



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2021 – 12:57 AM JST

PDB ID : 7DQV  
Title : Crystal structure of a CmABCB1 mutant  
Authors : Matsuoka, K.; Nakatsu, T.; Kato, H.  
Deposited on : 2020-12-24  
Resolution : 2.15 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

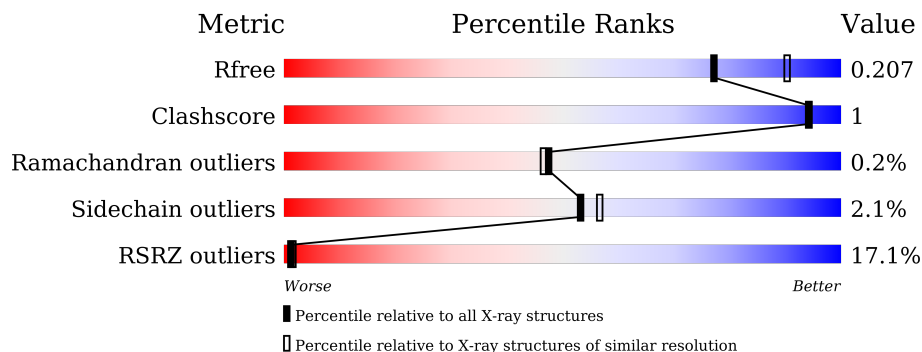
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 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	620	<div> <div>16%</div> <div>91%</div> <div>5%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4953 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.

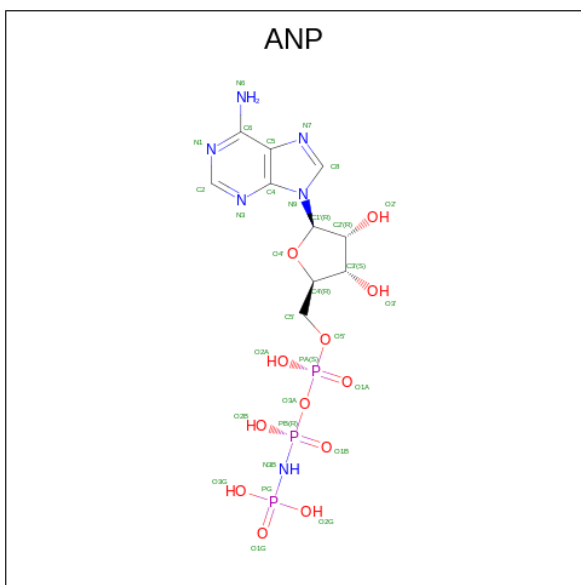
- Molecule 1 is a protein called Probable ATP-dependent transporter ycf16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	589	4497	2886	770	824	17	0	0	0

There are 17 discrepancies between the modelled and reference sequences:

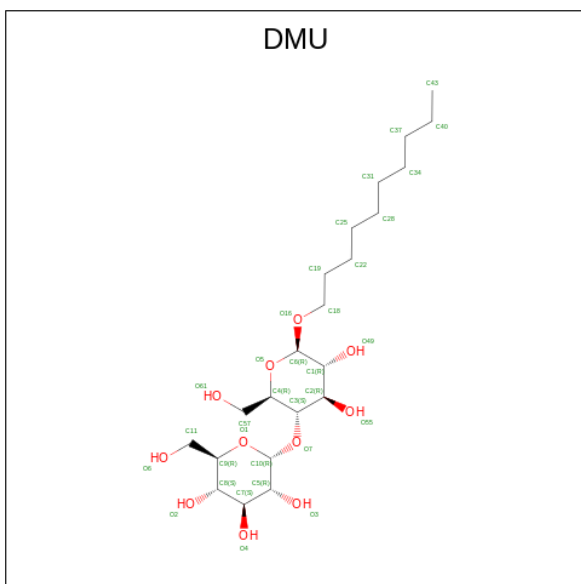
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	VAL	GLY	engineered mutation	UNP M1VAN7
A	697	GLY	-	expression tag	UNP M1VAN7
A	698	ARG	-	expression tag	UNP M1VAN7
A	699	ASP	-	expression tag	UNP M1VAN7
A	700	TYR	-	expression tag	UNP M1VAN7
A	701	LYS	-	expression tag	UNP M1VAN7
A	702	ASP	-	expression tag	UNP M1VAN7
A	703	ASP	-	expression tag	UNP M1VAN7
A	704	ASP	-	expression tag	UNP M1VAN7
A	705	ASP	-	expression tag	UNP M1VAN7
A	706	LYS	-	expression tag	UNP M1VAN7
A	707	HIS	-	expression tag	UNP M1VAN7
A	708	HIS	-	expression tag	UNP M1VAN7
A	709	HIS	-	expression tag	UNP M1VAN7
A	710	HIS	-	expression tag	UNP M1VAN7
A	711	HIS	-	expression tag	UNP M1VAN7
A	712	HIS	-	expression tag	UNP M1VAN7

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ) (labeled as "Ligand of Interest" by depositor).



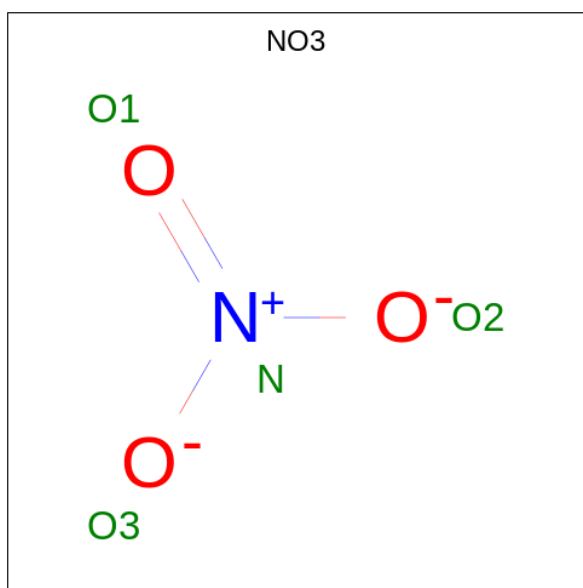
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 3 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 33	C 22	O 11	0	0
3	A	1	Total 33	C 22	O 11	0	0

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

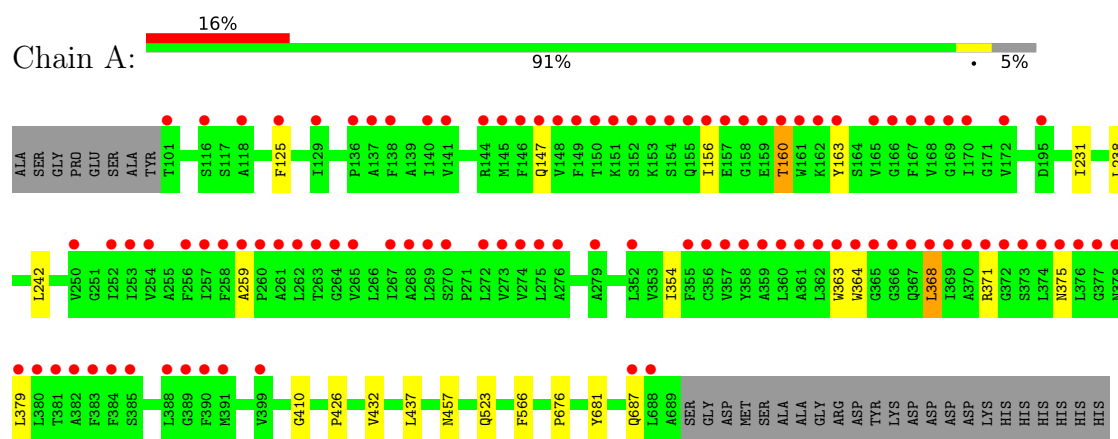
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	354	Total	O	0	0
			354	354		

### 3 Residue-property plots [i](#)

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: Probable ATP-dependent transporter ycf16



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.67Å 175.67Å 175.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.15 48.72 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.70-2.15) 99.8 (48.72-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.185 , 0.210 0.182 , 0.207	Depositor DCC
$R_{free}$ test set	2534 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4953	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, NO3, DMU, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.40	0/4580	0.55	0/6205

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4497	0	4562	11	0
2	A	31	0	13	0	0
3	A	66	0	84	2	0
4	A	4	0	0	0	0
5	A	1	0	0	0	0
6	A	354	0	0	0	0
All	All	4953	0	4659	12	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 1.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HD23	1:A:375:ASN:HB2	1.75	0.66
1:A:375:ASN:O	1:A:379:LEU:N	2.30	0.64
1:A:156:ILE:O	1:A:160:THR:N	2.38	0.56
1:A:437:LEU:O	1:A:523:GLN:HG3	2.07	0.54
1:A:426:PRO:HG2	1:A:432:VAL:HG22	1.89	0.53
1:A:125:PHE:CG	3:A:803:DMU:H16	2.45	0.52
1:A:125:PHE:HD1	1:A:242:LEU:HD13	1.75	0.51
3:A:803:DMU:H35	3:A:803:DMU:H29	1.95	0.49
1:A:231:ILE:HD11	1:A:410:GLY:HA2	1.96	0.47
1:A:676:PRO:HA	1:A:681:TYR:CD1	2.50	0.46
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.92	0.43
1:A:371:ARG:HA	1:A:371:ARG:NH1	2.36	0.41

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	587/620 (95%)	568 (97%)	18 (3%)	1 (0%)	47 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ALA

### 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	467/491 (95%)	457 (98%)	10 (2%)	53 57

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	160	THR
1	A	163	TYR
1	A	354	ILE
1	A	363	TRP
1	A	364	TRP
1	A	368	LEU
1	A	457	ASN
1	A	566	PHE
1	A	687	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	DMU	A	802	-	34,34,34	1.54	6 (17%)	45,45,45	1.01	1 (2%)
3	DMU	A	803	-	34,34,34	1.51	7 (20%)	45,45,45	1.12	3 (6%)
4	NO3	A	804	-	1,3,3	0.32	0	0,3,3	0.00	-
2	ANP	A	801	5	29,33,33	0.91	1 (3%)	31,52,52	1.25	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DMU	A	802	-	-	3/19/59/59	0/2/2/2
3	DMU	A	803	-	-	12/19/59/59	0/2/2/2
2	ANP	A	801	5	-	1/14/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	DMU	O1-C9	4.81	1.56	1.44
3	A	803	DMU	O1-C9	4.27	1.54	1.44
3	A	803	DMU	C11-C9	-3.35	1.40	1.51
2	A	801	ANP	PG-N3B	3.10	1.71	1.63
3	A	802	DMU	C11-C9	-3.09	1.41	1.51
3	A	802	DMU	O4-C7	2.81	1.49	1.43
3	A	802	DMU	O5-C6	2.81	1.49	1.41
3	A	803	DMU	O4-C7	2.53	1.48	1.43
3	A	803	DMU	O5-C6	2.43	1.48	1.41
3	A	802	DMU	C8-C9	2.34	1.58	1.53
3	A	803	DMU	C7-C5	-2.26	1.46	1.52
3	A	803	DMU	O1-C10	2.06	1.47	1.41
3	A	803	DMU	O3-C5	2.01	1.47	1.43
3	A	802	DMU	O3-C5	2.00	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ANP	O1G-PG-N3B	-4.28	105.47	111.77
3	A	802	DMU	C10-O7-C3	-2.91	110.76	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	DMU	C1-C2-C3	2.57	115.56	109.68
2	A	801	ANP	C5-C6-N6	2.46	124.09	120.35
3	A	803	DMU	C10-O7-C3	-2.31	112.25	117.96
2	A	801	ANP	O1B-PB-N3B	-2.25	108.46	111.77
2	A	801	ANP	O2B-PB-O3A	2.22	112.06	104.64
3	A	803	DMU	C6-C1-C2	2.11	114.38	110.00
2	A	801	ANP	O3A-PB-N3B	-2.03	100.95	106.59

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PG-N3B-PB-O1B
3	A	802	DMU	O6-C11-C9-O1
3	A	802	DMU	O6-C11-C9-C8
3	A	803	DMU	O6-C11-C9-O1
3	A	803	DMU	C3-C4-C57-O61
3	A	803	DMU	O5-C4-C57-O61
3	A	803	DMU	C25-C28-C31-C34
3	A	803	DMU	C31-C34-C37-C40
3	A	803	DMU	O1-C10-O7-C3
3	A	802	DMU	C25-C28-C31-C34
3	A	803	DMU	O6-C11-C9-C8
3	A	803	DMU	C2-C3-O7-C10
3	A	803	DMU	C5-C10-O7-C3
3	A	803	DMU	C18-C19-C22-C25
3	A	803	DMU	C4-C3-O7-C10
3	A	803	DMU	C34-C37-C40-C43

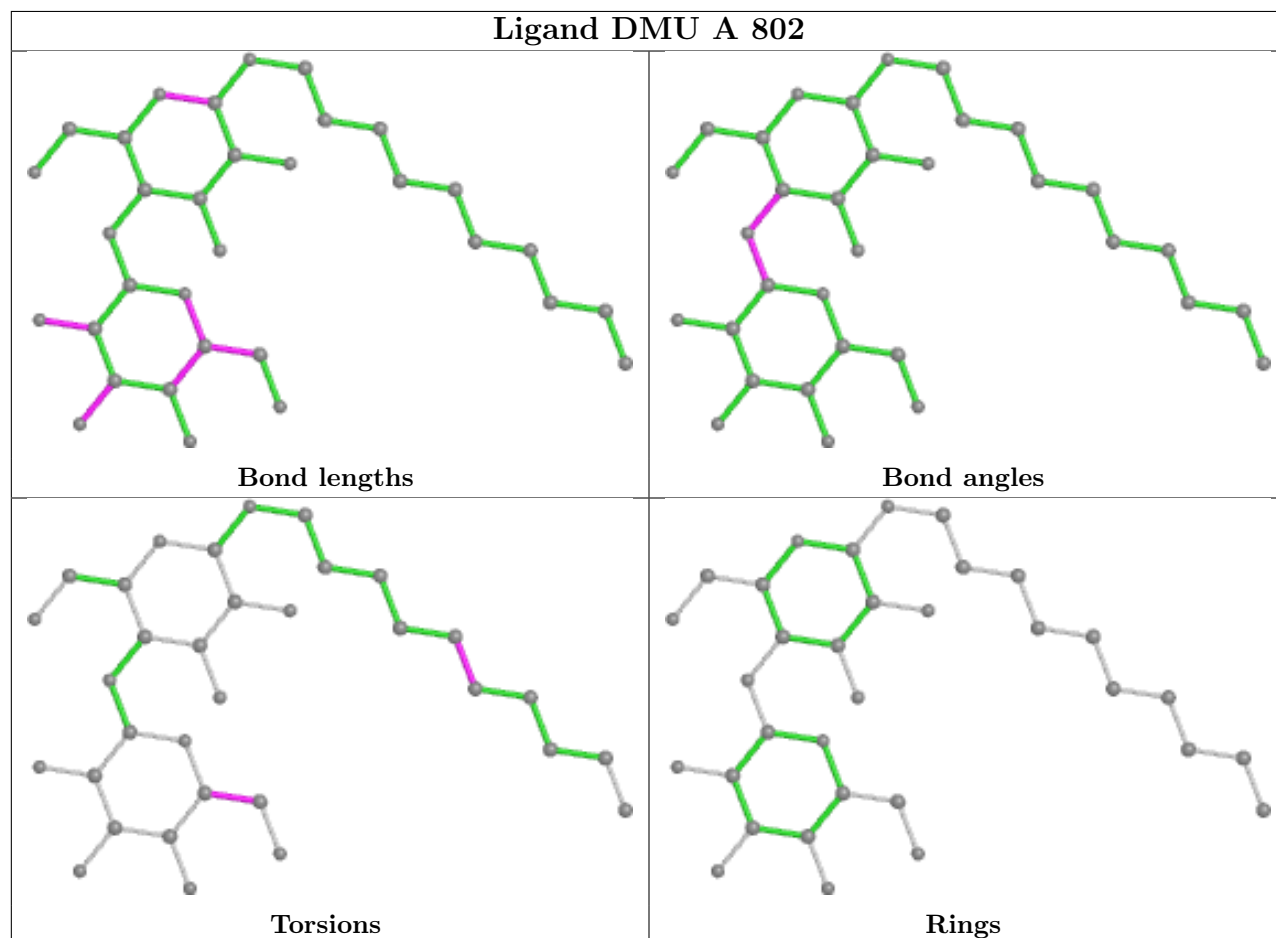
There are no ring outliers.

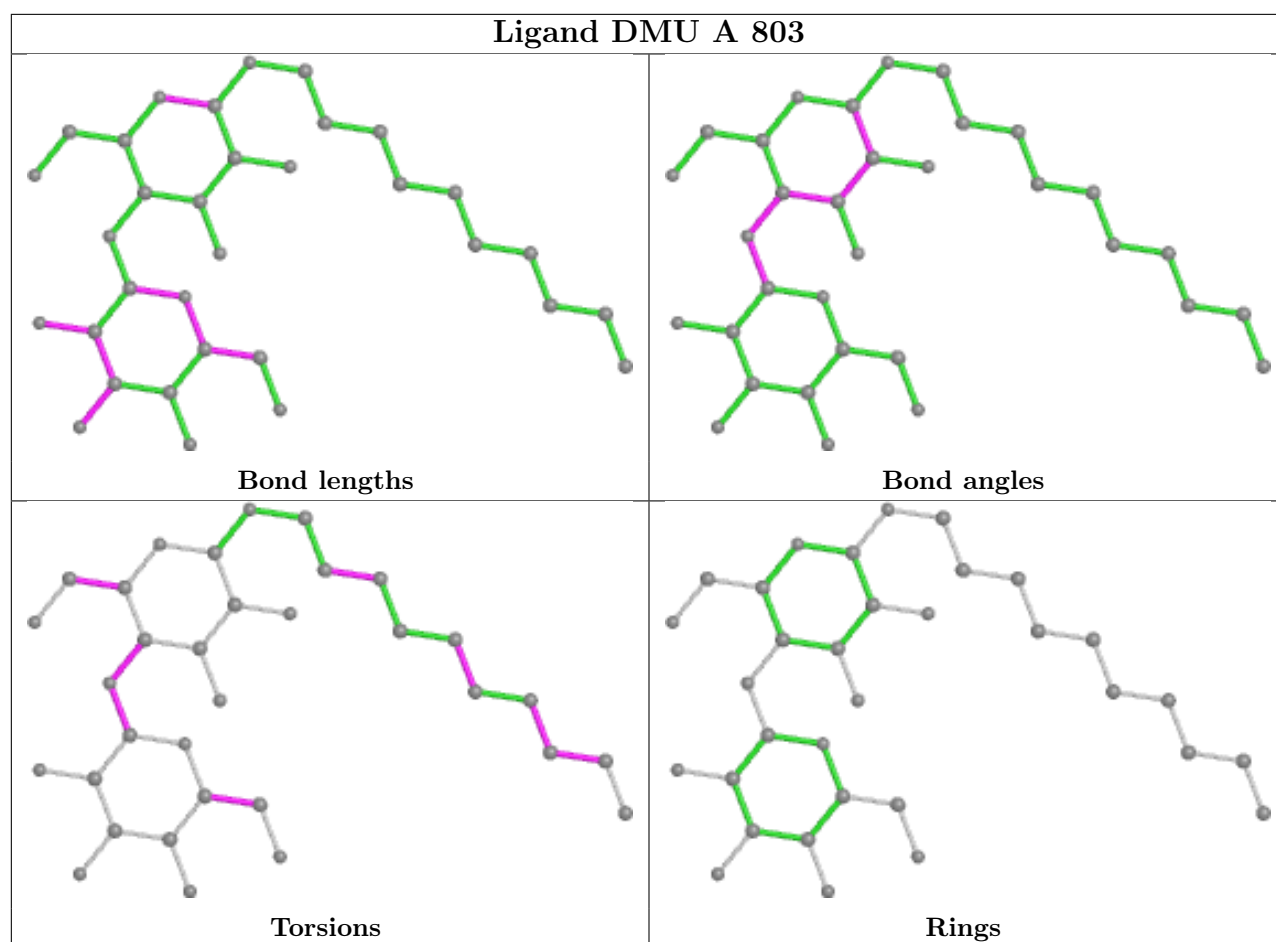
1 monomer is involved in 2 short contacts:

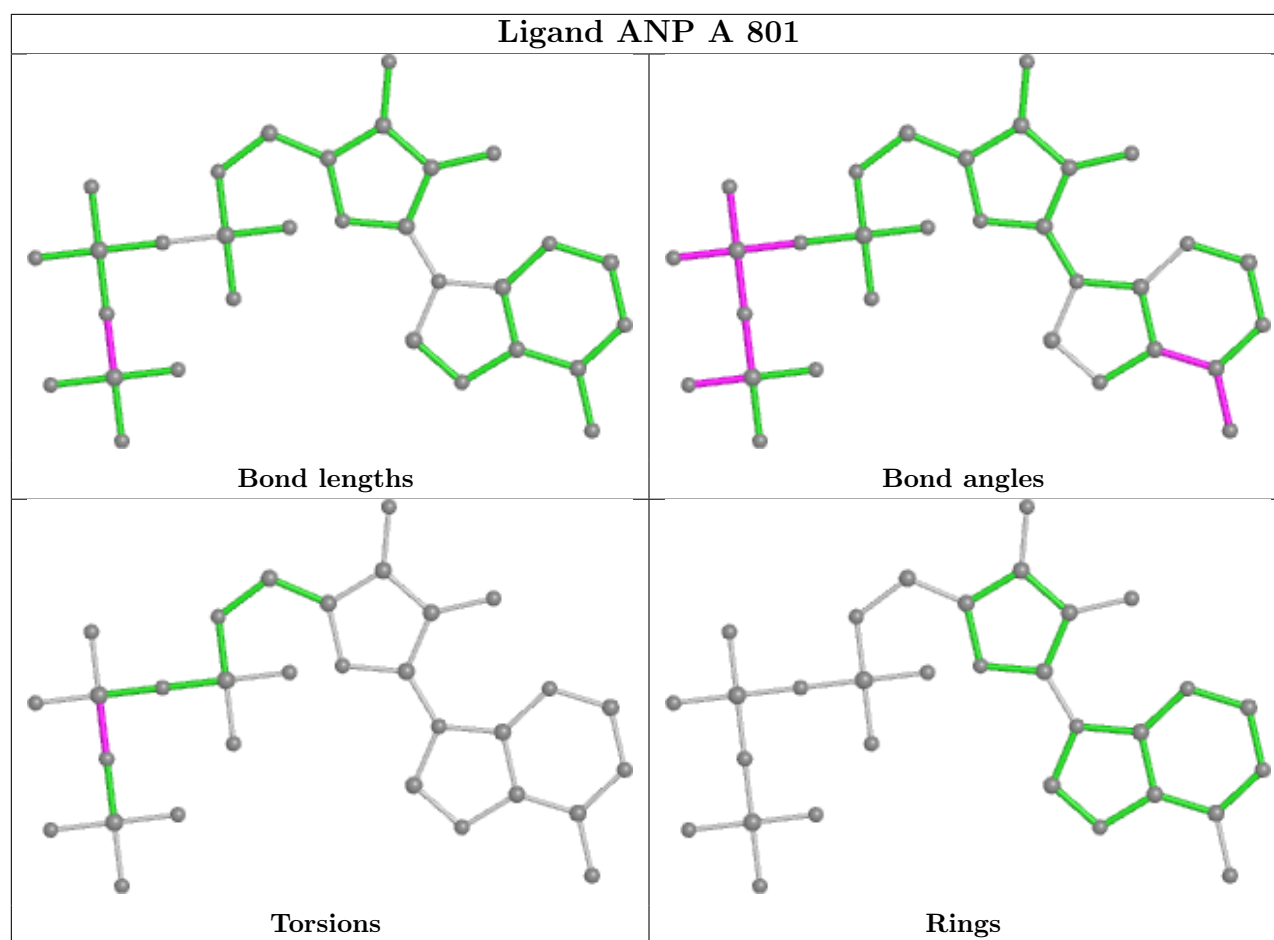
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	DMU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	589/620 (95%)	1.12	101 (17%) <b>1</b> <b>1</b>	29, 51, 216, 333	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	ALA	16.1
1	A	149	PHE	15.2
1	A	380	LEU	14.0
1	A	373	SER	13.5
1	A	369	ILE	13.0
1	A	372	GLY	13.0
1	A	374	LEU	12.6
1	A	382	ALA	12.2
1	A	379	LEU	11.6
1	A	377	GLY	11.3
1	A	261	ALA	11.1
1	A	272	LEU	10.6
1	A	366	GLY	10.1
1	A	381	THR	9.8
1	A	371	ARG	9.8
1	A	365	GLY	9.7
1	A	262	LEU	9.6
1	A	150	THR	9.1
1	A	364	TRP	8.9
1	A	152	SER	8.7
1	A	362	LEU	8.7
1	A	358	TYR	8.6
1	A	376	LEU	8.6
1	A	256	PHE	8.5
1	A	264	GLY	8.3
1	A	270	SER	8.3
1	A	161	TRP	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	269	LEU	8.1
1	A	355	PHE	7.9
1	A	154	SER	7.8
1	A	276	ALA	7.8
1	A	368	LEU	7.8
1	A	275	LEU	7.2
1	A	375	ASN	7.1
1	A	257	ILE	6.8
1	A	148	VAL	6.6
1	A	265	VAL	6.5
1	A	156	ILE	6.5
1	A	352	LEU	6.4
1	A	378	ASN	6.2
1	A	153	LYS	6.1
1	A	363	TRP	5.8
1	A	169	GLY	5.8
1	A	258	PHE	5.8
1	A	367	GLN	5.7
1	A	383	PHE	5.7
1	A	155	GLN	5.6
1	A	145	MET	5.6
1	A	385	SER	5.4
1	A	390	PHE	5.4
1	A	260	PRO	5.2
1	A	170	ILE	5.0
1	A	136	PRO	4.7
1	A	688	LEU	4.6
1	A	254	VAL	4.6
1	A	137	ALA	4.5
1	A	168	VAL	4.4
1	A	687	GLN	4.3
1	A	163	TYR	4.2
1	A	253	ILE	4.1
1	A	165	VAL	4.1
1	A	157	GLU	4.0
1	A	158	GLY	4.0
1	A	250	VAL	4.0
1	A	361	ALA	3.9
1	A	359	ALA	3.8
1	A	259	ALA	3.8
1	A	159	GLU	3.7
1	A	279	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	274	VAL	3.7
1	A	151	LYS	3.7
1	A	129	ILE	3.6
1	A	172	VAL	3.6
1	A	141	VAL	3.5
1	A	144	ARG	3.4
1	A	125	PHE	3.3
1	A	166	GLY	3.2
1	A	118	ALA	3.1
1	A	268	ALA	3.1
1	A	357	VAL	3.1
1	A	167	PHE	3.0
1	A	160	THR	3.0
1	A	360	LEU	3.0
1	A	263	THR	2.9
1	A	138	PHE	2.9
1	A	162	LYS	2.9
1	A	391	MET	2.9
1	A	146	PHE	2.8
1	A	147	GLN	2.8
1	A	388	LEU	2.8
1	A	273	VAL	2.7
1	A	252	ILE	2.6
1	A	399	VAL	2.4
1	A	389	GLY	2.3
1	A	267	ILE	2.3
1	A	384	PHE	2.3
1	A	356	CYS	2.2
1	A	140	ILE	2.2
1	A	101	THR	2.2
1	A	195	ASP	2.2
1	A	116	SER	2.0

## 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](#)

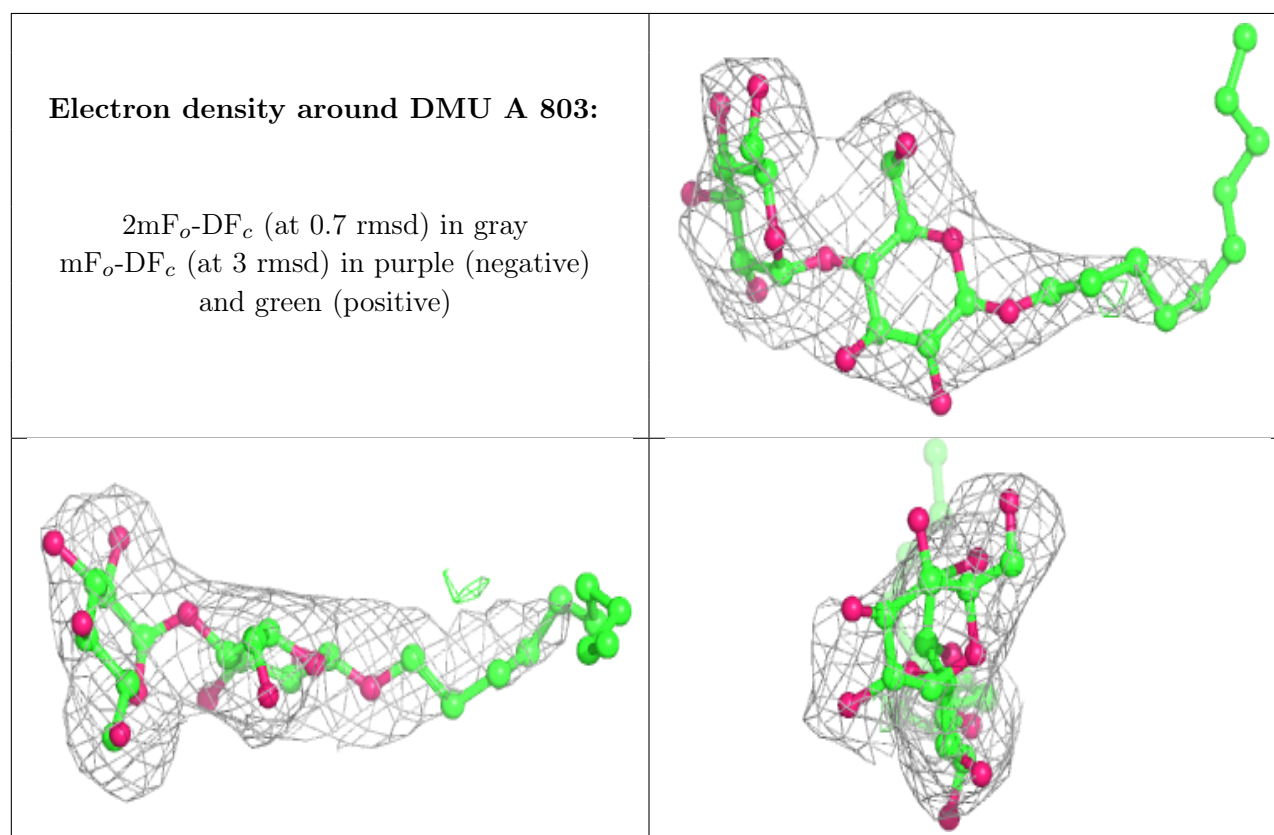
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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.

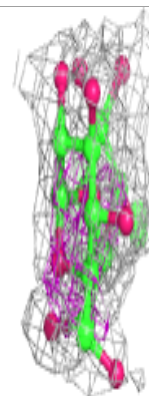
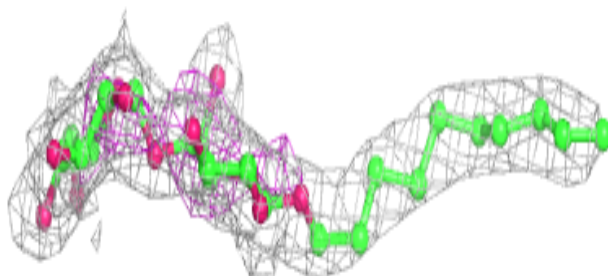
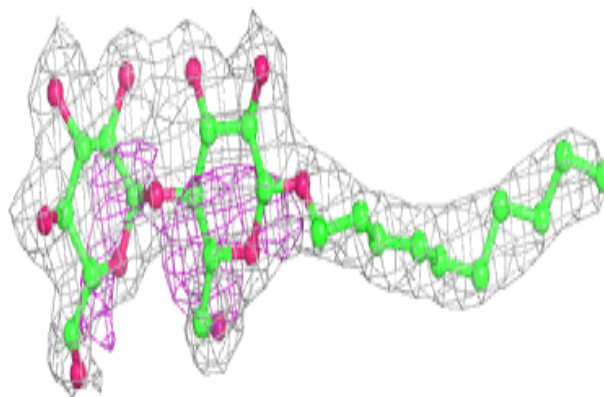
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	DMU	A	803	33/33	0.89	0.24	77,89,105,111	0
3	DMU	A	802	33/33	0.90	0.14	37,52,64,70	0
5	MG	A	805	1/1	0.95	0.07	32,32,32,32	0
2	ANP	A	801	31/31	0.99	0.13	28,31,35,36	0
4	NO3	A	804	4/4	1.00	0.12	35,37,38,42	0

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.



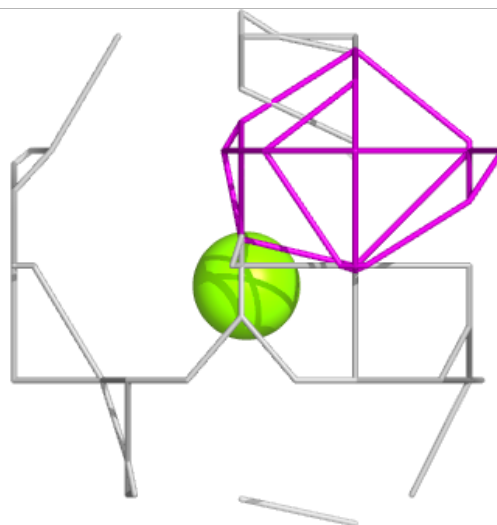
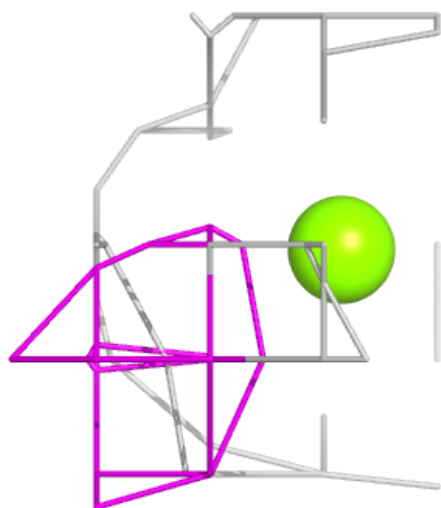
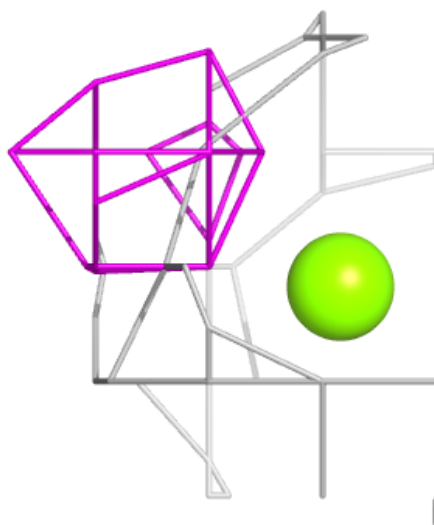
**Electron density around DMU A 802:**

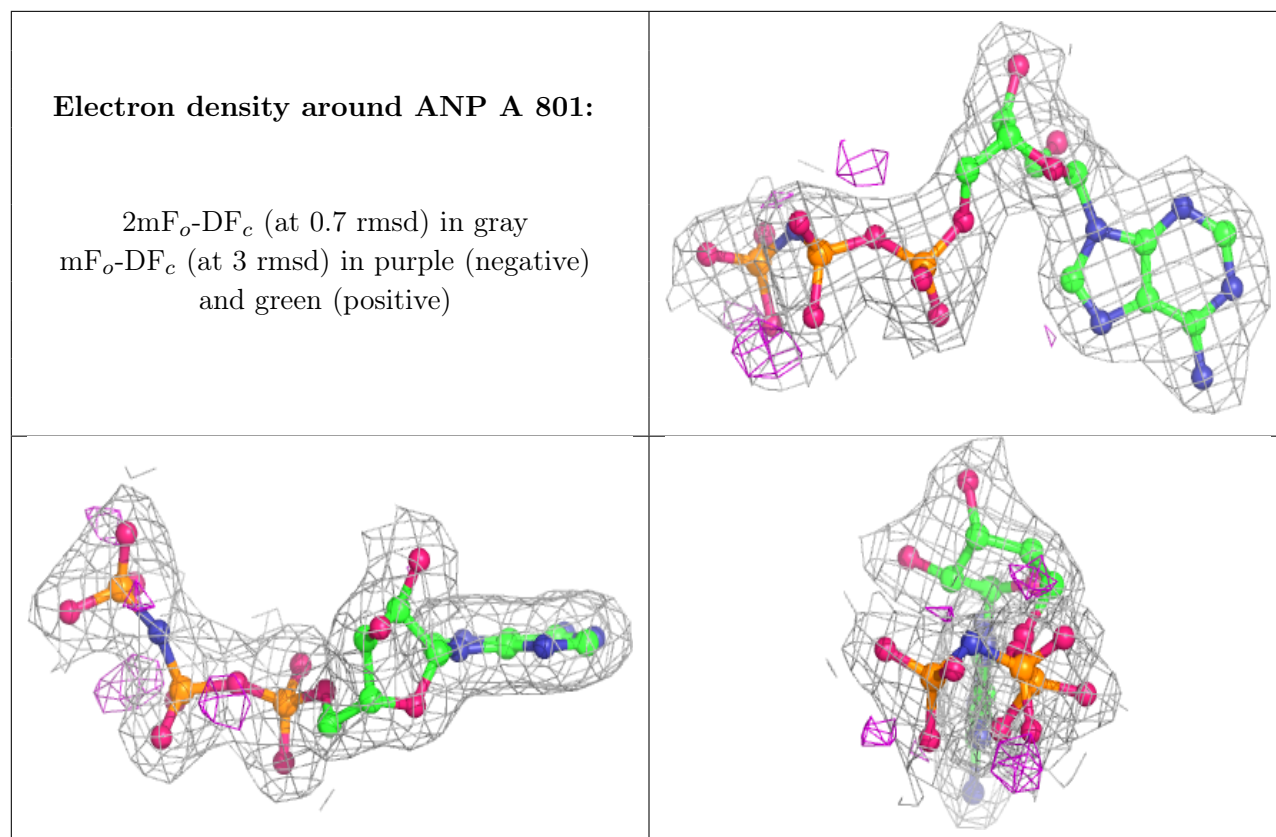
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MG A 805:**

$2mF_o-DF_c$  (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.