



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 10:47 AM UTC

PDB ID : 1E1C / pdb_00001e1c
Title : METHYLMALONYL-COA MUTASE H244A Mutant
Authors : Evans, P.R.; Thoma, N.H.
Deposited on : 2000-04-30
Resolution : 2.62 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)
Xtrriage (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

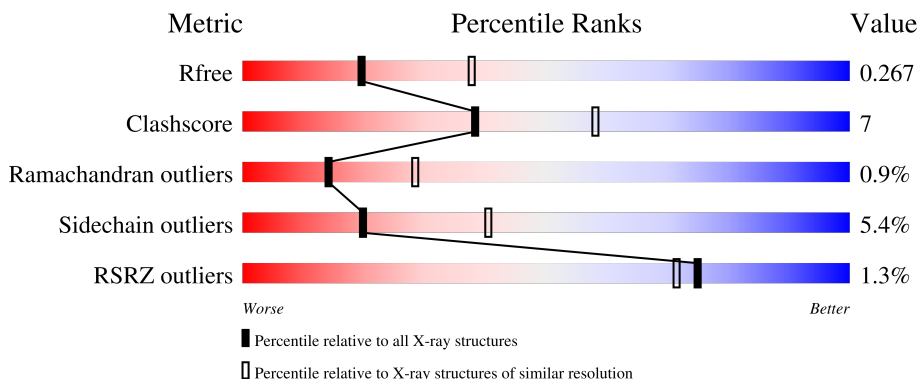
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	727	
1	C	727	
2	B	637	
2	D	637	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22307 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 METHYLMALONYL-COA MUTASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	Total	C	N	O	S	0	0	0
			5558	3511	958	1065	24			
1	C	727	Total	C	N	O	S	0	0	0
			5558	3511	958	1065	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	ALA	HIS	engineered mutation	UNP P11652
C	244	ALA	HIS	engineered mutation	UNP P11652

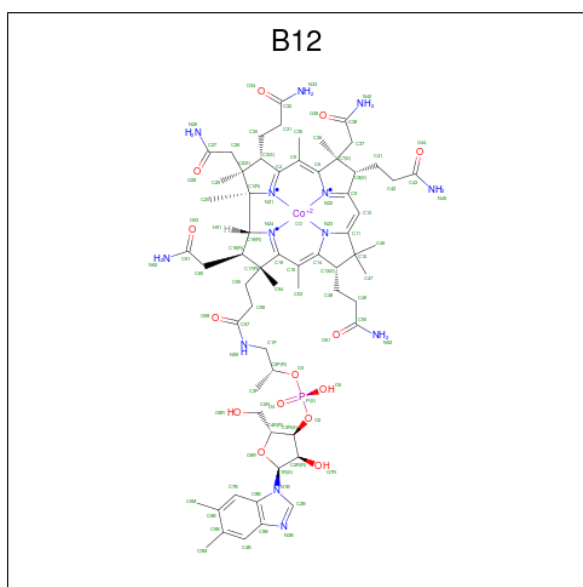
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	619	Total	C	N	O	S	0	0	0
			4695	2962	820	900	13			
2	D	619	Total	C	N	O	S	0	0	0
			4695	2962	820	900	13			

There are 6 discrepancies between the modelled and reference sequences:

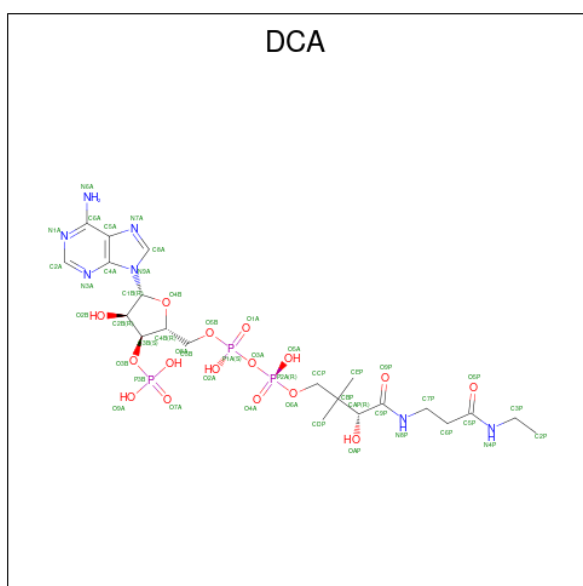
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
3	A	1	91	62	1	13	14	1	0	0
3	C	1	91	62	1	13	14	1	0	0

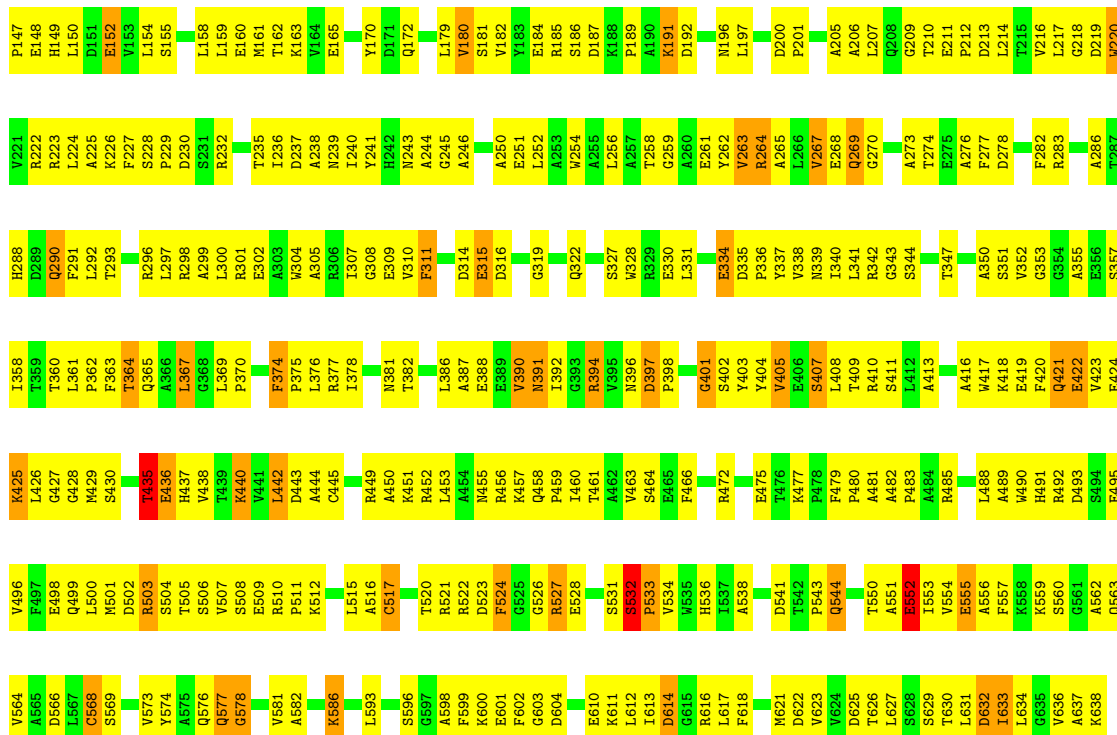
- Molecule 4 is DESULFO-COENZYME A (CCD ID: DCA) (formula: $C_{21}H_{36}N_7O_{16}P_3$).



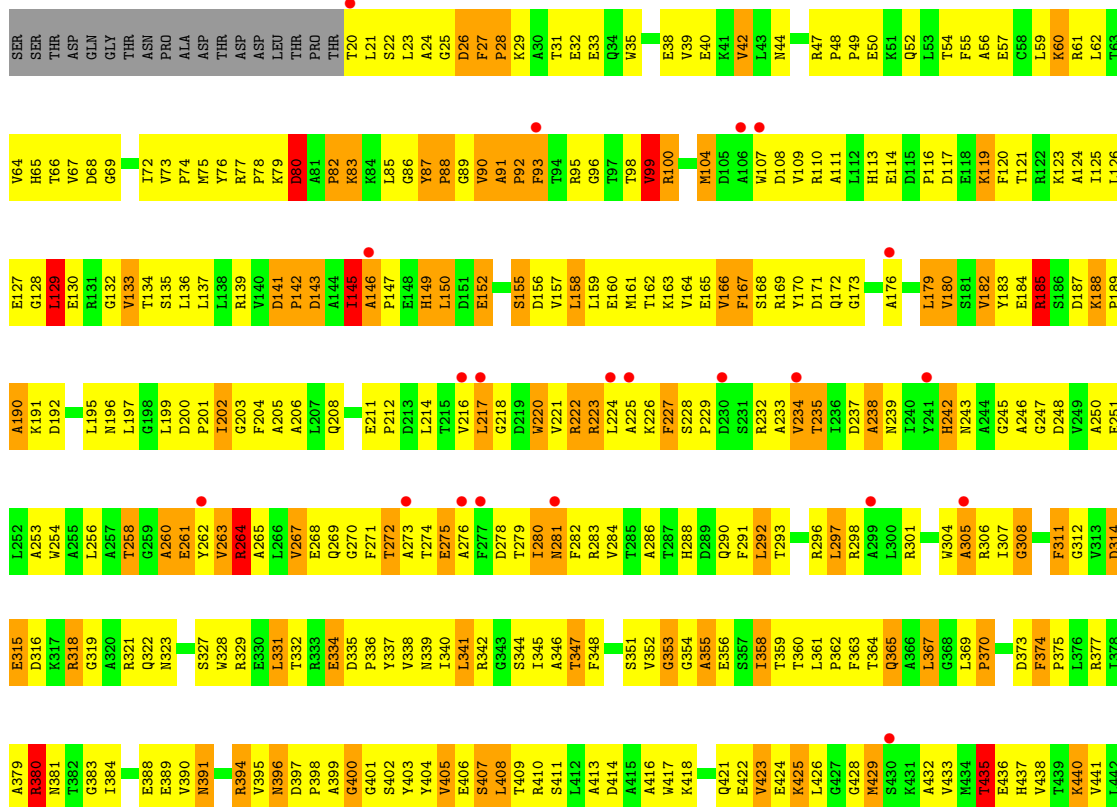
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	47	21	7	16	3	0	0
4	C	1	47	21	7	16	3	0	0

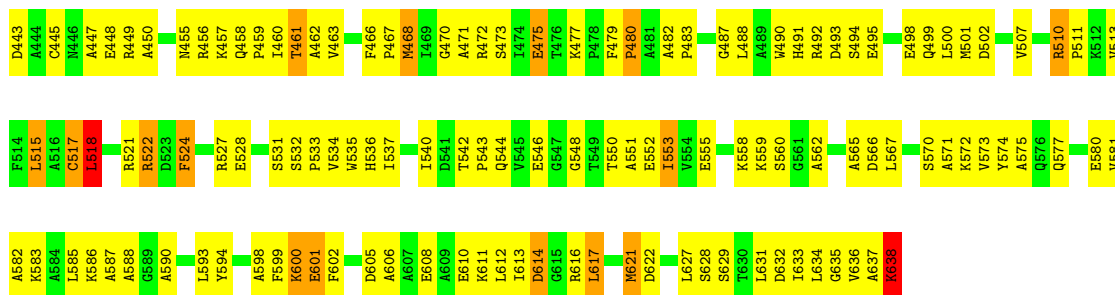
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	454	Total 454	O 454	0	0
5	B	316	Total 316	O 316	0	0
5	C	490	Total 490	O 490	0	0
5	D	265	Total 265	O 265	0	0



● Molecule 2: METHYLMALONYL-COA MUTASE BETA CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	125.40Å 161.83Å 166.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.20 – 2.62 29.20 – 2.62	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.20-2.62) 97.4 (29.20-2.62)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.61Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.283 0.201 , 0.267	Depositor DCC
R_{free} test set	5001 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtrriage
Anisotropy	0.488	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22307	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.59 % 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 1.7263e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DCA, B12

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	1.10	6/5673 (0.1%)	3.34	925/7710 (12.0%)
1	C	1.09	7/5673 (0.1%)	3.33	975/7710 (12.6%)
2	B	1.04	6/4785 (0.1%)	3.27	746/6499 (11.5%)
2	D	0.97	5/4785 (0.1%)	3.29	782/6499 (12.0%)
All	All	1.06	24/20916 (0.1%)	3.31	3428/28418 (12.1%)

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	A	0	1
1	C	0	1
2	B	0	1
All	All	0	3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	87	TYR	CA-CB	10.18	1.68	1.53
2	D	466	PHE	CA-CB	9.16	1.60	1.52
2	B	466	PHE	CA-CB	8.78	1.60	1.52
1	C	593	ALA	N-CA	-8.52	1.36	1.46
2	B	397	ASP	C-O	7.72	1.27	1.23

The worst 5 of 3428 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	485	ASN	CA-CB-CG	47.27	159.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	ARG	CD-NE-CZ	33.00	170.60	124.40
1	C	485	ASN	CA-CB-CG	29.43	142.03	112.60
1	C	131	ARG	CD-NE-CZ	23.95	157.93	124.40
1	A	642	ARG	CD-NE-CZ	23.91	157.87	124.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	GLY	Mainchain
2	B	401	GLY	Mainchain
1	C	593	ALA	Mainchain

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	5558	0	5441	72	0
1	C	5558	0	5440	75	0
2	B	4695	0	4610	44	0
2	D	4695	0	4610	83	0
3	A	91	0	88	16	0
3	C	91	0	88	16	0
4	A	47	0	32	0	0
4	C	47	0	32	0	0
5	A	454	0	0	3	0
5	B	316	0	0	1	0
5	C	490	0	0	4	0
5	D	265	0	0	0	0
All	All	22307	0	20341	283	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 7.

The worst 5 of 283 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:800:B12:H363	3:C:800:B12:H421	1.27	1.16
3:C:800:B12:H421	3:C:800:B12:C36	1.80	1.11
3:C:800:B12:H552	3:C:800:B12:H531	1.26	1.10
3:A:800:B12:H363	3:A:800:B12:H421	1.07	1.05
3:A:800:B12:H421	3:A:800:B12:C36	1.90	1.01

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	725/727 (100%)	671 (93%)	51 (7%)	3 (0%)	30	49
1	C	725/727 (100%)	652 (90%)	62 (9%)	11 (2%)	8	16
2	B	617/637 (97%)	566 (92%)	47 (8%)	4 (1%)	21	39
2	D	617/637 (97%)	554 (90%)	56 (9%)	7 (1%)	11	23
All	All	2684/2728 (98%)	2443 (91%)	216 (8%)	25 (1%)	14	28

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	56	LYS
2	B	578	GLY
1	C	3	THR
1	C	8	ASP
1	C	573	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	570/589 (97%)	542 (95%)	28 (5%)	22	44
1	C	570/589 (97%)	540 (95%)	30 (5%)	20	41
2	B	474/509 (93%)	456 (96%)	18 (4%)	29	54
2	D	474/509 (93%)	437 (92%)	37 (8%)	11	25
All	All	2088/2196 (95%)	1975 (95%)	113 (5%)	20	40

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	207	ARG
2	D	593	LEU
1	C	585	GLU
2	D	553	ILE
2	D	334	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	385	ASN
2	D	196	ASN
2	D	544	GLN
1	C	562	GLN
2	D	290	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	DCA	A	801	-	47,49,49	0.78	0	69,74,74	1.52	12 (17%)
3	B12	A	800	1	94,101,101	1.13	6 (6%)	149,166,166	2.38	49 (32%)
4	DCA	C	801	-	47,49,49	0.78	0	69,74,74	1.45	9 (13%)
3	B12	C	800	5,1	94,101,101	1.23	7 (7%)	149,166,166	2.28	53 (35%)

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	DCA	A	801	-	-	3/47/63/63	0/3/3/3
3	B12	A	800	1	-	13/56/223/223	0/3/11/11
4	DCA	C	801	-	-	2/47/63/63	0/3/3/3
3	B12	C	800	5,1	-	11/56/223/223	0/3/11/11

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	B12	CO-N22	-4.93	1.73	1.96
3	C	800	B12	C54-C17	4.13	1.61	1.54
3	C	800	B12	C2B-N1B	-3.35	1.31	1.37
3	A	800	B12	C54-C17	3.26	1.59	1.54
3	A	800	B12	CO-N22	-3.04	1.82	1.96

The worst 5 of 123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C9B-C8B-N1B	8.51	109.08	105.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	B12	C55-C17-C18	8.49	127.33	111.12
3	C	800	B12	C13-C14-N23	7.43	119.16	109.09
3	A	800	B12	C13-C14-C15	-6.89	113.84	124.32
3	A	800	B12	C13-C14-N23	6.70	118.17	109.09

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

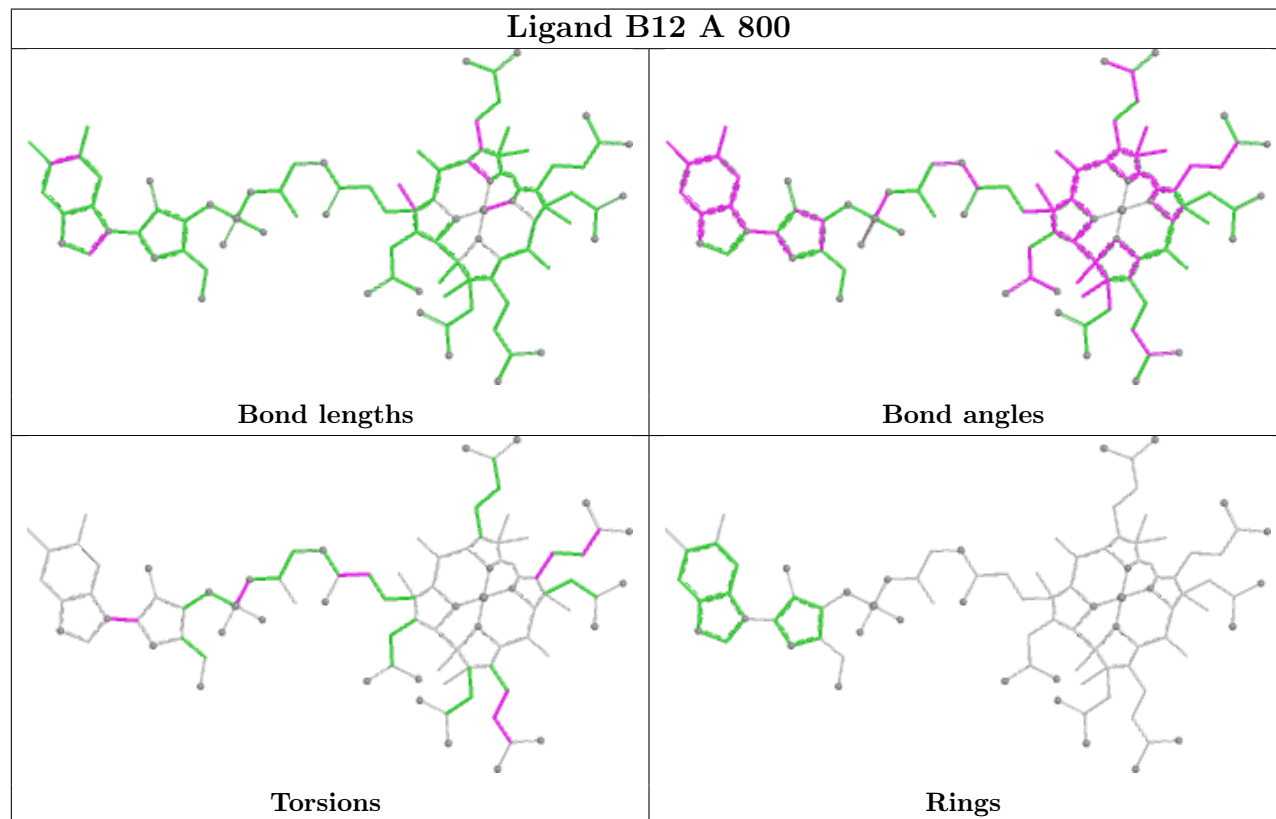
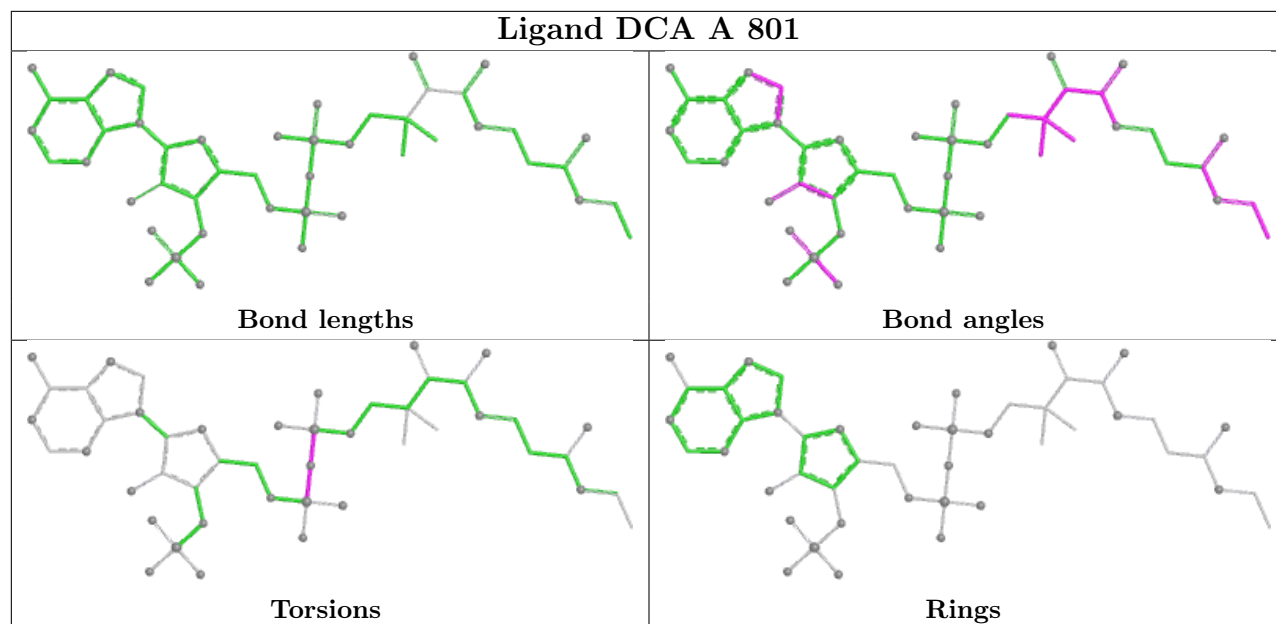
Mol	Chain	Res	Type	Atoms
3	A	800	B12	C2P-O3-P-O4
3	A	800	B12	C2R-C1R-N1B-C2B
3	C	800	B12	C2R-C1R-N1B-C2B
3	C	800	B12	C16-C17-C55-C56
3	A	800	B12	C2R-C1R-N1B-C8B

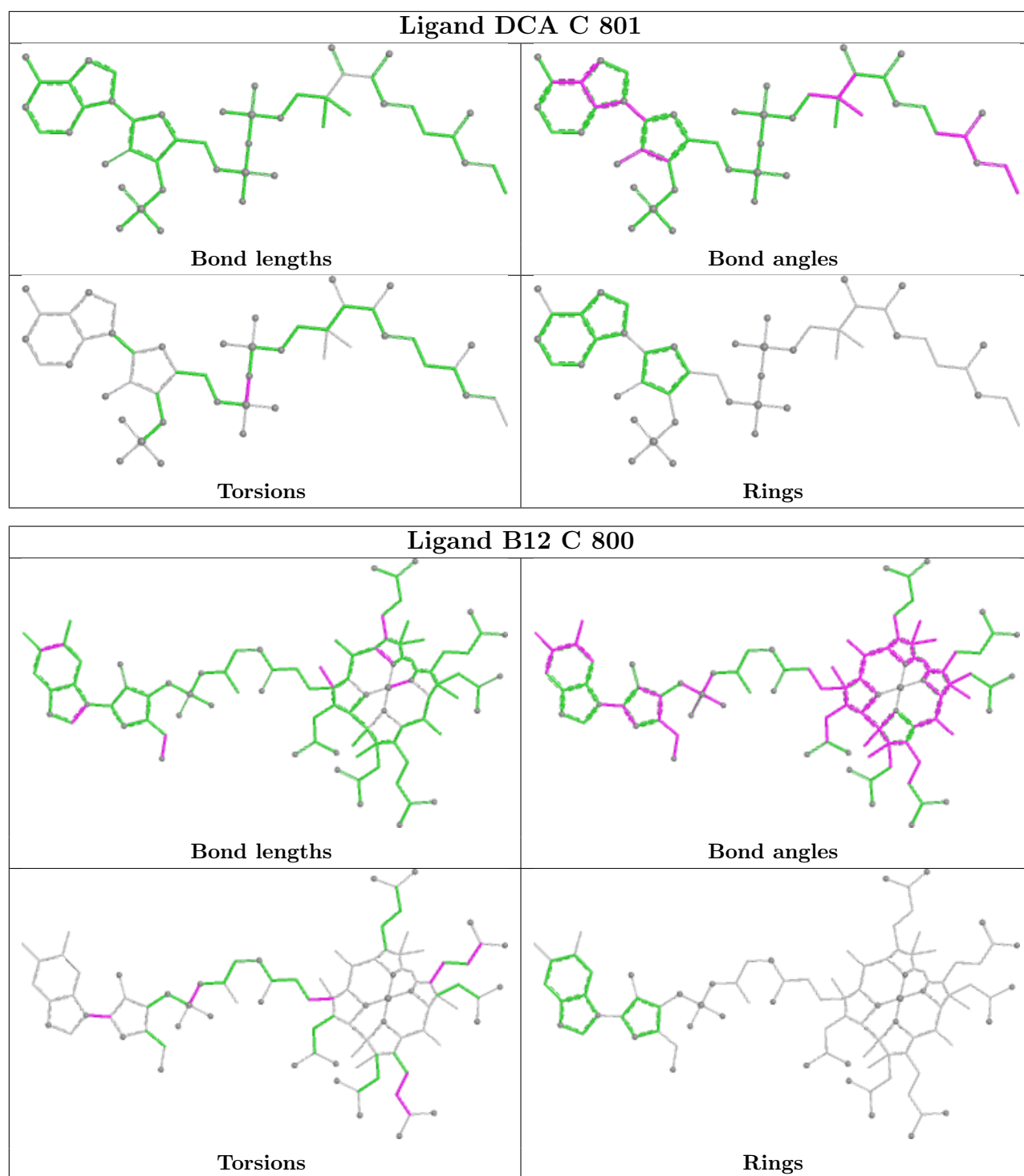
There are no ring outliers.

2 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	B12	16	0
3	C	800	B12	16	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.





5.7 Other polymers [\(i\)](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	727/727 (100%)	-0.67	3 (0%) 88 86	17, 36, 64, 145	0
1	C	727/727 (100%)	-0.45	6 (0%) 82 80	20, 41, 74, 145	0
2	B	619/637 (97%)	-0.34	4 (0%) 85 83	21, 49, 74, 103	0
2	D	619/637 (97%)	0.18	21 (3%) 48 43	27, 58, 88, 112	0
All	All	2692/2728 (98%)	-0.34	34 (1%) 75 71	17, 45, 80, 145	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	107	TRP	3.8
2	D	107	TRP	3.8
2	D	20	THR	3.3
2	D	224	LEU	3.3
1	C	4	LEU	3.0

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

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

6.3 Carbohydrates [i](#)

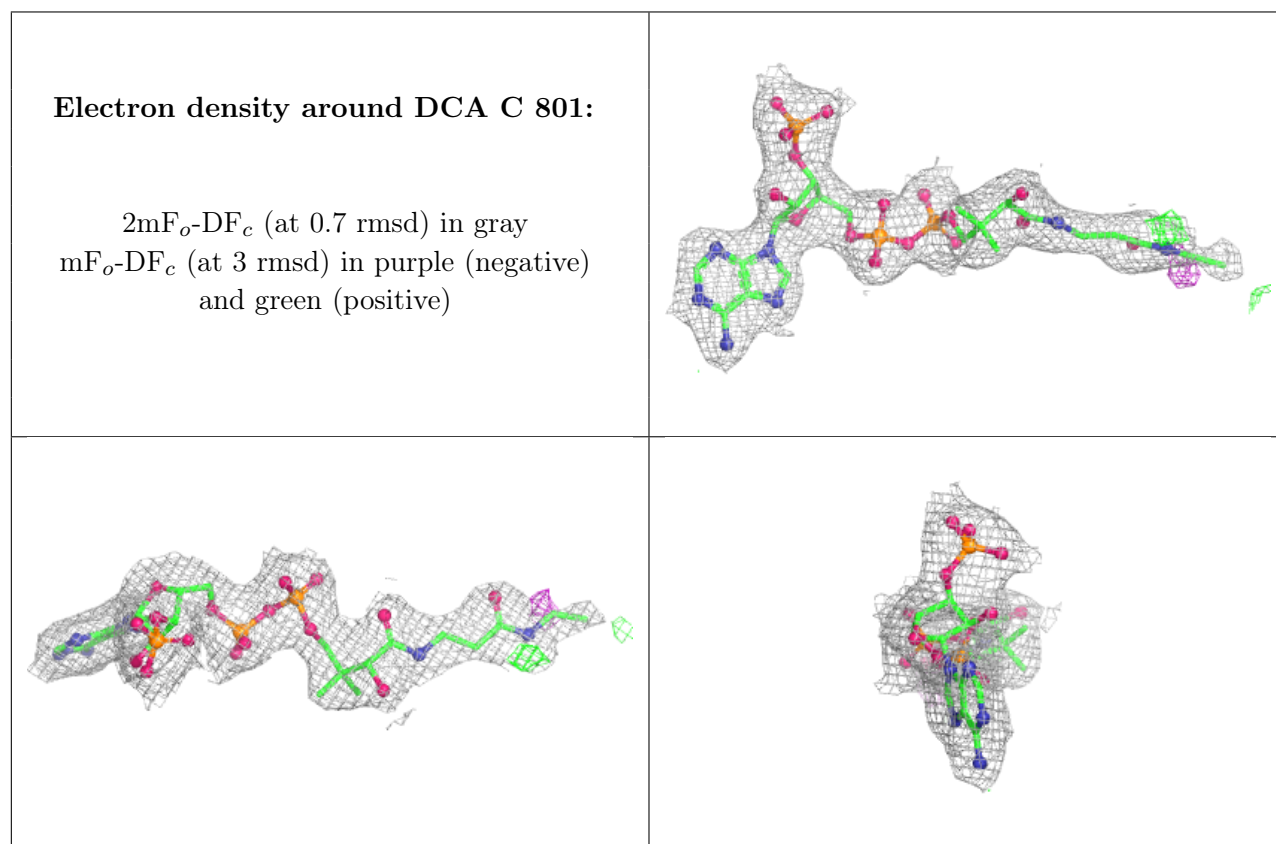
There are no oligosaccharides in this entry.

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.

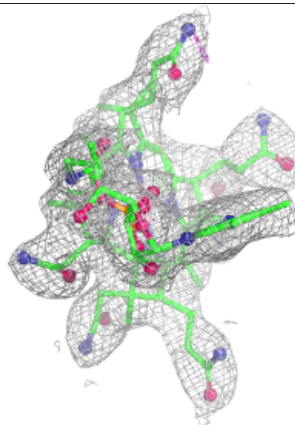
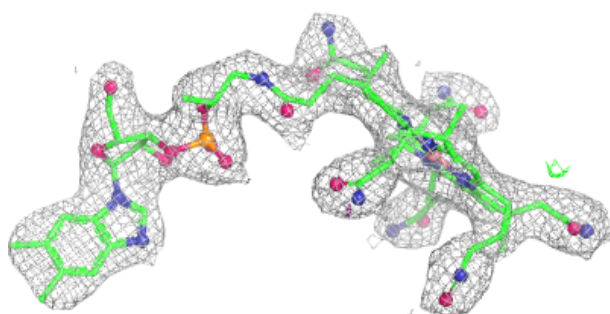
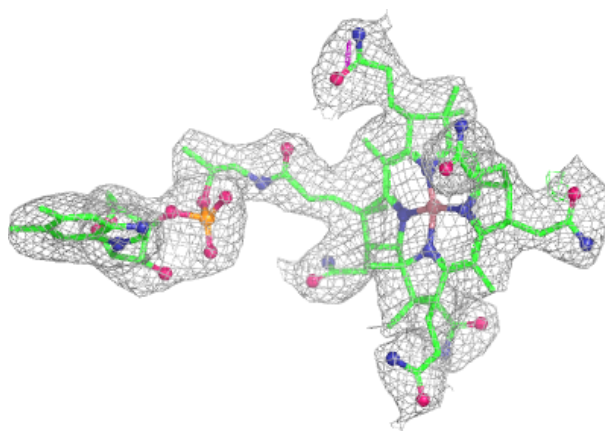
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DCA	C	801	47/47	0.97	0.06	21,28,32,35	0
3	B12	C	800	91/91	0.98	0.05	18,28,39,41	0
4	DCA	A	801	47/47	0.98	0.06	19,29,35,39	0
3	B12	A	800	91/91	0.98	0.05	13,27,35,38	0

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.

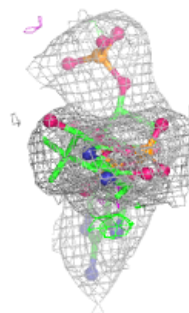
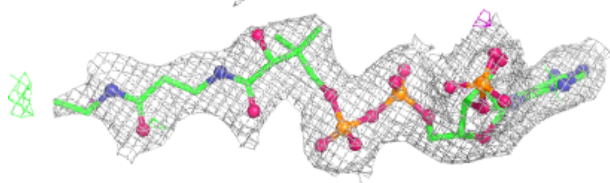
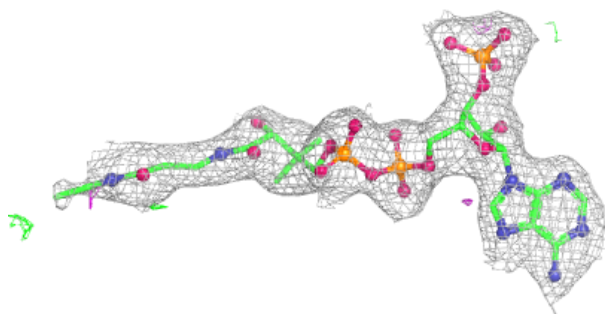


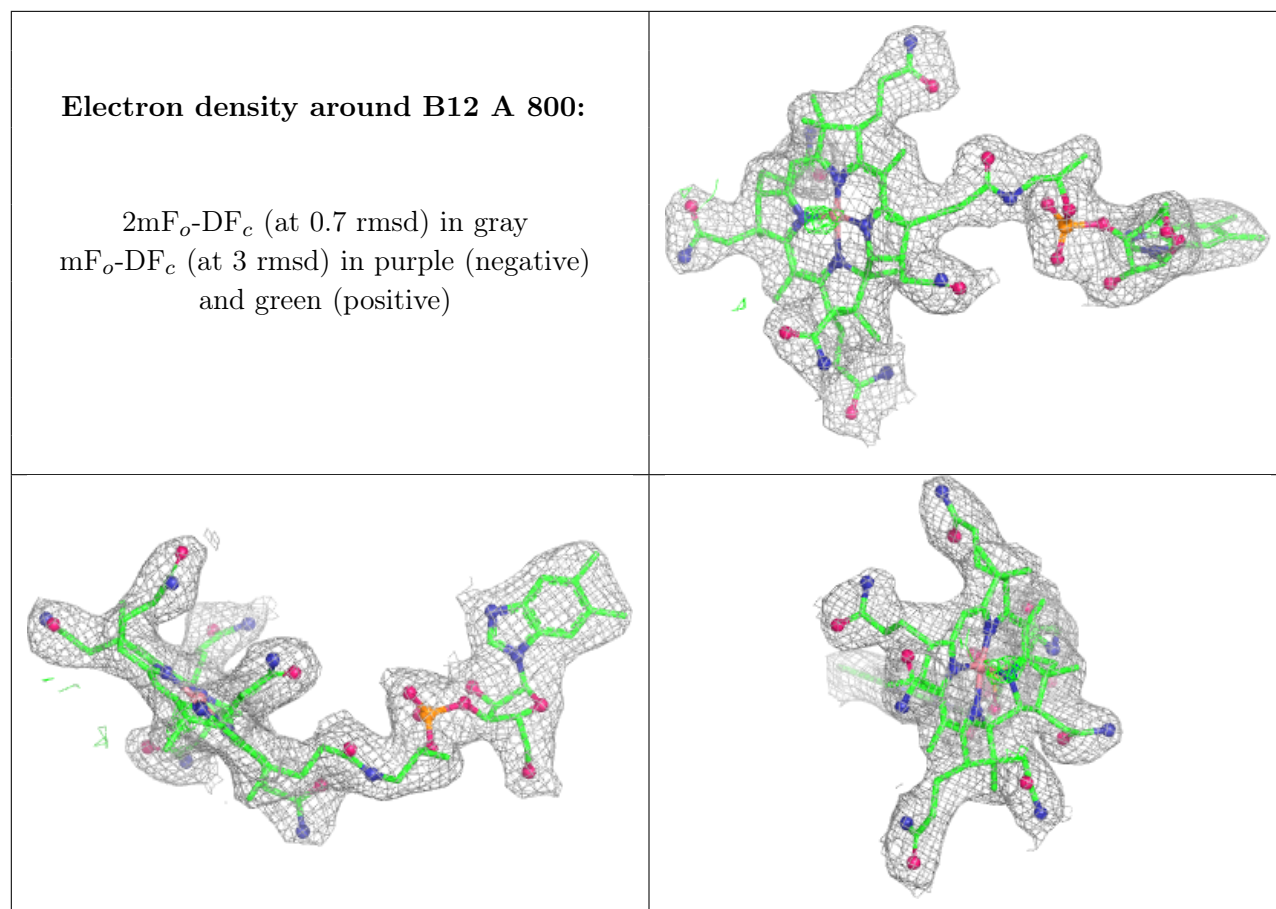
Electron density around B12 C 800:

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

**Electron density around DCA A 801:**

$2mF_o-DF_c$ (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.