Full wwPDB X-ray Structure Validation Report (i)

Apr 4, 2022 – 08:08 PM EDT

PDB ID	:	5T7E
Title	:	Crystal structure of Streptomyces hygroscopicus Bialaphos Resistance (BAR) protein in complex with Coenzyme A and L-phosphinothricin
Authors	:	Christ, B.; Weng, J.K.
Deposited on	:	2016-09-04
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11883 atoms, of which 5612 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 Phosphinothricin N-acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	174	2722	882	1340	245	251	4	0	0	0
1	B	174	2737	887	1346	246	254	4	0	1	0
1	C	175	2736	887	1347	246	252	4	0	0	0
1	D	175	2736	887	1347	246	252	4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P16426
A	-4	ALA	-	expression tag	UNP P16426
A	-3	MET	-	expression tag	UNP P16426
A	-2	ASP	-	expression tag	UNP P16426
A	-1	PRO	-	expression tag	UNP P16426
A	0	PHE	-	expression tag	UNP P16426
B	-5	GLY	-	expression tag	UNP P16426
B	-4	ALA	-	expression tag	UNP P16426
B	-3	MET	-	expression tag	UNP P16426
B	-2	ASP	-	expression tag	UNP P16426
B	-1	PRO	-	expression tag	UNP P16426
B	0	PHE	-	expression tag	UNP P16426
C	-5	GLY	-	expression tag	UNP P16426
C	-4	ALA	-	expression tag	UNP P16426
C	-3	MET	-	expression tag	UNP P16426
C	-2	ASP	-	expression tag	UNP P16426
C	-1	PRO	-	expression tag	UNP P16426
C	0	PHE	-	expression tag	UNP P16426
D	-5	GLY	-	expression tag	UNP P16426
D	-4	ALA	-	expression tag	UNP P16426
D	-3	MET	-	expression tag	UNP P16426

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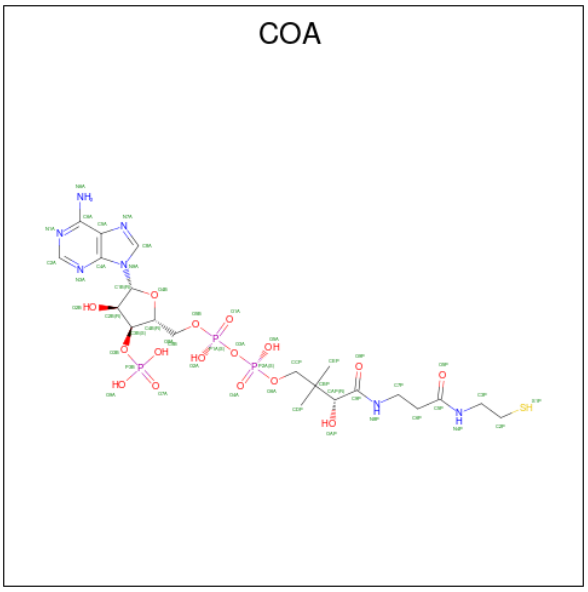
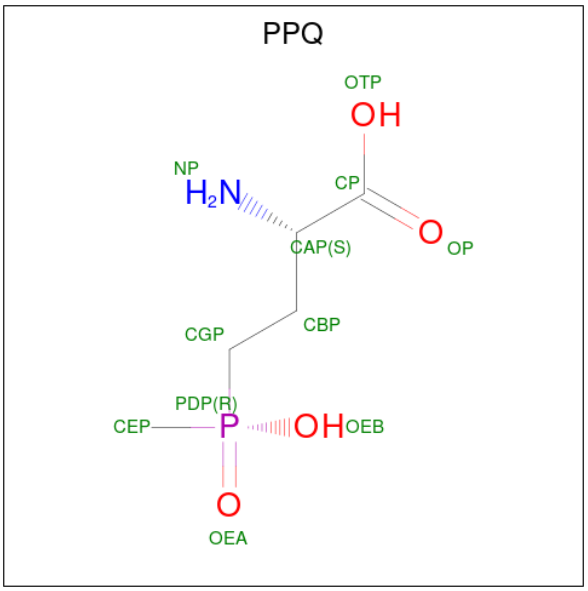
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	ASP	-	expression tag	UNP P16426
D	-1	PRO	-	expression tag	UNP P16426
D	0	PHE	-	expression tag	UNP P16426

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



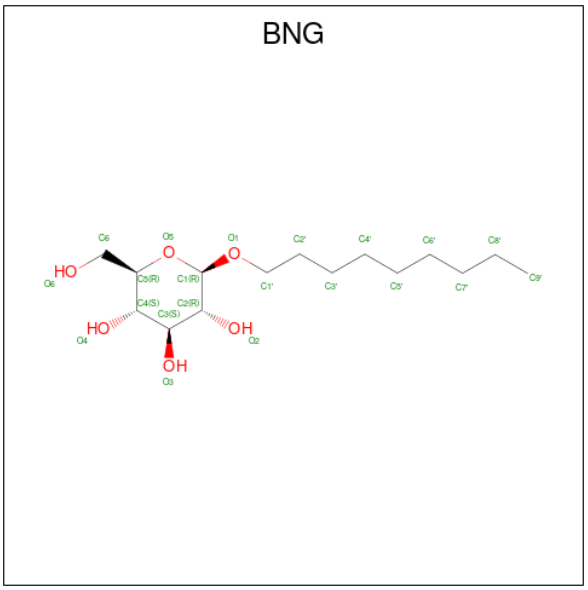
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	H	N	O	P	S		
2	A	1	80	21	32	7	16	3	1	0	0
2	B	1	80	21	32	7	16	3	1	0	0
2	C	1	80	21	32	7	16	3	1	0	0
2	D	1	80	21	32	7	16	3	1	0	0

- Molecule 3 is PHOSPHINOTHRICIN (three-letter code: PPQ) (formula: $C_5H_{12}NO_4P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
3	A	1	22	5	11	1	4	1	0	0
3	B	1	22	5	11	1	4	1	0	0
3	C	1	22	5	11	1	4	1	0	0
3	D	1	22	5	11	1	4	1	0	0

- Molecule 4 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	51	15	30	6	0	0
4	B	1	51	15	30	6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	106	106	106	0	0
5	B	101	101	101	0	0
5	C	124	124	124	0	0
5	D	111	111	111	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.18Å 66.11Å 86.15Å 90.00° 103.06° 90.00°	Depositor
Resolution (Å)	62.52 – 1.80	Depositor
% Data completeness (in resolution range)	72.3 (62.52-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 1.80Å)	Xtriage
Refinement program	PHENIX (dev_2499: ???)	Depositor
R, R_{free}	0.208 , 0.247	Depositor
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.732	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11883	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1860e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

10 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	$\#\|Z\| > 2$
4	BNG	A	802	-	21,21,21	1.27	2 (9%)	26,26,26	0.96	1 (3%)
3	PPQ	B	801	-	4,10,10	1.77	1 (25%)	2,14,14	2.02	1 (50%)
3	PPQ	A	801	-	4,10,10	1.86	1 (25%)	2,14,14	1.93	1 (50%)
4	BNG	B	802	-	21,21,21	1.25	2 (9%)	26,26,26	0.92	0
2	COA	C	800	-	41,50,50	3.91	11 (26%)	52,75,75	2.07	5 (9%)
2	COA	A	800	-	41,50,50	3.94	12 (29%)	52,75,75	2.06	4 (7%)
3	PPQ	D	801	-	4,10,10	1.70	1 (25%)	2,14,14	2.33	1 (50%)
2	COA	D	800	-	41,50,50	3.94	11 (26%)	52,75,75	2.03	5 (9%)
3	PPQ	C	801	-	4,10,10	1.78	1 (25%)	2,14,14	2.08	1 (50%)
2	COA	B	800	-	41,50,50	3.90	12 (29%)	52,75,75	2.08	5 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BNG	A	802	-	-	8/12/32/32	0/1/1/1
3	PPQ	B	801	-	-	0/6/10/10	-
3	PPQ	A	801	-	-	0/6/10/10	-
4	BNG	B	802	-	-	8/12/32/32	0/1/1/1
2	COA	C	800	-	-	5/44/64/64	0/3/3/3
2	COA	A	800	-	-	10/44/64/64	0/3/3/3
3	PPQ	D	801	-	-	0/6/10/10	-
2	COA	D	800	-	-	1/44/64/64	0/3/3/3
3	PPQ	C	801	-	-	0/6/10/10	-
2	COA	B	800	-	-	9/44/64/64	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	800	COA	O4B-C1B	17.14	1.65	1.41
2	C	800	COA	O4B-C1B	17.09	1.64	1.41
2	A	800	COA	O4B-C1B	16.96	1.64	1.41
2	B	800	COA	O4B-C1B	16.91	1.64	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	COA	C2B-C1B	-13.59	1.33	1.53
2	D	800	COA	C2B-C1B	-13.25	1.33	1.53
2	C	800	COA	C2B-C1B	-13.08	1.33	1.53
2	B	800	COA	C2B-C1B	-13.08	1.33	1.53
2	D	800	COA	O4B-C4B	-6.56	1.30	1.45
2	C	800	COA	O4B-C4B	-6.50	1.30	1.45
2	B	800	COA	O4B-C4B	-6.44	1.30	1.45
2	A	800	COA	O4B-C4B	-6.39	1.30	1.45
2	D	800	COA	C5P-N4P	5.89	1.46	1.33
2	B	800	COA	C5P-N4P	5.88	1.46	1.33
2	A	800	COA	C5P-N4P	5.86	1.46	1.33
2	C	800	COA	C5P-N4P	5.78	1.46	1.33
2	D	800	COA	C9P-N8P	5.67	1.46	1.33
2	B	800	COA	C9P-N8P	5.66	1.46	1.33
2	A	800	COA	C9P-N8P	5.59	1.45	1.33
2	C	800	COA	C9P-N8P	5.55	1.45	1.33
4	A	802	BNG	O5-C1	3.87	1.51	1.41
4	B	802	BNG	O5-C1	3.83	1.51	1.41
3	A	801	PPQ	PDP-CGP	2.80	1.82	1.79
2	D	800	COA	O3B-C3B	-2.77	1.34	1.44
2	A	800	COA	O3B-C3B	-2.75	1.34	1.44
2	B	800	COA	C2A-N3A	2.74	1.36	1.32
2	B	800	COA	O3B-C3B	-2.74	1.34	1.44
3	C	801	PPQ	PDP-CGP	2.72	1.82	1.79
2	C	800	COA	O3B-C3B	-2.71	1.34	1.44
2	D	800	COA	C2A-N3A	2.71	1.36	1.32
2	C	800	COA	C2A-N3A	2.68	1.36	1.32
2	A	800	COA	C2A-N3A	2.66	1.36	1.32
3	B	801	PPQ	PDP-CGP	2.63	1.82	1.79
2	B	800	COA	C6A-N6A	2.52	1.43	1.34
2	A	800	COA	OAP-CAP	-2.51	1.37	1.42
2	B	800	COA	OAP-CAP	-2.51	1.37	1.42
2	C	800	COA	C6A-N6A	2.50	1.43	1.34
2	A	800	COA	C6A-N6A	2.48	1.43	1.34
2	C	800	COA	OAP-CAP	-2.47	1.37	1.42
2	D	800	COA	C6A-N6A	2.46	1.43	1.34
2	D	800	COA	OAP-CAP	-2.43	1.37	1.42
2	D	800	COA	O2B-C2B	2.36	1.48	1.43
2	B	800	COA	O2B-C2B	2.30	1.48	1.43
3	D	801	PPQ	PDP-CGP	2.28	1.81	1.79
2	C	800	COA	O2B-C2B	2.28	1.48	1.43
2	A	800	COA	O2B-C2B	2.27	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	COA	C3B-C4B	2.11	1.58	1.52
2	A	800	COA	C3B-C4B	2.09	1.58	1.52
2	A	800	COA	C5A-C4A	-2.09	1.35	1.40
2	C	800	COA	C5A-C4A	-2.09	1.35	1.40
2	B	800	COA	C5A-C4A	-2.04	1.35	1.40
4	A	802	BNG	C3-C2	-2.03	1.47	1.52
2	D	800	COA	C5A-C4A	-2.02	1.35	1.40
4	B	802	BNG	C3-C2	-2.00	1.47	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	800	COA	C5A-C6A-N6A	10.06	135.63	120.35
2	B	800	COA	C5A-C6A-N6A	9.99	135.53	120.35
2	A	800	COA	C5A-C6A-N6A	9.98	135.51	120.35
2	D	800	COA	C5A-C6A-N6A	9.93	135.44	120.35
2	A	800	COA	N6A-C6A-N1A	-6.88	104.29	118.57
2	C	800	COA	N6A-C6A-N1A	-6.85	104.35	118.57
2	D	800	COA	N6A-C6A-N1A	-6.76	104.54	118.57
2	B	800	COA	N6A-C6A-N1A	-6.73	104.60	118.57
2	A	800	COA	N3A-C2A-N1A	-5.63	119.88	128.68
2	C	800	COA	N3A-C2A-N1A	-5.55	120.00	128.68
2	D	800	COA	N3A-C2A-N1A	-5.47	120.12	128.68
2	B	800	COA	N3A-C2A-N1A	-5.35	120.32	128.68
3	D	801	PPQ	PDP-CGP-CBP	-2.99	109.06	114.53
2	B	800	COA	C3B-C2B-C1B	2.75	105.99	99.89
2	A	800	COA	P2A-O3A-P1A	-2.71	123.52	132.83
4	A	802	BNG	O5-C1-C2	2.61	115.88	110.35
3	C	801	PPQ	PDP-CGP-CBP	-2.55	109.87	114.53
3	B	801	PPQ	PDP-CGP-CBP	-2.54	109.89	114.53
2	C	800	COA	P2A-O3A-P1A	-2.46	124.37	132.83
3	A	801	PPQ	PDP-CGP-CBP	-2.38	110.17	114.53
2	D	800	COA	C3B-C2B-C1B	2.36	105.11	99.89
2	B	800	COA	P2A-O3A-P1A	-2.23	125.16	132.83
2	D	800	COA	P2A-O3A-P1A	-2.20	125.29	132.83
2	C	800	COA	C3B-C2B-C1B	2.19	104.75	99.89

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	COA	C5B-O5B-P1A-O3A

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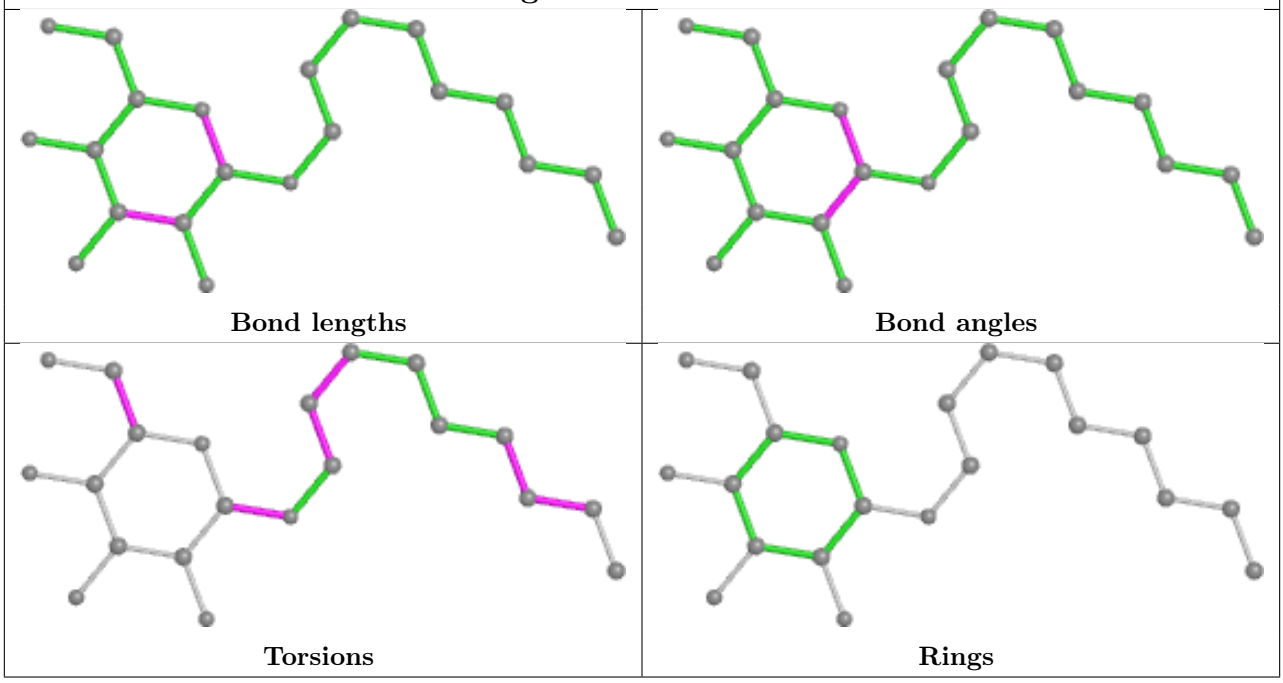
Mol	Chain	Res	Type	Atoms
2	B	800	COA	C5B-O5B-P1A-O1A
2	B	800	COA	C5B-O5B-P1A-O2A
2	B	800	COA	C5B-O5B-P1A-O3A
2	D	800	COA	C3B-O3B-P3B-O9A
4	A	802	BNG	O5-C1-O1-C1'
4	B	802	BNG	O5-C1-O1-C1'
4	B	802	BNG	O5-C5-C6-O6
4	B	802	BNG	C4-C5-C6-O6
2	A	800	COA	O4B-C4B-C5B-O5B
4	A	802	BNG	C4-C5-C6-O6
4	A	802	BNG	O5-C5-C6-O6
4	A	802	BNG	C2-C1-O1-C1'
4	B	802	BNG	C2-C1-O1-C1'
2	A	800	COA	C6P-C7P-N8P-C9P
4	A	802	BNG	O1-C1'-C2'-C3'
2	B	800	COA	C3B-C4B-C5B-O5B
2	B	800	COA	O4B-C4B-C5B-O5B
2	A	800	COA	C3B-C4B-C5B-O5B
4	B	802	BNG	O1-C1'-C2'-C3'
2	B	800	COA	C6P-C7P-N8P-C9P
2	B	800	COA	CEP-CBP-CCP-O6A
4	B	802	BNG	C1'-C2'-C3'-C4'
2	B	800	COA	CDP-CBP-CCP-O6A
2	C	800	COA	CEP-CBP-CCP-O6A
4	B	802	BNG	C6'-C7'-C8'-C9'
2	A	800	COA	P2A-O3A-P1A-O2A
4	B	802	BNG	C5'-C6'-C7'-C8'
4	A	802	BNG	C5'-C6'-C7'-C8'
2	A	800	COA	O9P-C9P-CAP-OAP
2	A	800	COA	N8P-C9P-CAP-OAP
4	A	802	BNG	C6'-C7'-C8'-C9'
2	C	800	COA	CDP-CBP-CCP-O6A
2	C	800	COA	C3B-O3B-P3B-O8A
2	C	800	COA	C5B-O5B-P1A-O3A
2	A	800	COA	P2A-O3A-P1A-O1A
2	B	800	COA	P2A-O3A-P1A-O2A
4	A	802	BNG	C1'-C2'-C3'-C4'
2	A	800	COA	CBP-CCP-O6A-P2A
2	A	800	COA	C5B-O5B-P1A-O2A
2	C	800	COA	C5B-O5B-P1A-O1A

There are no ring outliers.

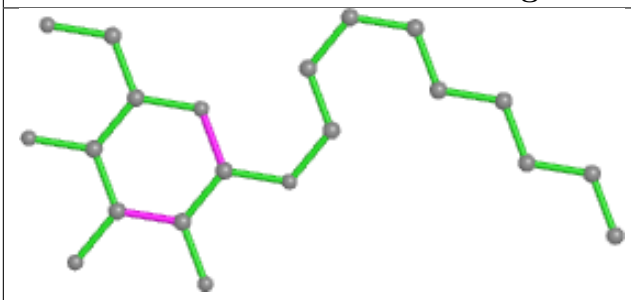
No monomer is involved in short contacts.

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 then 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.

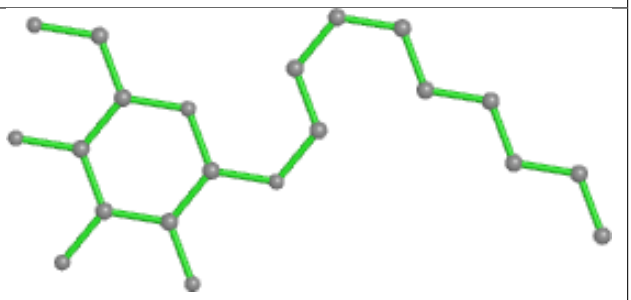
Ligand BNG A 802



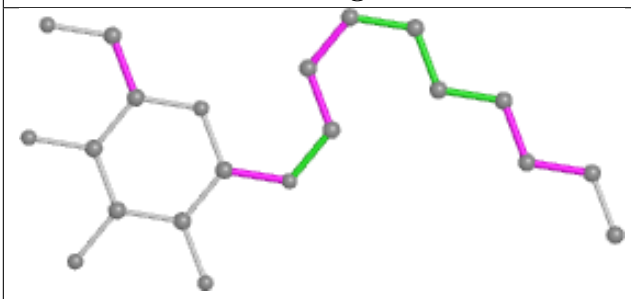
Ligand BNG B 802



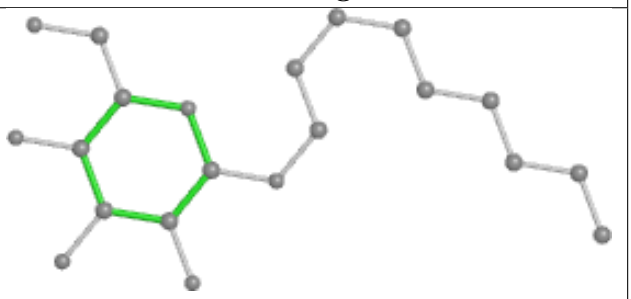
Bond lengths



Bond angles

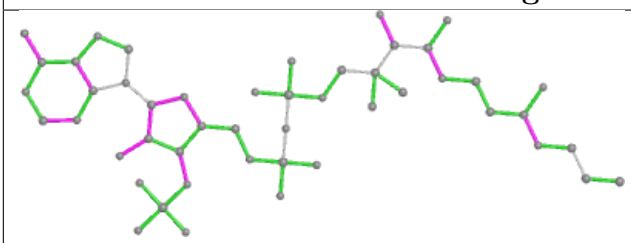


Torsions



Rings

Ligand COA C 800



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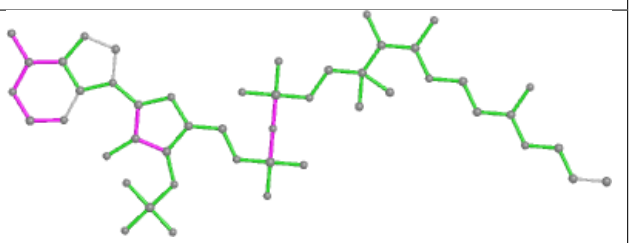
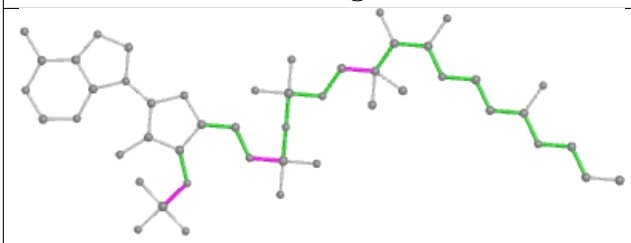
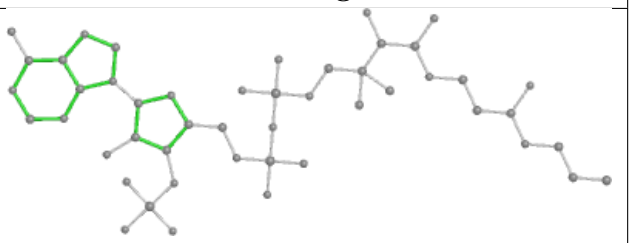


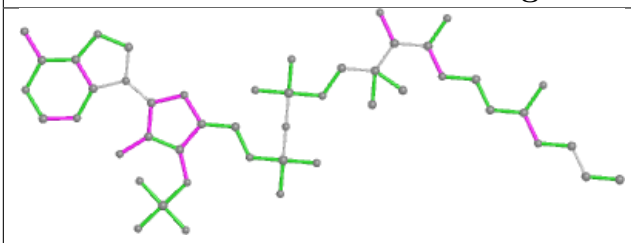
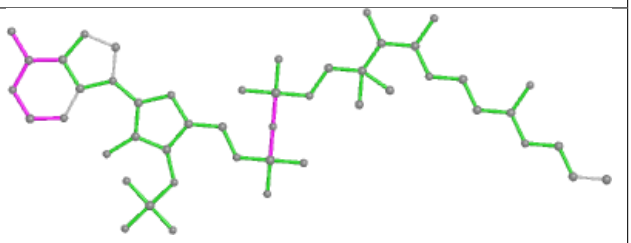
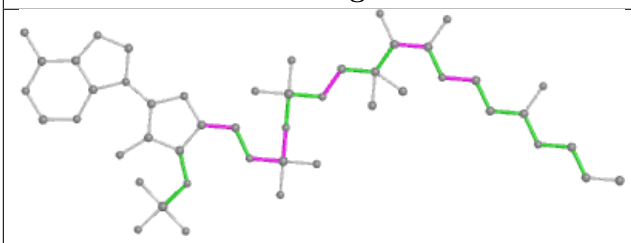
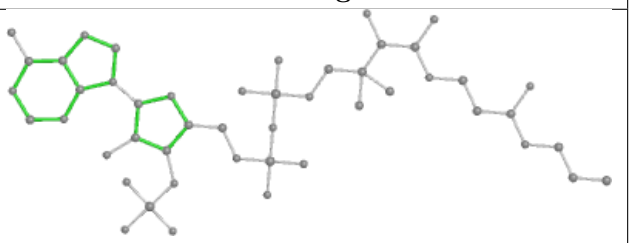
Bond angles

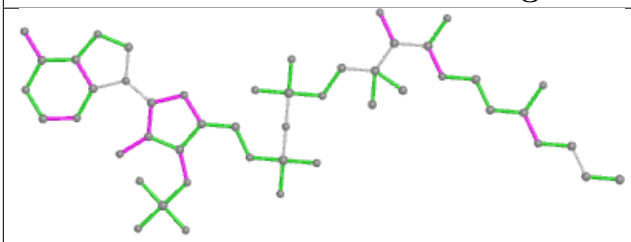
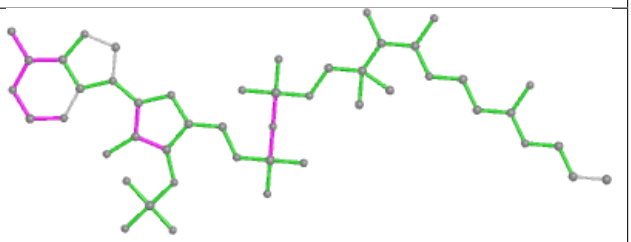
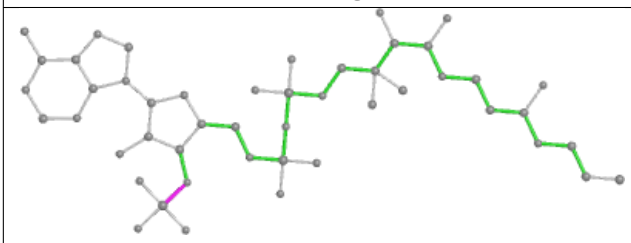
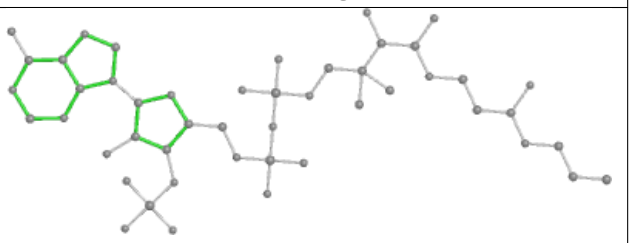


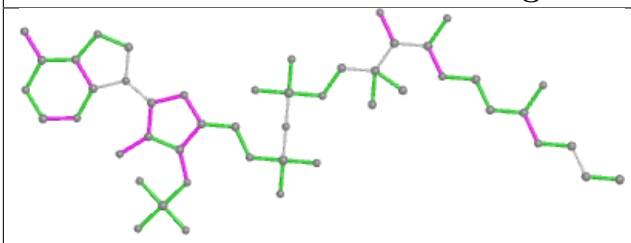
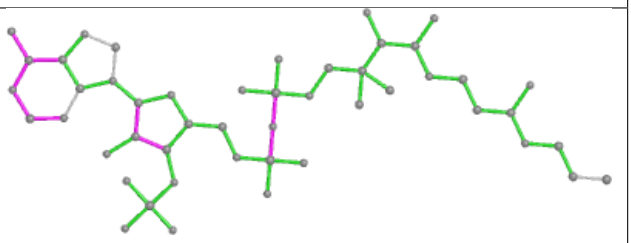
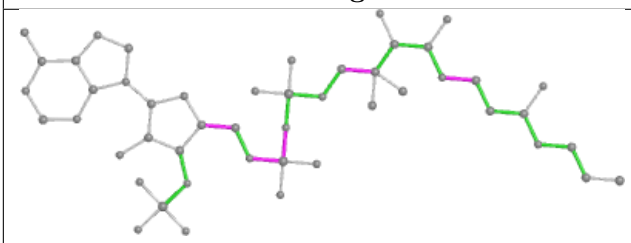
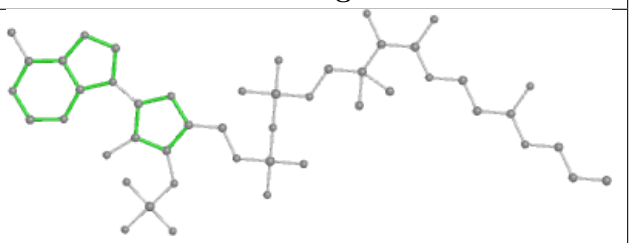
Torsions



Rings

Ligand COA A 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand COA D 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand COA B 800	
 Bond lengths	 Bond angles
 Torsions	 Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.