



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:22 PM UTC

PDB ID : 7DQV / pdb_00007dqv
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

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

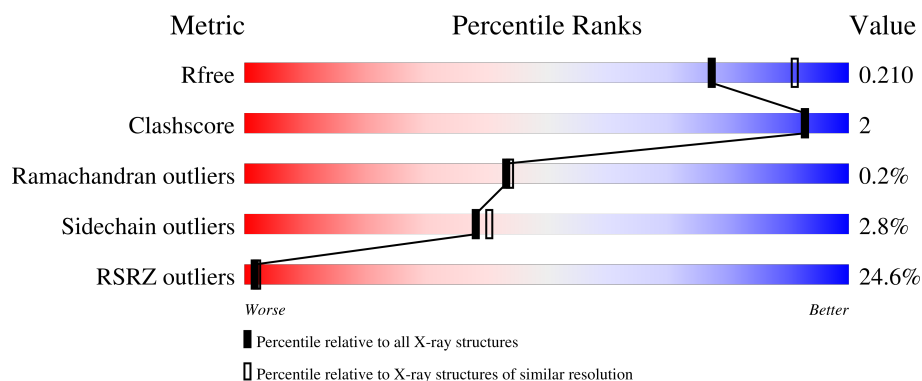
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 ≥ 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	23% 90% 5% 5%

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:

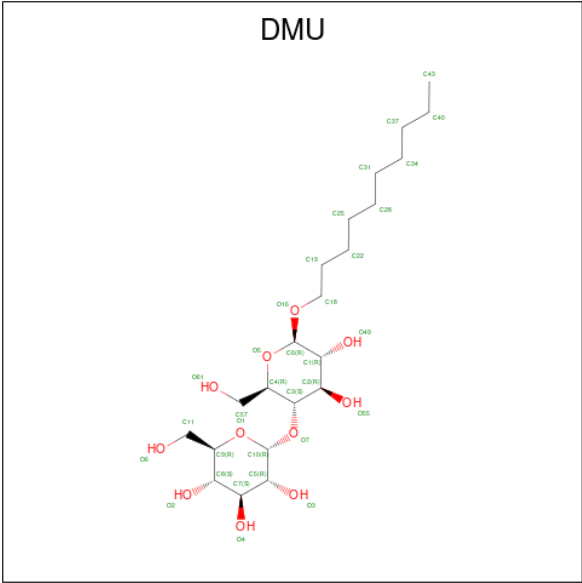
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	VAL	GLY	engineered mutation	UNP M1VAN7
A	697	GLY	-	expression tag	UNP M1VAN7
A	698	ARG	-	expression tag	UNP M1VAN7
A	699	ASP	-	expression tag	UNP M1VAN7
A	700	TYR	-	expression tag	UNP M1VAN7
A	701	LYS	-	expression tag	UNP M1VAN7
A	702	ASP	-	expression 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 (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



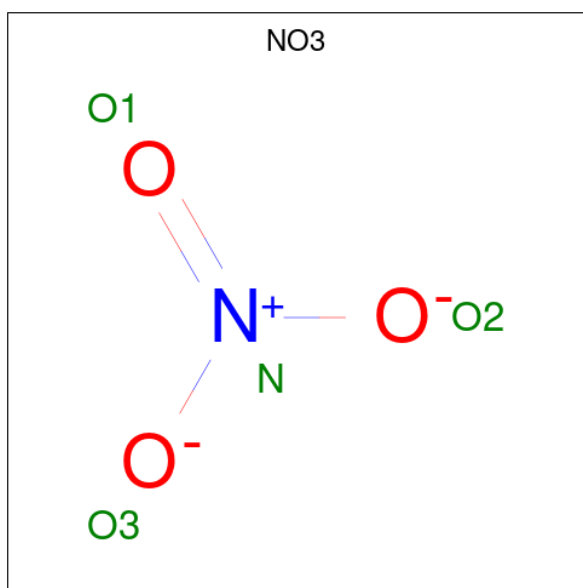
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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



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

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: 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		

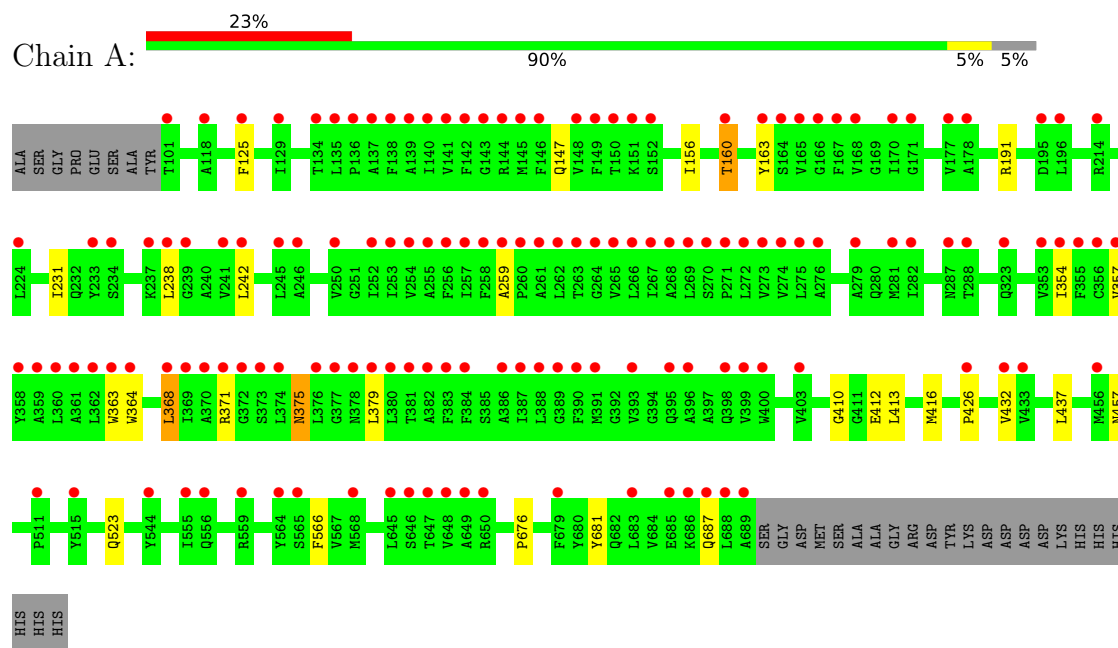
- Molecule 6 is water.

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, α , β , γ	175.67Å 175.67Å 175.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.15 48.70 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.70-2.15) 99.8 (48.70-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.185 , 0.210 0.185 , 0.210	Depositor DCC
R_{free} test set	2534 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: NO3, MG, 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	0.33	0/4580	0.45	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	13	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	14	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 2.

All (14) 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:413:LEU:HA	1:A:416:MET:HE3	1.87	0.57
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:412:GLU:HG2	1:A:416:MET:HE2	1.98	0.44
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%)	43	44

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%)	454 (97%)	13 (3%)	38	40

All (13) 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	191	ARG
1	A	354	ILE
1	A	357	VAL
1	A	363	TRP
1	A	364	TRP
1	A	368	LEU
1	A	375	ASN
1	A	457	ASN
1	A	566	PHE
1	A	687	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
1	A	280	GLN
1	A	470	ASN
1	A	518	HIS

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 [i](#)

There are no oligosaccharides 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	1.53	5 (14%)	45,45,45	1.03	2 (4%)
4	NO3	A	804	-	1,3,3	0.24	0	0,3,3	-	-
2	ANP	A	801	5	33,33,33	0.78	1 (3%)	45,52,52	1.00	5 (11%)
3	DMU	A	803	-	34,34,34	1.49	6 (17%)	45,45,45	1.14	3 (6%)

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
2	ANP	A	801	5	-	1/18/38/38	0/3/3/3
3	DMU	A	803	-	-	12/19/59/59	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	DMU	O1-C9	4.76	1.56	1.44
3	A	803	DMU	O1-C9	4.23	1.54	1.44
3	A	803	DMU	C11-C9	-3.34	1.40	1.51
2	A	801	ANP	PG-N3B	3.09	1.71	1.63
3	A	802	DMU	C11-C9	-3.08	1.41	1.51
3	A	802	DMU	O5-C6	2.79	1.49	1.41
3	A	802	DMU	O4-C7	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	DMU	O4-C7	2.41	1.48	1.43
3	A	803	DMU	O5-C6	2.41	1.48	1.41
3	A	802	DMU	C8-C9	2.32	1.58	1.53
3	A	803	DMU	C7-C5	-2.22	1.46	1.52
3	A	803	DMU	O1-C10	2.05	1.47	1.41

All (10) 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	-3.04	110.76	117.98
3	A	803	DMU	C1-C2-C3	2.59	115.56	109.68
3	A	803	DMU	C10-O7-C3	-2.42	112.25	117.98
2	A	801	ANP	O1B-PB-N3B	-2.25	108.46	111.77
2	A	801	ANP	O2A-PA-O3A	2.23	113.30	107.27
2	A	801	ANP	O2B-PB-O3A	2.22	112.06	104.64
3	A	803	DMU	C6-C1-C2	2.08	114.38	110.01
3	A	802	DMU	O49-C1-C6	-2.04	105.21	110.08
2	A	801	ANP	O3A-PB-N3B	-2.04	100.94	106.59

There are no chirality outliers.

All (16) torsion outliers are listed below:

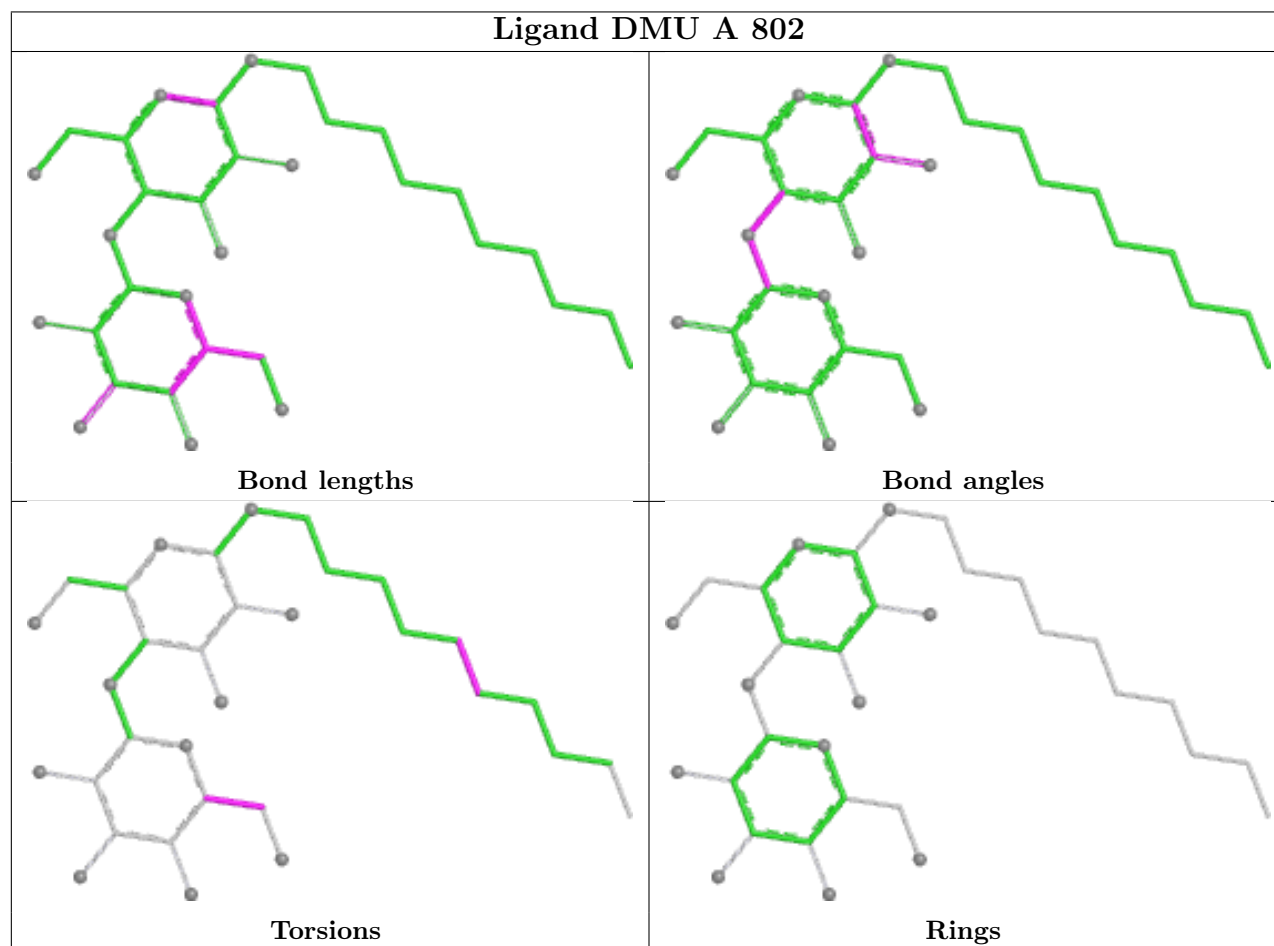
Mol	Chain	Res	Type	Atoms
2	A	801	ANP	PG-N3B-PB-O1B
3	A	802	DMU	O6-C11-C9-O1
3	A	802	DMU	O6-C11-C9-C8
3	A	803	DMU	O6-C11-C9-O1
3	A	803	DMU	C3-C4-C57-O61
3	A	803	DMU	O5-C4-C57-O61
3	A	803	DMU	C25-C28-C31-C34
3	A	803	DMU	C31-C34-C37-C40
3	A	803	DMU	O1-C10-O7-C3
3	A	803	DMU	O6-C11-C9-C8
3	A	802	DMU	C25-C28-C31-C34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

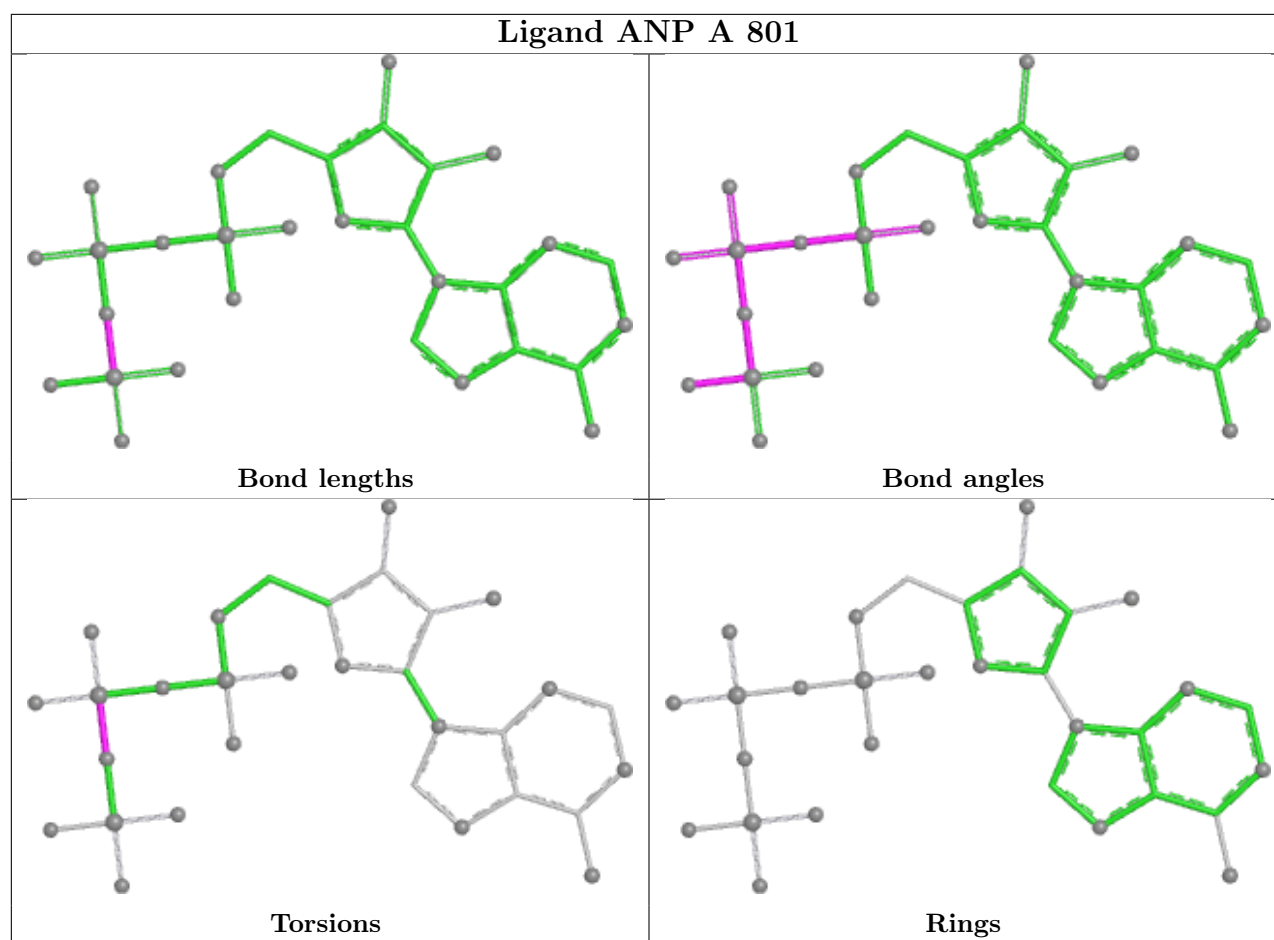
There are no ring outliers.

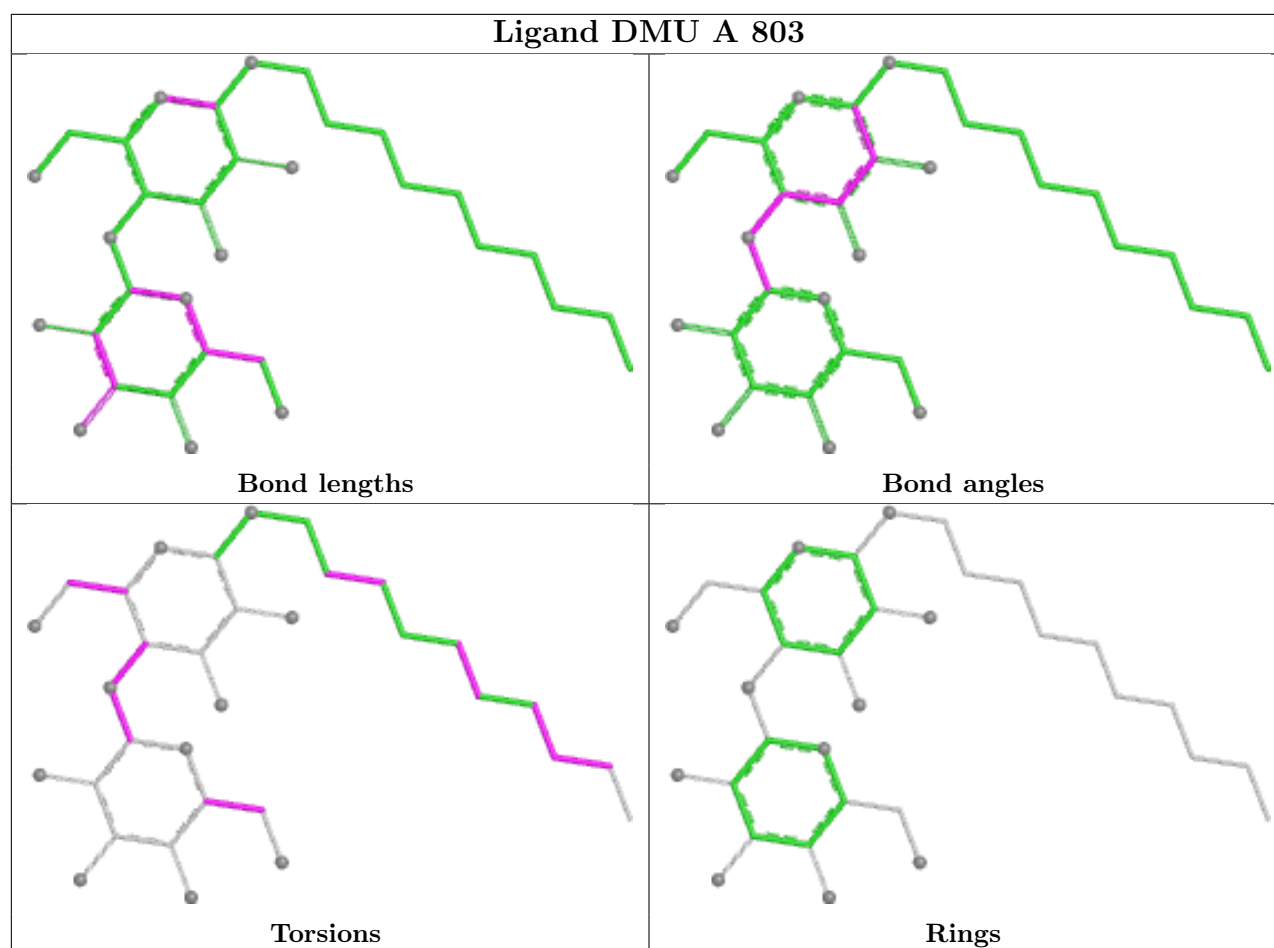
1 monomer is involved in 2 short contacts:

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, 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	589/620 (95%)	1.10	145 (24%) 2 2	29, 51, 216, 333	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	687	GLN	8.2
1	A	140	ILE	7.7
1	A	257	ILE	7.6
1	A	258	PHE	6.9
1	A	272	LEU	6.7
1	A	269	LEU	6.5
1	A	381	THR	6.3
1	A	390	PHE	5.9
1	A	273	VAL	5.9
1	A	125	PHE	5.8
1	A	383	PHE	5.7
1	A	266	LEU	5.5
1	A	270	SER	5.3
1	A	253	ILE	5.3
1	A	688	LEU	5.2
1	A	360	LEU	5.0
1	A	274	VAL	5.0
1	A	167	PHE	5.0
1	A	148	VAL	5.0
1	A	382	ALA	5.0
1	A	142	PHE	5.0
1	A	264	GLY	4.9
1	A	564	TYR	4.8
1	A	265	VAL	4.7
1	A	256	PHE	4.6
1	A	254	VAL	4.6
1	A	129	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	357	VAL	4.6
1	A	141	VAL	4.5
1	A	379	LEU	4.5
1	A	380	LEU	4.5
1	A	359	ALA	4.5
1	A	275	LEU	4.5
1	A	376	LEU	4.5
1	A	384	PHE	4.5
1	A	263	THR	4.4
1	A	138	PHE	4.4
1	A	146	PHE	4.4
1	A	358	TYR	4.2
1	A	144	ARG	4.2
1	A	267	ILE	4.2
1	A	250	VAL	4.1
1	A	139	ALA	3.9
1	A	387	ILE	3.9
1	A	386	ALA	3.9
1	A	245	LEU	3.9
1	A	234	SER	3.8
1	A	456	MET	3.8
1	A	364	TRP	3.8
1	A	242	LEU	3.8
1	A	399	VAL	3.8
1	A	260	PRO	3.7
1	A	238	LEU	3.7
1	A	362	LEU	3.7
1	A	388	LEU	3.7
1	A	149	PHE	3.7
1	A	370	ALA	3.6
1	A	276	ALA	3.6
1	A	559	ARG	3.6
1	A	233	TYR	3.6
1	A	164	SER	3.6
1	A	565	SER	3.6
1	A	433	VAL	3.5
1	A	288	THR	3.5
1	A	355	PHE	3.4
1	A	135	LEU	3.4
1	A	374	LEU	3.4
1	A	686	LYS	3.4
1	A	647	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	252	ILE	3.4
1	A	363	TRP	3.3
1	A	168	VAL	3.3
1	A	160	THR	3.3
1	A	323	GLN	3.3
1	A	372	GLY	3.3
1	A	354	ILE	3.3
1	A	361	ALA	3.2
1	A	262	LEU	3.2
1	A	136	PRO	3.2
1	A	395	GLN	3.2
1	A	170	ILE	3.1
1	A	237	LYS	3.1
1	A	287	ASN	3.0
1	A	261	ALA	3.0
1	A	368	LEU	3.0
1	A	389	GLY	3.0
1	A	259	ALA	3.0
1	A	544	TYR	3.0
1	A	214	ARG	3.0
1	A	373	SER	3.0
1	A	432	VAL	3.0
1	A	271	PRO	3.0
1	A	163	TYR	3.0
1	A	689	ALA	2.9
1	A	101	THR	2.9
1	A	145	MET	2.9
1	A	282	ILE	2.9
1	A	118	ALA	2.9
1	A	166	GLY	2.8
1	A	400	TRP	2.8
1	A	646	SER	2.8
1	A	649	ALA	2.8
1	A	143	GLY	2.7
1	A	195	ASP	2.7
1	A	150	THR	2.6
1	A	515	TYR	2.6
1	A	555	ILE	2.6
1	A	281	MET	2.6
1	A	371	ARG	2.6
1	A	391	MET	2.6
1	A	403	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	679	PHE	2.5
1	A	369	ILE	2.5
1	A	196	LEU	2.5
1	A	377	GLY	2.5
1	A	568	MET	2.5
1	A	239	GLY	2.5
1	A	353	VAL	2.5
1	A	378	ASN	2.5
1	A	137	ALA	2.5
1	A	268	ALA	2.5
1	A	685	GLU	2.4
1	A	556	GLN	2.4
1	A	279	ALA	2.4
1	A	151	LYS	2.4
1	A	650	ARG	2.4
1	A	134	THR	2.4
1	A	398	GLN	2.3
1	A	165	VAL	2.3
1	A	177	VAL	2.3
1	A	356	CYS	2.3
1	A	152	SER	2.3
1	A	648	VAL	2.3
1	A	511	PRO	2.2
1	A	178	ALA	2.2
1	A	224	LEU	2.2
1	A	683	LEU	2.2
1	A	241	VAL	2.2
1	A	255	ALA	2.2
1	A	645	LEU	2.1
1	A	393	VAL	2.1
1	A	426	PRO	2.1
1	A	396	ALA	2.1
1	A	171	GLY	2.0
1	A	246	ALA	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

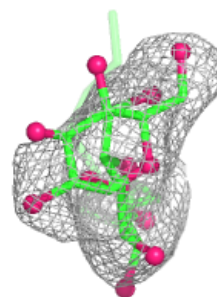
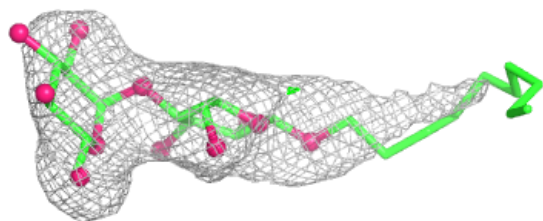
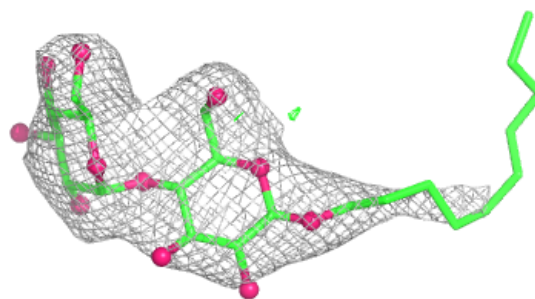
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	DMU	A	803	33/33	0.83	0.14	77,89,105,111	0
3	DMU	A	802	33/33	0.92	0.12	37,52,64,70	0
4	NO3	A	804	4/4	0.98	0.12	35,37,38,42	0
2	ANP	A	801	31/31	0.99	0.04	28,31,35,36	0
5	MG	A	805	1/1	0.99	0.03	32,32,32,32	0

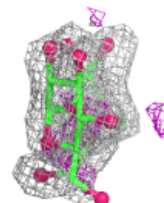
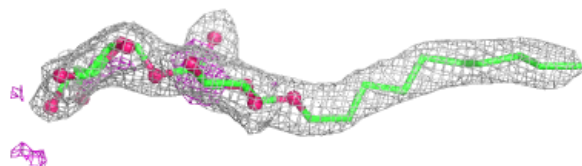
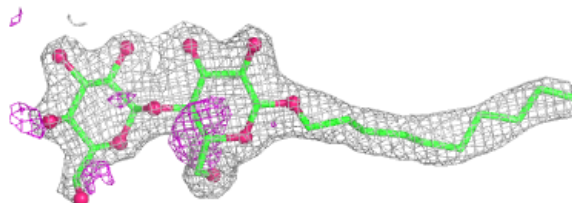
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

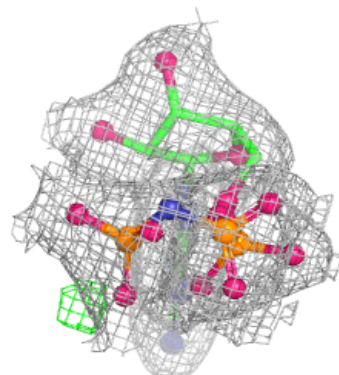
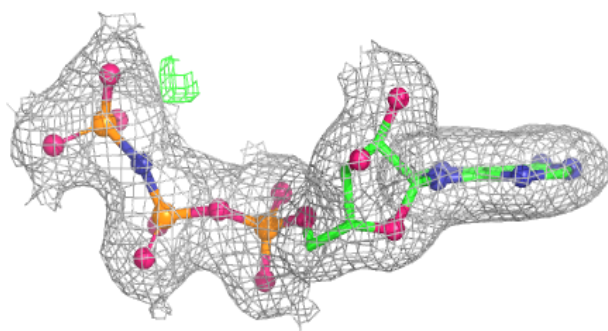
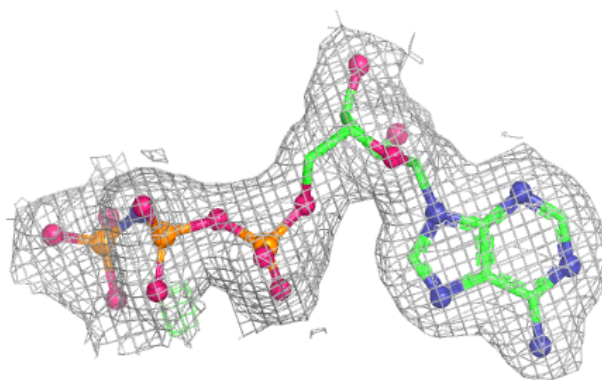
**Electron density around DMU A 802:**

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



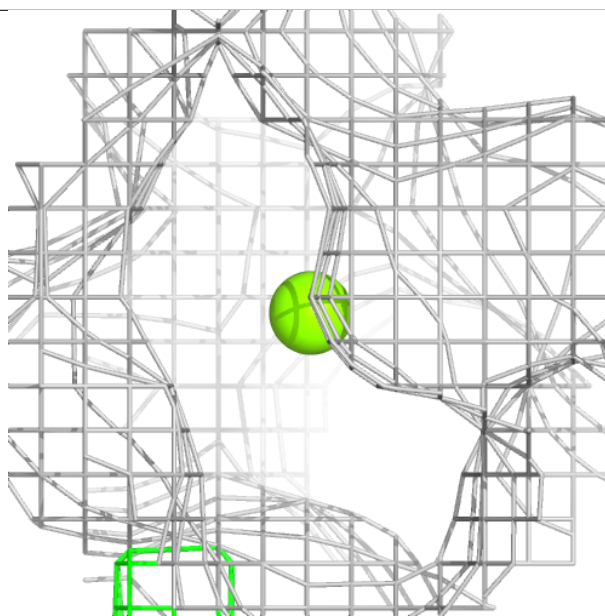
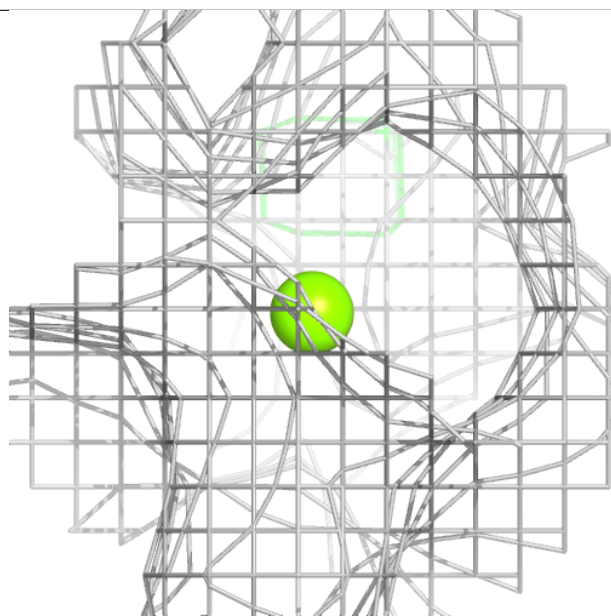
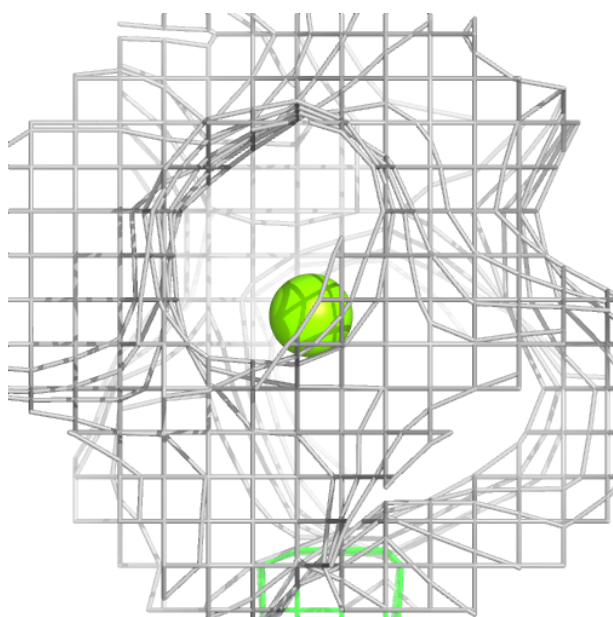
Electron density around ANP A 801:

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



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 ⓘ

There are no such residues in this entry.