



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2024 – 01:38 am BST

PDB ID : 2VAT
Title : Crystal structure of deacetylcephalosporin C acetyltransferase in complex with coenzyme A
Authors : Lejon, S.; Ellis, J.; Valegard, K.
Deposited on : 2007-09-04
Resolution : 2.20 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

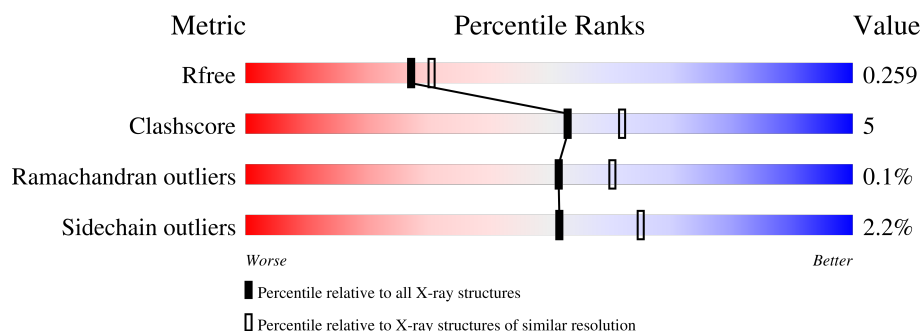
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	
1	F	444	
1	G	444	

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Mol	Chain	Length	Quality of chain
1	H	444	
1	I	444	
1	J	444	
1	K	444	
1	L	444	

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	ACT	H	1384	-	-	X	-
3	ACT	K	1386	-	-	X	-

2 Entry composition

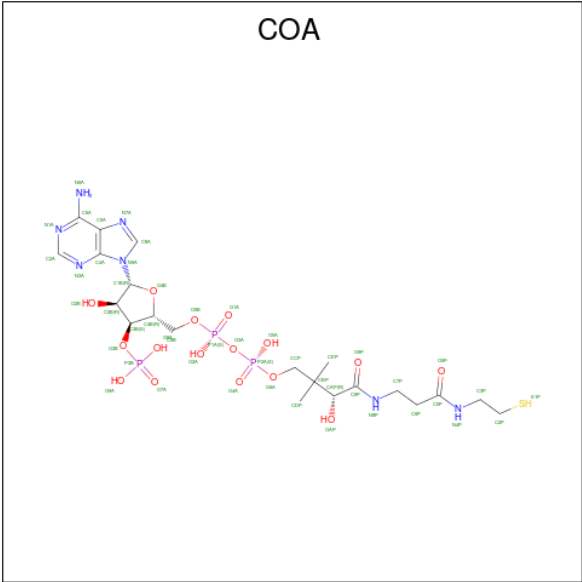
There are 5 unique types of molecules in this entry. The entry contains 35013 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	4	0
			2744	1731	485	509	19			
1	B	347	Total	C	N	O	S	0	3	0
			2744	1731	488	506	19			
1	C	345	Total	C	N	O	S	0	4	0
			2745	1730	488	508	19			
1	D	345	Total	C	N	O	S	0	4	0
			2748	1732	488	509	19			
1	E	346	Total	C	N	O	S	0	5	0
			2744	1732	487	506	19			
1	F	342	Total	C	N	O	S	0	2	0
			2694	1700	474	501	19			
1	G	342	Total	C	N	O	S	0	6	0
			2733	1724	484	506	19			
1	H	345	Total	C	N	O	S	0	8	0
			2760	1741	492	508	19			
1	I	347	Total	C	N	O	S	0	3	0
			2739	1728	485	507	19			
1	J	344	Total	C	N	O	S	0	4	0
			2724	1719	482	504	19			
1	K	344	Total	C	N	O	S	0	5	0
			2732	1724	485	504	19			
1	L	341	Total	C	N	O	S	0	3	0
			2697	1702	476	500	19			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		
3	J	1	Total	C	O	0	0
			4	2	2		
3	K	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total	O	0	0
			165	165		
5	B	171	Total	O	0	0
			171	171		
5	C	137	Total	O	0	0
			137	137		
5	D	123	Total	O	0	0
			123	123		
5	E	165	Total	O	0	0
			165	165		
5	F	102	Total	O	0	0
			102	102		
5	G	140	Total	O	0	0
			140	140		
5	H	144	Total	O	0	0
			144	144		
5	I	164	Total	O	0	0
			164	164		
5	J	80	Total	O	0	0
			80	80		

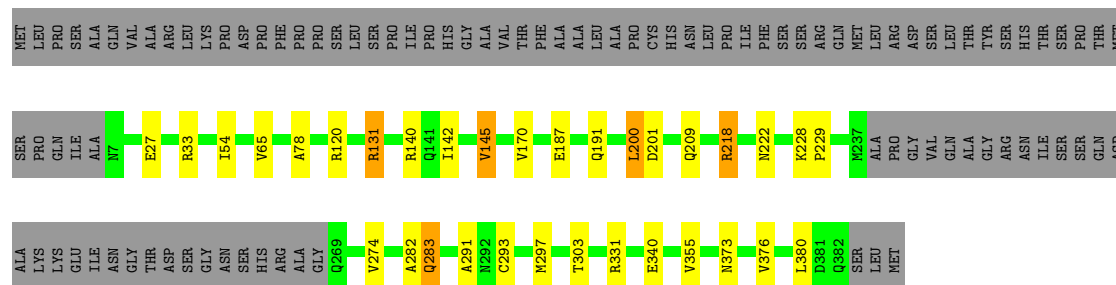
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	K	78	Total 78	O 78	0	0
5	L	104	Total 104	O 104	0	0

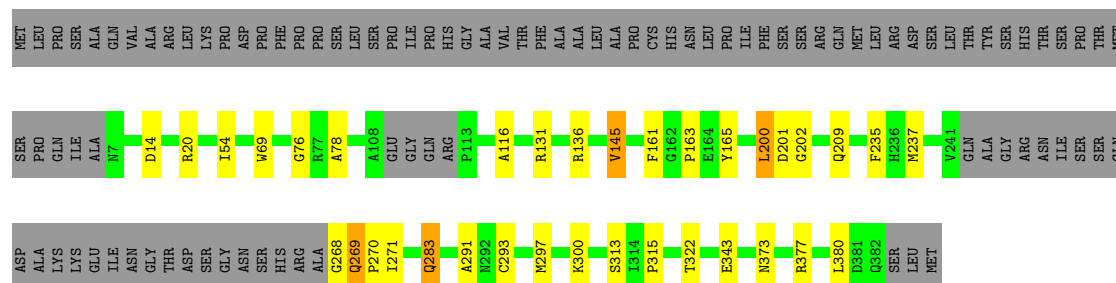
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain D:  70% 6% 22%



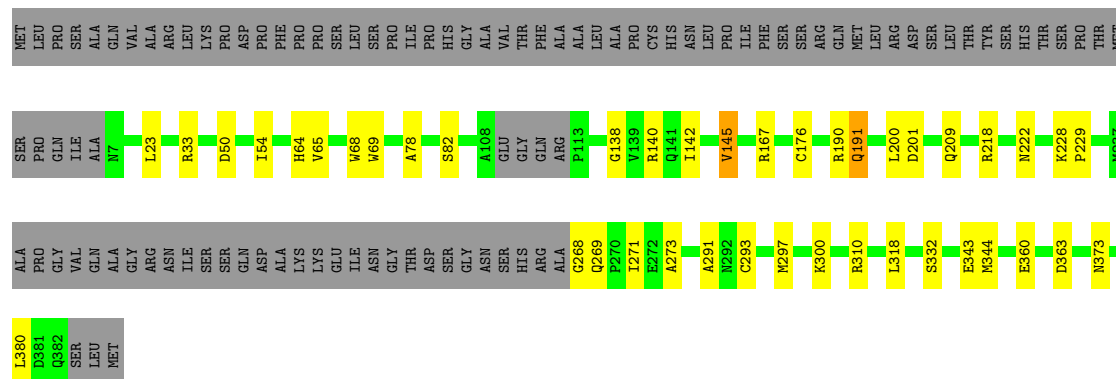
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain E:  70% 7% 22%



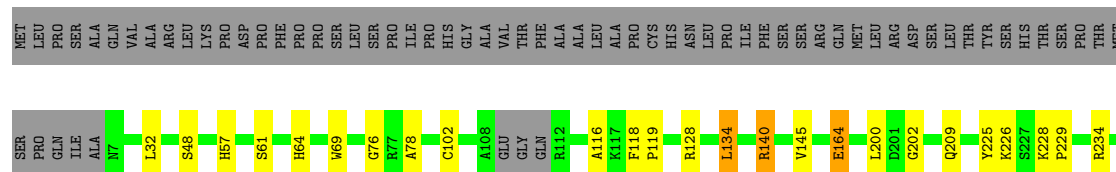
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain F:  68% 9% 23%



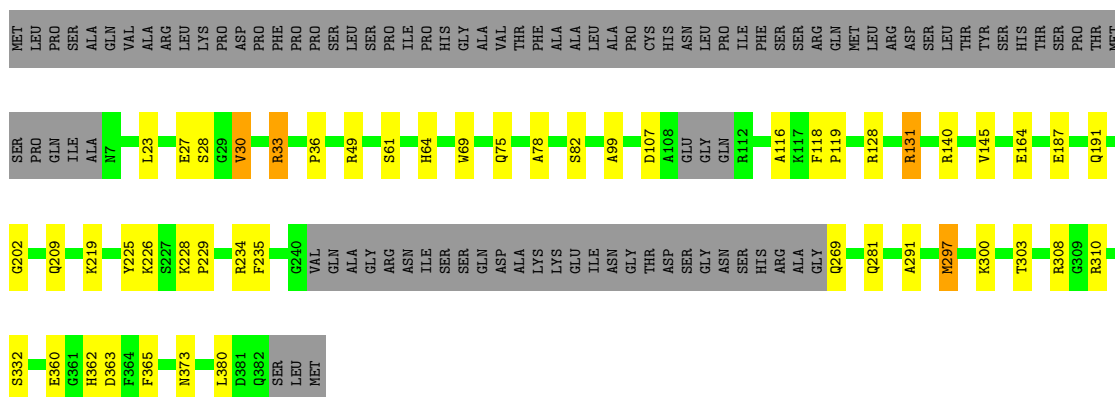
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain G:  68% 8% 23%



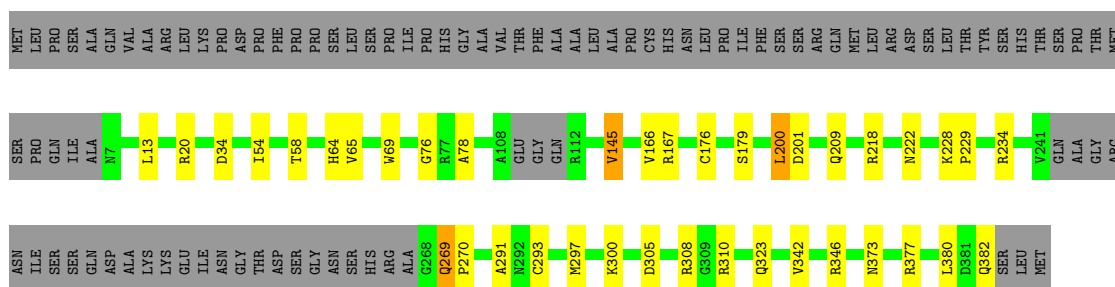
- Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain H: 67% 10% . 22%



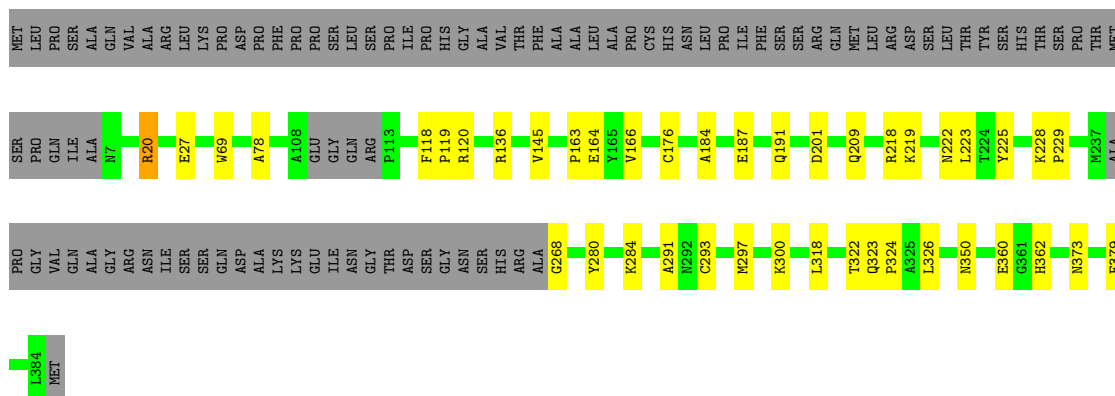
● Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain I: 69% 8% • 22%



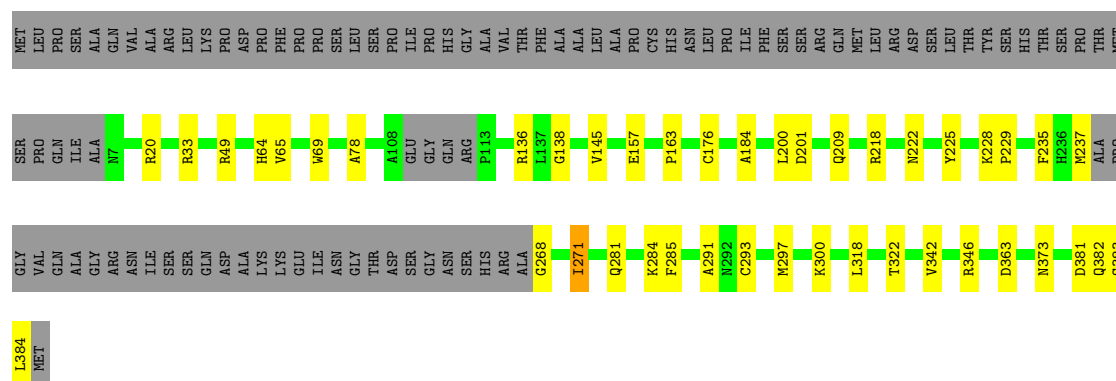
- Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain J:  68% 9% 23%



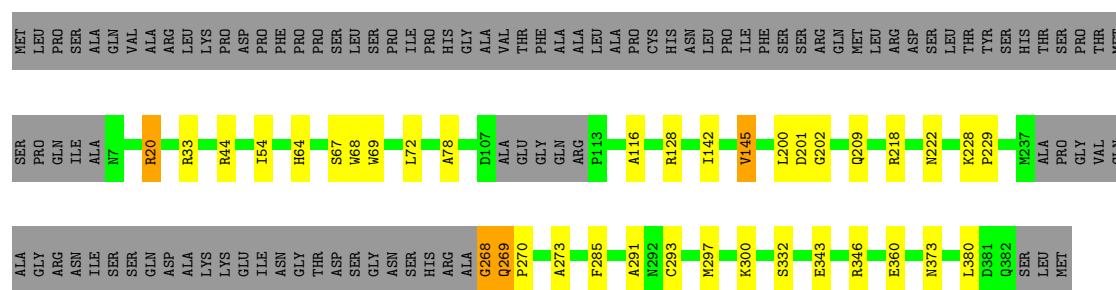
- Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain K:



- Molecule 1: ACETYL-COA--DEACETYLCEPHALOSPORIN C ACETYLTRANSFERASE

Chain L:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.96Å 109.28Å 197.00Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	122.17 – 2.20 27.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (122.17-2.20) 98.9 (27.45-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.230 0.263 , 0.259	Depositor DCC
R_{free} test set	10106 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 16.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	35013	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.77% 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

5.1 Standard geometry

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

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	0.89	3/2816 (0.1%)	0.75	4/3817 (0.1%)
1	B	0.99	10/2816 (0.4%)	0.76	3/3816 (0.1%)
1	C	0.89	6/2820 (0.2%)	0.71	1/3821 (0.0%)
1	D	0.94	5/2826 (0.2%)	0.74	2/3829 (0.1%)
1	E	0.85	1/2822 (0.0%)	0.70	0/3823
1	F	0.89	5/2759 (0.2%)	0.75	6/3739 (0.2%)
1	G	0.87	3/2813 (0.1%)	0.73	3/3811 (0.1%)
1	H	0.84	0/2844	0.73	4/3852 (0.1%)
1	I	0.87	2/2811 (0.1%)	0.73	3/3810 (0.1%)
1	J	0.89	2/2795 (0.1%)	0.72	1/3786 (0.0%)
1	K	0.86	1/2806 (0.0%)	0.69	0/3800
1	L	0.86	1/2765 (0.0%)	0.71	0/3746
All	All	0.89	39/33693 (0.1%)	0.73	27/45650 (0.1%)

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

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	PHE	CE1-CZ	-11.74	1.15	1.37
1	B	186	PHE	CG-CD2	-11.20	1.22	1.38
1	D	340	GLU	CD-OE1	-10.64	1.14	1.25
1	D	340	GLU	CD-OE2	-10.50	1.14	1.25
1	B	186	PHE	CE2-CZ	-9.88	1.18	1.37

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH1	11.47	126.04	120.30
1	B	8	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	D	340	GLU	OE1-CD-OE2	-10.00	111.30	123.30
1	D	27	GLU	OE1-CD-OE2	-9.88	111.44	123.30
1	J	27	GLU	OE1-CD-OE2	-9.78	111.56	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	268	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2744	0	2656	25	0
1	B	2744	0	2663	18	0
1	C	2745	0	2662	30	0
1	D	2748	0	2669	29	0
1	E	2744	0	2669	26	0
1	F	2694	0	2599	30	0
1	G	2733	0	2652	27	0
1	H	2760	0	2685	44	0
1	I	2739	0	2655	33	0
1	J	2724	0	2641	33	0
1	K	2732	0	2653	44	0
1	L	2697	0	2607	33	0
2	A	48	0	32	2	0
2	B	48	0	32	2	0
2	C	48	0	32	0	0
2	D	48	0	32	0	0
2	E	48	0	31	1	0
2	F	48	0	32	3	0
2	G	48	0	32	5	0
2	H	48	0	32	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	48	0	32	1	0
2	J	48	0	32	3	0
2	K	48	0	32	4	0
2	L	48	0	32	1	0
3	A	4	0	3	0	0
3	B	4	0	3	1	0
3	C	4	0	3	0	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	0	0
3	G	4	0	3	1	0
3	H	4	0	3	3	0
3	I	4	0	3	0	0
3	J	4	0	3	0	0
3	K	4	0	3	2	0
3	L	4	0	3	1	0
4	B	6	0	8	0	0
4	I	6	0	8	0	0
5	A	165	0	0	0	0
5	B	171	0	0	6	0
5	C	137	0	0	8	0
5	D	123	0	0	5	0
5	E	165	0	0	3	0
5	F	102	0	0	7	0
5	G	140	0	0	3	0
5	H	144	0	0	5	0
5	I	164	0	0	3	0
5	J	80	0	0	3	0
5	K	78	0	0	5	0
5	L	104	0	0	7	0
All	All	35013	0	32246	357	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 357 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:K:218[A]:ARG:NE	1:K:222[A]:ASN:HD21	1.04	1.42
1:K:218[A]:ARG:NE	1:K:222[A]:ASN:ND2	1.78	1.29
1:J:218:ARG:CZ	1:J:222[A]:ASN:OD1	1.98	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:363[A]:ASP:OD1	2:H:1383:COA:C6P	1.99	1.11
1:E:14:ASP:OD1	5:E:2005:HOH:O	1.72	1.08

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	343/444 (77%)	332 (97%)	11 (3%)	0	100	100
1	B	343/444 (77%)	332 (97%)	10 (3%)	1 (0%)	41	46
1	C	344/444 (78%)	334 (97%)	10 (3%)	0	100	100
1	D	345/444 (78%)	335 (97%)	10 (3%)	0	100	100
1	E	344/444 (78%)	333 (97%)	10 (3%)	1 (0%)	41	46
1	F	336/444 (76%)	325 (97%)	11 (3%)	0	100	100
1	G	341/444 (77%)	332 (97%)	9 (3%)	0	100	100
1	H	345/444 (78%)	334 (97%)	11 (3%)	0	100	100
1	I	343/444 (77%)	333 (97%)	9 (3%)	1 (0%)	41	46
1	J	340/444 (77%)	327 (96%)	13 (4%)	0	100	100
1	K	341/444 (77%)	328 (96%)	13 (4%)	0	100	100
1	L	336/444 (76%)	327 (97%)	8 (2%)	1 (0%)	41	46
All	All	4101/5328 (77%)	3972 (97%)	125 (3%)	4 (0%)	51	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	269	GLN
1	E	269	GLN

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Mol	Chain	Res	Type
1	I	269	GLN
1	L	269	GLN

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	293/372 (79%)	286 (98%)	7 (2%)	49	62
1	B	292/372 (78%)	286 (98%)	6 (2%)	53	67
1	C	293/372 (79%)	286 (98%)	7 (2%)	49	62
1	D	294/372 (79%)	286 (97%)	8 (3%)	44	57
1	E	293/372 (79%)	287 (98%)	6 (2%)	55	69
1	F	287/372 (77%)	280 (98%)	7 (2%)	49	62
1	G	293/372 (79%)	283 (97%)	10 (3%)	37	47
1	H	295/372 (79%)	286 (97%)	9 (3%)	40	51
1	I	292/372 (78%)	287 (98%)	5 (2%)	60	74
1	J	291/372 (78%)	287 (99%)	4 (1%)	67	80
1	K	292/372 (78%)	286 (98%)	6 (2%)	53	67
1	L	288/372 (77%)	281 (98%)	7 (2%)	49	62
All	All	3503/4464 (78%)	3421 (98%)	82 (2%)	52	63

5 of 82 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	140[B]	ARG
1	K	145	VAL
1	H	380	LEU
1	J	20	ARG
1	L	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	373	ASN
1	K	64	HIS
1	I	209	GLN
1	J	64	HIS
1	K	373	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 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	1383	-	41,50,50	2.13	15 (36%)	52,75,75	1.43	7 (13%)
3	ACT	D	1384	-	3,3,3	0.74	0	3,3,3	1.09	0
3	ACT	G	1384	-	3,3,3	0.95	0	3,3,3	0.37	0
2	COA	B	1383	-	41,50,50	1.73	4 (9%)	52,75,75	1.28	3 (5%)
2	COA	D	1383	-	41,50,50	1.85	4 (9%)	52,75,75	1.18	3 (5%)
2	COA	K	1385	-	41,50,50	1.80	4 (9%)	52,75,75	1.22	2 (3%)
2	COA	I	1383	-	41,50,50	1.73	4 (9%)	52,75,75	1.27	4 (7%)
3	ACT	E	1384	-	3,3,3	0.80	0	3,3,3	0.99	0
3	ACT	F	1384	-	3,3,3	0.71	0	3,3,3	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	C	1383	-	41,50,50	1.84	4 (9%)	52,75,75	1.25	4 (7%)
3	ACT	B	1385	-	3,3,3	0.66	0	3,3,3	1.19	0
2	COA	H	1383	-	41,50,50	2.02	10 (24%)	52,75,75	1.77	8 (15%)
4	GOL	B	1384	-	5,5,5	0.36	0	5,5,5	0.36	0
2	COA	F	1383	-	41,50,50	1.87	3 (7%)	52,75,75	1.22	3 (5%)
3	ACT	J	1386	-	3,3,3	0.77	0	3,3,3	1.09	0
4	GOL	I	1384	-	5,5,5	0.39	0	5,5,5	0.20	0
3	ACT	I	1385	-	3,3,3	0.78	0	3,3,3	0.67	0
2	COA	L	1383	-	41,50,50	1.82	3 (7%)	52,75,75	1.26	2 (3%)
3	ACT	H	1384	-	3,3,3	0.91	0	3,3,3	0.36	0
2	COA	G	1383	-	41,50,50	1.80	3 (7%)	52,75,75	1.20	3 (5%)
3	ACT	A	1384	-	3,3,3	0.73	0	3,3,3	1.03	0
3	ACT	K	1386	-	3,3,3	0.85	0	3,3,3	0.61	0
3	ACT	L	1384	-	3,3,3	0.69	0	3,3,3	0.94	0
2	COA	E	1383	-	41,50,50	2.08	12 (29%)	52,75,75	1.49	9 (17%)
3	ACT	C	1384	-	3,3,3	0.77	0	3,3,3	0.91	0
2	COA	J	1385	-	41,50,50	1.79	4 (9%)	52,75,75	1.14	2 (3%)

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	A	1383	-	-	13/44/64/64	0/3/3/3
2	COA	H	1383	-	-	20/44/64/64	0/3/3/3
2	COA	B	1383	-	-	18/44/64/64	0/3/3/3
4	GOL	B	1384	-	-	1/4/4/4	-
2	COA	E	1383	-	-	11/44/64/64	0/3/3/3
2	COA	F	1383	-	-	18/44/64/64	0/3/3/3
2	COA	D	1383	-	-	7/44/64/64	0/3/3/3
2	COA	L	1383	-	-	8/44/64/64	0/3/3/3
2	COA	J	1385	-	-	13/44/64/64	0/3/3/3
2	COA	K	1385	-	-	14/44/64/64	0/3/3/3
2	COA	G	1383	-	-	14/44/64/64	0/3/3/3
2	COA	I	1383	-	-	15/44/64/64	0/3/3/3
4	GOL	I	1384	-	-	2/4/4/4	-
2	COA	C	1383	-	-	10/44/64/64	0/3/3/3

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1383	COA	O9P-C9P	9.84	1.42	1.23
2	C	1383	COA	O9P-C9P	9.63	1.42	1.23
2	L	1383	COA	O9P-C9P	9.55	1.42	1.23
2	G	1383	COA	O9P-C9P	9.49	1.42	1.23
2	K	1385	COA	O9P-C9P	9.45	1.42	1.23

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1383	COA	N3A-C2A-N1A	-6.41	118.66	128.68
2	K	1385	COA	N3A-C2A-N1A	-6.19	119.00	128.68
2	I	1383	COA	N3A-C2A-N1A	-6.04	119.24	128.68
2	F	1383	COA	N3A-C2A-N1A	-5.91	119.44	128.68
2	B	1383	COA	N3A-C2A-N1A	-5.87	119.50	128.68

There are no chirality outliers.

5 of 164 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1383	COA	C3B-O3B-P3B-O8A
2	A	1383	COA	OAP-CAP-CBP-CCP
2	A	1383	COA	C9P-CAP-CBP-CCP
2	A	1383	COA	C9P-CAP-CBP-CDP
2	A	1383	COA	OAP-CAP-CBP-CEP

There are no ring outliers.

15 monomers are involved in 36 short contacts:

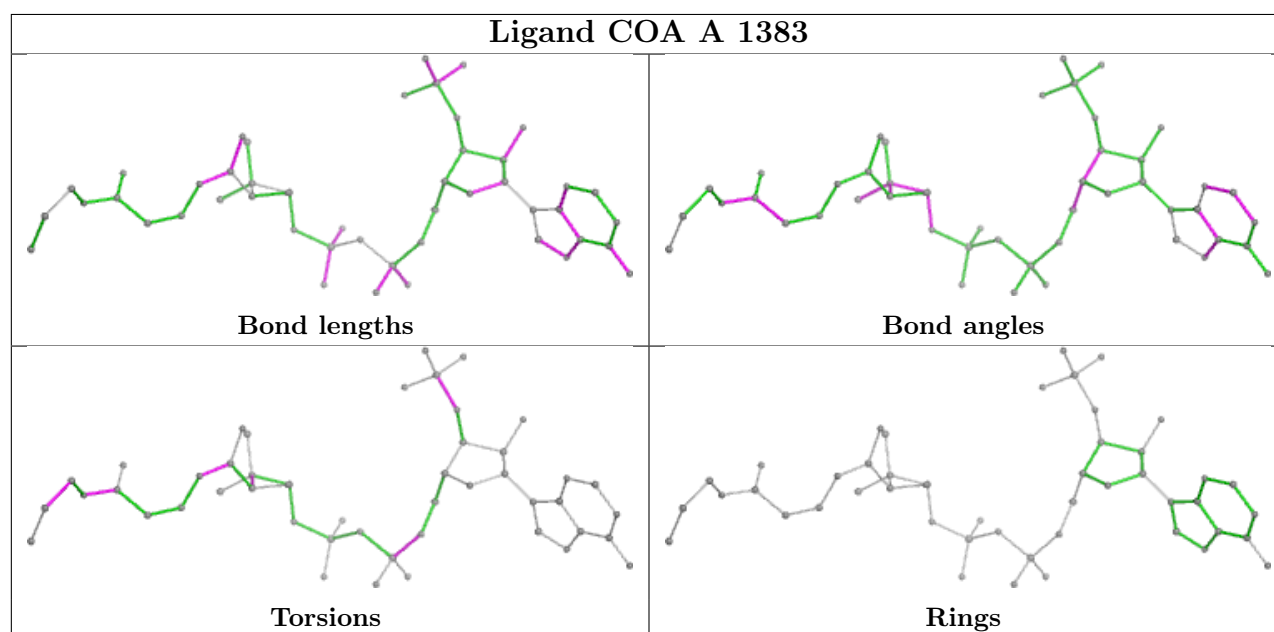
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1383	COA	2	0
3	G	1384	ACT	1	0
2	B	1383	COA	2	0
2	K	1385	COA	4	0
2	I	1383	COA	1	0
3	B	1385	ACT	1	0
2	H	1383	COA	6	0
2	F	1383	COA	3	0
2	L	1383	COA	1	0
3	H	1384	ACT	3	0
2	G	1383	COA	5	0

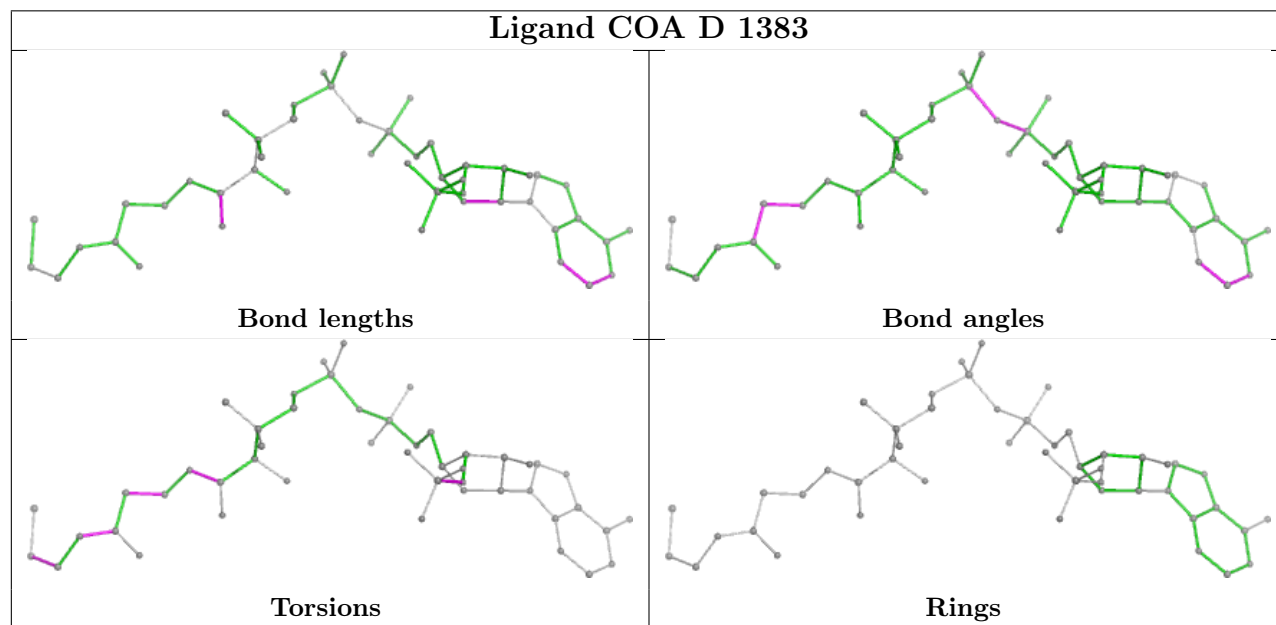
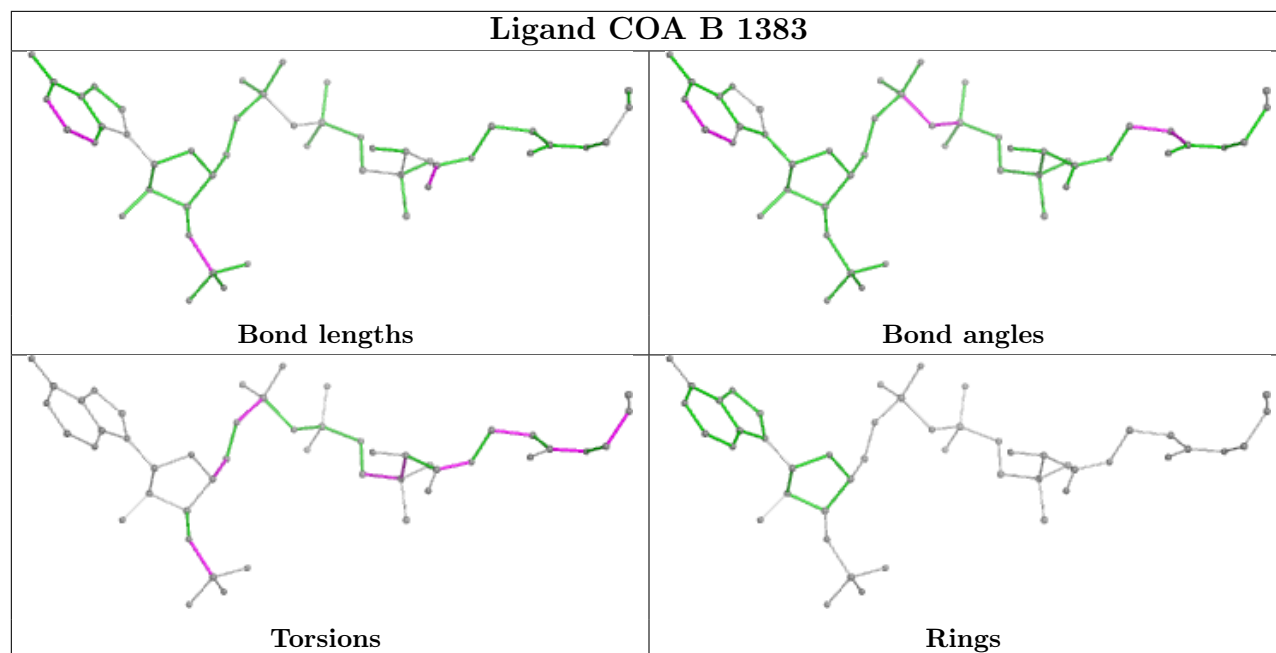
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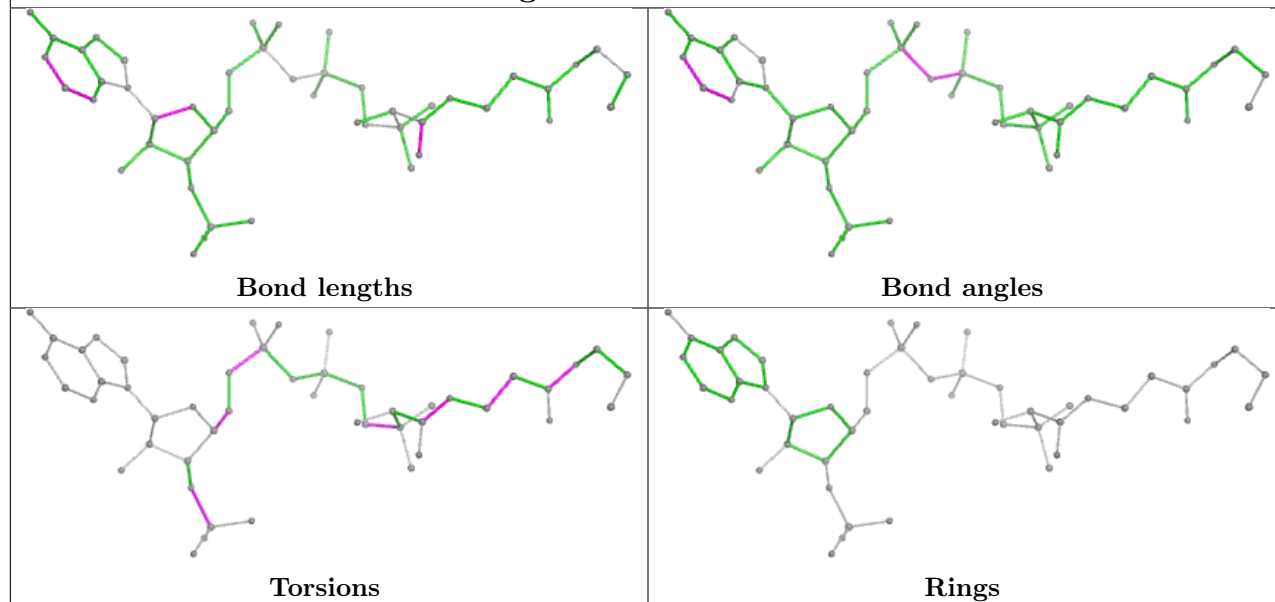
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1386	ACT	2	0
3	L	1384	ACT	1	0
2	E	1383	COA	1	0
2	J	1385	COA	3	0

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.

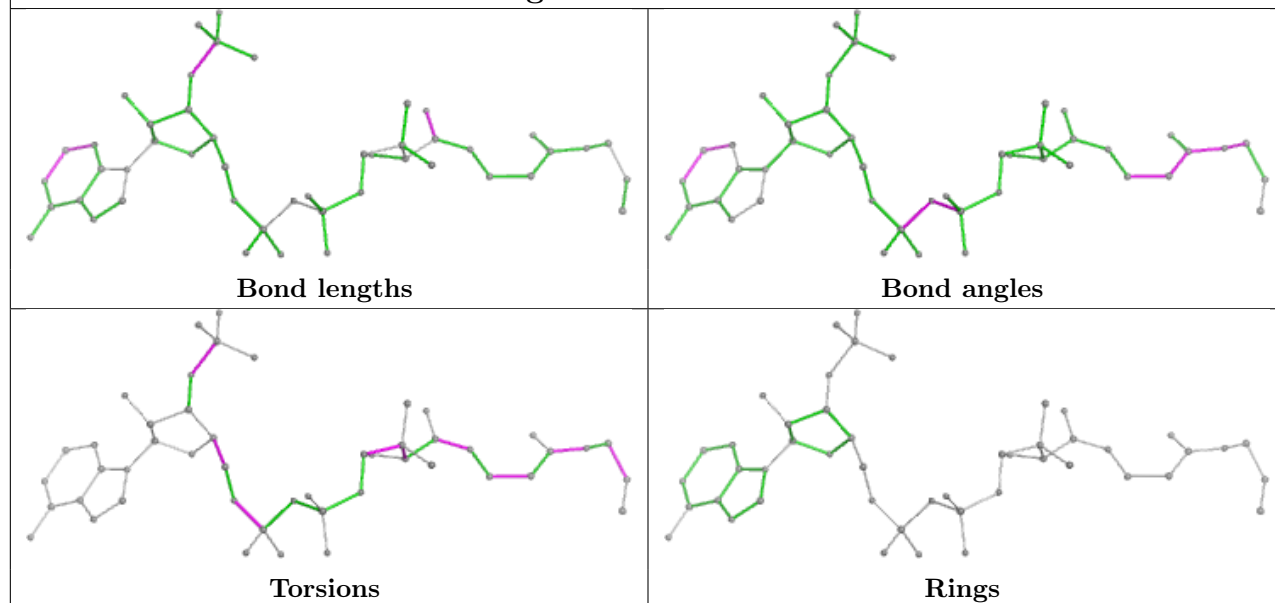


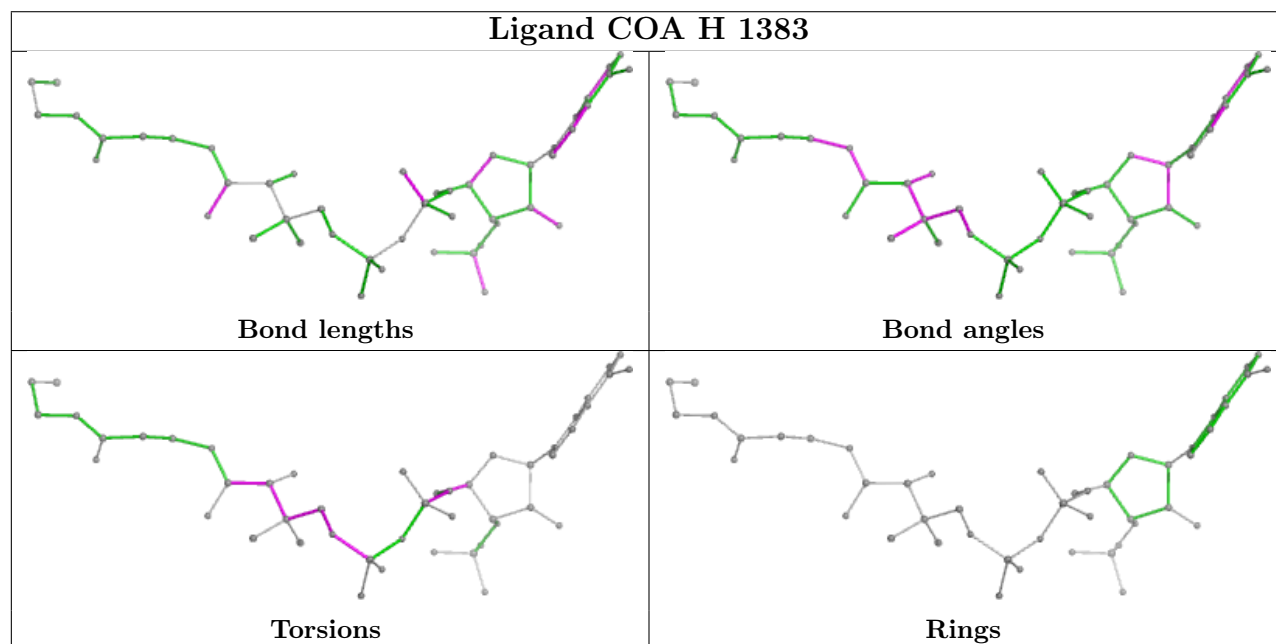
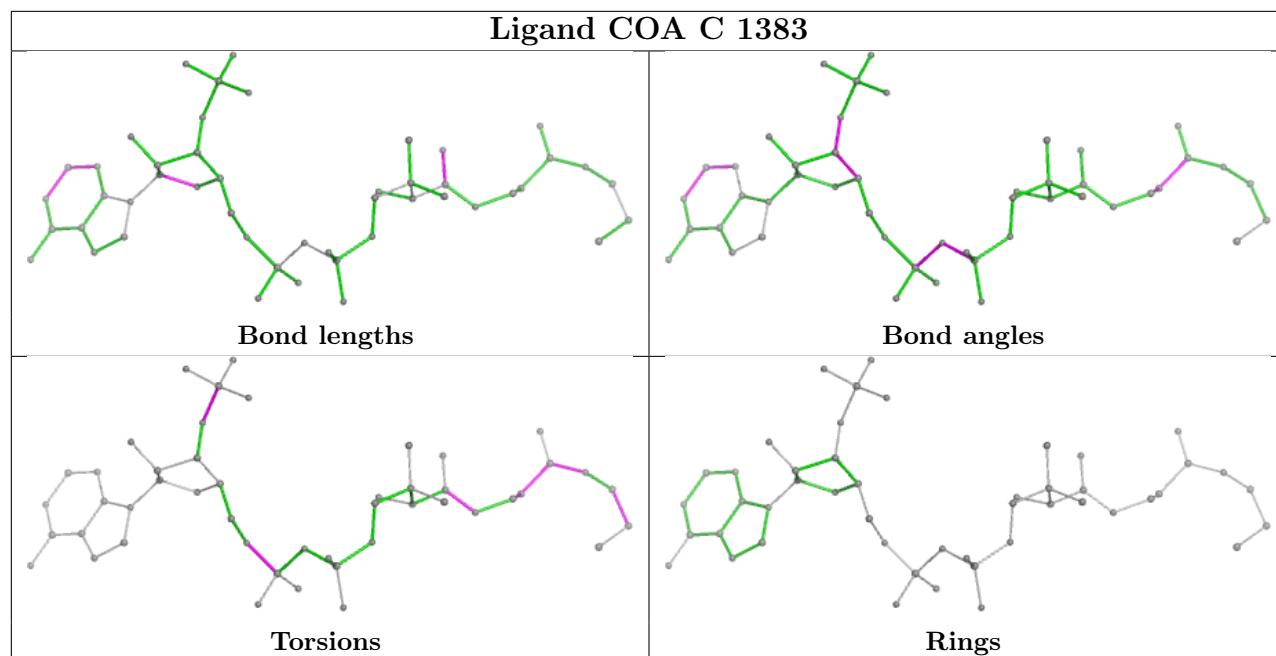


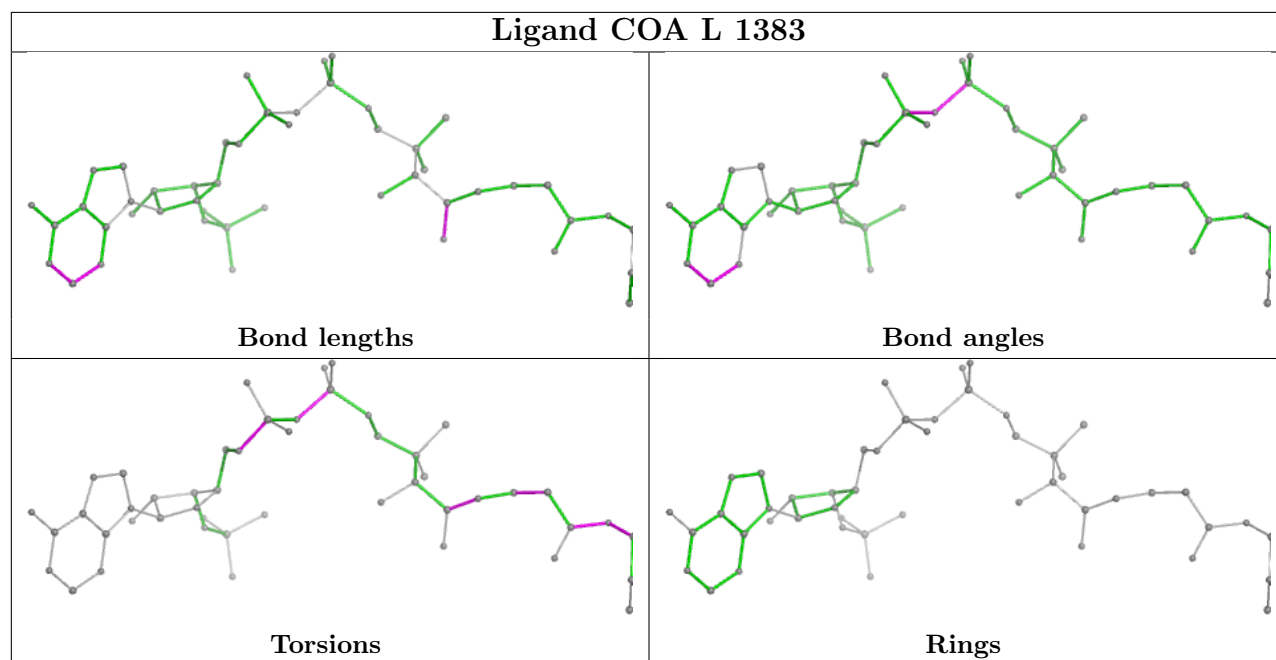
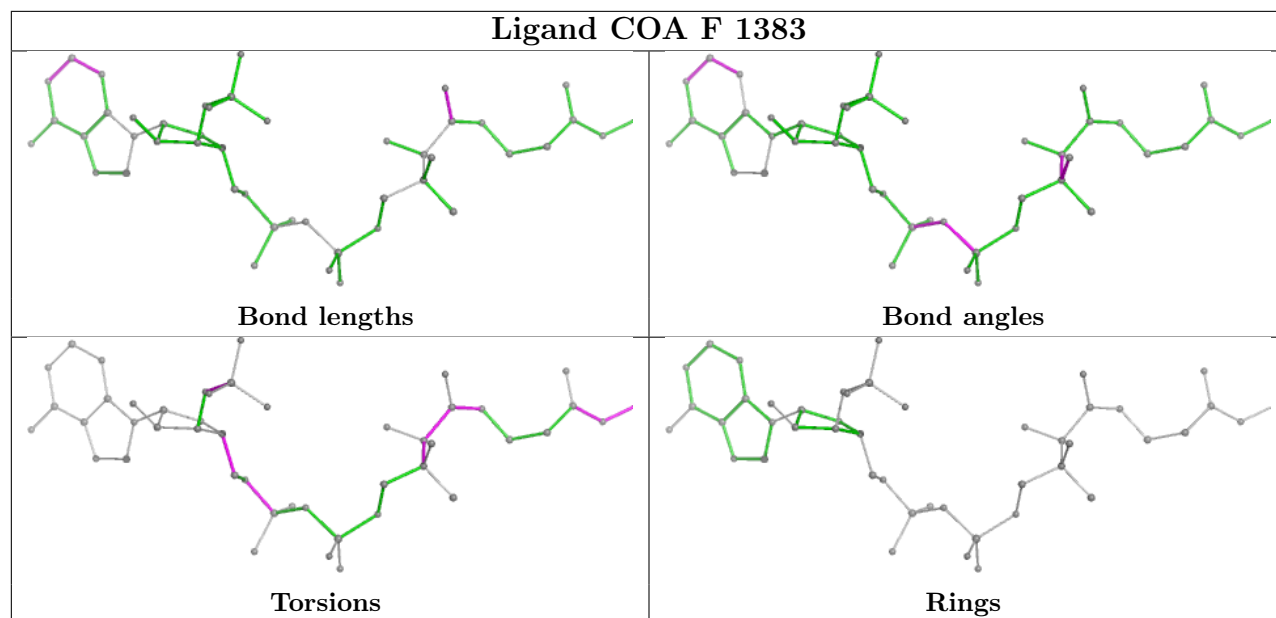
Ligand COA K 1385

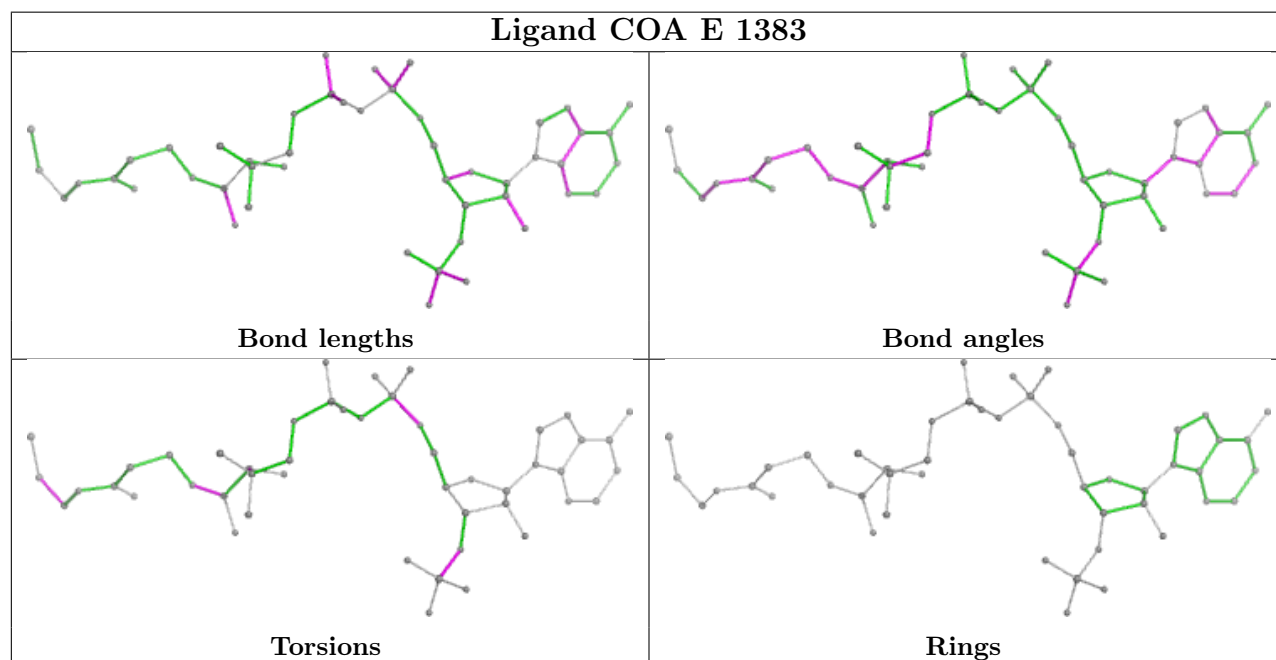
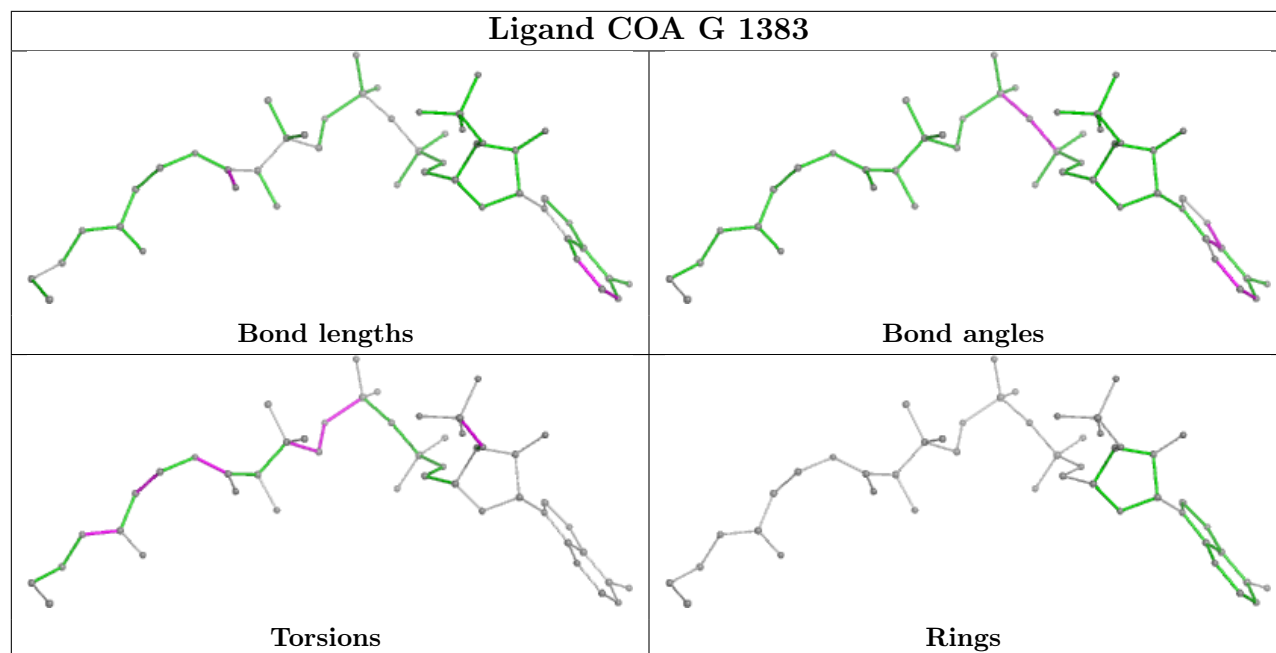


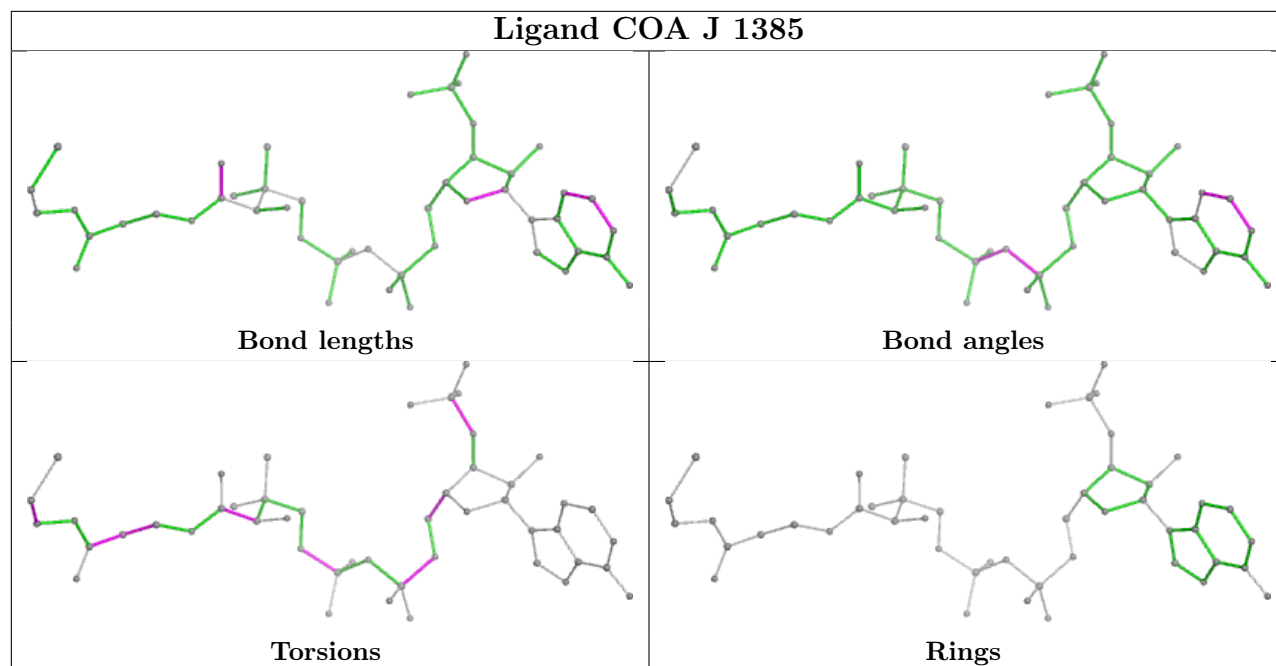
Ligand COA I 1383











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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

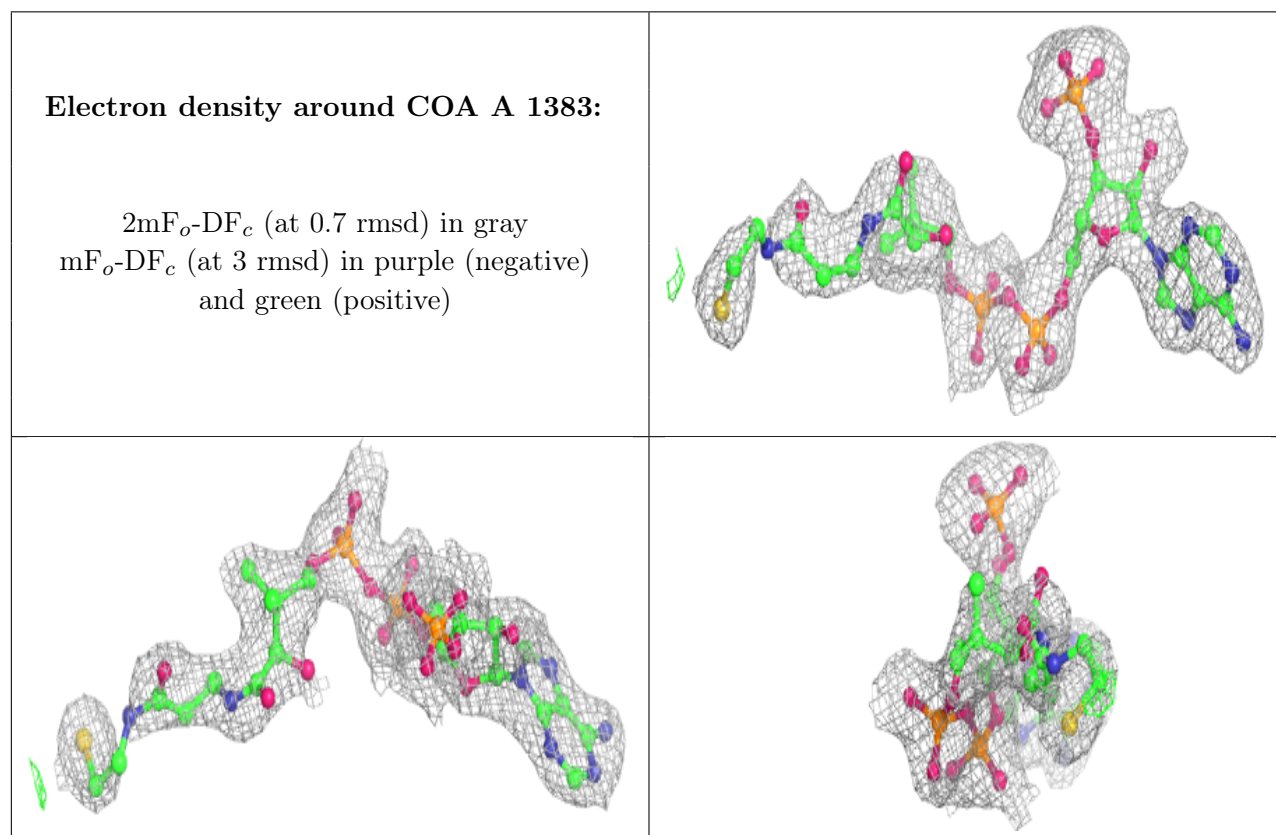
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

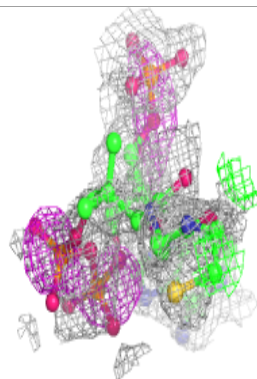
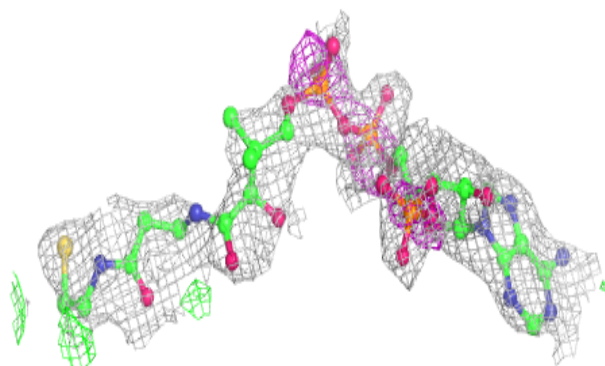
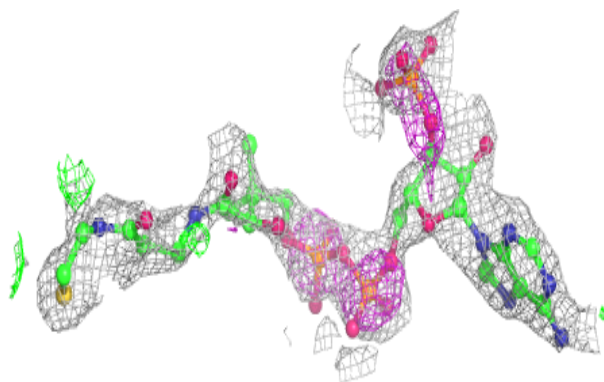
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

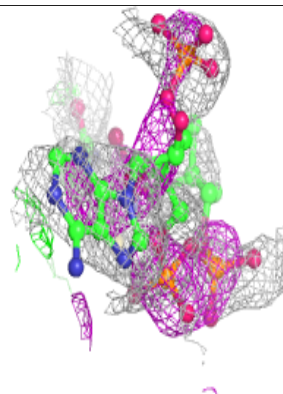
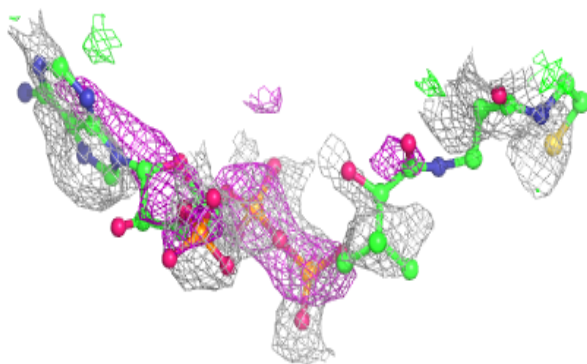
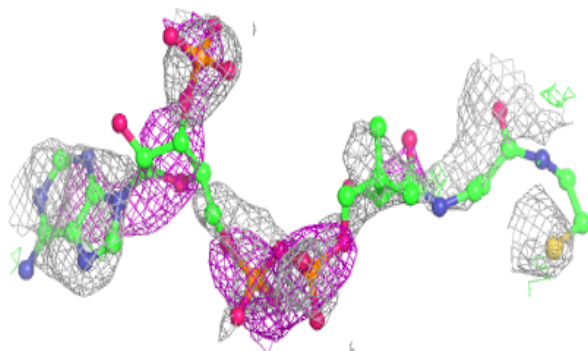


Electron density around COA B 1383:

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

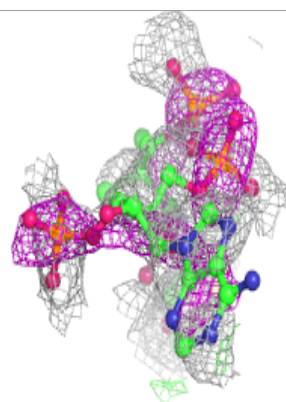
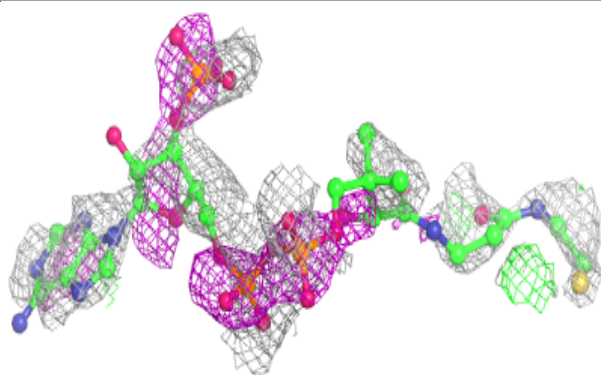
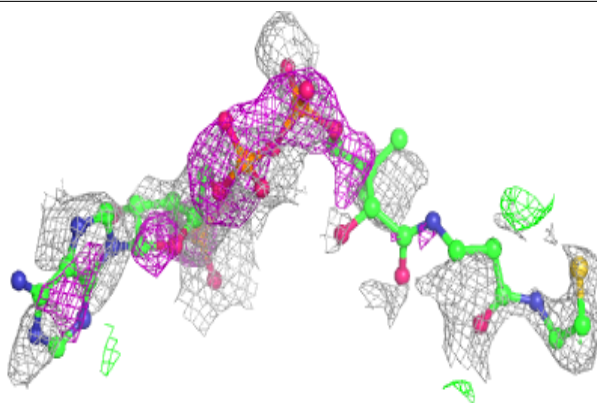
**Electron density around COA C 1383:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

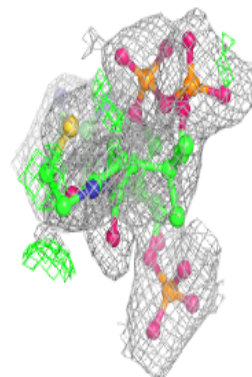
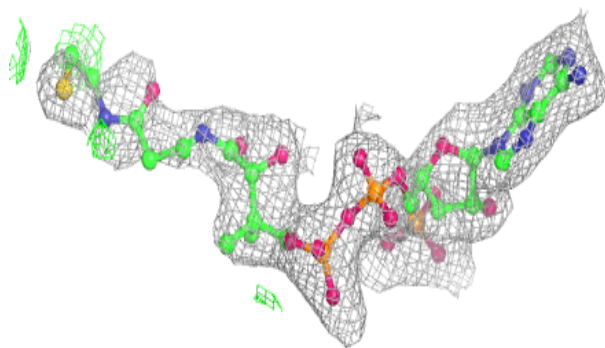
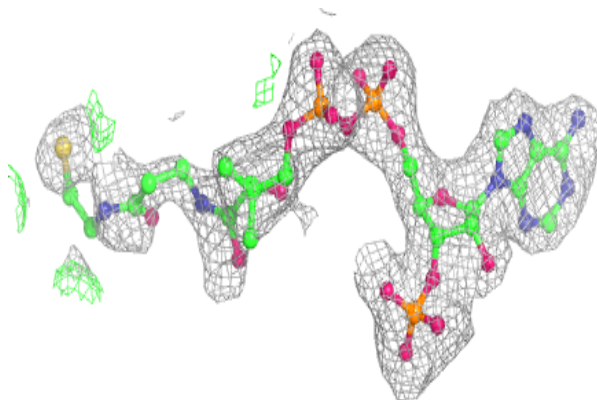


Electron density around COA D 1383:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

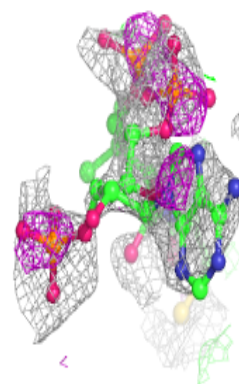
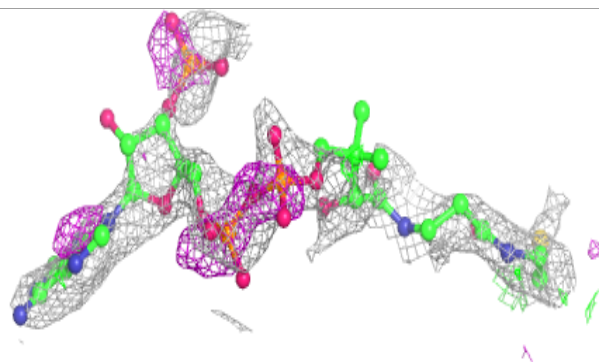
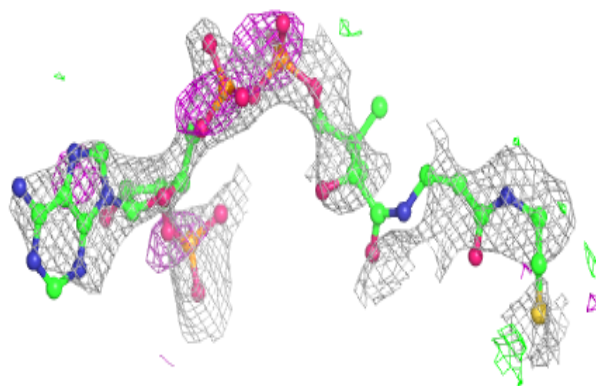
**Electron density around COA E 1383:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

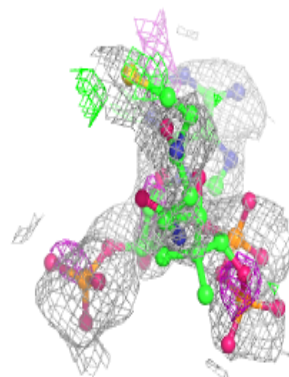
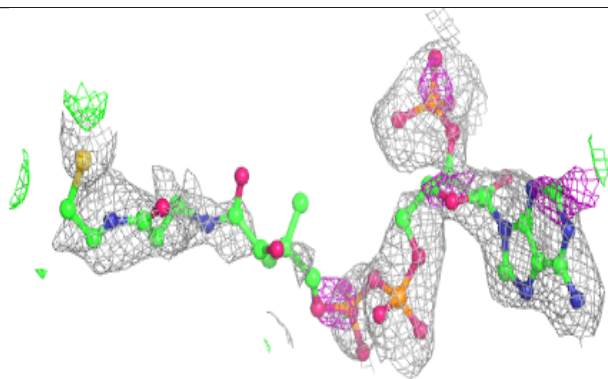
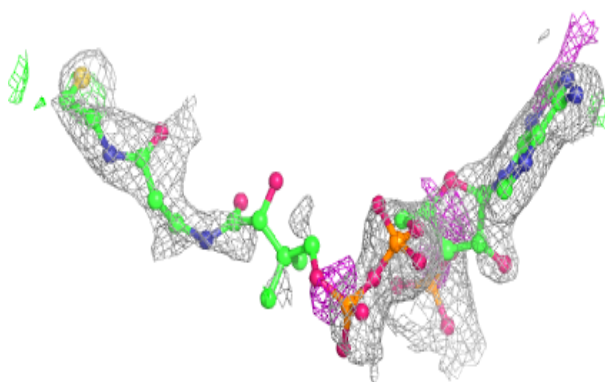


Electron density around COA F 1383:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

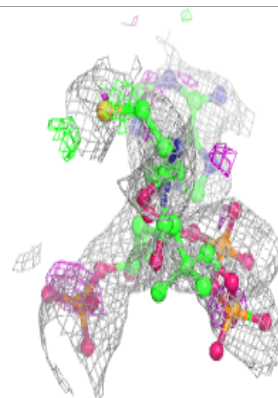
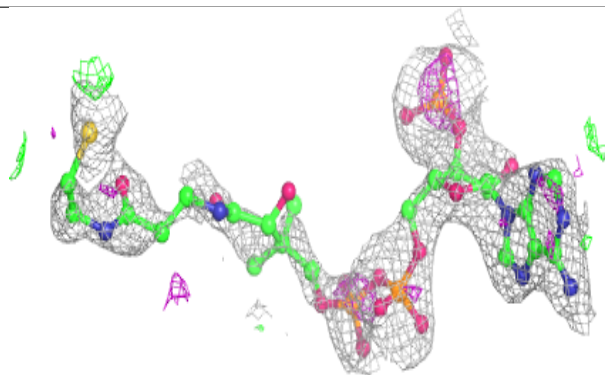
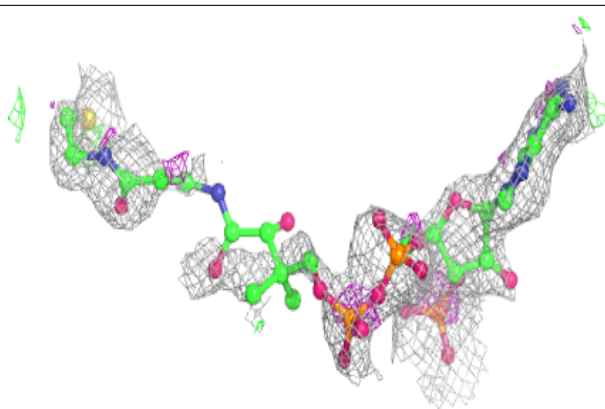
**Electron density around COA G 1383:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

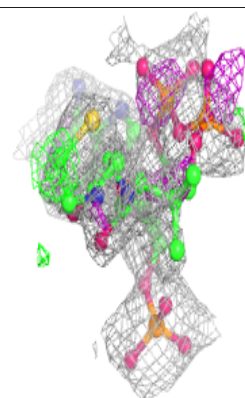
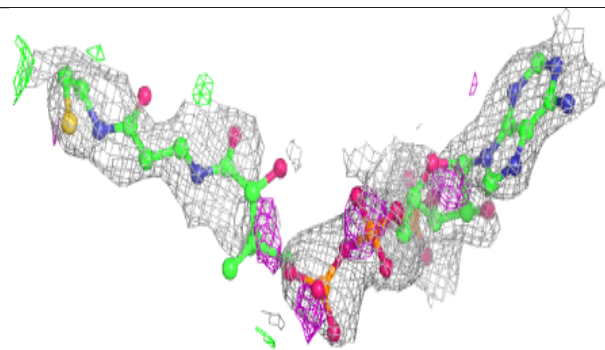
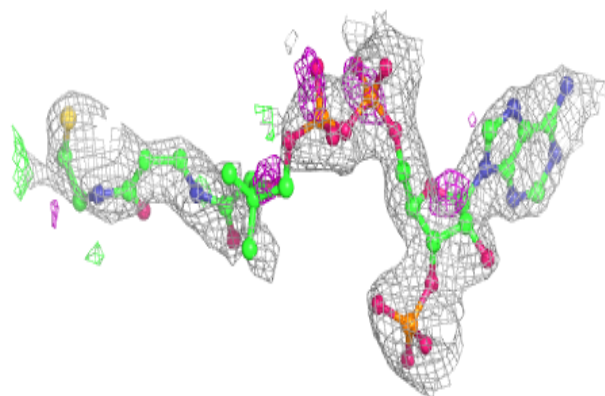


Electron density around COA H 1383:

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

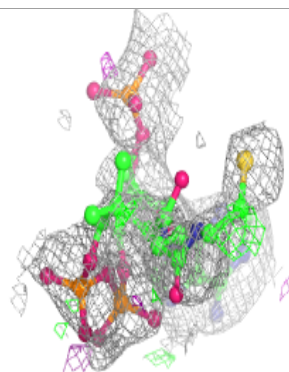
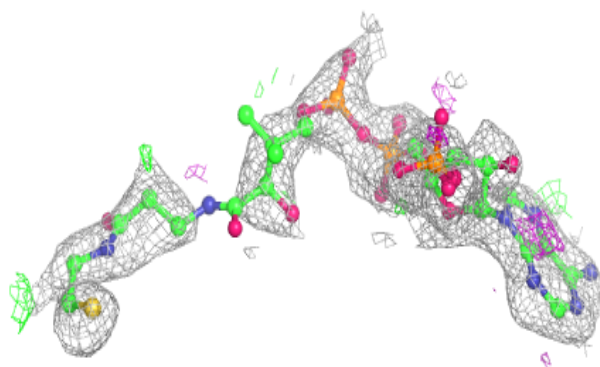
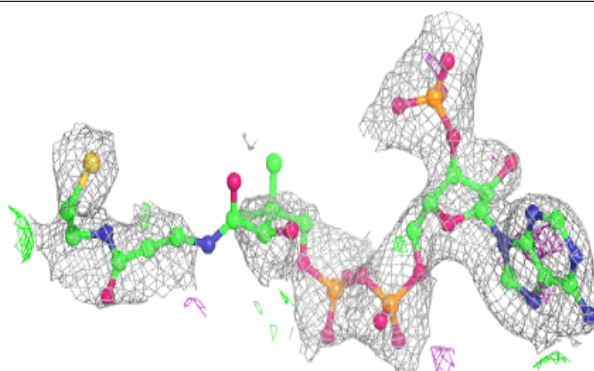
**Electron density around COA I 1383:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

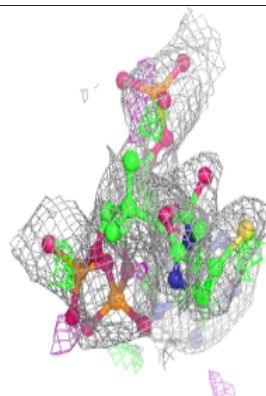
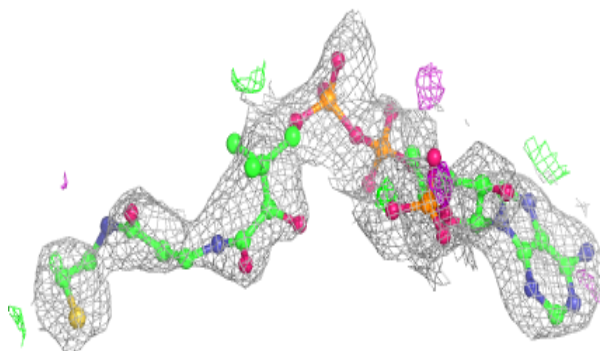
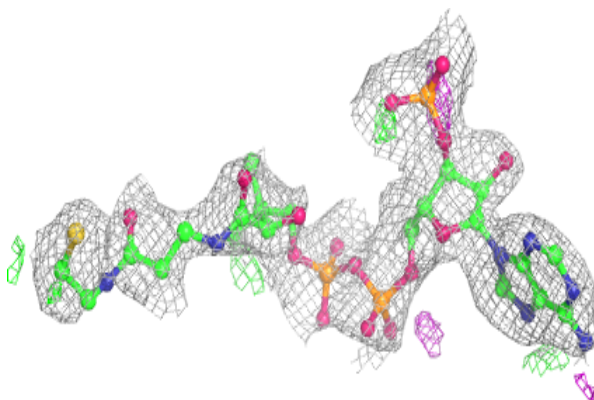


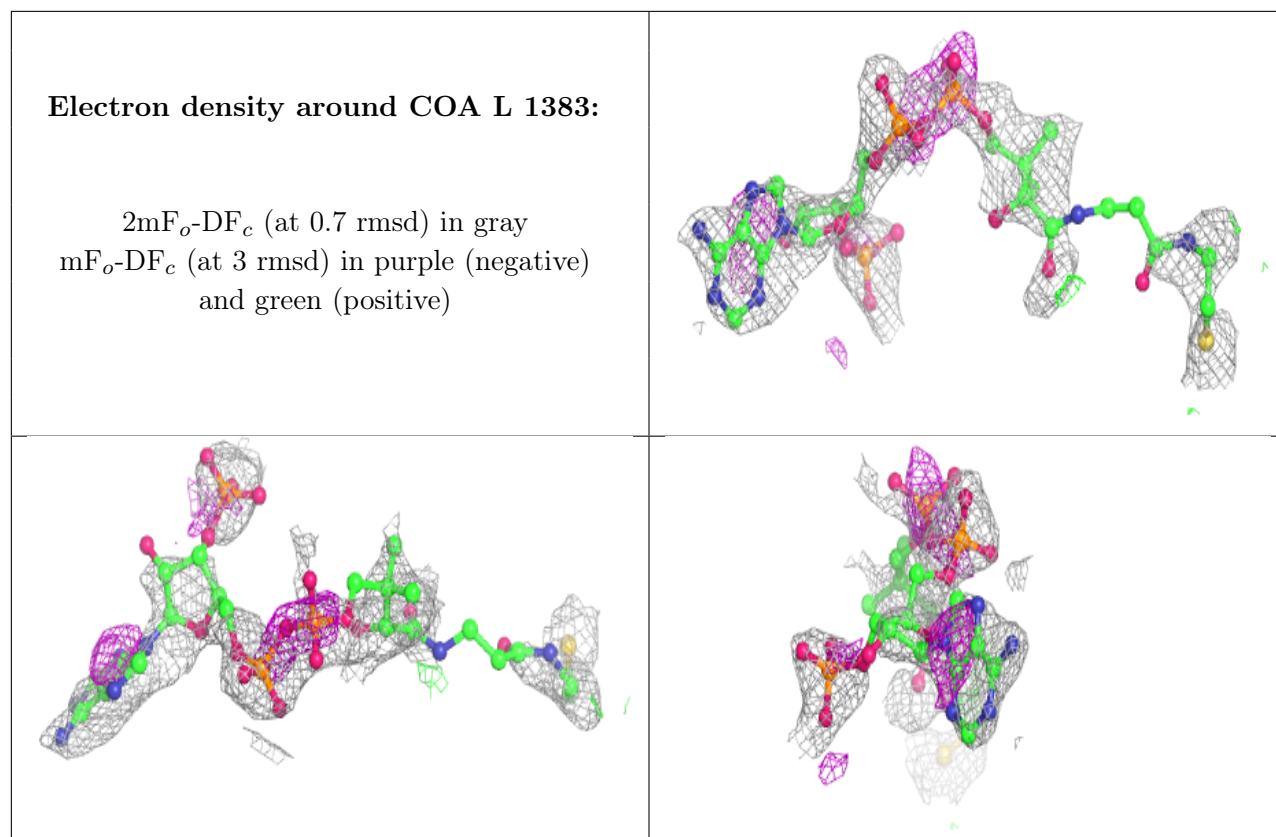
Electron density around COA J 1385:

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

**Electron density around COA K 1385:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.