



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:50 pm BST

PDB ID : 6A6M
Title : Crystal structure of an outward-open nucleotide-bound state of the eukaryotic ABC multidrug transporter CmABCB1
Authors : Kato, H.; Nakatsu, T.; Kodan, A.
Deposited on : 2018-06-28
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.11
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) : 2.11

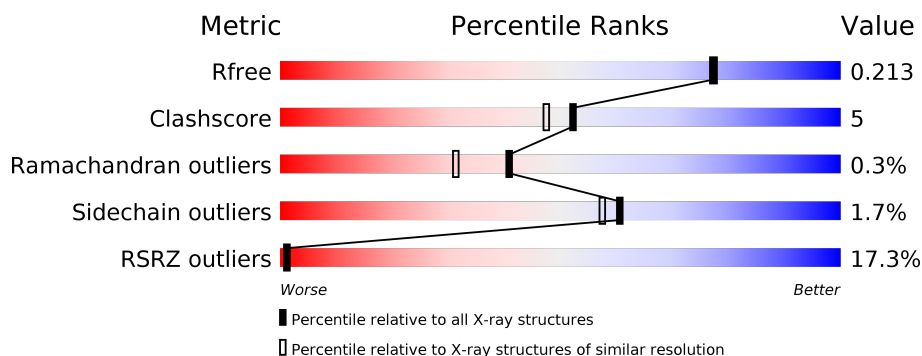
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	612	<div> <div>17%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5073 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 ATP-binding cassette, sub-family B, member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	7	0
			4535	2907	782	829	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	GLN	engineered mutation	UNP M1VAN7
A	381	ALA	THR	engineered mutation	UNP M1VAN7
A	697	GLY	-	expression tag	UNP M1VAN7
A	698	SER	-	expression tag	UNP M1VAN7
A	699	GLU	-	expression tag	UNP M1VAN7
A	700	ASN	-	expression tag	UNP M1VAN7
A	701	LEU	-	expression tag	UNP M1VAN7
A	702	TYR	-	expression tag	UNP M1VAN7
A	703	PHE	-	expression tag	UNP M1VAN7
A	704	GLN	-	expression tag	UNP M1VAN7

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

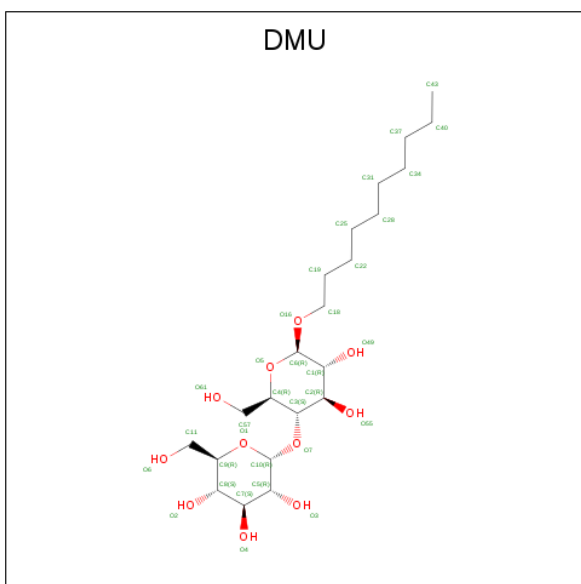


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

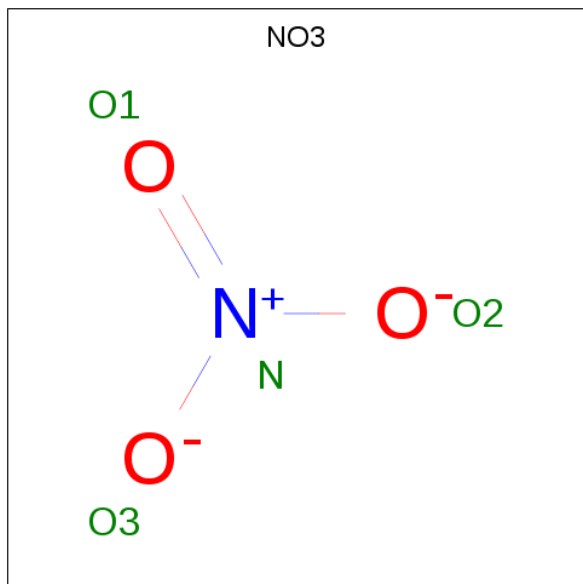
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 33 22 11	0	0
4	A	1	Total C O 26 15 11	0	0
4	A	1	Total C 8 8	0	0

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



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

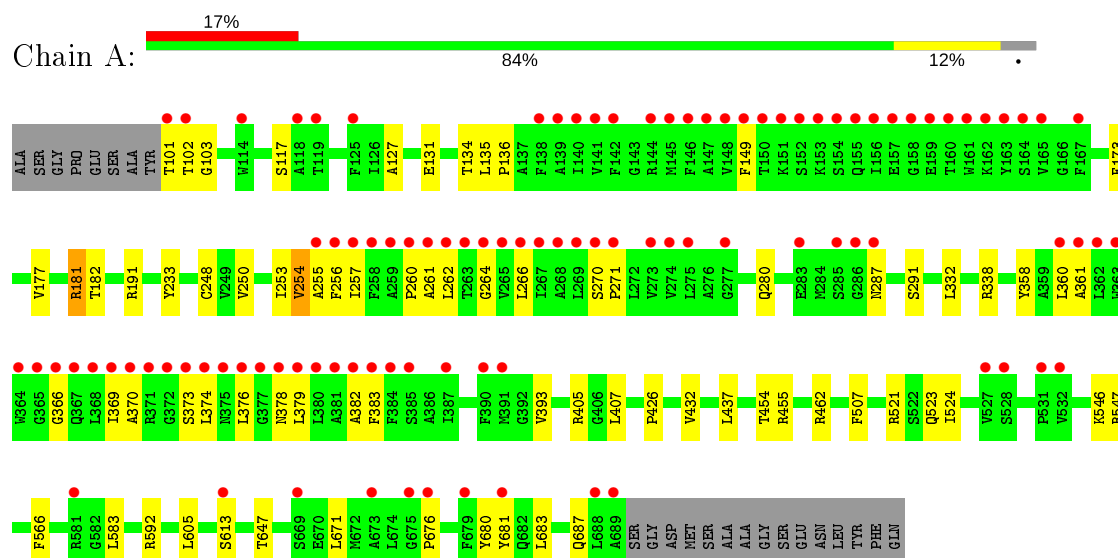
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	435	Total O 435 435	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: ATP-binding cassette, sub-family B, member 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	174.34Å 174.34Å 174.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.62 – 1.90 43.58 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.62-1.90) 99.6 (43.58-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.165 , 0.208 0.174 , 0.213	Depositor DCC
R_{free} test set	3606 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5073	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: MG, ANP, DMU, NO3

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	0.62	1/4630 (0.0%)	0.73	3/6269 (0.0%)

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	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	613	SER	CB-OG	6.27	1.50	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	A	455	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	592	ARG	NE-CZ-NH1	-6.99	116.81	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	181	ARG	Sidechain
1	A	338	ARG	Sidechain
1	A	405	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	462	ARG	Sidechain
1	A	547[A]	ARG	Sidechain

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	4535	0	4608	51	1
2	A	31	0	13	0	0
3	A	1	0	0	0	0
4	A	67	0	82	1	0
5	A	4	0	0	0	0
6	A	435	0	0	1	0
All	All	5073	0	4703	51	1

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.

All (51) 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:253:ILE:HD12	1:A:257:ILE:HD12	1.55	0.88
1:A:253:ILE:CD1	1:A:257:ILE:HD12	2.05	0.87
1:A:266:LEU:HD11	1:A:360:LEU:HG	1.59	0.83
1:A:255:ALA:HB1	1:A:264:GLY:HA3	1.67	0.76
1:A:256:PHE:H	1:A:260:PRO:HB3	1.48	0.76
1:A:253:ILE:CD1	1:A:257:ILE:CD1	2.65	0.75
1:A:253:ILE:HD12	1:A:257:ILE:CD1	2.18	0.74
1:A:266:LEU:HD21	1:A:360:LEU:HD23	1.70	0.74
1:A:437:LEU:O	1:A:523:GLN:HG3	1.91	0.70
1:A:134:THR:HG22	1:A:173:PHE:CD2	2.32	0.64
1:A:426:PRO:HG2	1:A:432:VAL:HG22	1.82	0.62
1:A:262:LEU:HD23	1:A:379:LEU:HD23	1.83	0.59
1:A:369:ILE:HG23	1:A:373:SER:HB2	1.86	0.57
1:A:253:ILE:HD11	1:A:257:ILE:CD1	2.37	0.55
1:A:270:SER:N	1:A:271:PRO:HD3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:THR:HG22	1:A:173:PHE:HD2	1.71	0.54
1:A:127:ALA:O	1:A:131:GLU:HB2	2.11	0.51
1:A:262:LEU:CD2	1:A:379:LEU:HD23	2.41	0.51
1:A:131:GLU:OE1	1:A:181:ARG:NE	2.38	0.51
1:A:262:LEU:HD22	1:A:262:LEU:N	2.26	0.50
1:A:358:TYR:CE1	1:A:383:PHE:CZ	3.00	0.50
1:A:255:ALA:HB1	1:A:264:GLY:CA	2.39	0.49
1:A:134:THR:CG2	1:A:173:PHE:CD2	2.96	0.49
1:A:671:LEU:HD13	1:A:680:TYR:CG	2.48	0.48
1:A:101:THR:HG22	1:A:103:GLY:H	1.80	0.47
1:A:454:THR:HG21	6:A:1201:HOH:O	2.14	0.47
1:A:117:SER:OG	1:A:191:ARG:HD2	2.14	0.47
1:A:250:VAL:HG12	1:A:250:VAL:O	2.14	0.47
1:A:134:THR:HG22	1:A:173:PHE:CE2	2.51	0.46
1:A:256:PHE:N	1:A:260:PRO:HB3	2.25	0.46
1:A:248:CYS:SG	1:A:393:VAL:HG23	2.57	0.45
1:A:524:ILE:HG12	1:A:605:LEU:HD23	1.97	0.45
1:A:254:VAL:HG11	1:A:382:ALA:HB1	1.99	0.45
1:A:671:LEU:HB3	1:A:680:TYR:CD2	2.52	0.45
1:A:134:THR:CG2	1:A:173:PHE:CE2	3.00	0.44
1:A:135:LEU:N	1:A:136:PRO:HD2	2.32	0.44
1:A:378:ASN:HB3	1:A:379:LEU:HD12	1.98	0.44
1:A:102:THR:HB	1:A:407:LEU:HD13	1.99	0.44
1:A:266:LEU:HD13	1:A:361:ALA:HA	1.99	0.44
1:A:583:LEU:O	1:A:583:LEU:HD12	2.18	0.43
1:A:131:GLU:HG3	1:A:177:VAL:HG23	2.01	0.43
1:A:332:LEU:HA	1:A:332:LEU:HD23	1.94	0.42
1:A:676:PRO:HA	1:A:681:TYR:CD1	2.54	0.42
1:A:250:VAL:O	1:A:253:ILE:HG22	2.20	0.42
1:A:101:THR:HG22	1:A:103:GLY:N	2.35	0.42
1:A:683:LEU:HB3	4:A:803:DMU:H18	2.03	0.41
1:A:374:LEU:HD23	1:A:379:LEU:CD1	2.51	0.41
1:A:181:ARG:HG3	1:A:182:THR:N	2.36	0.40
1:A:366:GLY:O	1:A:370:ALA:HB2	2.21	0.40
1:A:261:ALA:HB3	1:A:379:LEU:HG	2.03	0.40
1:A:437:LEU:HD21	1:A:507:PHE:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:TYR:OH	1:A:233:TYR:OH[22_564]	1.86	0.34

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	594/612 (97%)	562 (95%)	30 (5%)	2 (0%)	41 31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	546	LYS
1	A	254	VAL

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	471/480 (98%)	463 (98%)	8 (2%)	60 57

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	PHE
1	A	280	GLN
1	A	287	ASN
1	A	291	SER

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Mol	Chain	Res	Type
1	A	376	LEU
1	A	566	PHE
1	A	647	THR
1	A	687	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	A	624	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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
4	DMU	A	804	-	27,27,34	0.80	1 (3%)	37,38,45	1.62	5 (13%)
2	ANP	A	801	3	29,33,33	1.54	5 (17%)	31,52,52	1.85	6 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMU	A	805	-	7,7,34	0.35	0	6,6,45	0.45	0
5	NO3	A	806	-	1,3,3	1.26	0	0,3,3	0.00	-
4	DMU	A	803	-	34,34,34	0.85	1 (2%)	45,45,45	1.70	9 (20%)

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	DMU	A	803	-	-	2/19/59/59	0/2/2/2
2	ANP	A	801	3	-	1/14/38/38	0/3/3/3
4	DMU	A	804	-	-	6/12/52/59	0/2/2/2
4	DMU	A	805	-	-	0/5/5/59	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	PG-O2G	-3.91	1.46	1.56
2	A	801	ANP	PG-N3B	3.87	1.73	1.63
4	A	804	DMU	O5-C6	2.45	1.48	1.41
2	A	801	ANP	C5-C4	2.44	1.47	1.40
2	A	801	ANP	O4'-C1'	-2.39	1.37	1.41
4	A	803	DMU	C3-C4	2.33	1.59	1.52
2	A	801	ANP	PG-O3G	-2.27	1.50	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ANP	O1G-PG-N3B	-5.71	103.36	111.77
4	A	804	DMU	O5-C6-O16	5.53	123.08	109.97
4	A	803	DMU	O5-C6-O16	4.25	120.04	109.97
2	A	801	ANP	O3G-PG-O2G	4.09	118.53	107.64
4	A	803	DMU	O3-C5-C10	3.77	119.19	110.05
4	A	803	DMU	O5-C6-C1	3.65	118.07	110.35
4	A	803	DMU	O7-C10-C5	-3.27	99.63	108.10
4	A	803	DMU	C10-C5-C7	3.20	116.66	110.00
4	A	803	DMU	O3-C5-C7	3.07	117.45	110.35
4	A	804	DMU	O3-C5-C7	3.00	117.28	110.35
2	A	801	ANP	O2B-PB-O1B	2.99	116.18	109.92
4	A	804	DMU	O5-C6-C1	2.95	116.59	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	DMU	O1-C10-C5	2.82	116.32	110.35
4	A	803	DMU	C6-O5-C4	2.80	119.19	113.69
4	A	804	DMU	C6-O5-C4	-2.77	108.26	113.69
2	A	801	ANP	O3A-PB-N3B	-2.61	99.35	106.59
2	A	801	ANP	N3-C2-N1	-2.39	124.94	128.68
2	A	801	ANP	C4-C5-N7	-2.14	107.17	109.40
4	A	804	DMU	C18-O16-C6	2.10	117.32	113.84
4	A	803	DMU	O49-C1-C6	2.07	115.08	110.05

There are no chirality outliers.

All (9) torsion outliers are listed below:

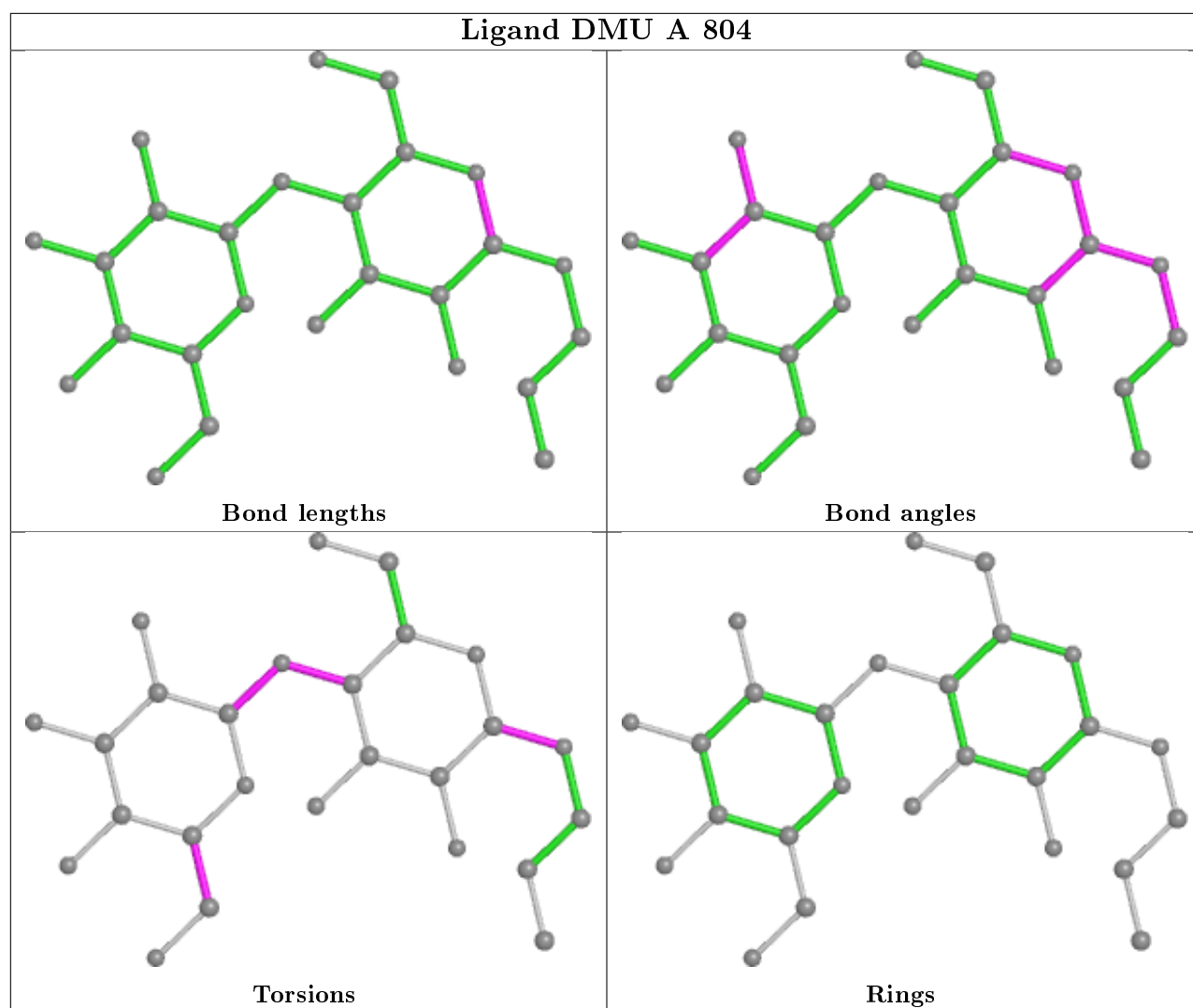
Mol	Chain	Res	Type	Atoms
4	A	804	DMU	O5-C6-O16-C18
2	A	801	ANP	PG-N3B-PB-O1B
4	A	803	DMU	O6-C11-C9-O1
4	A	804	DMU	O6-C11-C9-O1
4	A	803	DMU	O6-C11-C9-C8
4	A	804	DMU	O6-C11-C9-C8
4	A	804	DMU	C4-C3-O7-C10
4	A	804	DMU	C2-C3-O7-C10
4	A	804	DMU	O1-C10-O7-C3

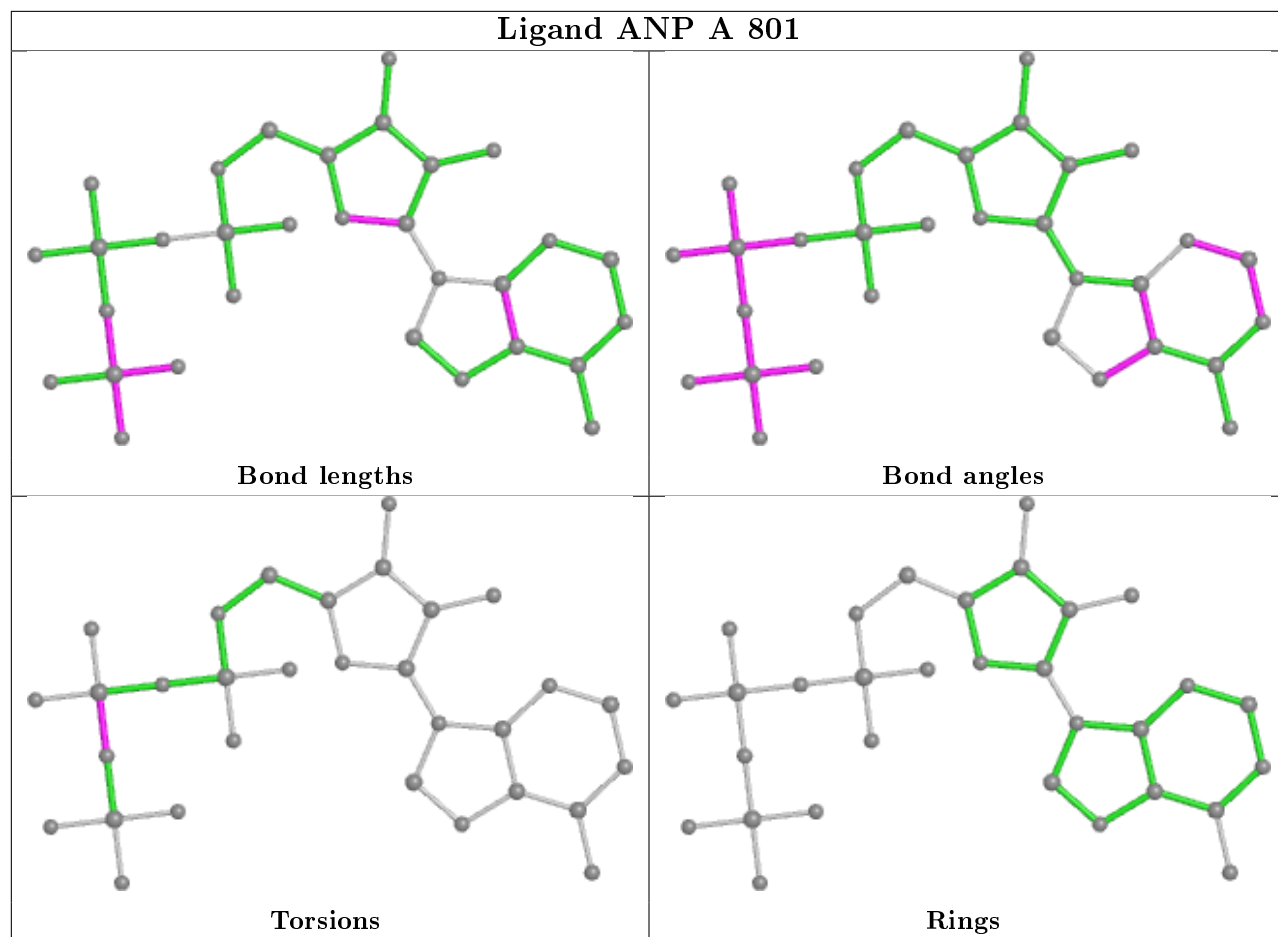
There are no ring outliers.

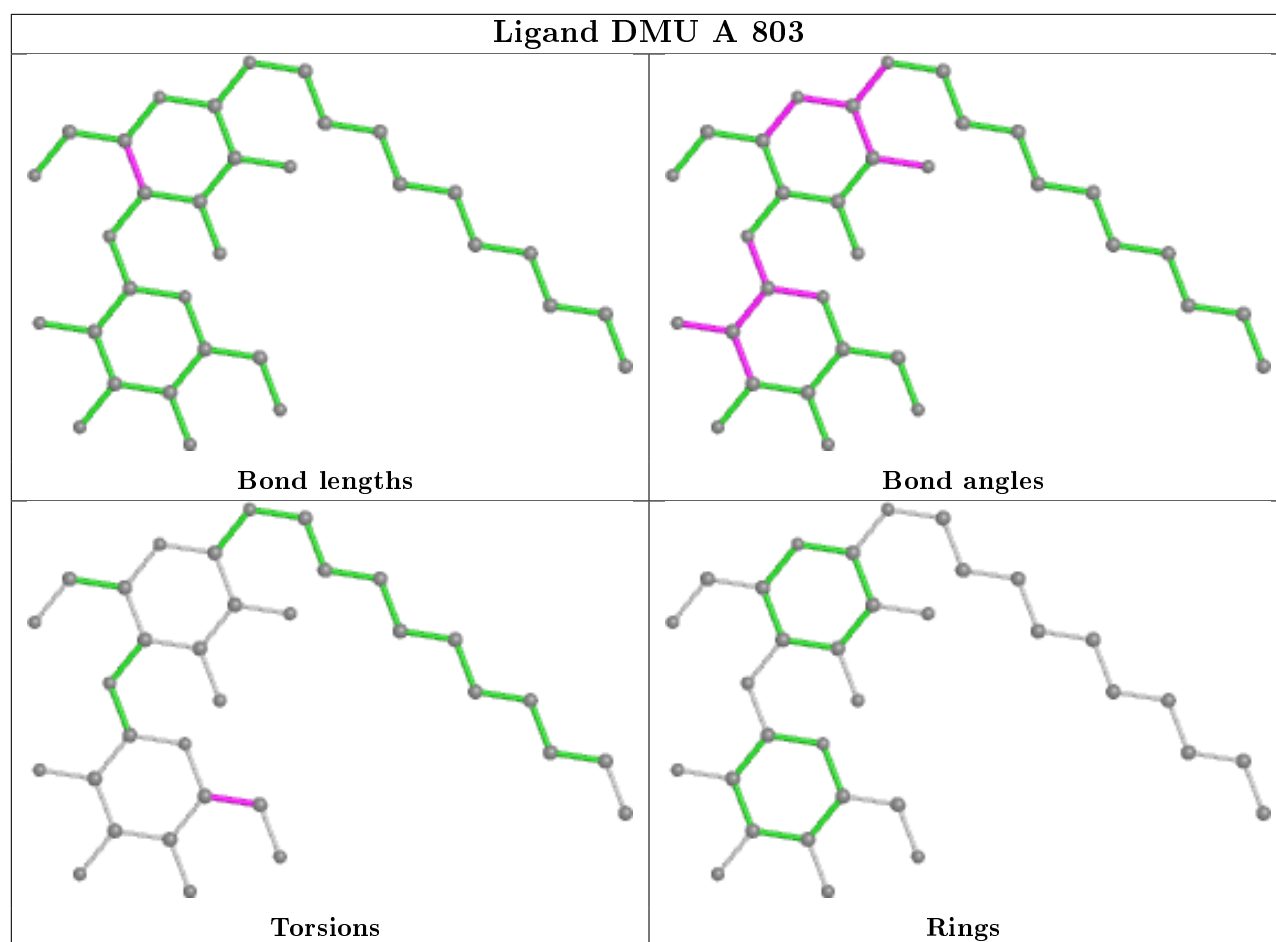
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	DMU	1	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, 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	589/612 (96%)	1.45	102 (17%) 1 1	21, 42, 183, 243	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	374	LEU	39.4
1	A	259	ALA	28.8
1	A	372	GLY	26.8
1	A	261	ALA	22.6
1	A	383	PHE	22.2
1	A	380	LEU	19.6
1	A	257	ILE	18.1
1	A	376	LEU	18.0
1	A	258	PHE	17.8
1	A	379	LEU	17.3
1	A	364	TRP	16.0
1	A	260	PRO	15.9
1	A	154	SER	15.8
1	A	378	ASN	15.7
1	A	366	GLY	15.4
1	A	368	LEU	14.8
1	A	262	LEU	13.9
1	A	371	ARG	13.6
1	A	377	GLY	13.3
1	A	147	ALA	12.5
1	A	256	PHE	12.1
1	A	148	VAL	12.1
1	A	375	ASN	11.9
1	A	161	TRP	11.8
1	A	370	ALA	11.6
1	A	265	VAL	11.3
1	A	363	TRP	11.0

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Mol	Chain	Res	Type	RSRZ
1	A	153	LYS	10.9
1	A	373	SER	10.9
1	A	149	PHE	10.9
1	A	155	GLN	9.9
1	A	268	ALA	9.9
1	A	269	LEU	9.3
1	A	274	VAL	9.2
1	A	150	THR	8.5
1	A	163	TYR	8.4
1	A	158	GLY	8.2
1	A	369	ILE	8.2
1	A	160	THR	8.1
1	A	387	ILE	8.1
1	A	367	GLN	7.9
1	A	156	ILE	7.9
1	A	381	ALA	7.8
1	A	145	MET	7.4
1	A	138	PHE	7.1
1	A	152	SER	6.9
1	A	151	LYS	6.8
1	A	162	LYS	6.7
1	A	157	GLU	6.7
1	A	263	THR	6.6
1	A	365	GLY	6.6
1	A	360	LEU	6.5
1	A	266	LEU	5.7
1	A	146	PHE	5.7
1	A	390	PHE	5.7
1	A	275	LEU	5.6
1	A	159	GLU	5.3
1	A	382	ALA	5.2
1	A	270	SER	5.2
1	A	384	PHE	5.1
1	A	264	GLY	4.6
1	A	142	PHE	4.5
1	A	675	GLY	4.1
1	A	286	GLY	4.0
1	A	144	ARG	3.8
1	A	673	ALA	3.7
1	A	273	VAL	3.7
1	A	362	LEU	3.6
1	A	141	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	676	PRO	3.5
1	A	167	PHE	3.4
1	A	255	ALA	3.3
1	A	681	TYR	3.3
1	A	669	SER	3.2
1	A	532	VAL	3.2
1	A	165	VAL	3.2
1	A	391	MET	3.0
1	A	688	LEU	2.9
1	A	101	THR	2.8
1	A	102	THR	2.7
1	A	139	ALA	2.7
1	A	271	PRO	2.6
1	A	140	ILE	2.6
1	A	114	TRP	2.6
1	A	277	GLY	2.5
1	A	285	SER	2.5
1	A	531	PRO	2.4
1	A	287	ASN	2.4
1	A	689	ALA	2.4
1	A	164	SER	2.3
1	A	385	SER	2.3
1	A	125	PHE	2.3
1	A	119	THR	2.3
1	A	527	VAL	2.2
1	A	267	ILE	2.2
1	A	361	ALA	2.2
1	A	581	ARG	2.1
1	A	528	SER	2.1
1	A	118	ALA	2.1
1	A	679	PHE	2.1
1	A	283	GLU	2.1
1	A	613	SER	2.0

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

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

6.3 Carbohydrates ⓘ

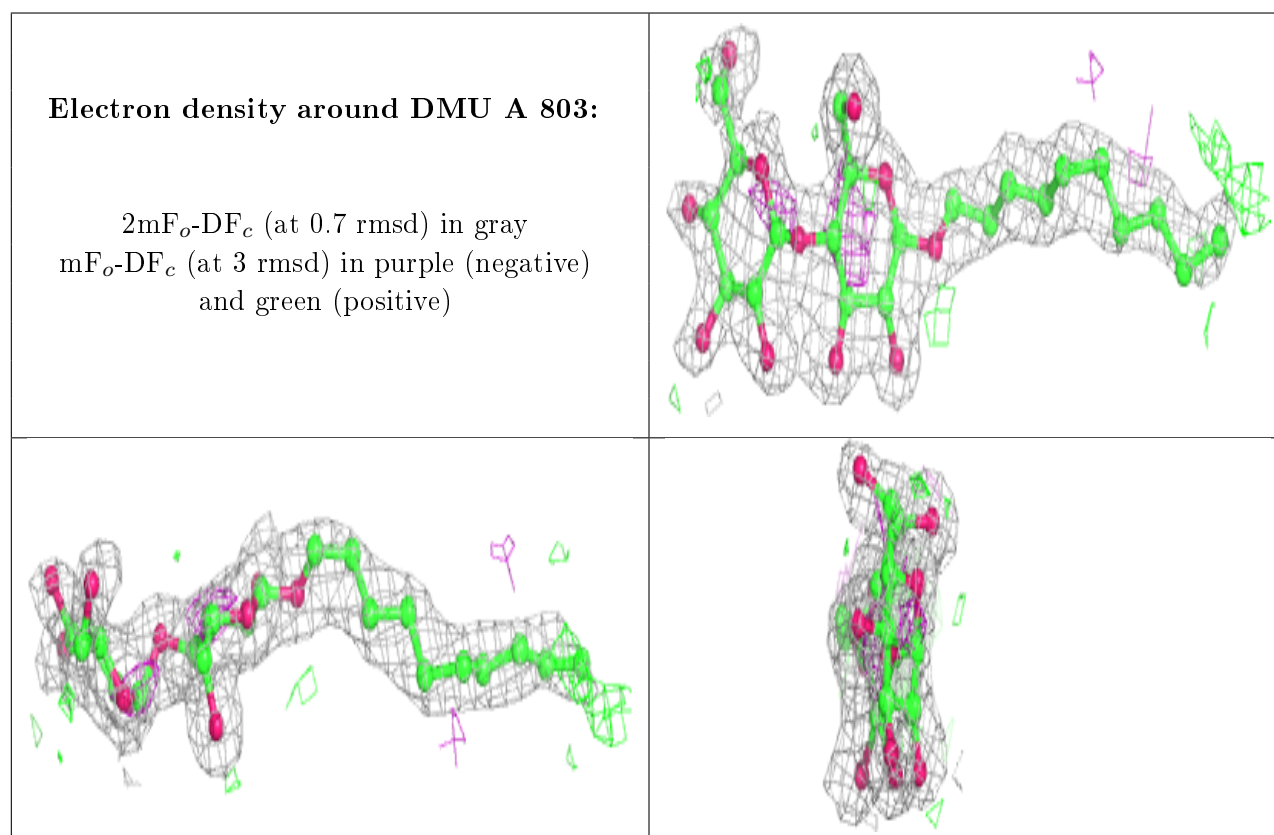
There are no carbohydrates in this entry.

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, 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.

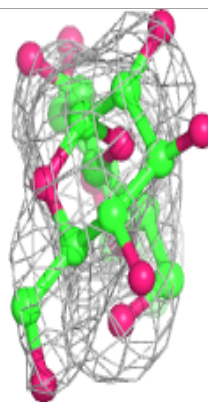
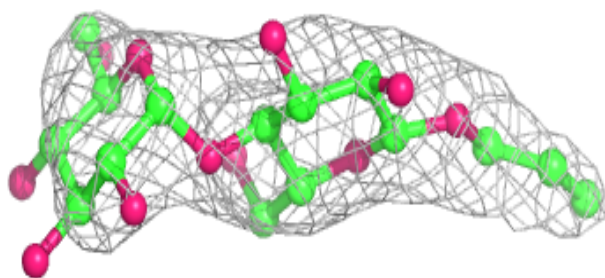
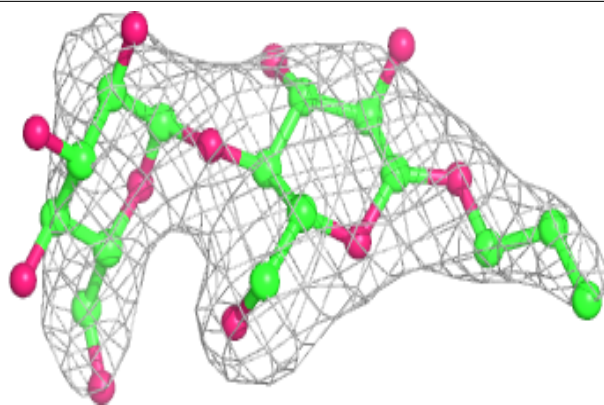
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DMU	A	805	8/33	0.85	0.15	66,72,77,79	0
4	DMU	A	803	33/33	0.88	0.17	29,48,68,72	0
4	DMU	A	804	26/33	0.91	0.31	65,88,102,104	0
5	NO3	A	806	4/4	0.98	0.10	29,29,32,33	0
3	MG	A	802	1/1	0.98	0.10	22,22,22,22	0
2	ANP	A	801	31/31	0.99	0.12	19,23,25,27	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.

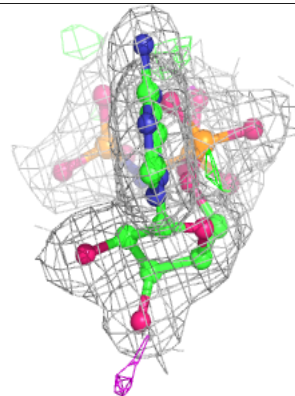
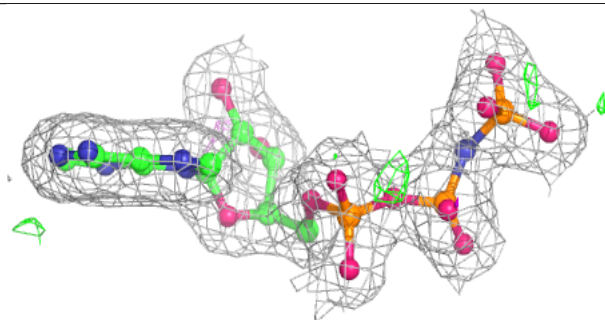
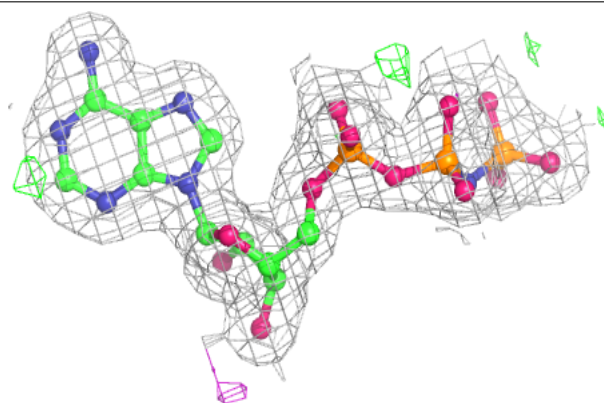


Electron density around DMU A 804:

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

**Electron density around ANP 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.