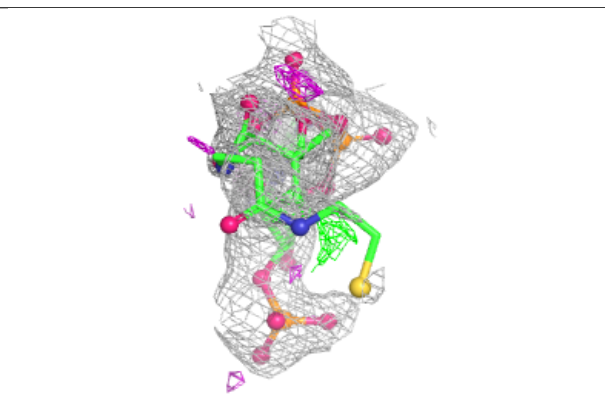
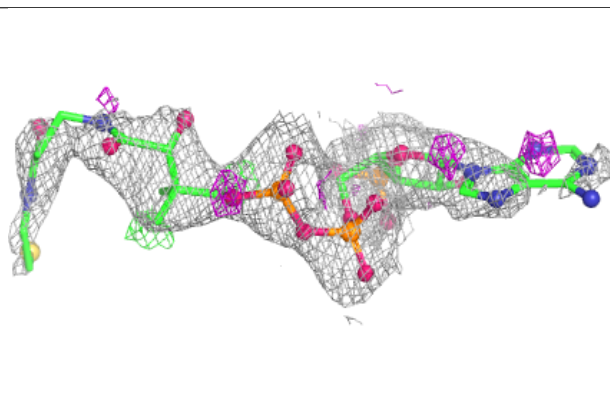
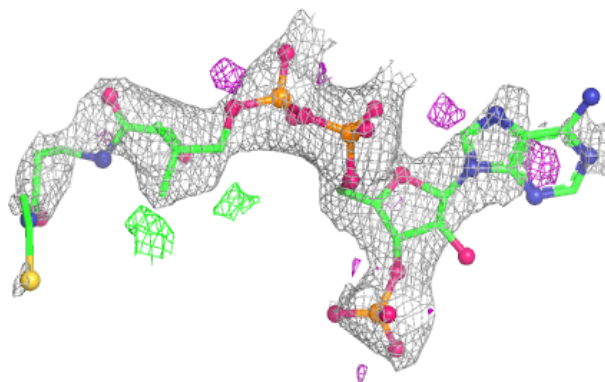


Electron density around 8MM I 201:

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

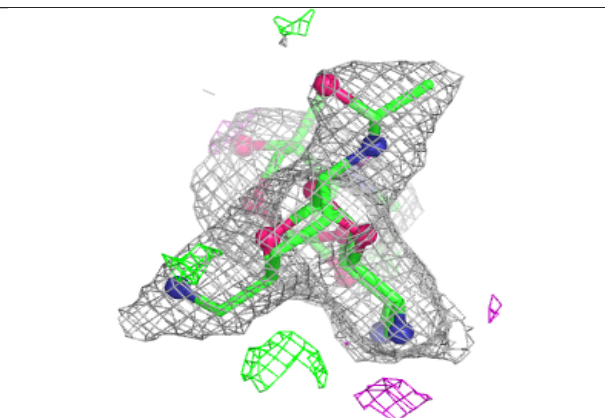
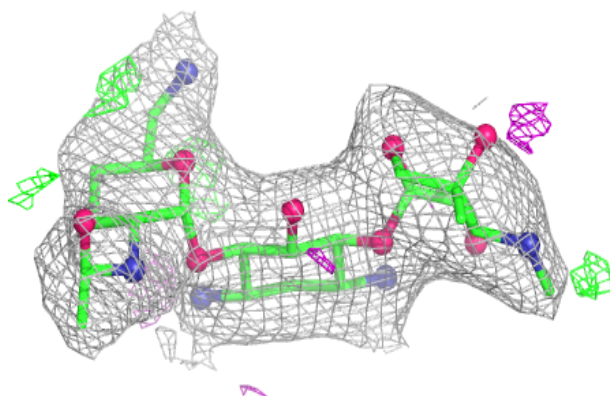
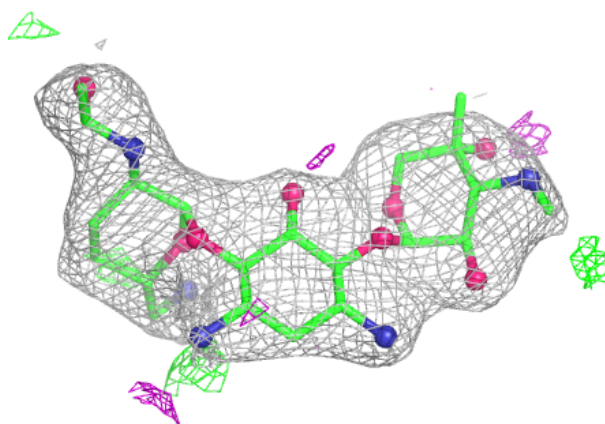
**Electron density around COA E 202:**

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

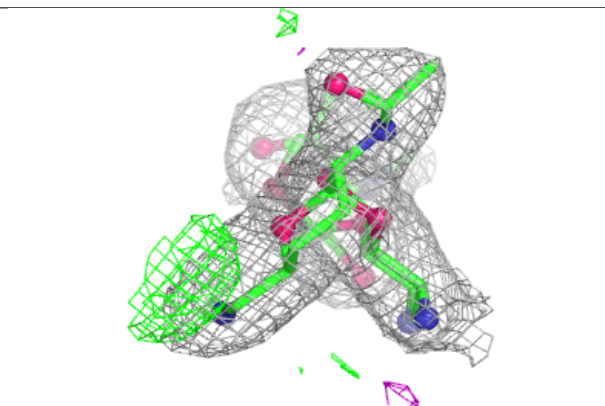
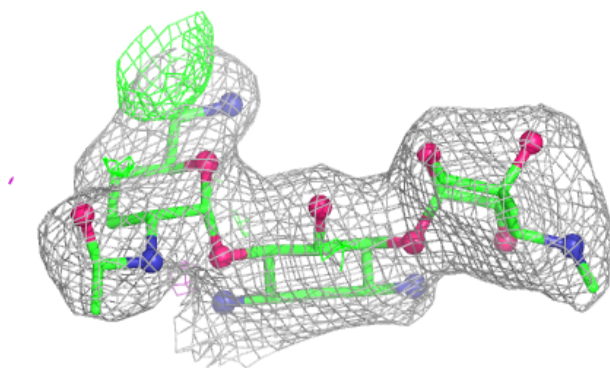
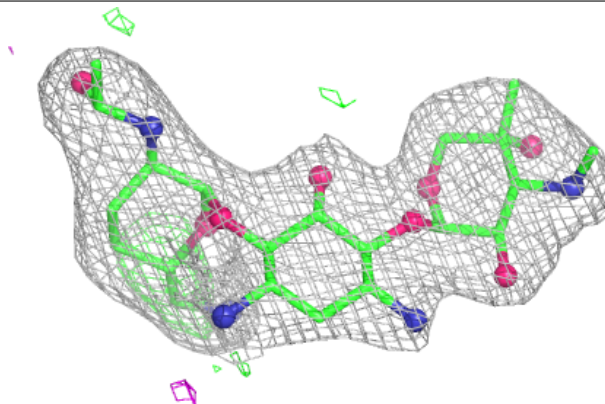


Electron density around 8MM B 400:

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

**Electron density around 8MM G 400:**

$2mF_o-DF_c$ (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.