



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 03:25 pm BST

PDB ID : 4A0S
Title : STRUCTURE OF THE 2-OCTENOYL-COA CARBOXYLASE REDUCTASE CINF IN COMPLEX WITH NADP AND 2-OCTENOYL-COA
Authors : Quade, N.; Huo, L.; Rachid, S.; Heinz, D.W.; Muller, R.
Deposited on : 2011-09-12
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

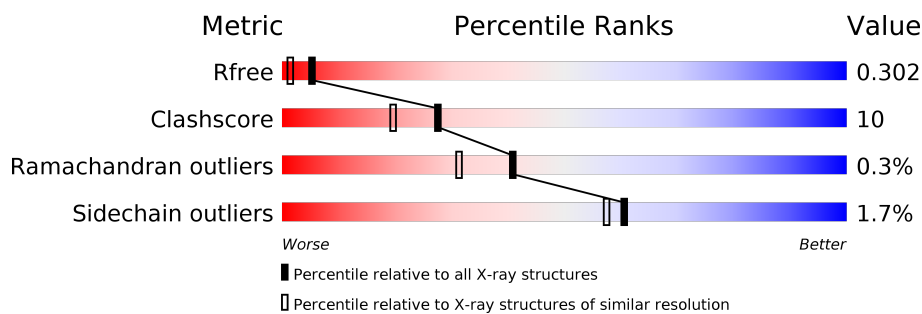
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	447	
1	B	447	
1	C	447	
1	D	447	

2 Entry composition [i](#)

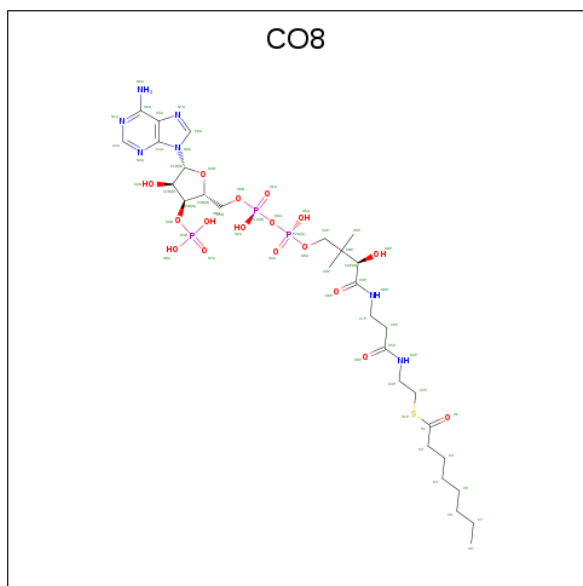
There are 4 unique types of molecules in this entry. The entry contains 15766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 OCTENOYL-COA REDUCTASE/CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	3	0
			3375	2115	613	631	16			
1	B	445	Total	C	N	O	S	0	2	0
			3371	2112	615	628	16			
1	C	444	Total	C	N	O	S	0	2	0
			3360	2106	609	629	16			
1	D	444	Total	C	N	O	S	0	0	0
			3348	2098	608	626	16			

- Molecule 2 is OCTANOYL-COENZYME A (three-letter code: CO8) (formula: $C_{29}H_{50}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			57	29	7	17	3 1		
2	B	1	Total	C	N	O	P S	0	0
			57	29	7	17	3 1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total 57	C 29	N 7	O 17	P 3	S 1	0	0
2	D	1	Total 57	C 29	N 7	O 17	P 3	S 1	0	0

- [illegible]

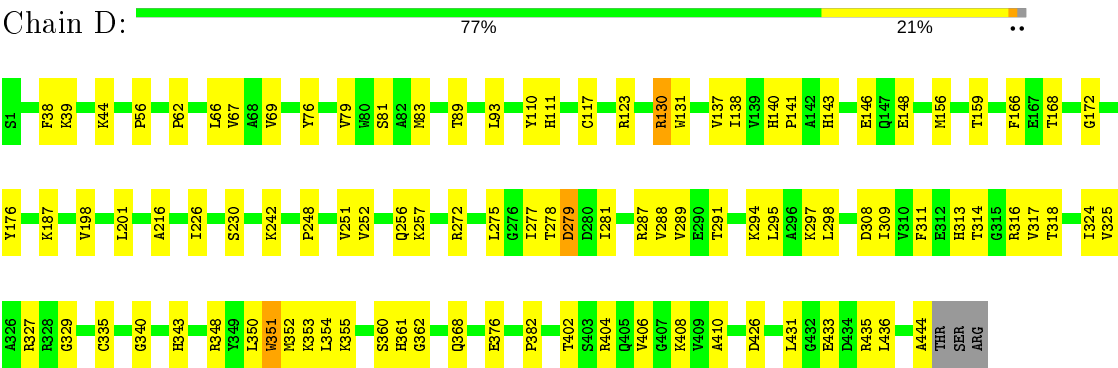
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	522	Total O 522 522	0	0
4	B	482	Total O 482 482	0	0
4	C	457	Total O 457 457	0	0

WORLDWIDE
PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	431	Total 431	O 431	0	0

● Molecule 1: OCTENOYL-COA REDUCTASE/CARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.01Å 83.30Å 122.74Å 90.00° 110.96° 90.00°	Depositor
Resolution (Å)	47.21 – 1.90 47.21 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.21-1.90) 98.9 (47.21-1.90)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.250 0.256 , 0.302	Depositor DCC
R_{free} test set	7037 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 15.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15766	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.55% 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: CO8, NAP

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	0.53	0/3452	0.66	0/4687
1	B	0.54	0/3445	0.67	0/4677
1	C	0.52	0/3434	0.67	0/4663
1	D	0.51	0/3416	0.68	3/4639 (0.1%)
All	All	0.53	0/13747	0.67	3/18666 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	130	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	D	275	LEU	CA-CB-CG	5.06	126.93	115.30
1	D	130	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3375	0	3369	59	0
1	B	3371	0	3368	70	0
1	C	3360	0	3349	80	0
1	D	3348	0	3335	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	57	0	46	2	0
2	B	57	0	46	4	0
2	C	57	0	46	5	0
2	D	57	0	46	5	0
3	A	48	0	25	7	0
3	B	48	0	25	9	0
3	C	48	0	25	6	0
3	D	48	0	25	5	0
4	A	522	0	0	6	0
4	B	482	0	0	8	0
4	C	457	0	0	6	0
4	D	431	0	0	9	0
All	All	15766	0	13705	276	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 10.

The worst 5 of 276 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:VAL:HG12	1:D:83:MET:HE2	1.28	1.07
1:D:79:VAL:HG12	1:D:83:MET:CE	1.91	0.99
1:B:228:GLY:H	1:B:272[B]:ARG:HH22	1.11	0.97
1:C:362:GLY:H	3:C:1445:NAP:H72N	1.13	0.94
1:D:362:GLY:H	3:D:1445:NAP:H72N	1.06	0.94

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	446/447 (100%)	433 (97%)	12 (3%)	1 (0%)	47	38
1	B	445/447 (100%)	433 (97%)	11 (2%)	1 (0%)	47	38
1	C	444/447 (99%)	429 (97%)	14 (3%)	1 (0%)	47	38
1	D	442/447 (99%)	427 (97%)	13 (3%)	2 (0%)	29	18
All	All	1777/1788 (99%)	1722 (97%)	50 (3%)	5 (0%)	41	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	HIS
1	C	313	HIS
1	D	313	HIS
1	B	313	HIS
1	D	277	ILE

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	351/350 (100%)	346 (99%)	5 (1%)	67	65
1	B	350/350 (100%)	344 (98%)	6 (2%)	60	57
1	C	349/350 (100%)	344 (99%)	5 (1%)	67	65
1	D	347/350 (99%)	340 (98%)	7 (2%)	55	51
All	All	1397/1400 (100%)	1374 (98%)	23 (2%)	60	60

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	435	ARG
1	C	279	ASP
1	D	351	TRP
1	C	116	ASP
1	C	286	ARG

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

Mol	Chain	Res	Type
1	B	95	GLN
1	B	217	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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$
3	NAP	C	1445	-	45,52,52	1.63	8 (17%)	56,80,80	2.30	10 (17%)
2	CO8	C	1446	-	51,59,59	2.18	9 (17%)	62,85,85	1.36	6 (9%)
2	CO8	B	1447	-	51,59,59	2.09	6 (11%)	62,85,85	1.29	5 (8%)
2	CO8	D	1446	-	51,59,59	2.09	6 (11%)	62,85,85	1.45	9 (14%)
3	NAP	A	1447	-	45,52,52	1.67	5 (11%)	56,80,80	1.75	12 (21%)
3	NAP	D	1445	-	45,52,52	1.75	8 (17%)	56,80,80	2.45	17 (30%)
3	NAP	B	1446	-	45,52,52	1.60	7 (15%)	56,80,80	1.38	6 (10%)
2	CO8	A	1446	-	51,59,59	2.34	10 (19%)	62,85,85	1.64	10 (16%)

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
3	NAP	C	1445	-	-	6/31/67/67	0/5/5/5
2	CO8	C	1446	-	-	13/54/74/74	0/3/3/3
2	CO8	B	1447	-	-	9/54/74/74	0/3/3/3
2	CO8	D	1446	-	-	12/54/74/74	0/3/3/3
3	NAP	A	1447	-	-	4/31/67/67	0/5/5/5
3	NAP	D	1445	-	-	3/31/67/67	0/5/5/5
3	NAP	B	1446	-	-	4/31/67/67	0/5/5/5
2	CO8	A	1446	-	-	13/54/74/74	0/3/3/3

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1446	CO8	C2'-C1'	-12.38	1.38	1.50
2	B	1447	CO8	C2'-C1'	-11.27	1.39	1.50
2	C	1446	CO8	C2'-C1'	-11.03	1.39	1.50
2	D	1446	CO8	C2'-C1'	-10.99	1.39	1.50
3	A	1447	NAP	O4B-C1B	6.58	1.50	1.41

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1445	NAP	O3X-P2B-O1X	-9.67	72.81	110.68
3	D	1445	NAP	O3X-P2B-O2X	-9.64	70.78	107.64
3	C	1445	NAP	O3X-P2B-O2X	-7.22	80.03	107.64
3	D	1445	NAP	O3X-P2B-O1X	-6.25	86.19	110.68
3	D	1445	NAP	N3A-C2A-N1A	-6.00	119.31	128.68

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

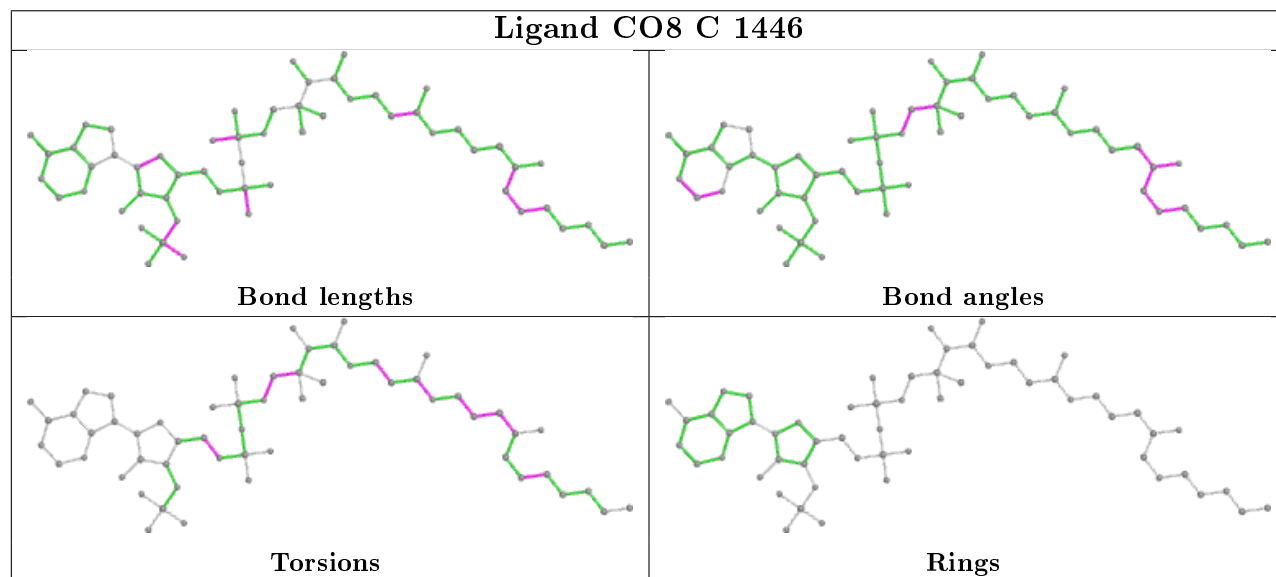
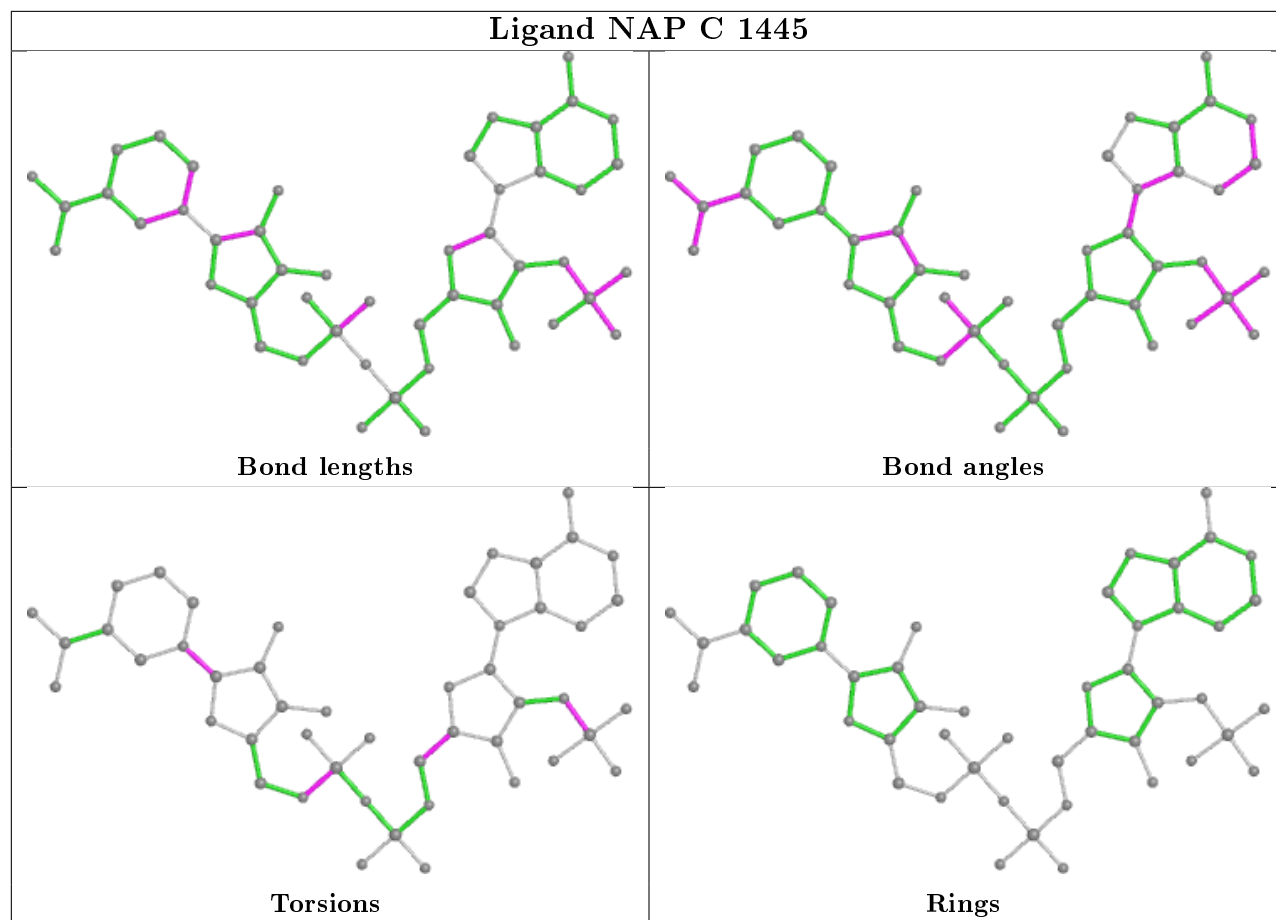
Mol	Chain	Res	Type	Atoms
3	C	1445	NAP	C2B-O2B-P2B-O1X
3	C	1445	NAP	C5D-O5D-PN-O1N
3	C	1445	NAP	O4D-C1D-N1N-C6N
2	C	1446	CO8	CAP-CBP-CCP-O6A
2	C	1446	CO8	C5P-C6P-C7P-N8P

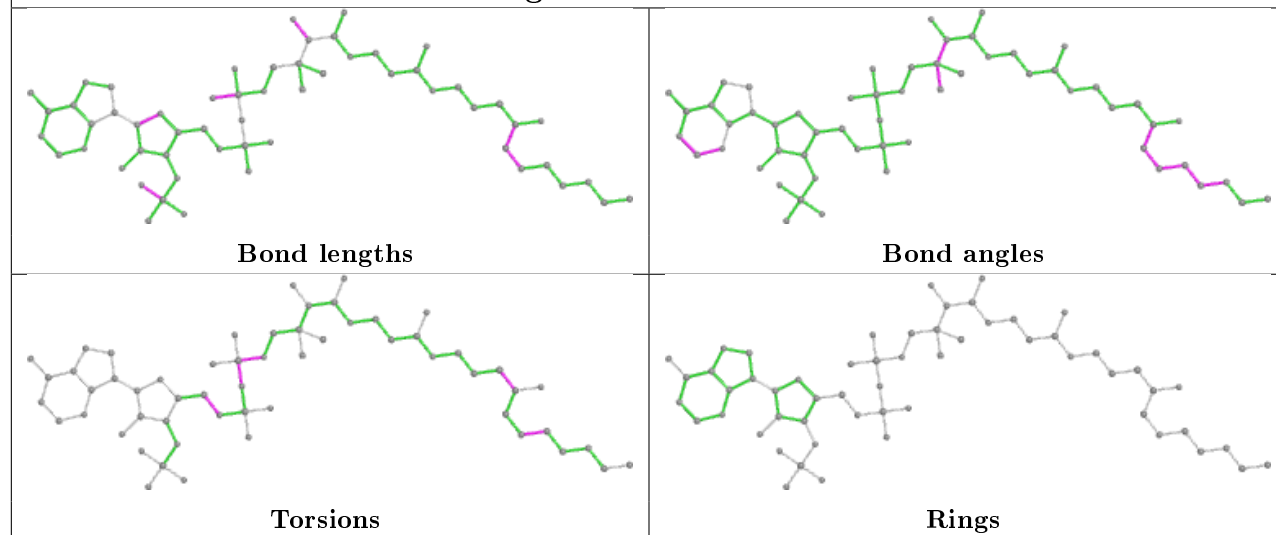
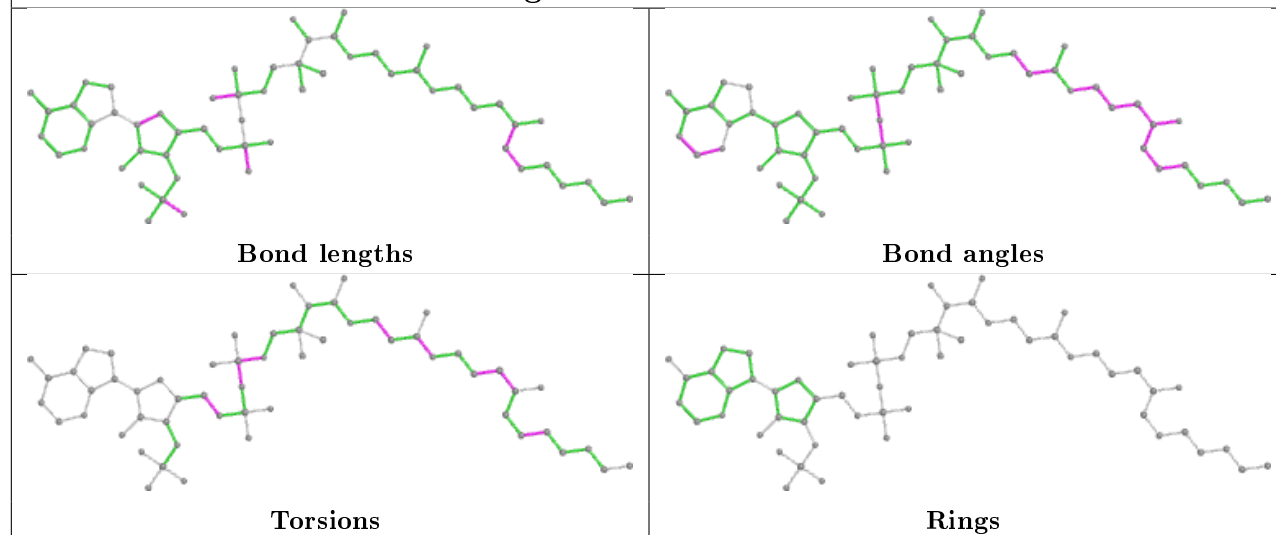
There are no ring outliers.

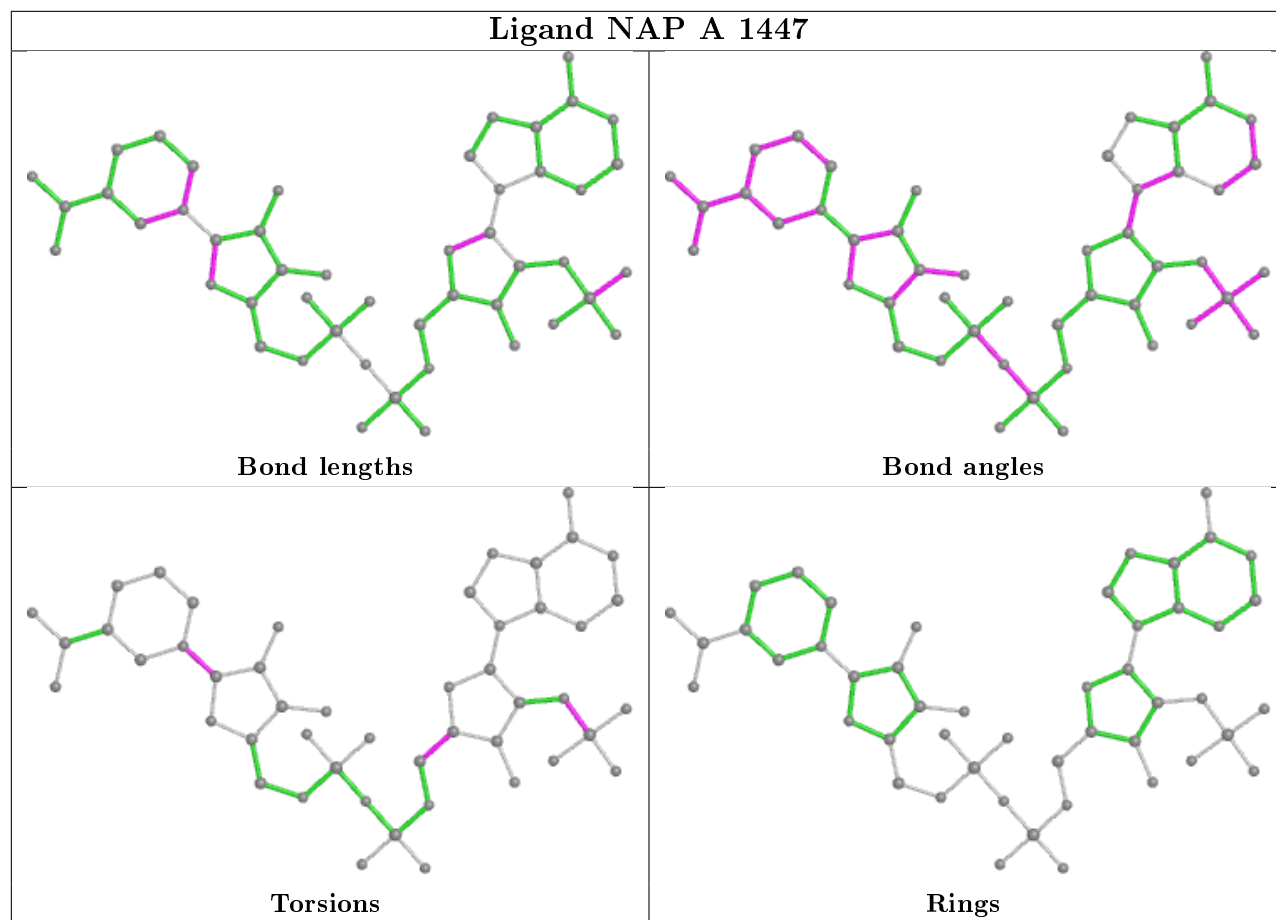
8 monomers are involved in 38 short contacts:

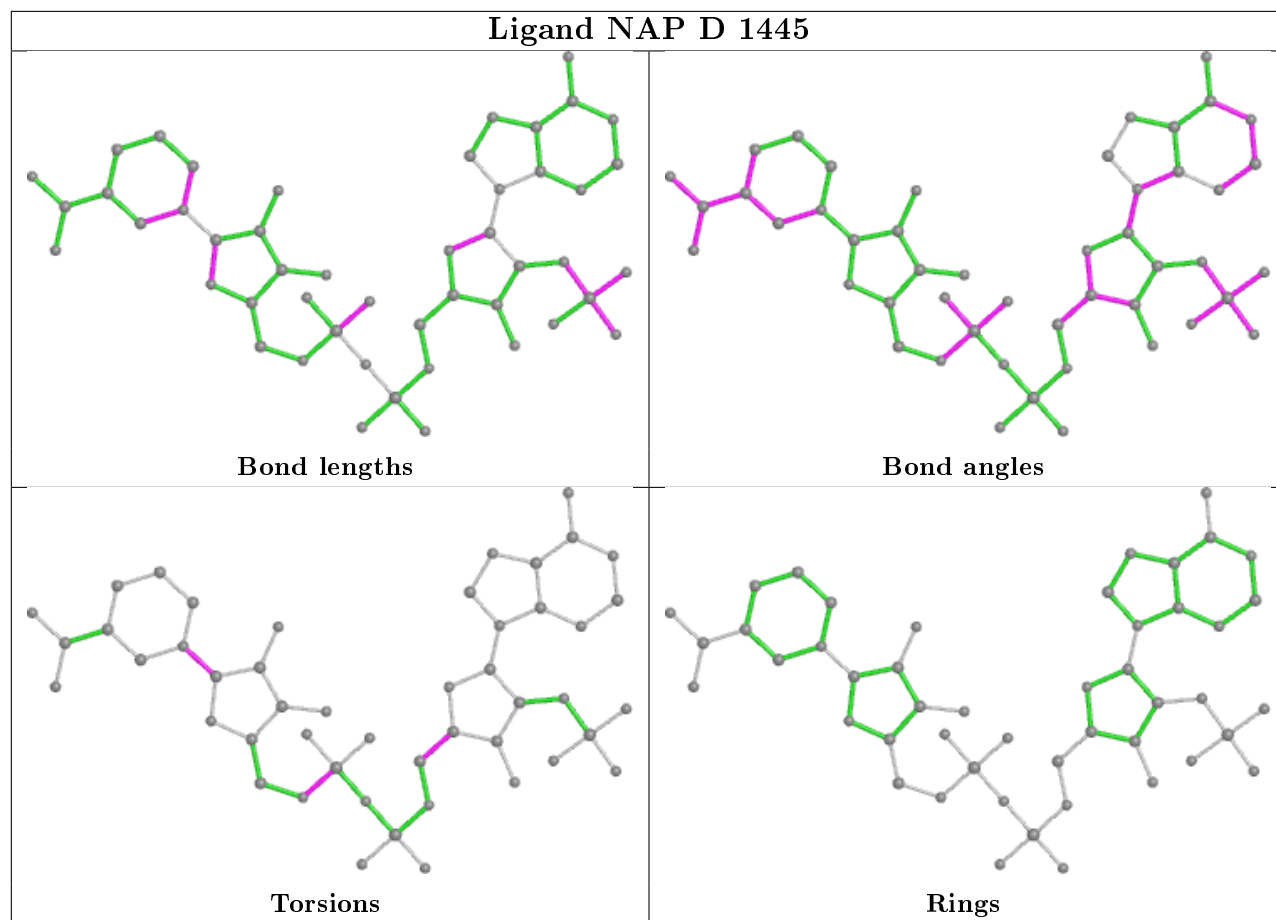
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1445	NAP	6	0
2	C	1446	CO8	5	0
2	B	1447	CO8	4	0
2	D	1446	CO8	5	0
3	A	1447	NAP	7	0
3	D	1445	NAP	5	0
3	B	1446	NAP	9	0
2	A	1446	CO8	2	0

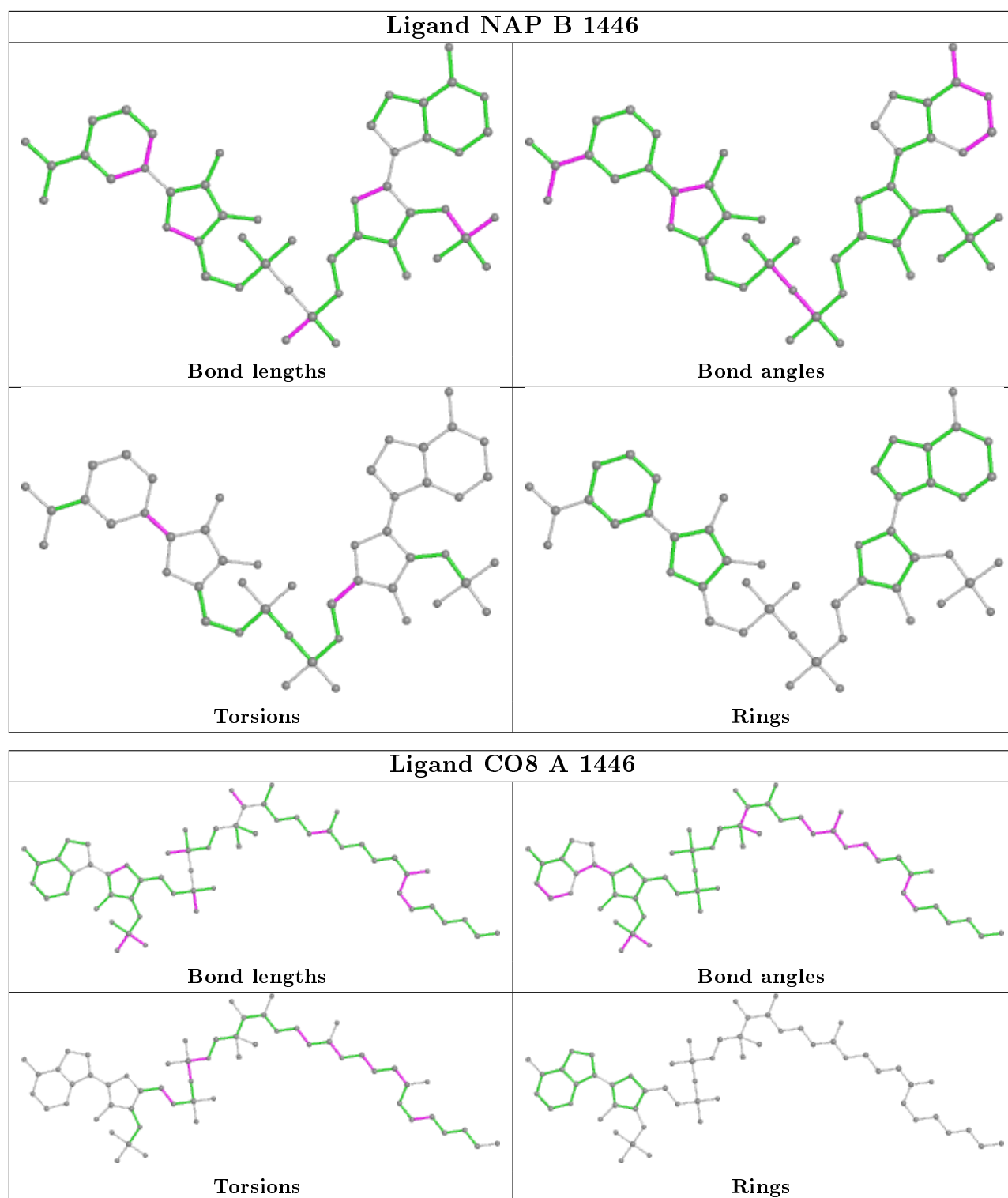
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand CO8 B 1447**Ligand CO8 D 1446**







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

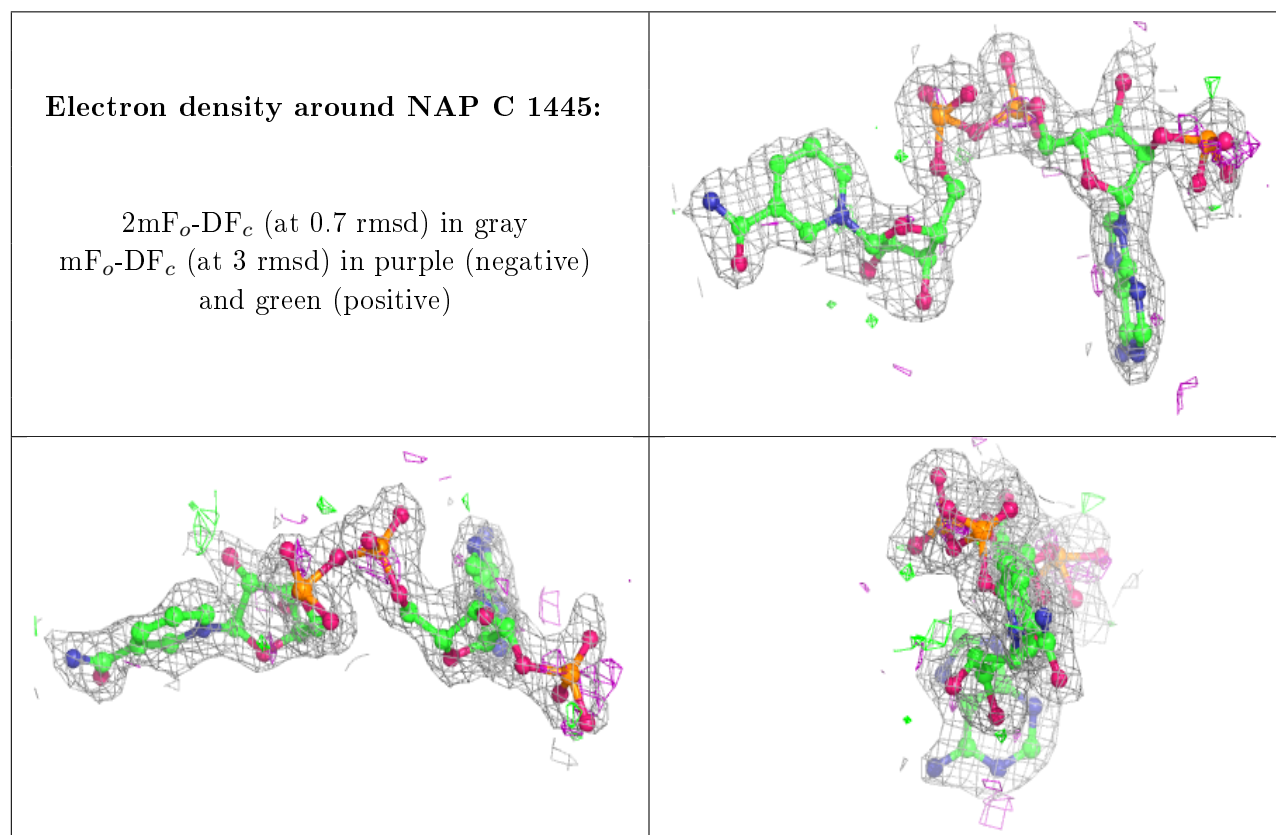
6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

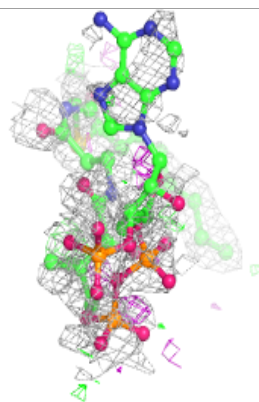
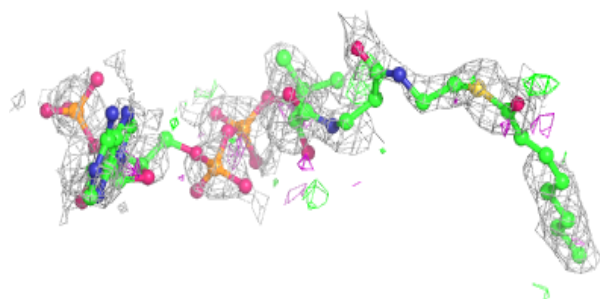
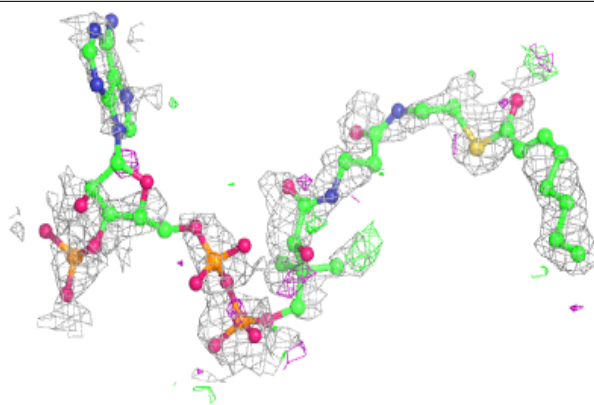
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

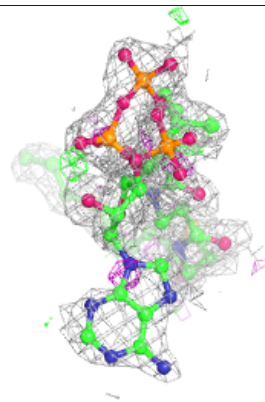
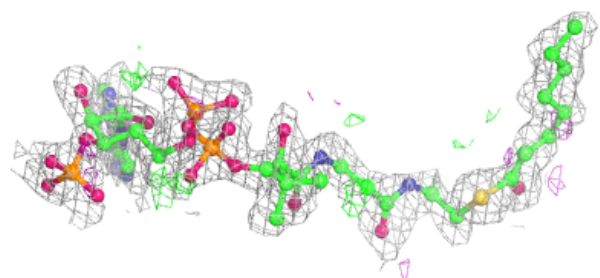
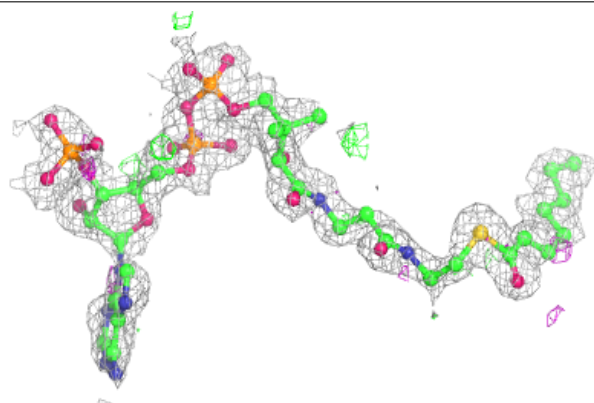


Electron density around CO8 C 1446:

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

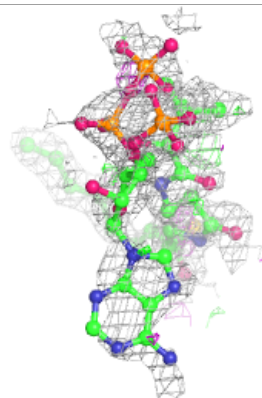
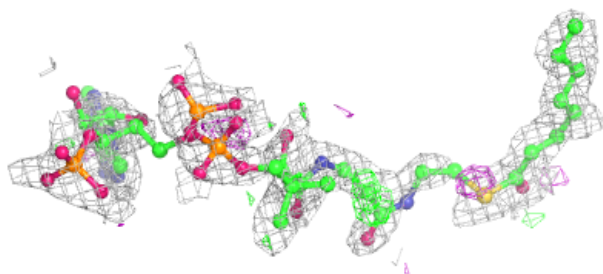
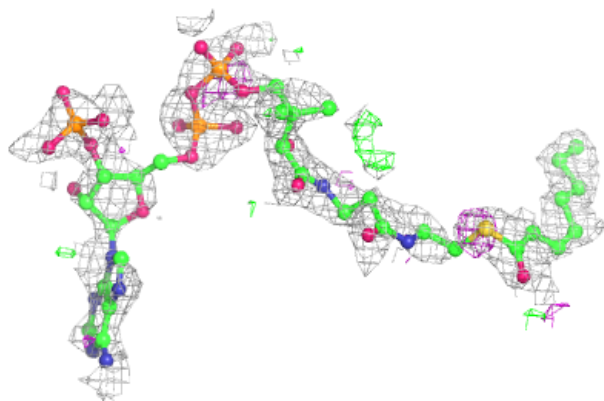
**Electron density around CO8 B 1447:**

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

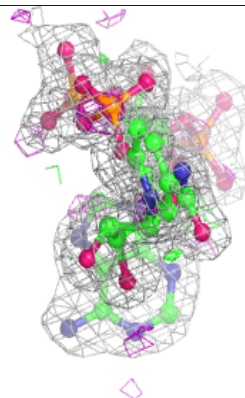
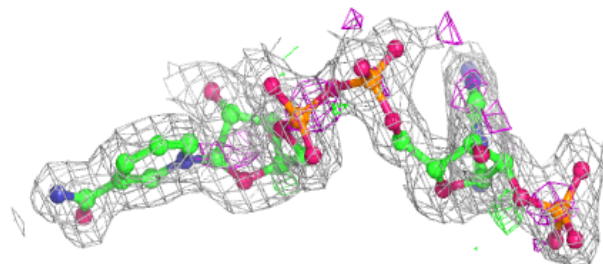
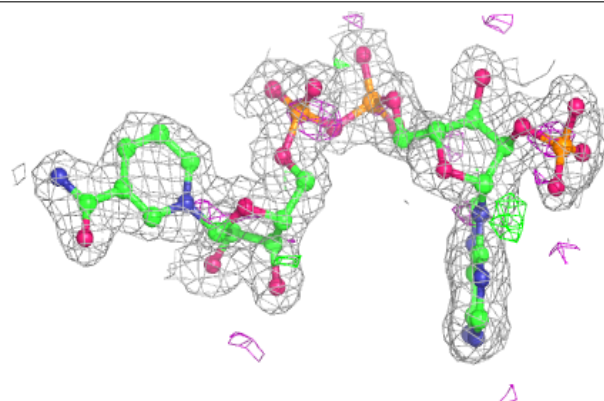


Electron density around CO8 D 1446:

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

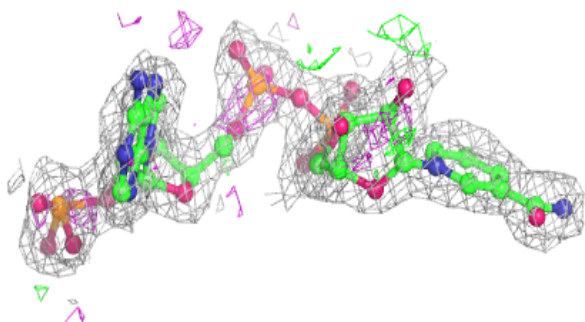
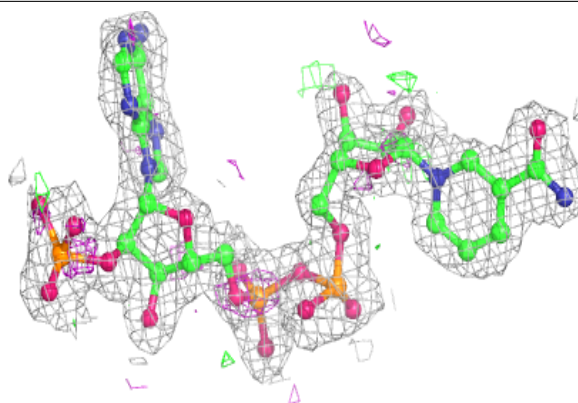
**Electron density around NAP A 1447:**

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

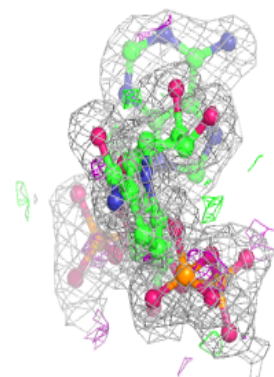
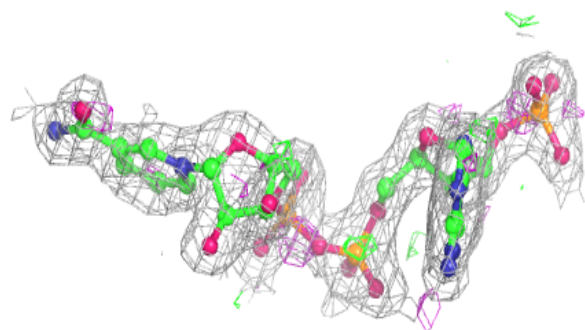
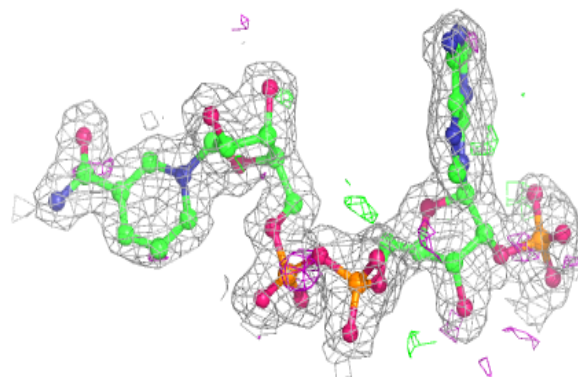


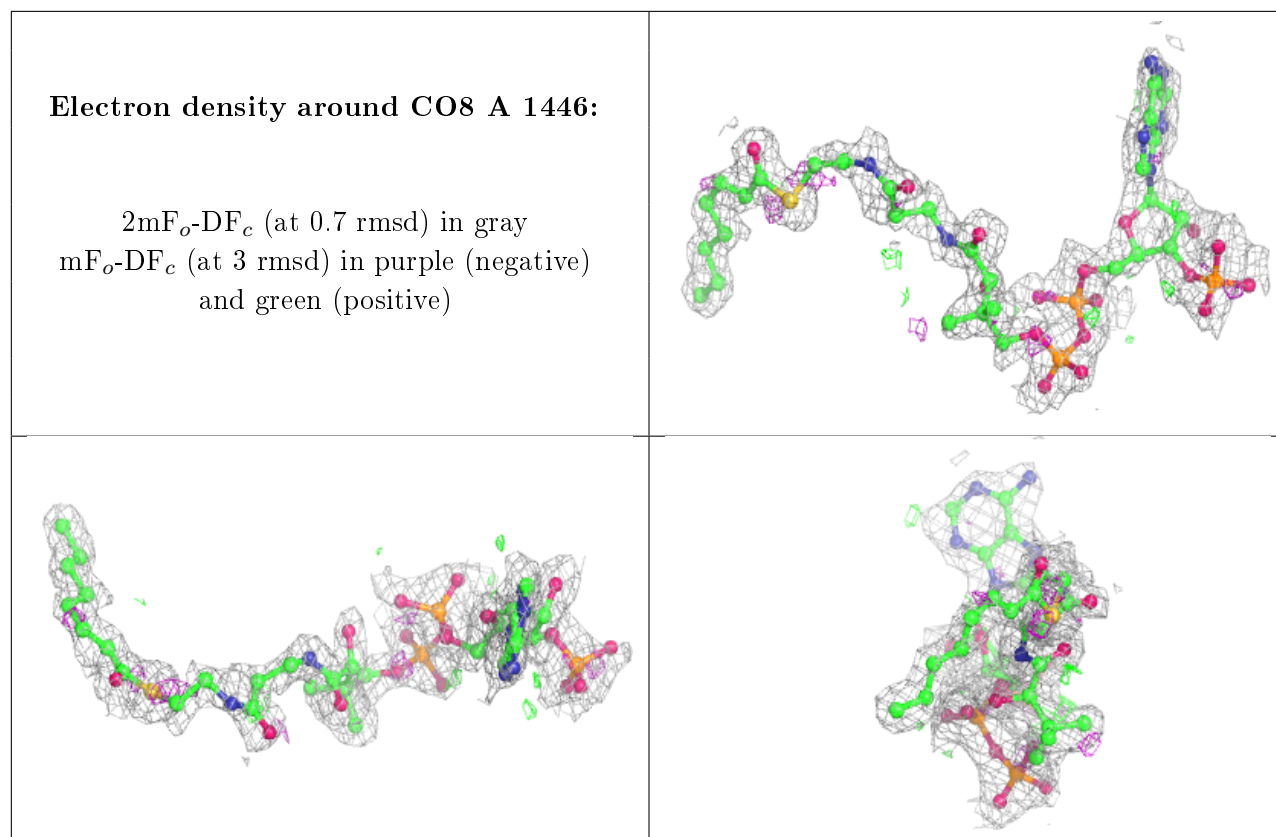
Electron density around NAP D 1445:

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

**Electron density around NAP B 1446:**

$2mF_o-DF_c$ (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.