



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 10:33 PM EDT

PDB ID : 1REQ / pdb_00001req
Title : METHYLMALONYL-COA MUTASE
Authors : Evans, P.R.; Mancina, F.
Deposited on : 1996-01-19
Resolution : 2.00 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)
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

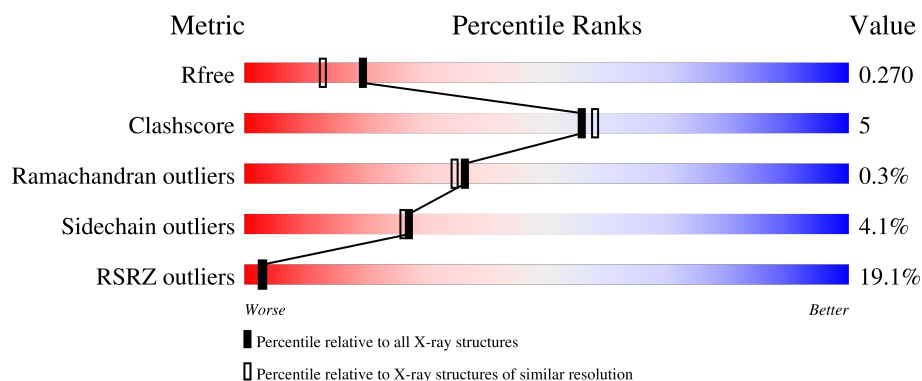
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	12% 53% 41% 5%
1	C	727	11% 50% 39% 9%
2	B	637	16% 53% 36% 8%
2	D	637	39% 54% 35% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22372 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5563	3514	960	1065	24			
1	C	727	Total	C	N	O	S	0	0	0
			5560	3515	960	1061	24			

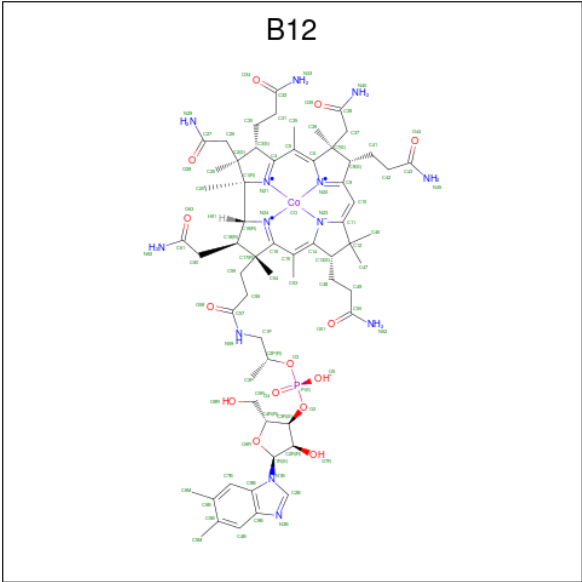
- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

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	622	Total	C	N	O	S	0	0	0
			4692	2958	818	903	13			

There are 6 discrepancies between the modelled and reference sequences:

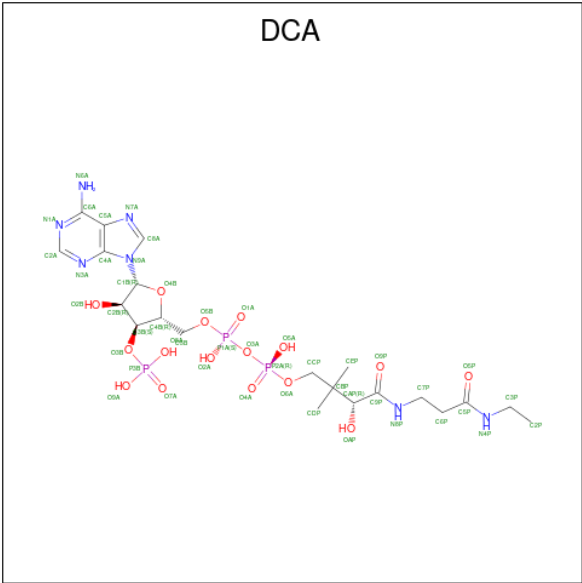
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	conflict	UNP P11652
B	330	GLU	ASP	conflict	UNP P11652
B	331	LEU	VAL	conflict	UNP P11652
D	203	GLY	ALA	conflict	UNP P11652
D	330	GLU	ASP	conflict	UNP P11652
D	331	LEU	VAL	conflict	UNP P11652

- Molecule 3 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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: C₂₁H₃₆N₇O₁₆P₃).



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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	457	Total	O	0	0
			457	457		
6	B	318	Total	O	0	0
			318	318		

Continued on next page...

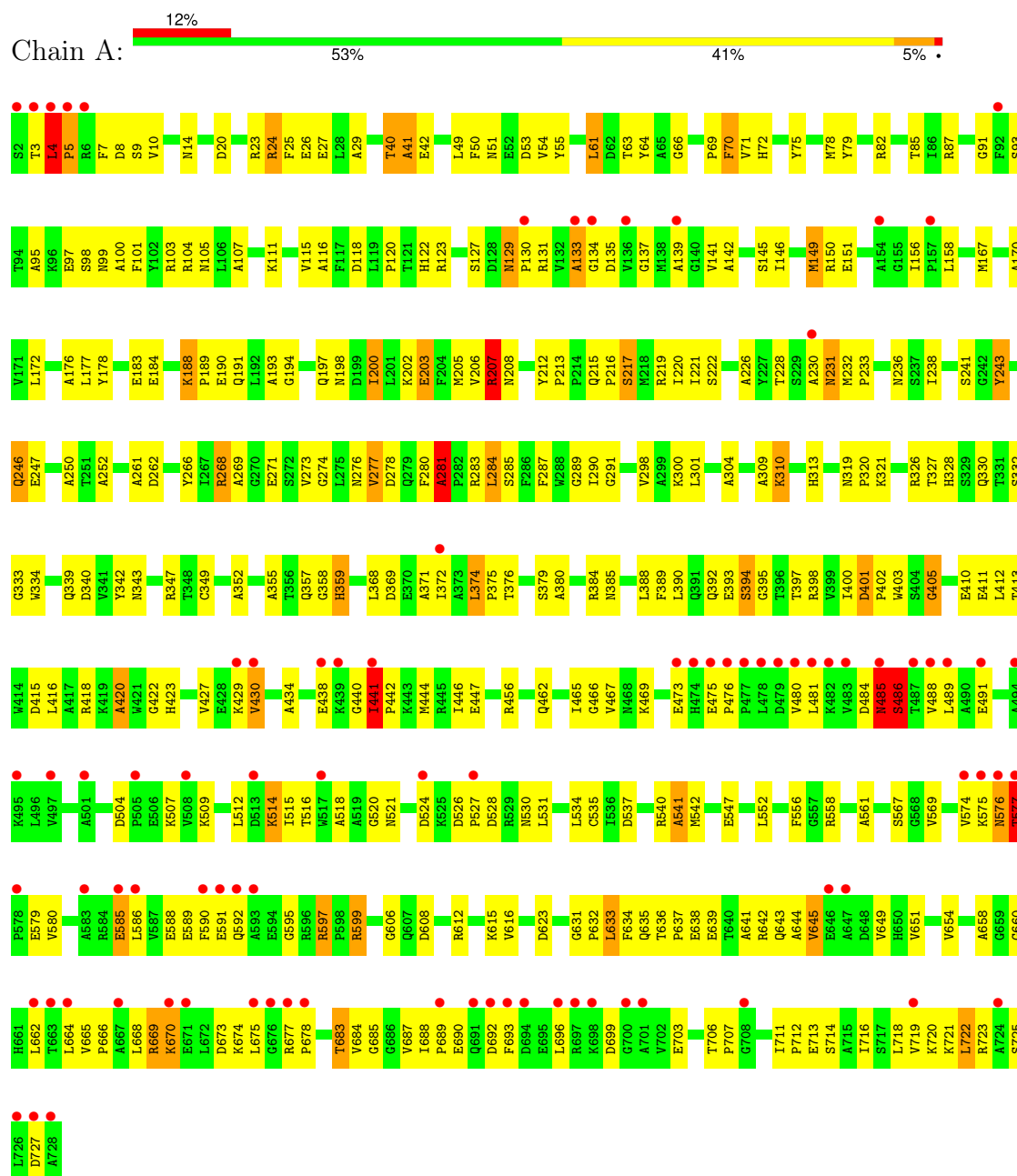
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	493	Total 493	O 493	0	0
6	D	264	Total 264	O 264	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



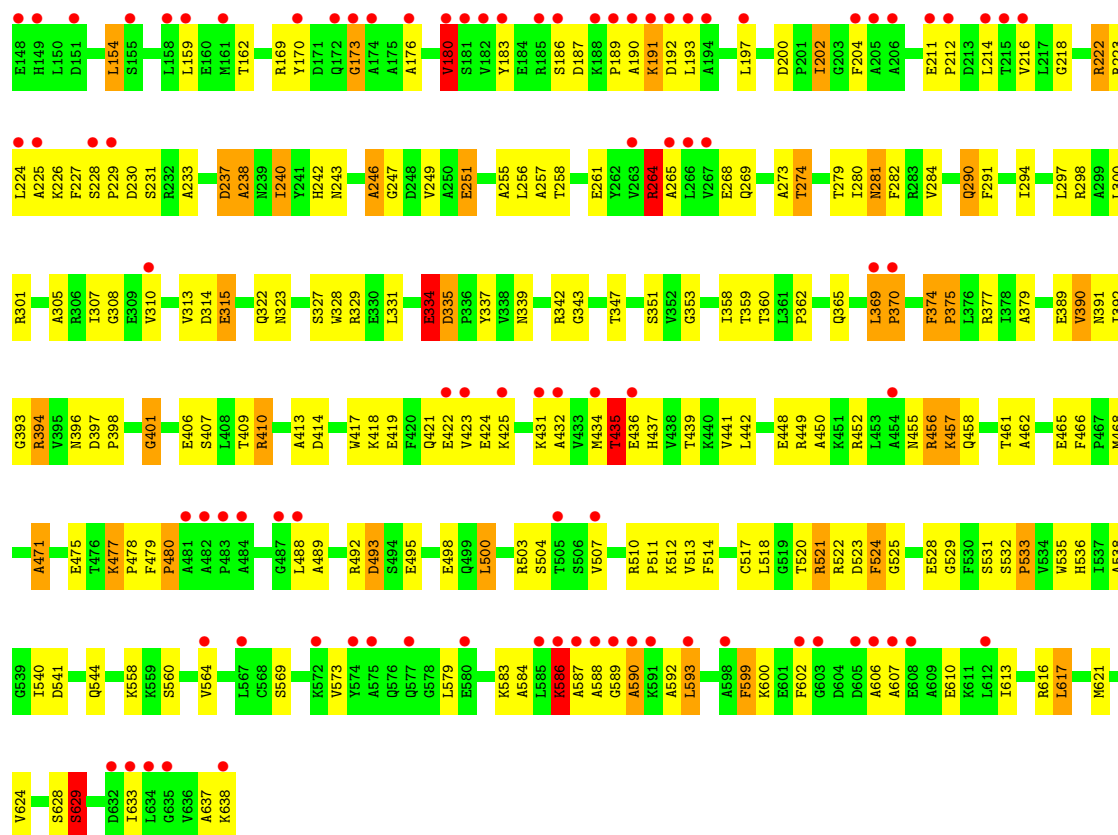
Chain C: 11% 50% 39% 9%

The visualization displays a sequence of 100 nodes, each represented by a colored square with a unique ID. The nodes are arranged in a grid that is 10 columns wide and 10 rows high. The nodes are labeled with IDs that are unique to each node. The nodes are arranged in a way that shows the flow of the chain from left to right and top to bottom. The nodes are labeled with IDs that are unique to each node.

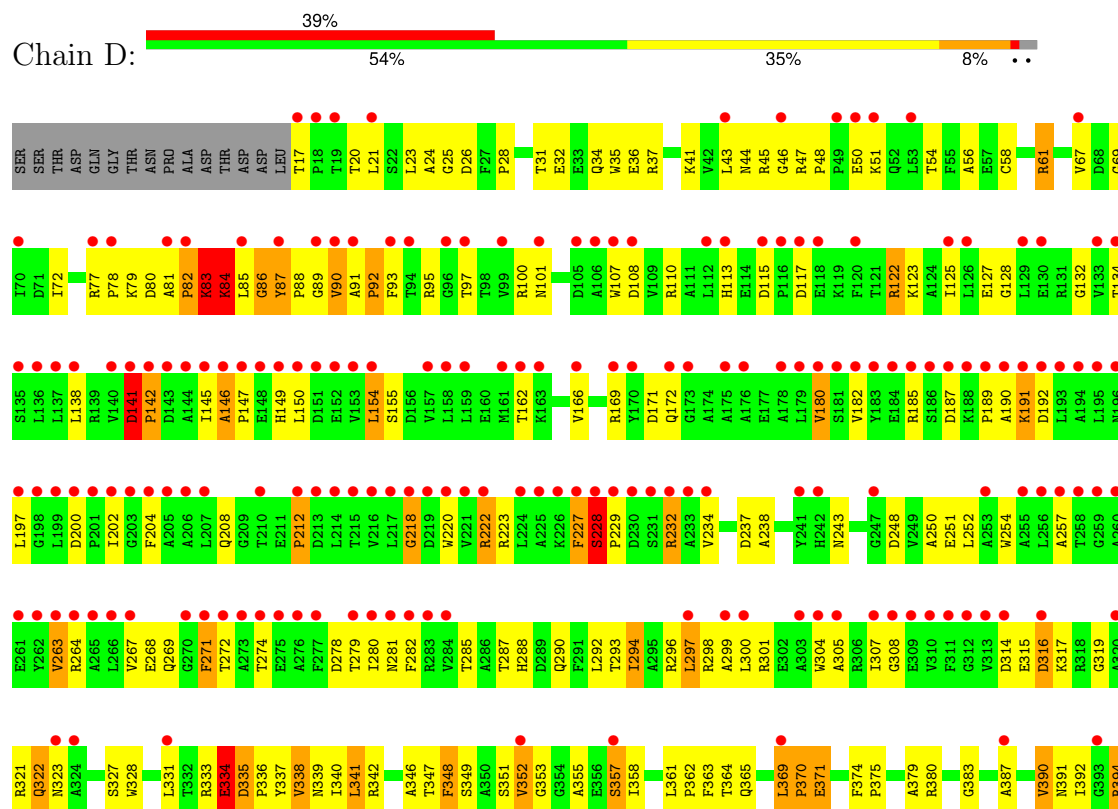
Chain B:

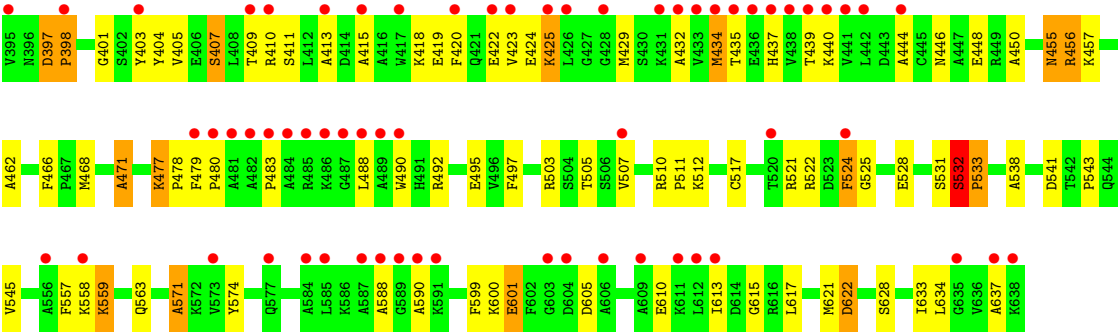
16% 53% 36% 8%

SER THR ASP GLN GLY THR ASN ALA ASP ASP ASP LEU THR PRO THR T20 L21 S22 L23 A24 G25 D26 F27 P28 T31 E32 E36 V39 R44 R45 P48 P49 E50 T54 F55 L59 K60 R61 L62 T63 T66 D71 I72 V73 P74 R77 D78



● Molecule 2: METHYLMALONYL-COA MUTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.80Å 161.30Å 88.40Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 99.7 (20.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.28 (at 1.98Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.275 0.250 , 0.270	Depositor DCC
R_{free} test set	10942 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	22372	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: DCA, B12, GOL

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	1.22	5/5679 (0.1%)	2.63	495/7718 (6.4%)
1	C	1.30	8/5676 (0.1%)	2.66	539/7711 (7.0%)
2	B	1.12	8/4785 (0.2%)	2.56	405/6499 (6.2%)
2	D	0.99	1/4783 (0.0%)	2.61	399/6503 (6.1%)
All	All	1.17	22/20923 (0.1%)	2.62	1838/28431 (6.5%)

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	25
1	C	0	37
2	B	0	21
2	D	0	17
All	All	0	100

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	466	PHE	CA-CB	8.06	1.59	1.52
2	B	466	PHE	CA-CB	6.68	1.58	1.52
1	C	122	HIS	N-CA	-6.36	1.38	1.46
1	C	300	LYS	CA-C	-6.09	1.44	1.52
1	A	72	HIS	CE1-NE2	-6.01	1.26	1.32

The worst 5 of 1838 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	264	ARG	CD-NE-CZ	38.39	178.14	124.40
2	D	169	ARG	CD-NE-CZ	29.83	166.16	124.40
1	C	384	ARG	CD-NE-CZ	24.97	159.35	124.40
1	A	384	ARG	CD-NE-CZ	24.42	158.59	124.40
1	C	596	ARG	CD-NE-CZ	19.42	151.59	124.40

There are no chirality outliers.

5 of 100 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	THR	Mainchain
1	A	41	ALA	Mainchain
1	A	61	LEU	Mainchain
1	A	70	PHE	Mainchain
1	A	87	ARG	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	5563	0	5443	41	0
1	C	5560	0	5456	53	0
2	B	4695	0	4610	45	0
2	D	4692	0	4580	53	0
3	A	91	0	88	13	0
3	C	91	0	88	10	0
4	A	47	0	32	0	0
4	C	47	0	32	0	0
5	A	12	0	16	3	0
5	B	18	0	24	2	0
5	C	12	0	16	3	0
5	D	12	0	15	1	0
6	A	457	0	0	0	0
6	B	318	0	0	1	0
6	C	493	0	0	2	0
6	D	264	0	0	0	0
All	All	22372	0	20400	195	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 195 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:A:800:B12:H421	3:A:800:B12:C36	1.67	1.23
3:A:800:B12:H421	3:A:800:B12:H363	1.18	1.12
3:A:800:B12:H552	3:A:800:B12:H531	1.24	1.10
3:A:800:B12:H363	3:A:800:B12:C42	1.93	0.96
3:A:800:B12:C36	3:A:800:B12:C42	2.36	0.90

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%)	698 (96%)	26 (4%)	1 (0%)	48	46
1	C	725/727 (100%)	685 (94%)	37 (5%)	3 (0%)	30	27
2	B	617/637 (97%)	595 (96%)	21 (3%)	1 (0%)	43	42
2	D	620/637 (97%)	580 (94%)	38 (6%)	2 (0%)	36	35
All	All	2687/2728 (98%)	2558 (95%)	122 (4%)	7 (0%)	36	35

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	15	ALA
1	C	16	PRO
2	D	228	SER
1	A	486	SER
1	C	486	SER

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	571/590 (97%)	550 (96%)	21 (4%)	30	30
1	C	571/590 (97%)	549 (96%)	22 (4%)	28	28
2	B	474/509 (93%)	455 (96%)	19 (4%)	28	27
2	D	472/509 (93%)	449 (95%)	23 (5%)	22	20
All	All	2088/2198 (95%)	2003 (96%)	85 (4%)	27	26

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	596	ARG
2	D	297	LEU
1	C	671	GLU
2	D	141	ASP
2	D	371	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	391	ASN
2	D	365	GLN
1	C	191	GLN
1	C	643	GLN
1	C	14	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
5	GOL	A	802	-	5,5,5	0.79	0	5,5,5	1.76	1 (20%)
5	GOL	C	803	-	5,5,5	0.52	0	5,5,5	0.61	0
4	DCA	C	801	-	47,49,49	1.32	7 (14%)	69,74,74	1.50	13 (18%)
5	GOL	A	803	-	5,5,5	0.82	0	5,5,5	0.66	0
5	GOL	D	639	-	5,5,5	0.21	0	5,5,5	0.91	0
5	GOL	C	802	-	5,5,5	1.09	0	5,5,5	2.93	1 (20%)
5	GOL	B	1	-	5,5,5	0.66	0	5,5,5	0.24	0
3	B12	C	800	1	94,101,101	1.59	19 (20%)	149,166,166	2.58	59 (39%)
5	GOL	B	640	-	5,5,5	0.44	0	5,5,5	0.45	0
5	GOL	B	639	-	5,5,5	0.31	0	5,5,5	0.58	0
5	GOL	D	1	-	5,5,5	0.61	0	5,5,5	2.14	1 (20%)
3	B12	A	800	1	94,101,101	1.61	19 (20%)	149,166,166	2.34	48 (32%)
4	DCA	A	801	-	47,49,49	1.64	4 (8%)	69,74,74	1.14	5 (7%)

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
5	GOL	A	802	-	-	0/4/4/4	-
5	GOL	C	803	-	-	0/4/4/4	-
4	DCA	C	801	-	-	2/47/63/63	0/3/3/3
5	GOL	A	803	-	-	0/4/4/4	-
5	GOL	D	639	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	C	802	-	-	0/4/4/4	-
5	GOL	B	1	-	-	0/4/4/4	-
3	B12	C	800	1	-	10/56/223/223	0/3/11/11
5	GOL	B	640	-	-	4/4/4/4	-
5	GOL	B	639	-	-	2/4/4/4	-
5	GOL	D	1	-	-	3/4/4/4	-
3	B12	A	800	1	-	12/56/223/223	0/3/11/11
4	DCA	A	801	-	-	2/47/63/63	0/3/3/3

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	B12	C14-N23	7.91	1.45	1.35
4	A	801	DCA	P1A-O3A	-6.76	1.52	1.59
3	C	800	B12	C14-N23	5.38	1.42	1.35
4	A	801	DCA	P3B-O3B	4.95	1.68	1.59
4	A	801	DCA	P2A-O3A	4.26	1.64	1.59

The worst 5 of 128 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800	B12	C9-N22-C6	9.74	117.00	105.28
3	C	800	B12	C19-N24-C16	7.90	115.92	107.29
3	C	800	B12	C13-C14-C15	-6.92	113.80	124.32
3	A	800	B12	C13-C14-N23	6.78	118.27	109.09
5	C	802	GOL	O3-C3-C2	6.38	139.09	110.38

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

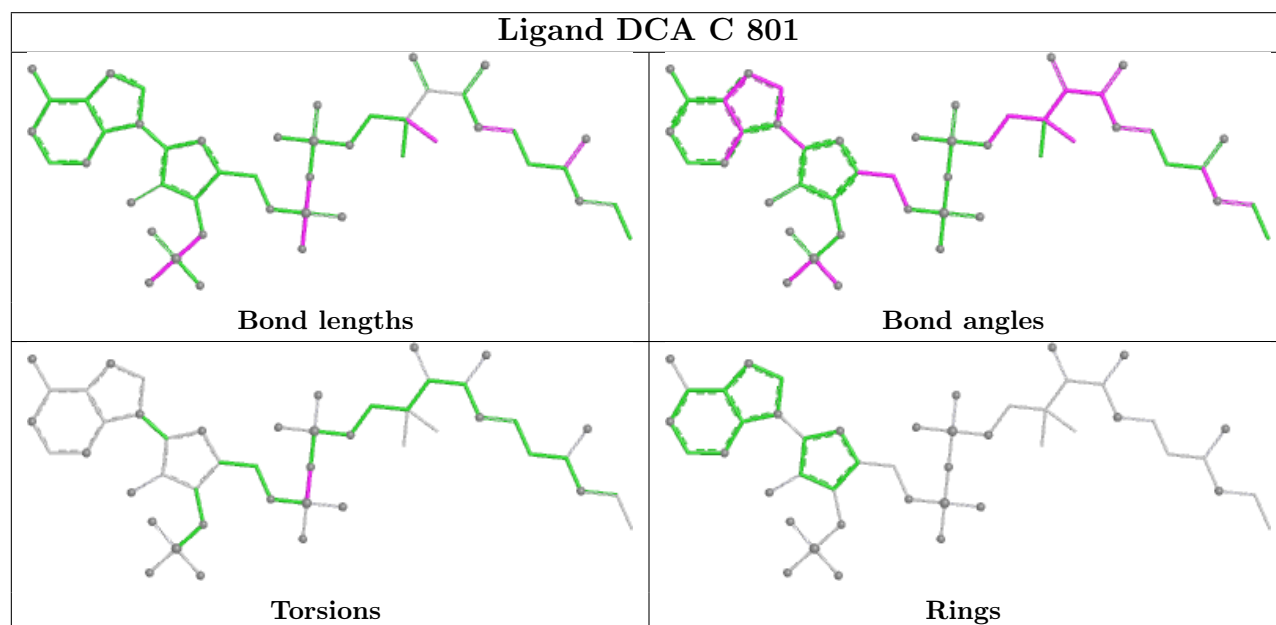
Mol	Chain	Res	Type	Atoms
3	A	800	B12	C2R-C1R-N1B-C2B
3	C	800	B12	C42-C41-C8-C9
3	C	800	B12	C2R-C1R-N1B-C2B
5	B	639	GOL	C1-C2-C3-O3
5	B	640	GOL	C1-C2-C3-O3

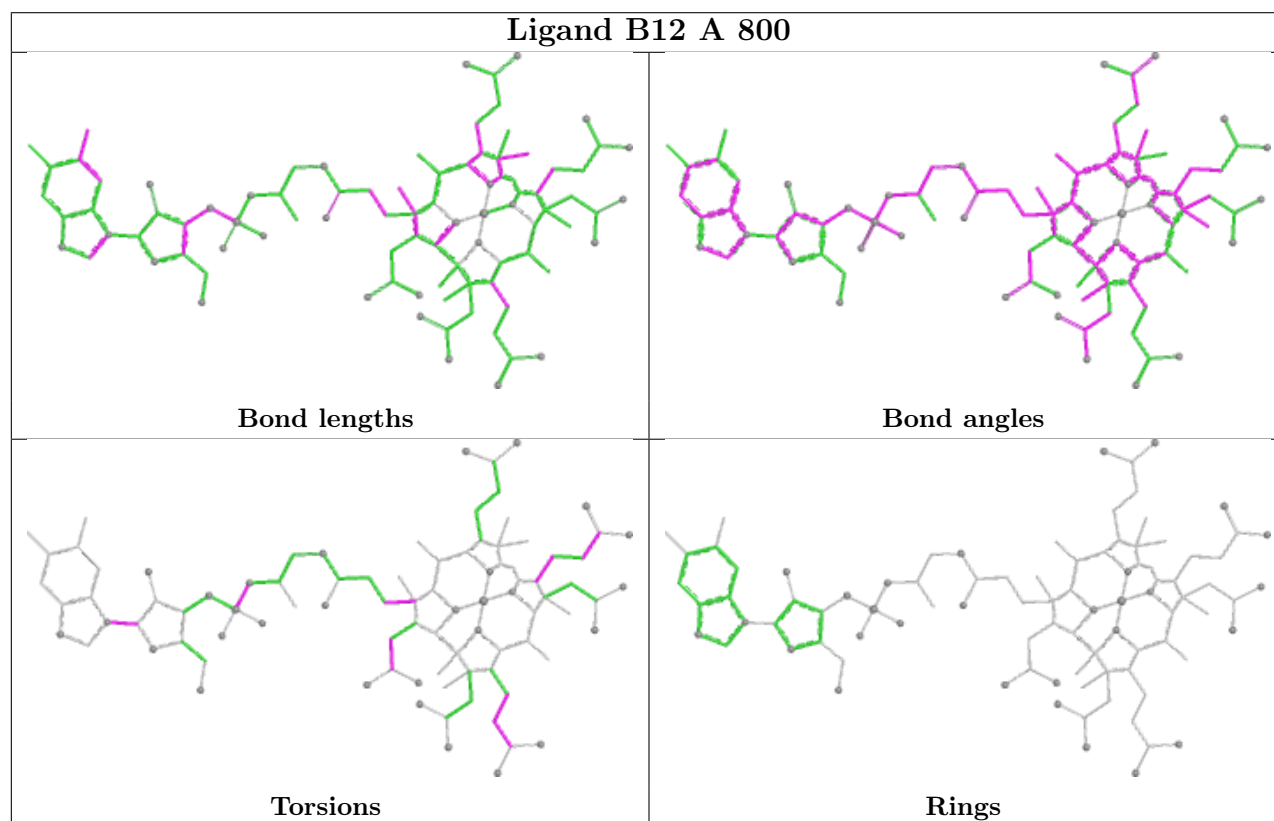
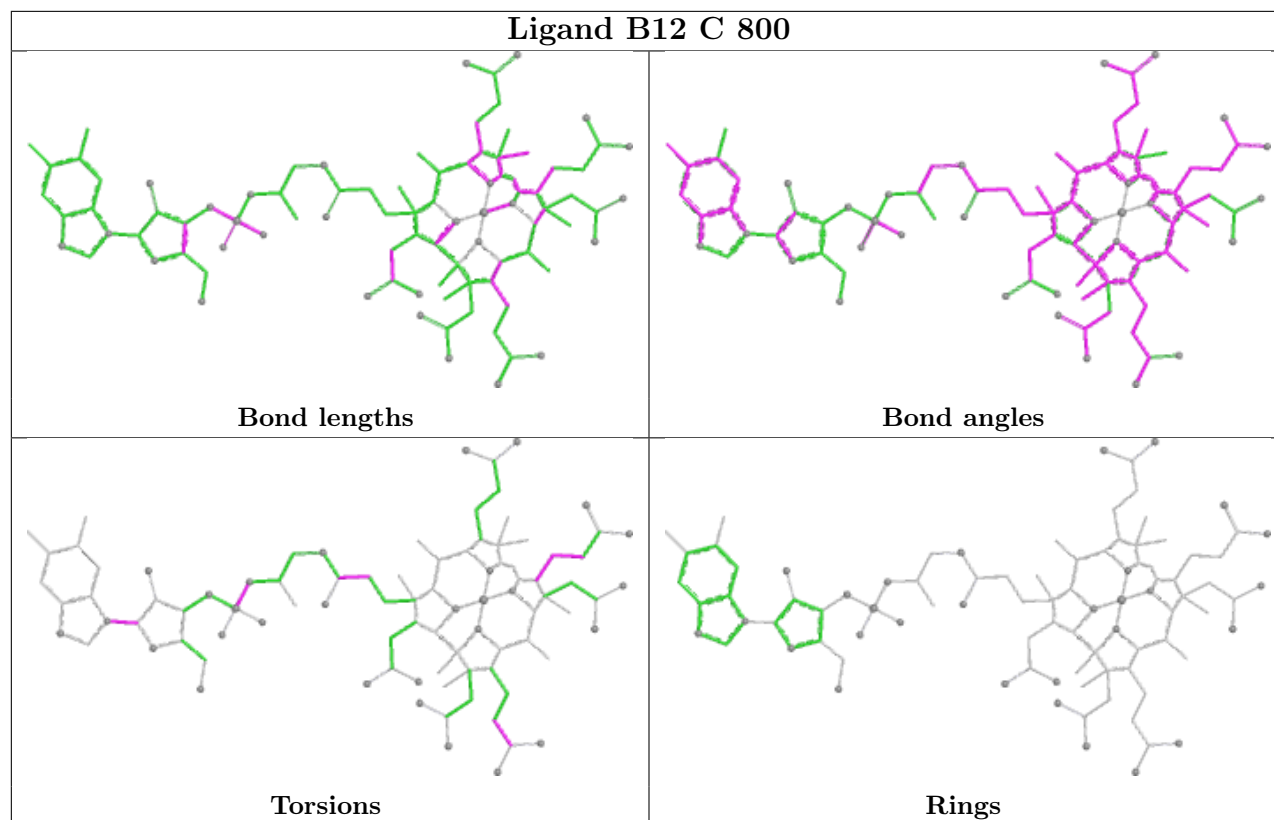
There are no ring outliers.

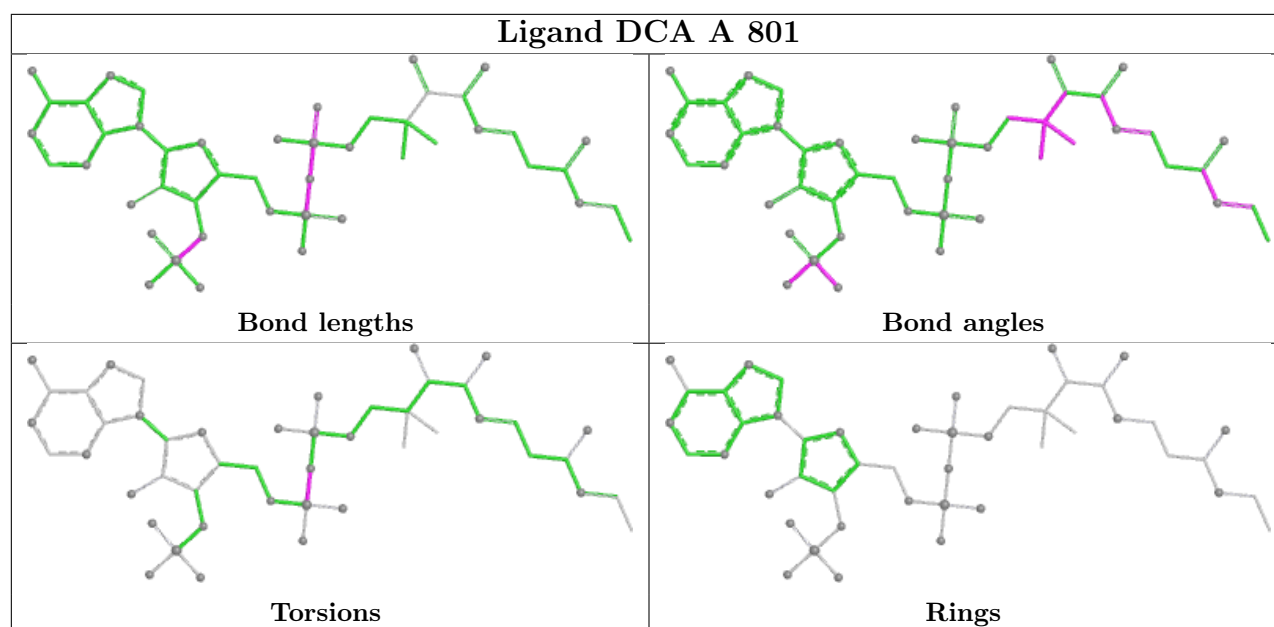
7 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	802	GOL	3	0
5	C	802	GOL	3	0
3	C	800	B12	10	0
5	B	640	GOL	1	0
5	B	639	GOL	1	0
5	D	1	GOL	1	0
3	A	800	B12	13	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 [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%)	0.75	86 (11%) 9 8	19, 35, 61, 89	0
1	C	727/727 (100%)	0.76	79 (10%) 10 9	18, 34, 60, 105	0
2	B	619/637 (97%)	1.06	103 (16%) 4 4	23, 41, 61, 82	0
2	D	622/637 (97%)	1.83	247 (39%) 1 1	23, 50, 75, 103	0
All	All	2695/2728 (98%)	1.08	515 (19%) 3 3	18, 39, 67, 105	0

The worst 5 of 515 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	THR	7.4
2	D	190	ALA	6.9
1	A	3	THR	6.5
2	D	183	TYR	6.5
1	C	2	SER	5.8

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](#)

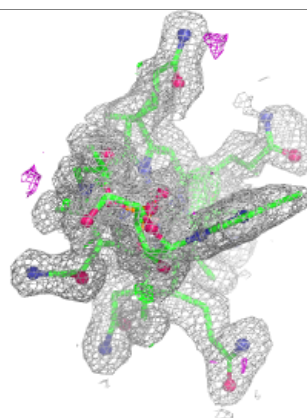
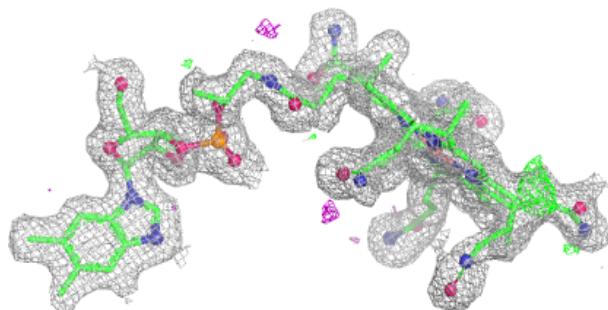
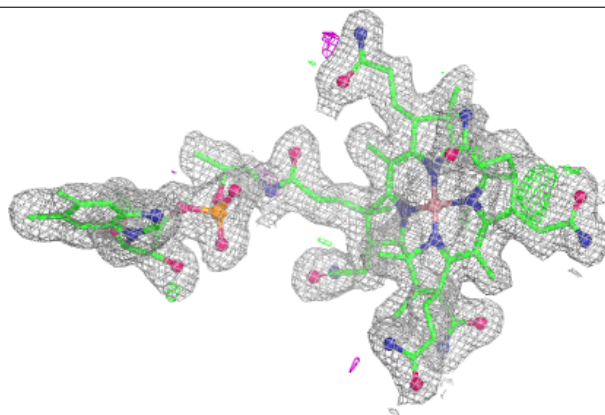
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
5	GOL	B	1	6/6	0.75	0.22	54,59,61,61	0
5	GOL	D	1	6/6	0.81	0.21	61,62,64,68	0
5	GOL	D	639	6/6	0.82	0.19	53,61,64,70	0
5	GOL	B	640	6/6	0.86	0.15	50,60,62,68	0
5	GOL	B	639	6/6	0.88	0.16	44,48,53,53	0
5	GOL	A	802	6/6	0.89	0.19	29,41,45,48	0
5	GOL	A	803	6/6	0.92	0.12	34,38,42,46	0
5	GOL	C	802	6/6	0.93	0.15	21,32,43,45	0
5	GOL	C	803	6/6	0.93	0.10	38,39,41,45	0
3	B12	A	800	91/91	0.97	0.09	17,29,48,68	0
3	B12	C	800	91/91	0.98	0.08	15,26,40,53	0
4	DCA	A	801	47/47	0.98	0.07	20,25,28,31	0
4	DCA	C	801	47/47	0.98	0.06	14,23,30,32	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.

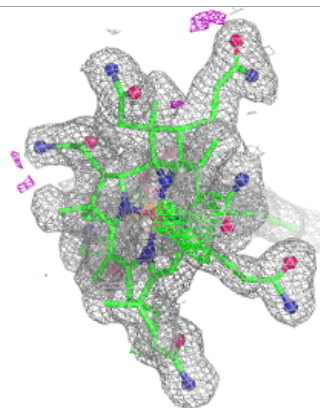
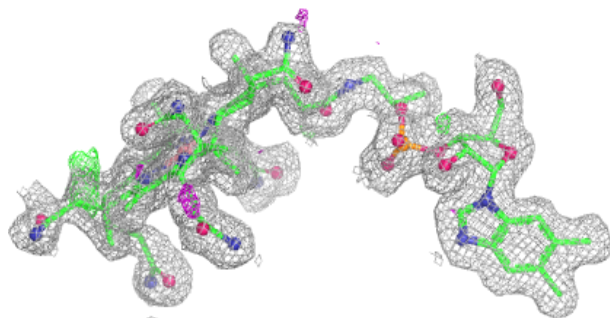
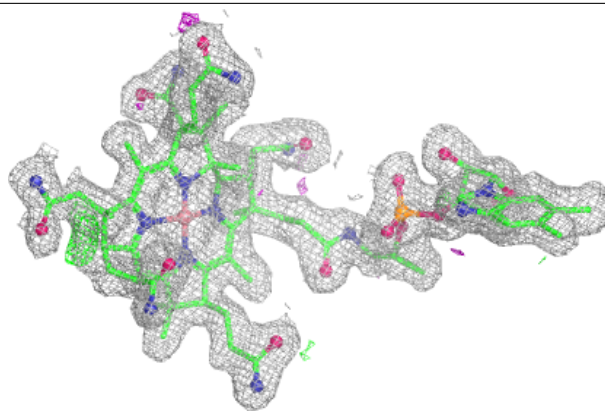
Electron density around B12 A 800:

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

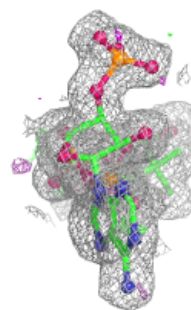
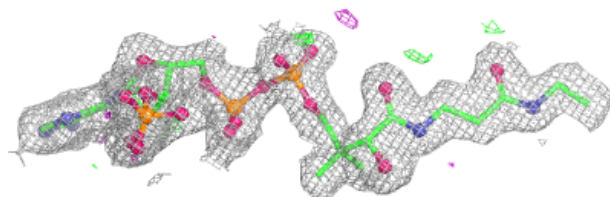
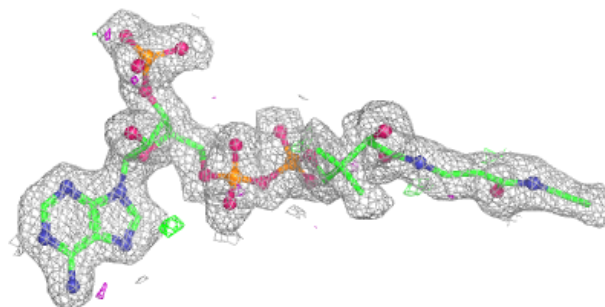


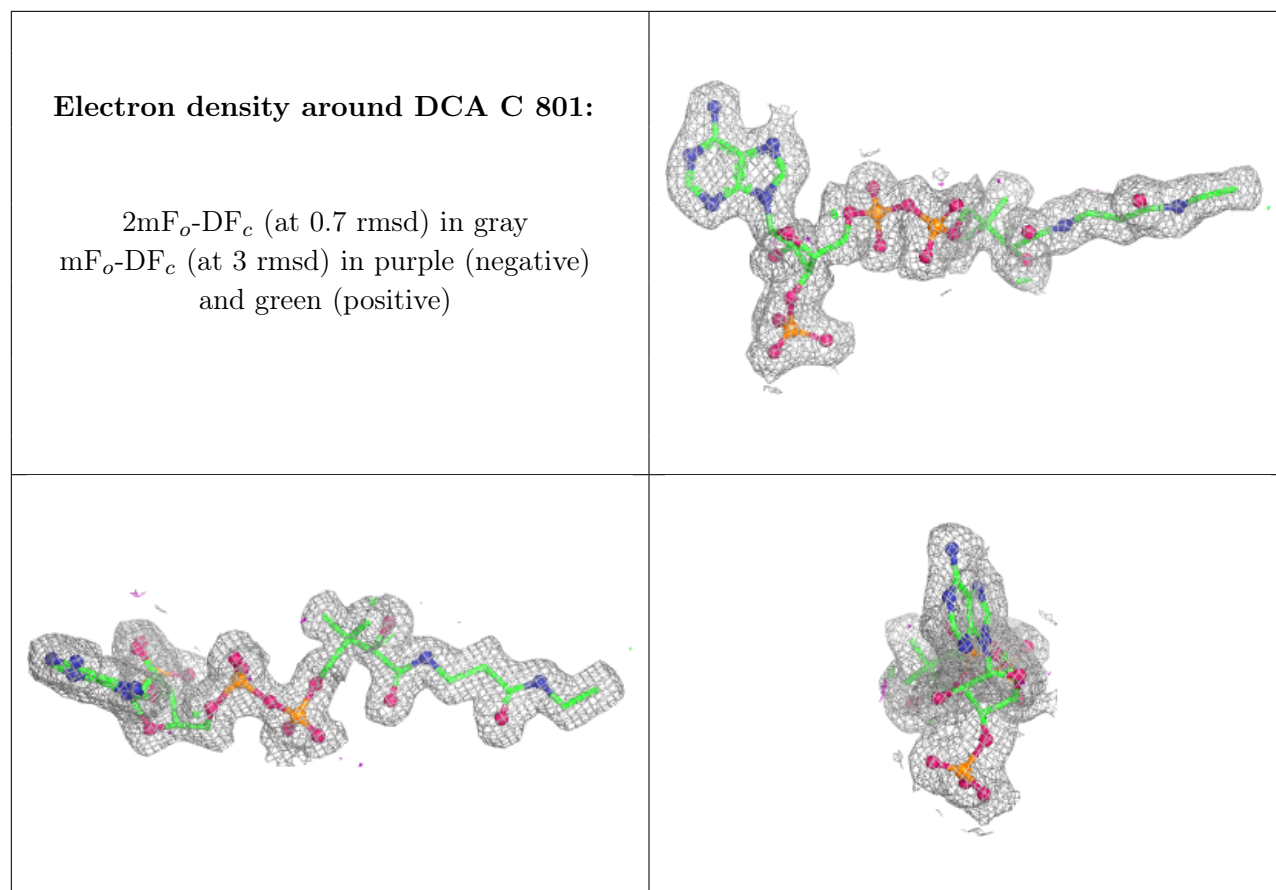
Electron density around B12 C 800:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.