



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2026 – 07:51 am BST

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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

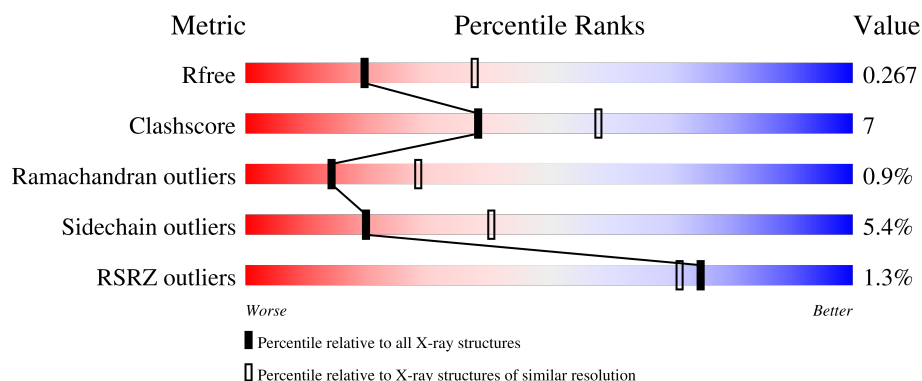
1 Overall quality at a glance

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

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
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

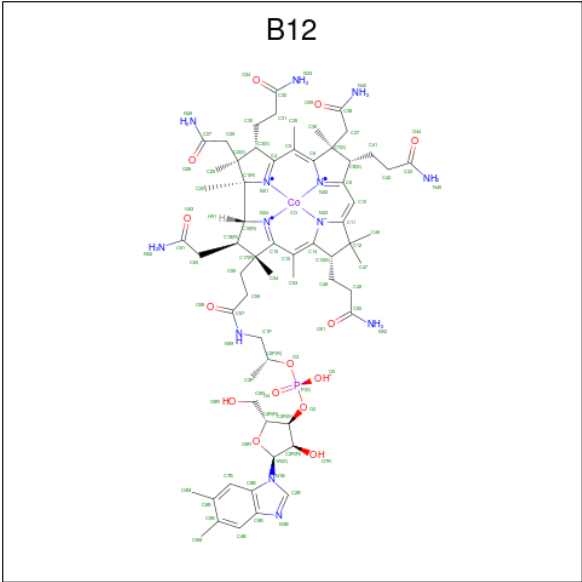
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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:

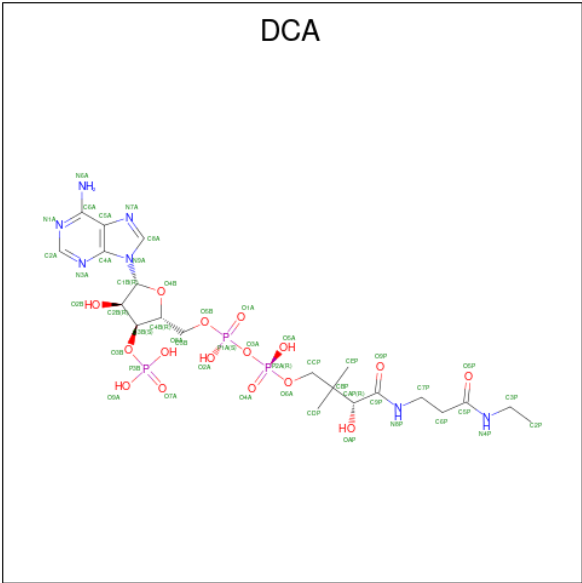
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

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



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

- 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
4	A	1	Total	C	N	O	P	0	0
			47	21	7	16	3		
4	C	1	Total	C	N	O	P	0	0
			47	21	7	16	3		

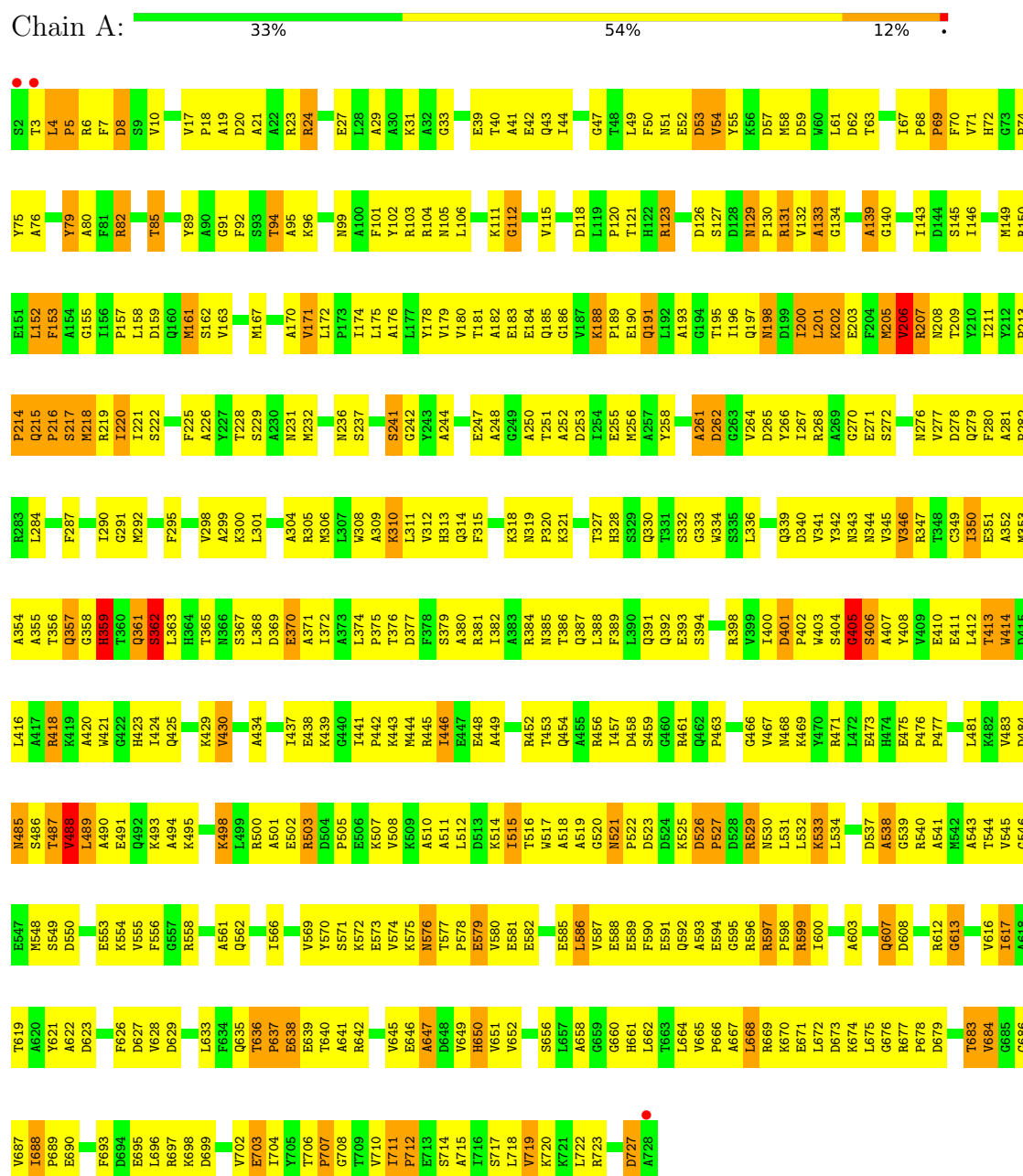
- Molecule 5 is water.

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

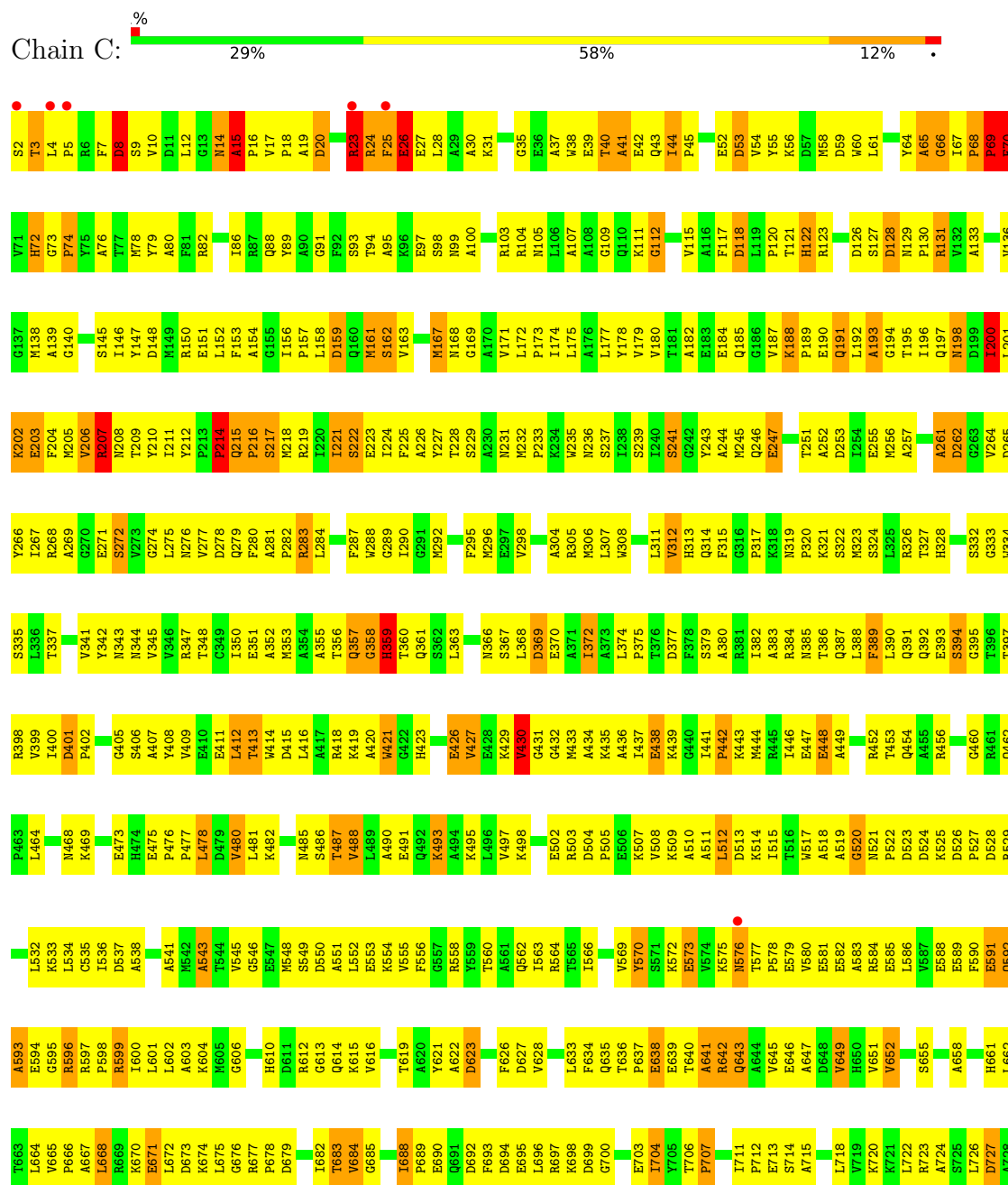
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

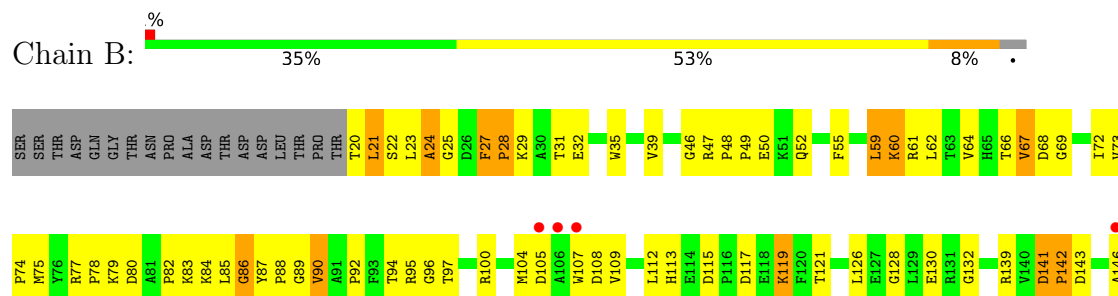
• Molecule 1: METHYLMALONYL-COA MUTASE ALPHA CHAIN

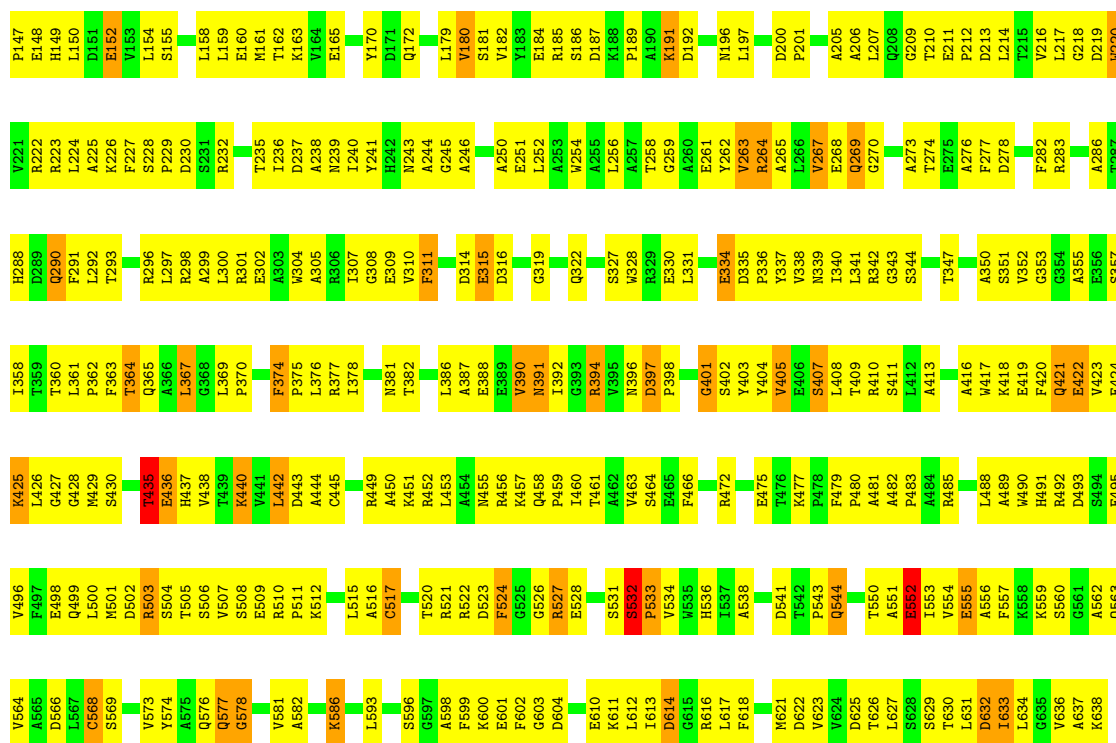


● Molecule 1: METHYLMALONYL-COA MUTASE ALPHA CHAIN

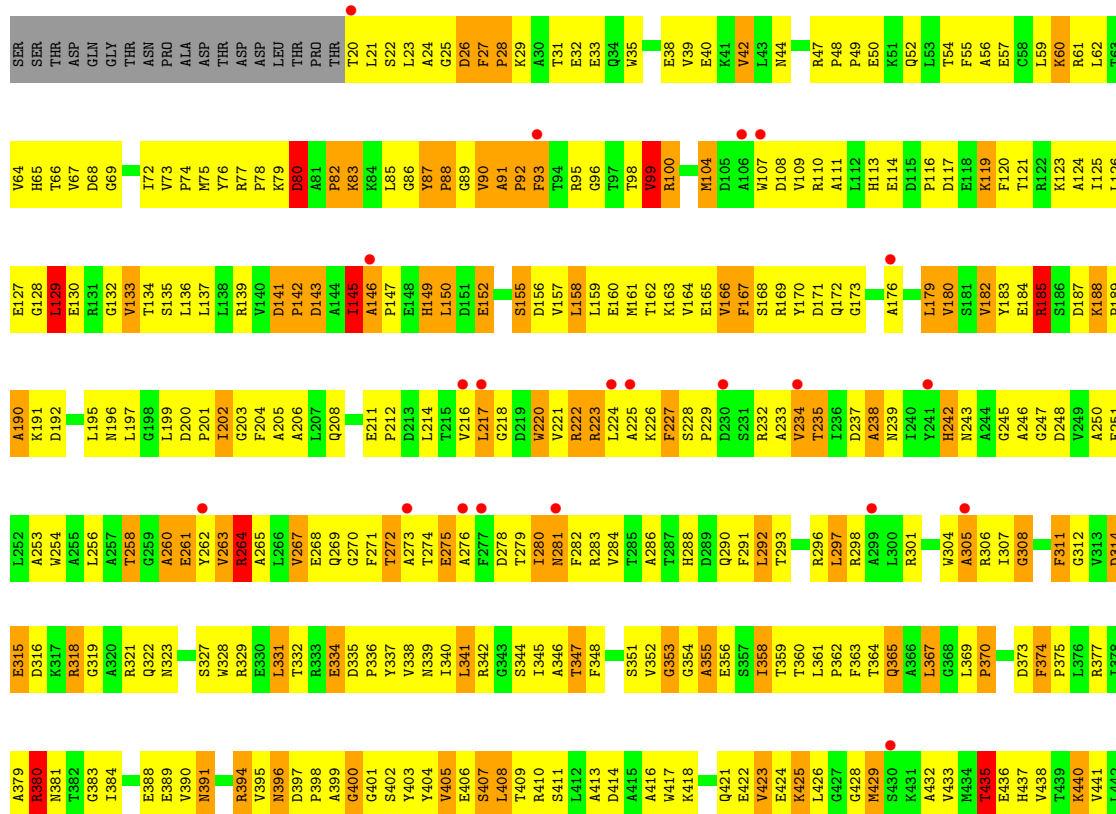


● Molecule 2: METHYLMALONYL-COA MUTASE BETA CHAIN





● Molecule 2: METHYLMALONYL-COA MUTASE BETA CHAIN



A582	K583	A584	L585	K586	A587	A588	G589	A590	L593	Y594	A598	F599	K600	E601	F602	D605	A606	A607	E608	A609	E610	K611	L612	I613	D614	G615	R616	L617	M621	D622	L627	S628	S629	T630	L631	D632	I633	L634	G635	V636	A637	K638											
F514	L515	A516	C517	I518	R521	R522	D523	F524	R527	E528	S531	S532	P533	V534	W535	H536	I537	I540	D541	T542	P543	Q544	V545	E546	G547	G548	T549	T550	A551	E552	I553	V554	E555	K558	K559	S560	G561	A562	A565	D566	L567	S570	A571	K572	V573	Y574	A575	Q576	Q577	E580	V581		
D443	A444	C445	N446	A447	E448	R449	A450	N455	R456	K457	Q458	P459	I460	T461	A462	V463	F466	P467	M468	I469	G470	A471	R472	S473	I474	E475	T476	K477	R478	F479	P480	A481	A482	P483	G487	L488	A489	W490	H491	R492	D493	S494	E495	E498	Q499	L500	M501	D502	V507	R510	P511	K512	V513

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)	Xtriage
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	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
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

Xtriage'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: B12, DCA

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	C	801	-	44,49,49	0.78	0	64,74,74	1.49	9 (14%)
3	B12	C	800	5,1	93,101,101	1.09	6 (6%)	146,166,166	2.26	49 (33%)
3	B12	A	800	1	93,101,101	1.07	5 (5%)	146,166,166	2.38	49 (33%)
4	DCA	A	801	-	44,49,49	0.72	0	64,74,74	1.53	12 (18%)

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	C	801	-	-	2/47/63/63	0/3/3/3
3	B12	C	800	5,1	-	11/56/223/223	0/3/11/11
3	B12	A	800	1	-	12/56/223/223	0/3/11/11
4	DCA	A	801	-	-	3/47/63/63	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	800	B12	C54-C17	3.93	1.61	1.54
3	C	800	B12	C2B-N1B	-3.16	1.31	1.37
3	A	800	B12	C54-C17	3.10	1.59	1.54
3	A	800	B12	C14-N23	3.04	1.39	1.35
3	A	800	B12	C2B-N1B	-2.50	1.33	1.37

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	B12	C9B-C8B-N1B	8.83	109.08	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	B12	C55-C17-C18	8.37	127.33	111.15
3	C	800	B12	C13-C14-N23	7.39	119.16	109.10
3	A	800	B12	C13-C14-C15	-6.85	113.84	124.32
3	A	800	B12	C13-C14-N23	6.66	118.17	109.10

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

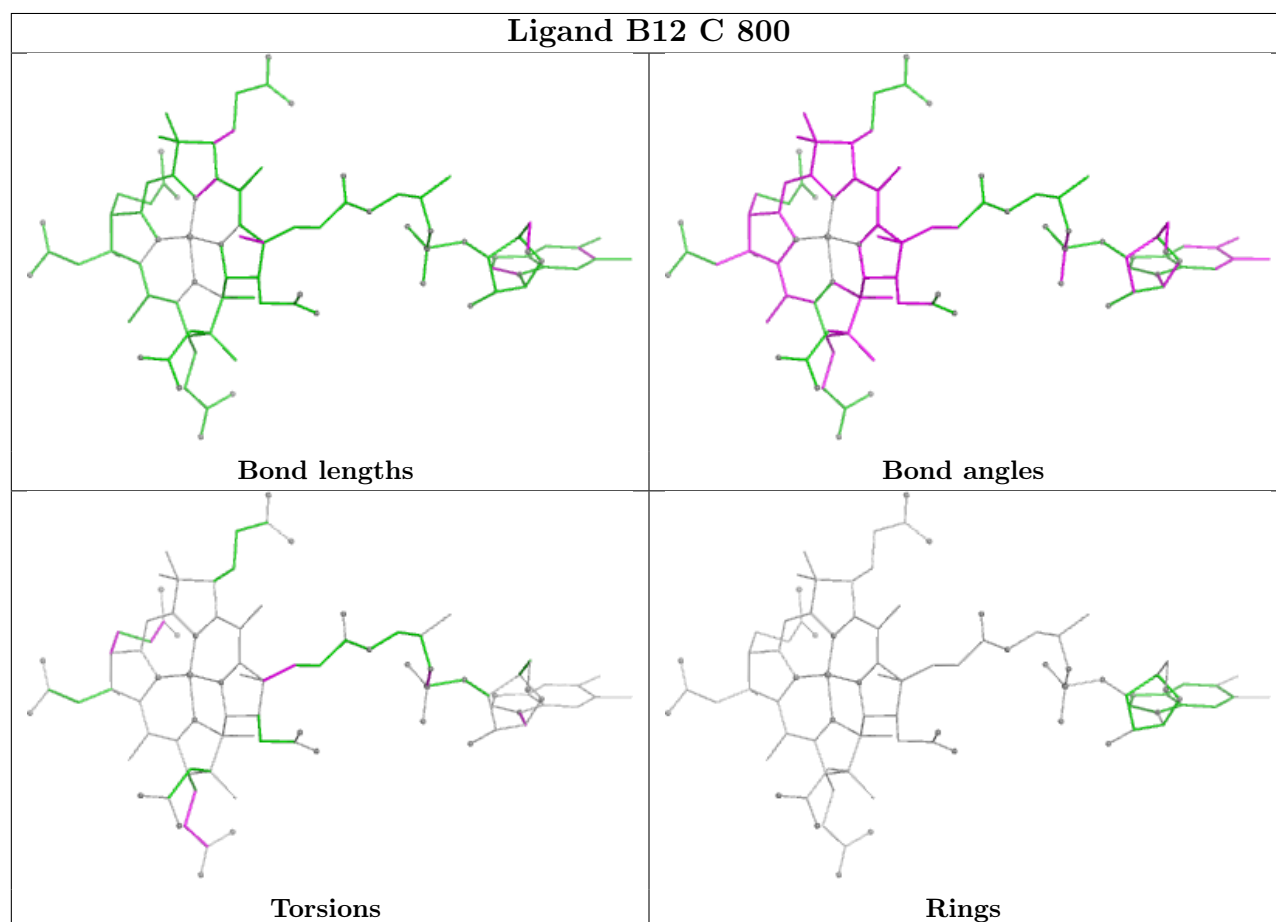
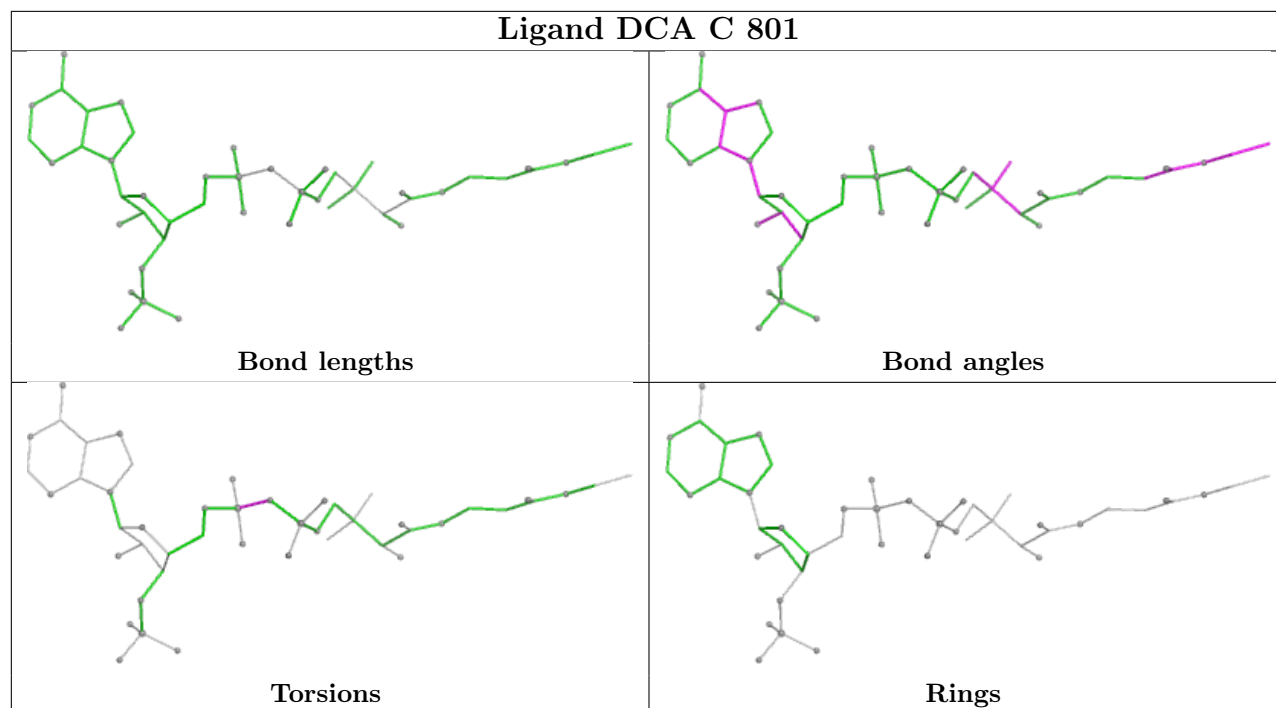
Mol	Chain	Res	Type	Atoms
3	A	800	B12	C2R-C1R-N1B-C2B
3	C	800	B12	C2R-C1R-N1B-C2B
3	C	800	B12	C16-C17-C55-C56
3	A	800	B12	C2R-C1R-N1B-C8B
3	C	800	B12	C2R-C1R-N1B-C8B

There are no ring outliers.

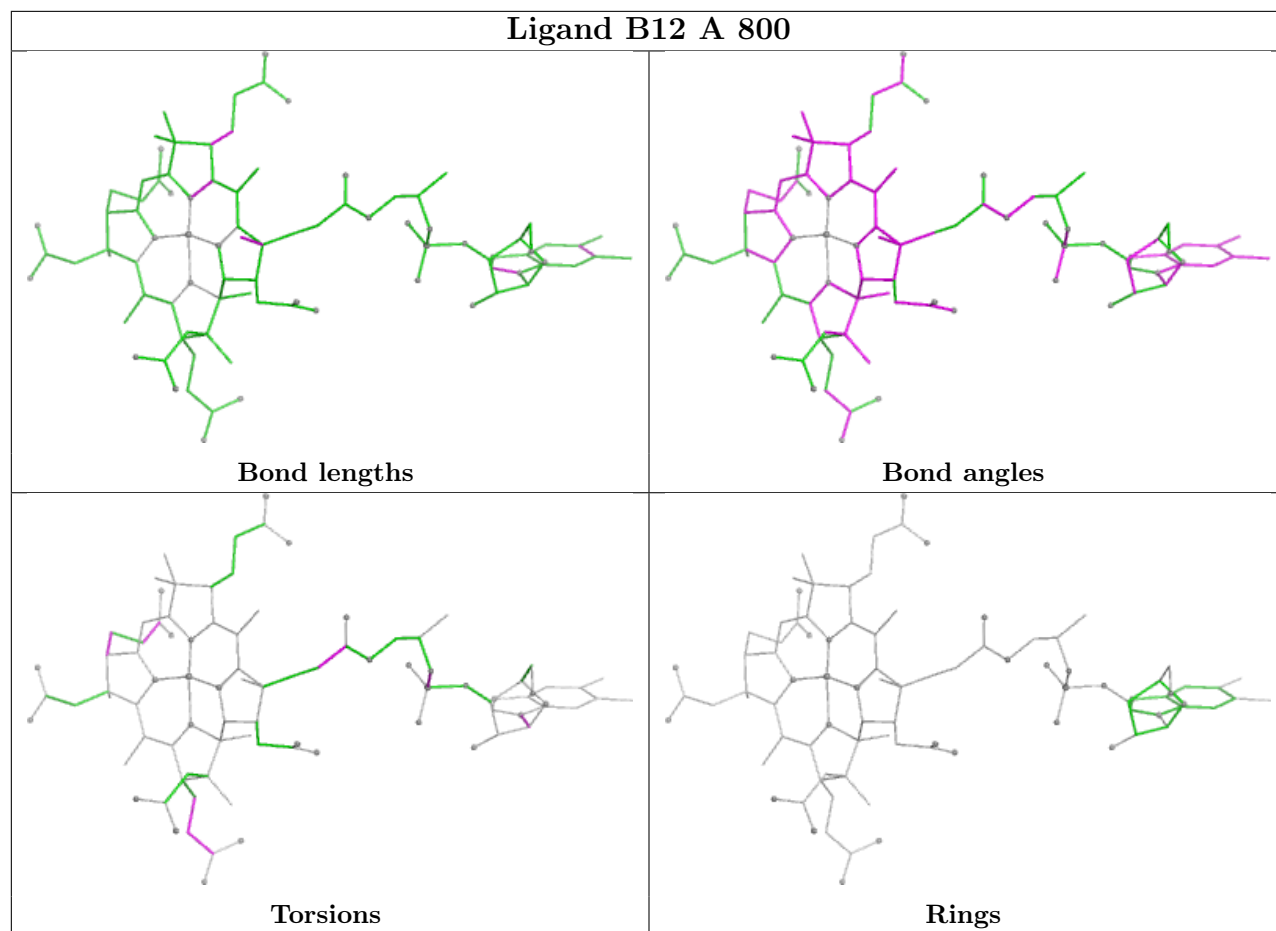
2 monomers are involved in 32 short contacts:

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

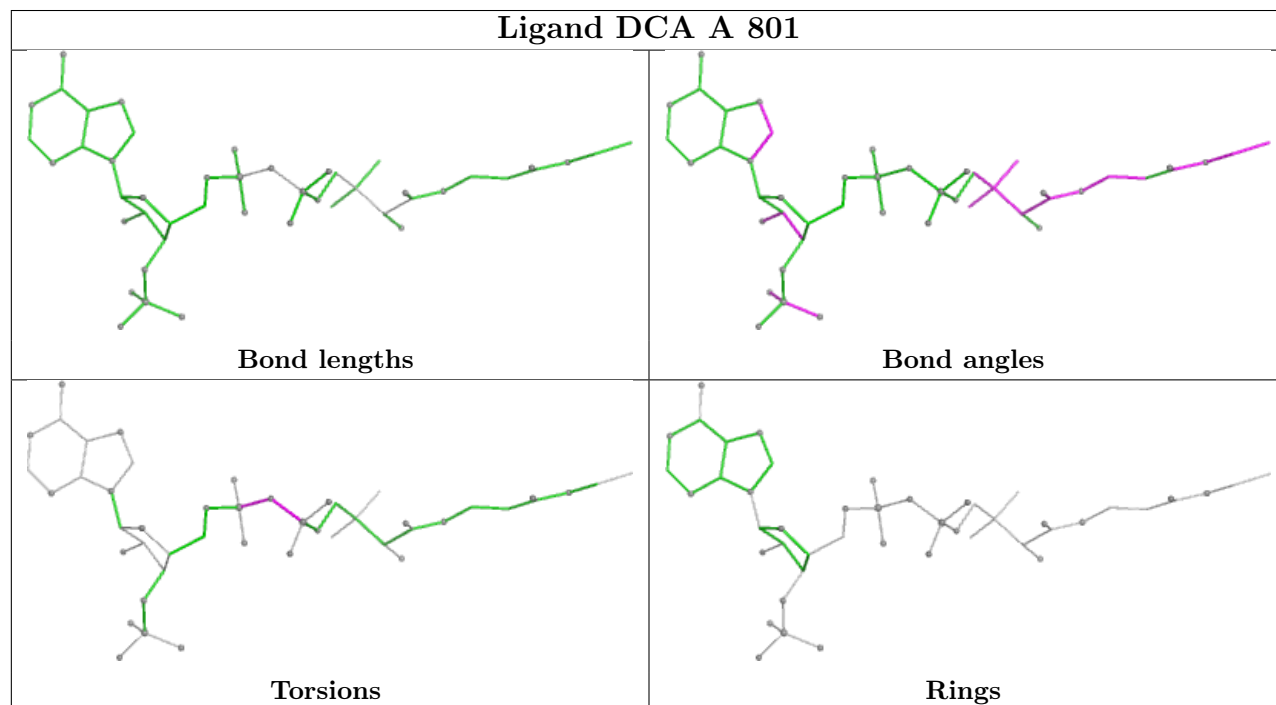
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand B12 A 800



Ligand DCA A 801



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](#)

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](#)

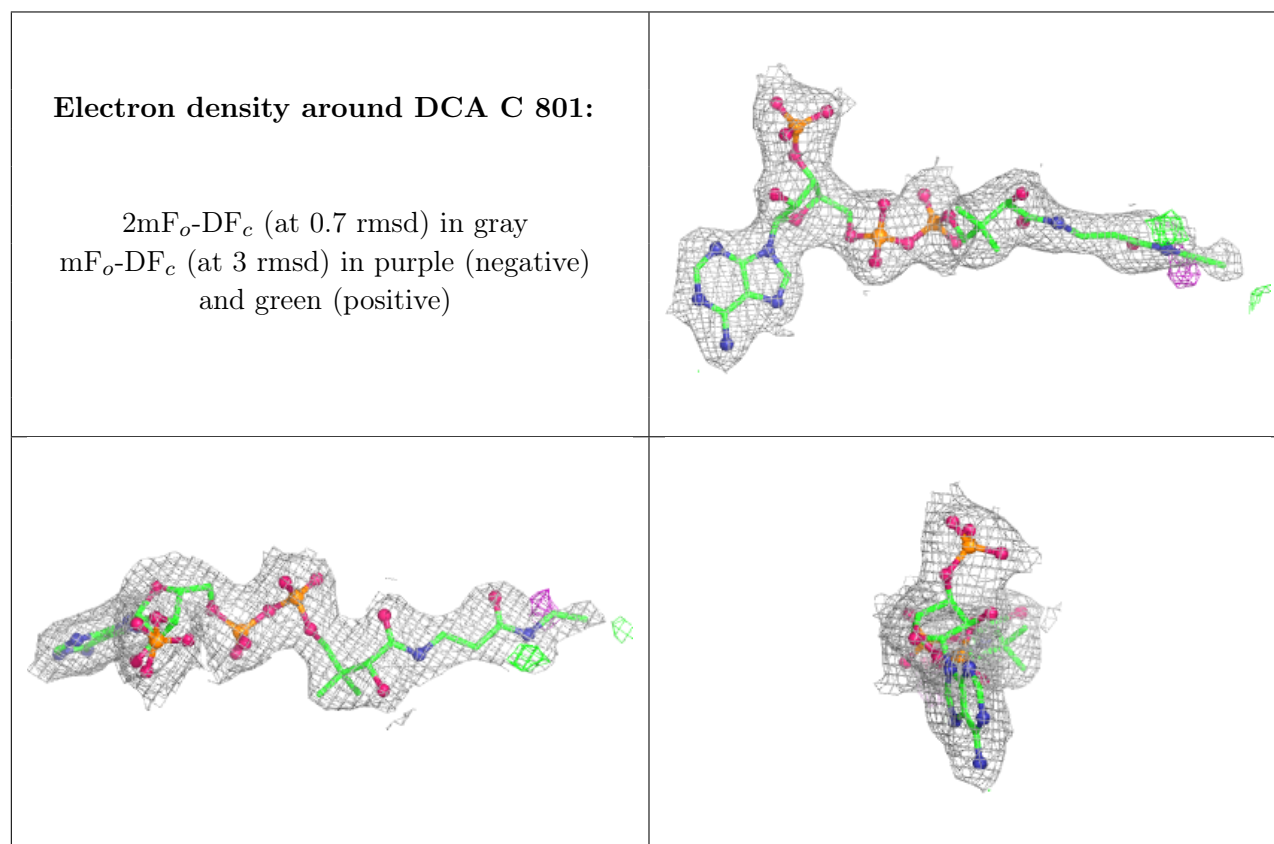
There are no oligosaccharides in this entry.

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.

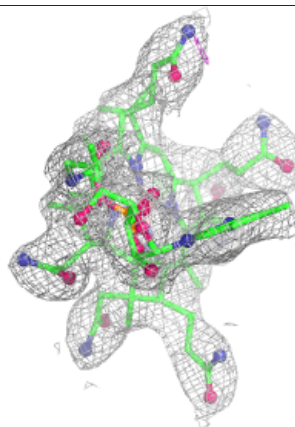
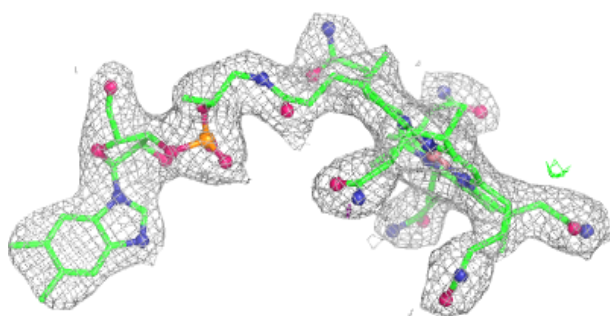
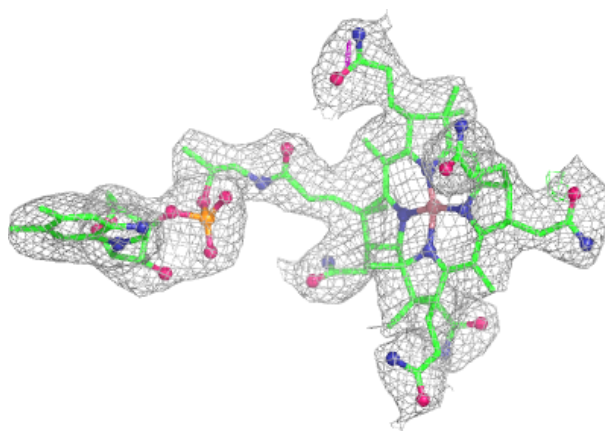
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DCA	C	801	47/47	0.97	0.06	21,28,32,35	0
3	B12	C	800	91/91	0.98	0.05	18,28,39,41	0
4	DCA	A	801	47/47	0.98	0.06	19,29,35,39	0
3	B12	A	800	91/91	0.98	0.05	13,27,35,38	0

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.

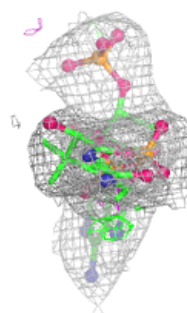
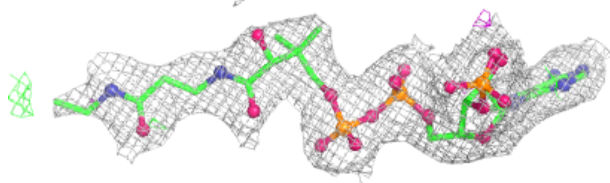
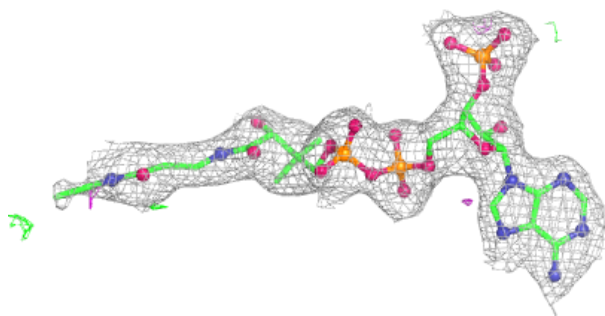


Electron density around B12 C 800:

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

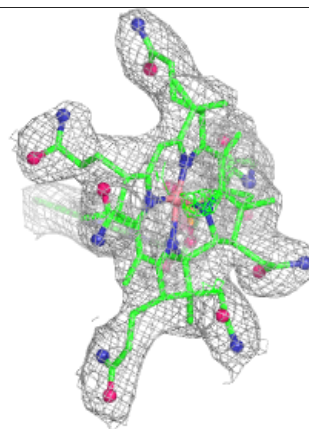
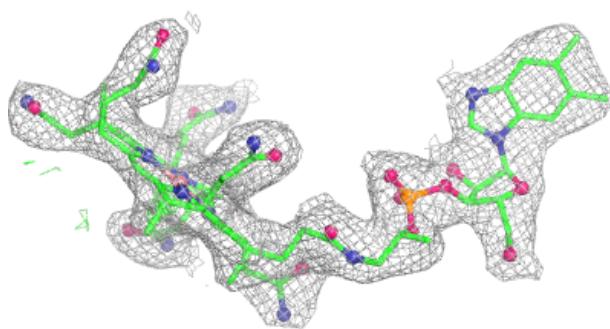
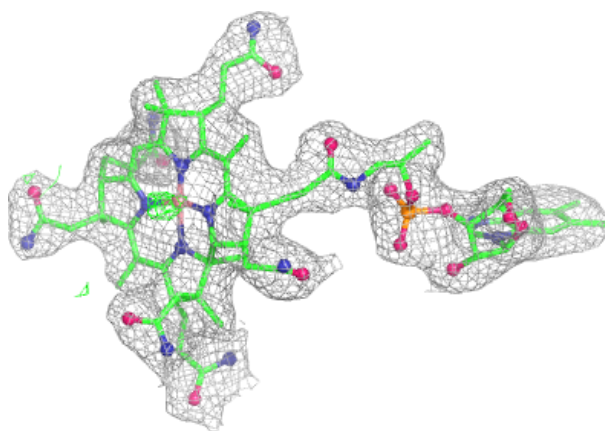
**Electron density around DCA A 801:**

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



Electron density around B12 A 800:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.