



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:15 PM EDT

PDB ID : 6A6M / pdb_00006a6m
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 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

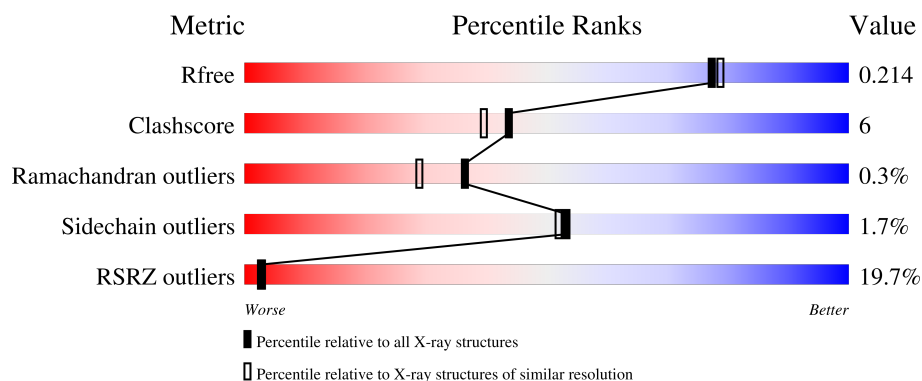
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	612	19% 83% 13% ••

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 (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

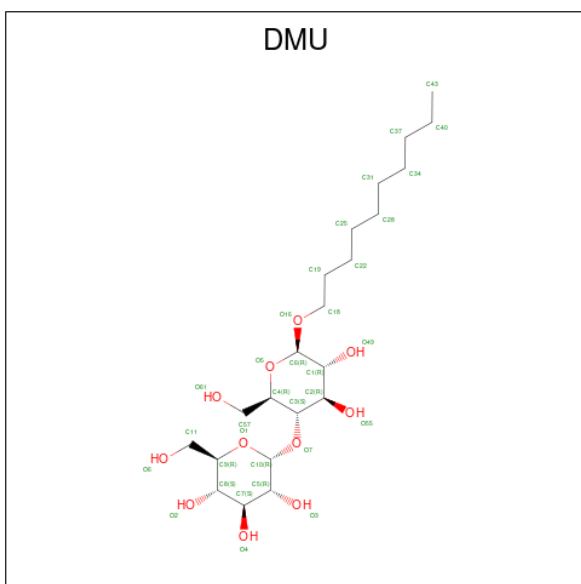


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

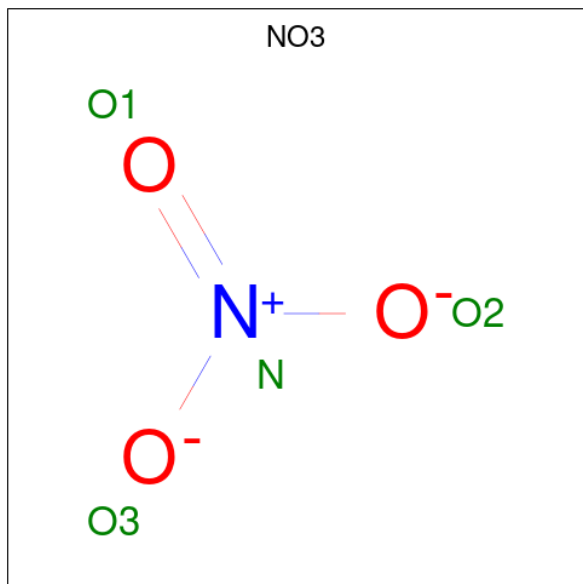
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: 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 (CCD ID: NO3) (formula: NO₃).



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

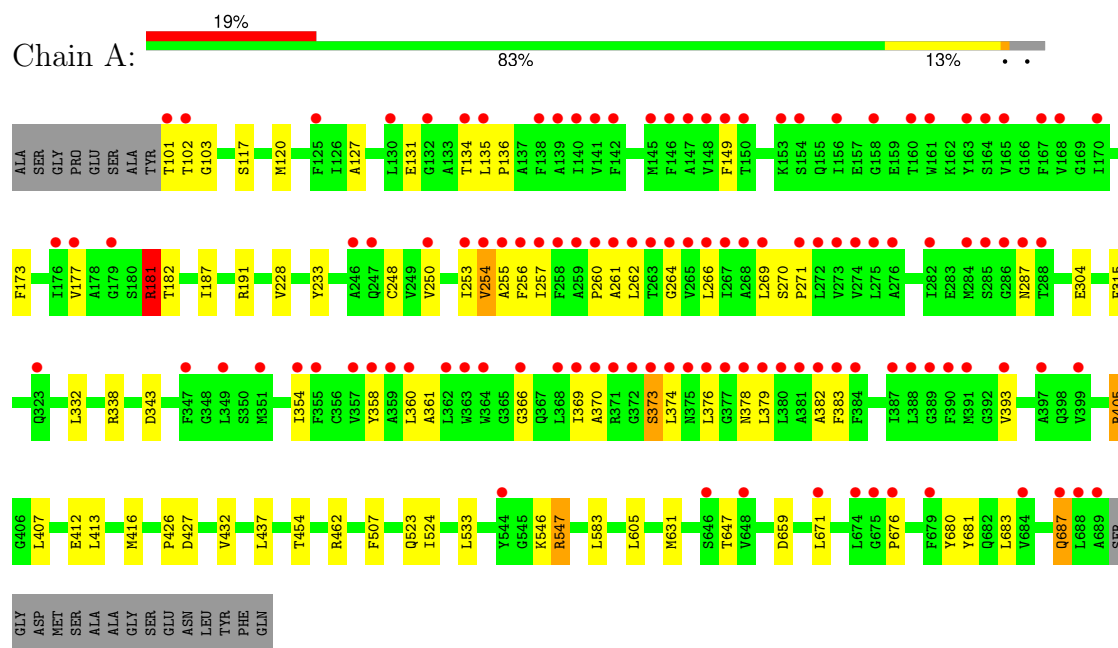
- Molecule 6 is water.

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

3 Residue-property plots

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: 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 43.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (43.62-1.90) 99.6 (43.62-1.90)	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 , 0.214	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 , 52.8	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, NO3, DMU

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	0.92	4/4630 (0.1%)	1.05	6/6269 (0.1%)

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	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	533	LEU	C-O	-5.73	1.16	1.23
1	A	228	VAL	N-CA	-5.50	1.39	1.46
1	A	304	GLU	C-O	-5.34	1.18	1.24
1	A	631	MET	N-CA	-5.33	1.40	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	SER	N-CA-C	6.73	118.41	111.14
1	A	427	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	659	ASP	CA-C-N	5.66	131.75	120.77
1	A	659	ASP	C-N-CA	5.66	131.75	120.77
1	A	687	GLN	CB-CG-CD	5.54	122.02	112.60
1	A	315	PHE	CA-CB-CG	-5.00	108.80	113.80

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
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	57	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	57	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 6.

All (57) 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:413:LEU:HA	1:A:416:MET:HE3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:134:THR:HG22	1:A:173:PHE:HD2	1.71	0.54
1:A:412:GLU:HG2	1:A:416:MET:HE2	1.90	0.53
1:A:120:MET:HE1	1:A:187:ILE:HG21	1.91	0.53
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: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:454:THR:HG21	6:A:1201:HOH: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:102:THR:HB	1:A:407:LEU:HD13	1.99	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:266:LEU:HD13	1:A:361:ALA:HA	1.99	0.44
1:A:583:LEU:HD12	1:A:583:LEU:O	2.18	0.43
1:A:131:GLU:HG3	1:A:177:VAL:HG23	2.01	0.43
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.94	0.42
1:A:676:PRO:HA	1:A:681:TYR:CD1	2.54	0.42
1:A:269:LEU:C	1:A:271:PRO:HD3	2.45	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:261:ALA:C	1:A:262:LEU:HD22	2.45	0.41
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:343:ASP:CG	1:A:405:ARG:HH22	2.30	0.40
1:A:181:ARG:HG3	1:A:182:THR:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	29

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%)	462 (98%)	9 (2%)	50 47

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	PHE
1	A	181	ARG
1	A	287	ASN
1	A	354	ILE
1	A	376	LEU
1	A	547[A]	ARG
1	A	547[B]	ARG
1	A	647	THR
1	A	687	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	GLN
1	A	395	GLN
1	A	624	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.79	1 (3%)	38,38,45	1.61	5 (13%)
5	NO3	A	806	-	1,3,3	1.24	0	0,3,3	-	-
4	DMU	A	803	-	34,34,34	0.84	1 (2%)	45,45,45	1.72	9 (20%)
2	ANP	A	801	3	33,33,33	1.76	7 (21%)	45,52,52	1.99	11 (24%)
4	DMU	A	805	-	7,7,34	0.36	0	6,6,45	0.46	0

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	804	-	-	7/12/52/59	0/2/2/2
4	DMU	A	805	-	-	0/5/5/59	-
4	DMU	A	803	-	-	2/19/59/59	0/2/2/2
2	ANP	A	801	3	-	1/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	ANP	C5-C4	4.65	1.47	1.39
2	A	801	ANP	PG-O2G	-3.98	1.46	1.56
2	A	801	ANP	PG-N3B	3.87	1.73	1.63
2	A	801	ANP	C4-N9	-3.05	1.31	1.37
2	A	801	ANP	C5-N7	-2.76	1.34	1.39
4	A	804	DMU	O5-C6	2.43	1.48	1.41
2	A	801	ANP	PG-O3G	-2.32	1.50	1.56
4	A	803	DMU	C3-C4	2.28	1.59	1.52
2	A	801	ANP	PA-O3A	-2.22	1.57	1.59

All (25) 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	5.51	123.08	110.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	ANP	C5-C4-N3	-4.52	120.49	126.72
4	A	803	DMU	O5-C6-O16	4.23	120.04	110.04
2	A	801	ANP	N3-C4-N9	4.11	134.16	127.17
2	A	801	ANP	O2G-PG-O3G	4.07	118.53	107.59
4	A	803	DMU	O3-C5-C10	3.83	119.19	110.08
4	A	803	DMU	O5-C6-C1	3.75	118.07	110.37
4	A	803	DMU	O7-C10-C5	-3.44	99.63	108.09
2	A	801	ANP	C4-N9-C8	3.20	109.09	105.74
4	A	803	DMU	C10-C5-C7	3.16	116.66	110.01
4	A	804	DMU	O5-C6-C1	3.03	116.59	110.37
4	A	803	DMU	O3-C5-C7	3.00	117.45	110.38
2	A	801	ANP	C4-C5-N7	-2.99	107.17	110.58
2	A	801	ANP	O2B-PB-O1B	2.94	116.18	109.87
4	A	804	DMU	O3-C5-C7	2.93	117.28	110.38
4	A	803	DMU	O1-C10-C5	2.89	116.32	110.37
4	A	803	DMU	C6-O5-C4	2.80	119.19	113.72
4	A	804	DMU	C6-O5-C4	-2.80	108.26	113.72
2	A	801	ANP	O3A-PB-N3B	-2.61	99.35	106.59
2	A	801	ANP	C2-N3-C4	2.47	117.88	111.83
2	A	801	ANP	C5-N7-C8	2.42	107.25	103.45
2	A	801	ANP	N3-C2-N1	-2.40	124.94	128.58
4	A	804	DMU	C18-O16-C6	2.13	117.32	113.68
4	A	803	DMU	O49-C1-C6	2.10	115.08	110.08

There are no chirality outliers.

All (10) torsion outliers are listed below:

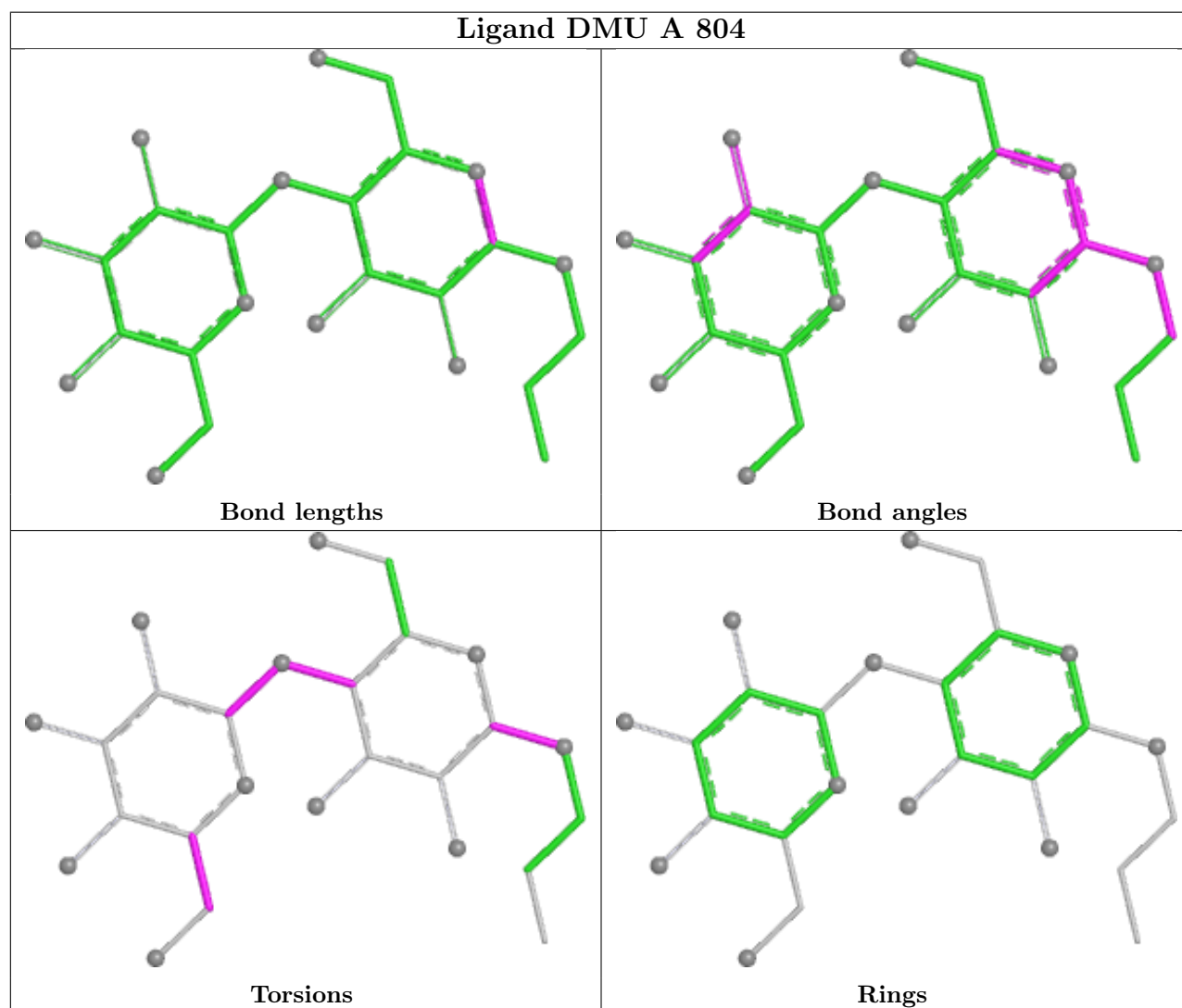
Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PG-N3B-PB-O1B
4	A	804	DMU	O5-C6-O16-C18
4	A	803	DMU	O6-C11-C9-O1
4	A	803	DMU	O6-C11-C9-C8
4	A	804	DMU	O6-C11-C9-O1
4	A	804	DMU	O6-C11-C9-C8
4	A	804	DMU	C4-C3-O7-C10
4	A	804	DMU	C2-C3-O7-C10
4	A	804	DMU	O1-C10-O7-C3
4	A	804	DMU	C5-C10-O7-C3

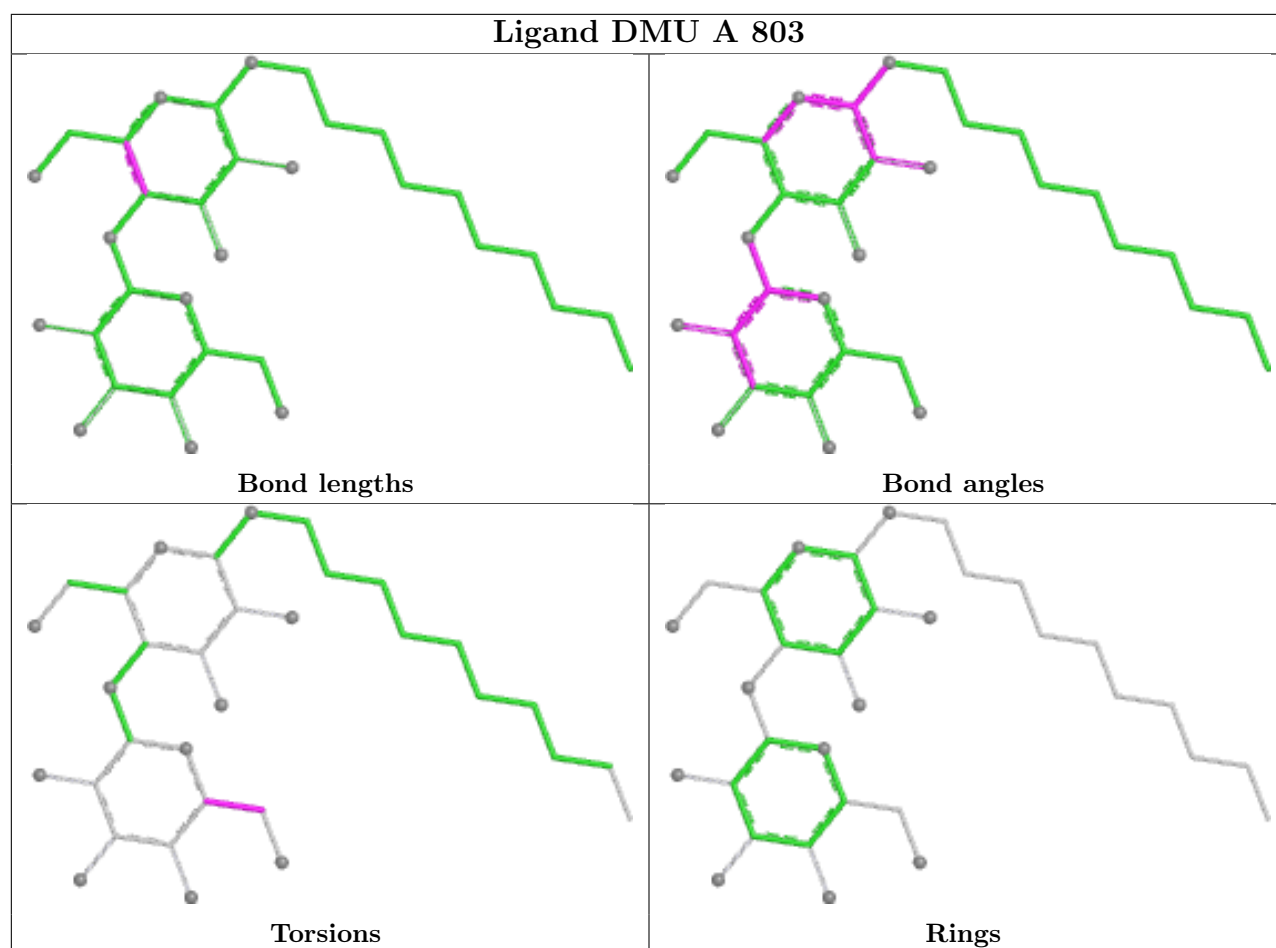
There are no ring outliers.

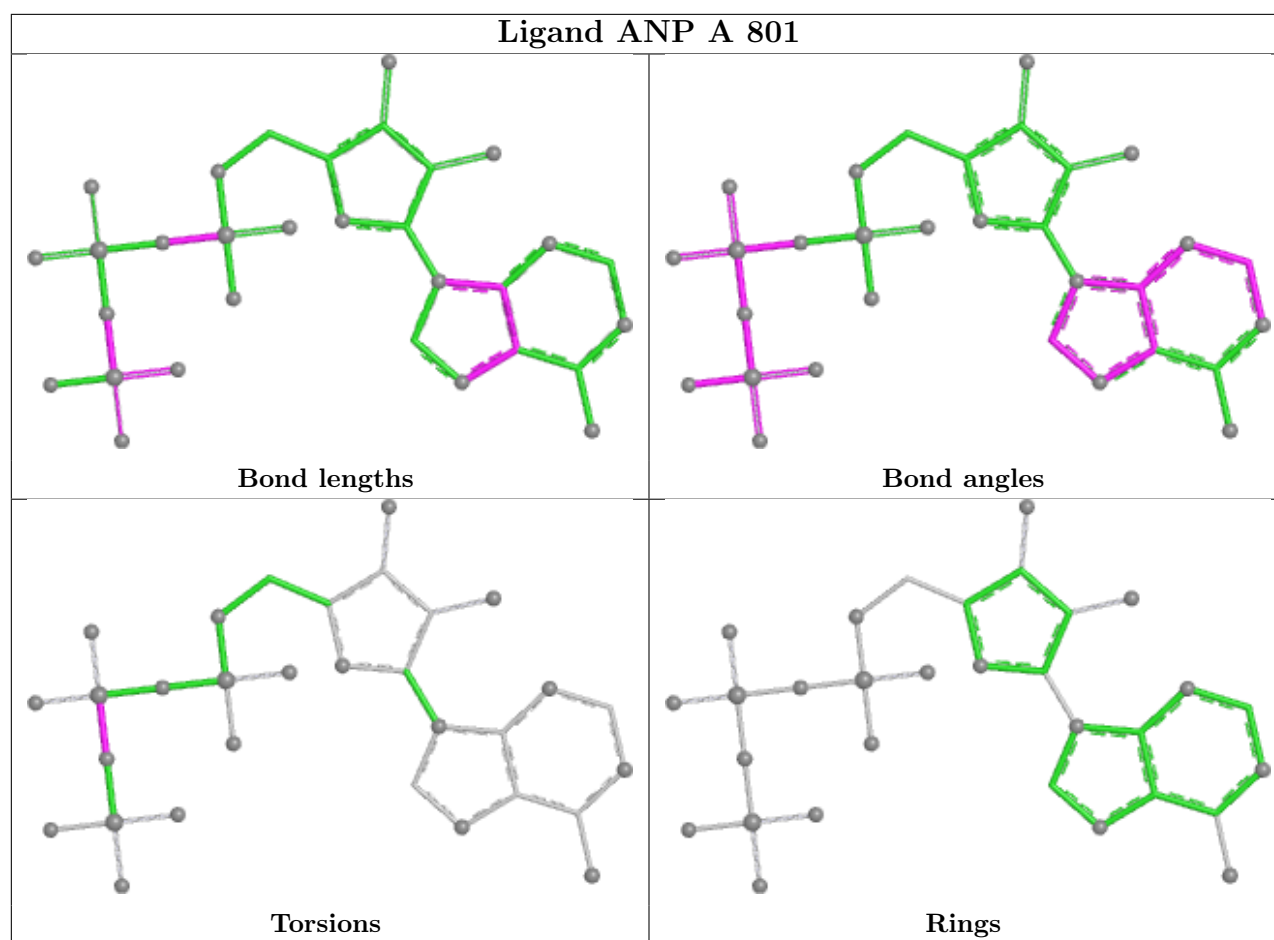
1 monomer is involved in 1 short contact:

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%)	0.77	116 (19%) 3 3	18, 42, 183, 243	7 (1%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	LEU	10.9
1	A	374	LEU	8.8
1	A	259	ALA	8.4
1	A	265	VAL	7.0
1	A	387	ILE	6.8
1	A	258	PHE	6.6
1	A	383	PHE	6.5
1	A	379	LEU	6.1
1	A	138	PHE	6.0
1	A	161	TRP	5.9
1	A	163	TYR	5.8
1	A	376	LEU	5.6
1	A	274	VAL	5.2
1	A	148	VAL	5.2
1	A	149	PHE	5.0
1	A	261	ALA	4.9
1	A	366	GLY	4.9
1	A	267	ILE	4.8
1	A	262	LEU	4.8
1	A	364	TRP	4.6
1	A	260	PRO	4.6
1	A	390	PHE	4.6
1	A	372	GLY	4.6
1	A	254	VAL	4.3
1	A	369	ILE	4.3
1	A	377	GLY	4.3
1	A	675	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	263	THR	4.3
1	A	264	GLY	4.3
1	A	256	PHE	4.2
1	A	273	VAL	4.2
1	A	275	LEU	4.1
1	A	373	SER	4.0
1	A	378	ASN	3.9
1	A	362	LEU	3.9
1	A	363	TRP	3.8
1	A	145	MET	3.8
1	A	272	LEU	3.7
1	A	370	ALA	3.7
1	A	391	MET	3.6
1	A	268	ALA	3.6
1	A	689	ALA	3.6
1	A	168	VAL	3.6
1	A	357	VAL	3.6
1	A	359	ALA	3.5
1	A	288	THR	3.5
1	A	101	THR	3.5
1	A	688	LEU	3.5
1	A	257	ILE	3.4
1	A	388	LEU	3.4
1	A	156	ILE	3.4
1	A	154	SER	3.3
1	A	253	ILE	3.2
1	A	397	ALA	3.2
1	A	375	ASN	3.2
1	A	646	SER	3.2
1	A	160	THR	3.2
1	A	368	LEU	3.2
1	A	347	PHE	3.2
1	A	360	LEU	3.1
1	A	102	THR	3.1
1	A	147	ALA	3.1
1	A	687	GLN	3.0
1	A	389	GLY	3.0
1	A	150	THR	2.9
1	A	146	PHE	2.9
1	A	371	ARG	2.9
1	A	266	LEU	2.9
1	A	384	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	LEU	2.8
1	A	135	LEU	2.8
1	A	141	VAL	2.8
1	A	158	GLY	2.8
1	A	354	ILE	2.8
1	A	679	PHE	2.7
1	A	286	GLY	2.7
1	A	142	PHE	2.7
1	A	176	ILE	2.7
1	A	250	VAL	2.7
1	A	382	ALA	2.6
1	A	323	GLN	2.6
1	A	167	PHE	2.6
1	A	284	MET	2.6
1	A	132	GLY	2.6
1	A	674	LEU	2.5
1	A	381	ALA	2.5
1	A	648	VAL	2.5
1	A	170	ILE	2.5
1	A	358	TYR	2.4
1	A	271	PRO	2.4
1	A	676	PRO	2.4
1	A	276	ALA	2.4
1	A	269	LEU	2.3
1	A	671	LEU	2.3
1	A	351	MET	2.3
1	A	164	SER	2.2
1	A	287	ASN	2.2
1	A	125	PHE	2.2
1	A	393	VAL	2.2
1	A	134	THR	2.2
1	A	139	ALA	2.2
1	A	246	ALA	2.2
1	A	349	LEU	2.1
1	A	153	LYS	2.1
1	A	247	GLN	2.1
1	A	282	ILE	2.1
1	A	684	VAL	2.1
1	A	140	ILE	2.1
1	A	285	SER	2.1
1	A	165	VAL	2.1
1	A	399	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	177	VAL	2.0
1	A	255	ALA	2.0
1	A	355	PHE	2.0
1	A	179	GLY	2.0
1	A	544	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

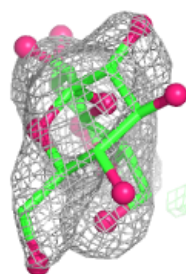
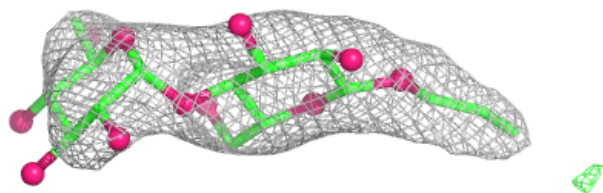
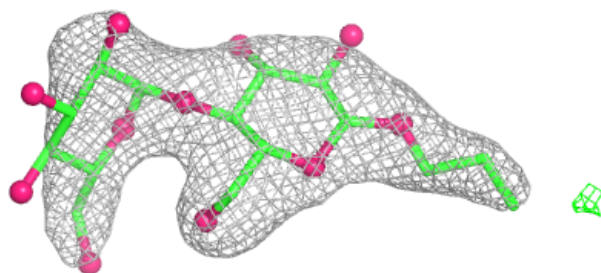
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	DMU	A	804	26/33	0.84	0.12	65,88,102,104	0
4	DMU	A	803	33/33	0.89	0.13	29,48,68,72	0
4	DMU	A	805	8/33	0.89	0.23	66,72,77,79	0
5	NO3	A	806	4/4	0.97	0.08	29,29,32,33	0
3	MG	A	802	1/1	0.98	0.03	22,22,22,22	0
2	ANP	A	801	31/31	0.99	0.03	19,23,25,27	0

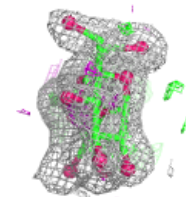
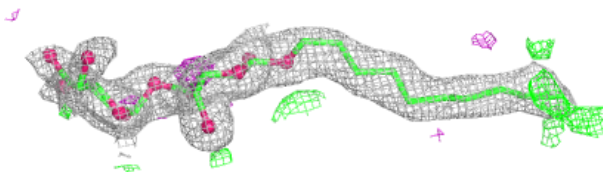
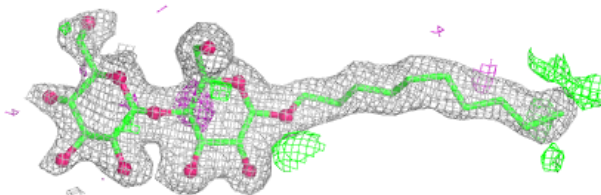
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

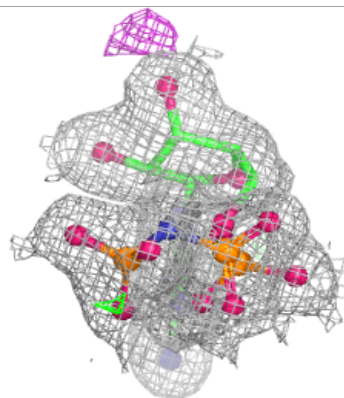
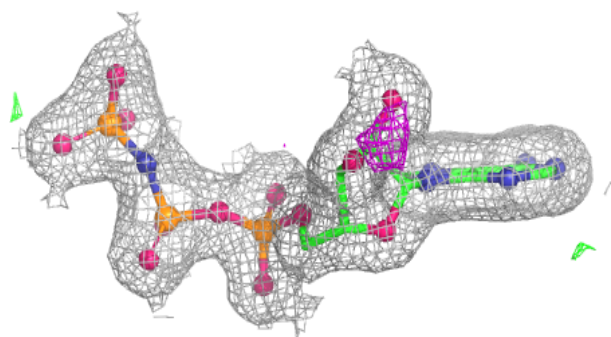
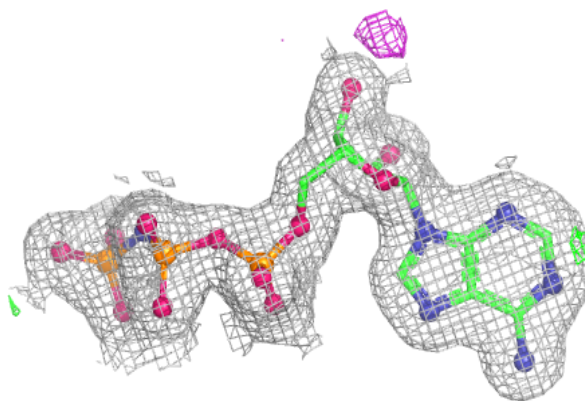
**Electron density around DMU A 803:**

$2mF_o-DF_c$ (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.