



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:35 PM UTC

PDB ID : 8OVS / pdb_00008ovs
Title : Crystal structure of YeGT glycosyltransferase with bound UDP
Authors : Wirth, C.; Hunte, C.
Deposited on : 2023-04-26
Resolution : 1.12 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

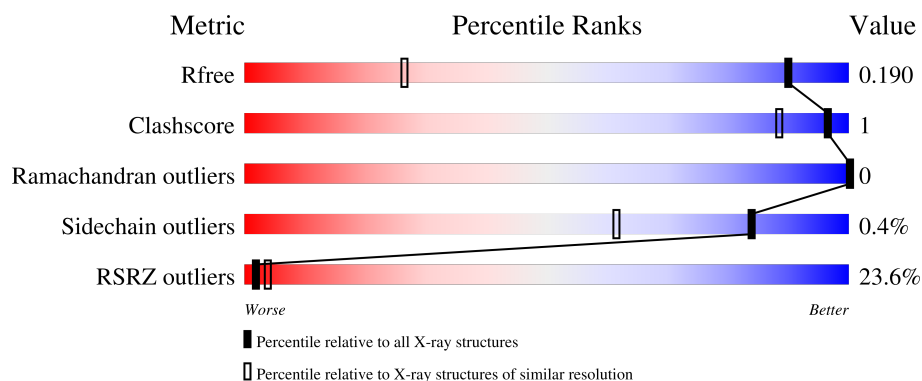
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.12 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	1985 (1.14-1.10)
Clashscore	190562	2021 (1.14-1.10)
Ramachandran outliers	187476	1978 (1.14-1.10)
Sidechain outliers	187428	1974 (1.14-1.10)
RSRZ outliers	180081	1984 (1.14-1.10)

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	AAA	299	18% 89% 8%
1	BBB	299	25% 89% 9%

2 Entry composition [i](#)

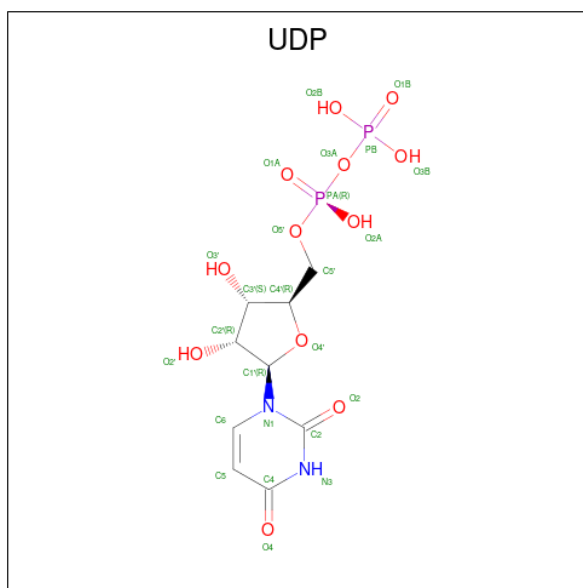
There are 8 unique types of molecules in this entry. The entry contains 5565 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 YeGT glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	276	Total	C	N	O	S	24	13	0
			2306	1472	399	428	7			
1	BBB	271	Total	C	N	O	S	21	12	0
			2252	1445	386	414	7			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	BBB	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	AAA	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	BBB	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	AAA	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 8 4 4	0	1
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0
4	BBB	1	Total C O 4 2 2	0	0

- Molecule 5 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	10	Total Cd 10 10	0	0
5	BBB	7	Total Cd 7 7	0	0

- Molecule 6 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total Mn 1 1	0	0
6	BBB	1	Total Mn 1 1	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	2	Total Na 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	BBB	1	Total	Na	0	0
			1	1		

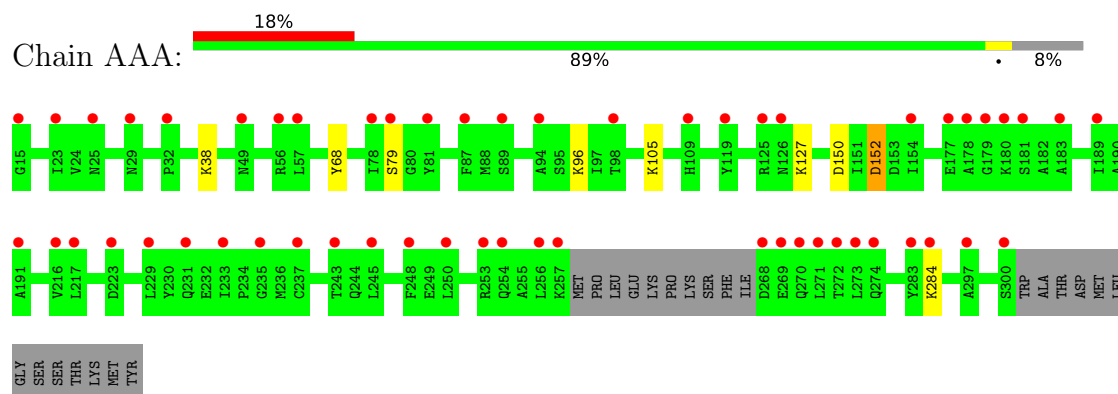
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	428	Total	O	0	0
			428	428		
8	BBB	443	Total	O	0	0
			443	443		

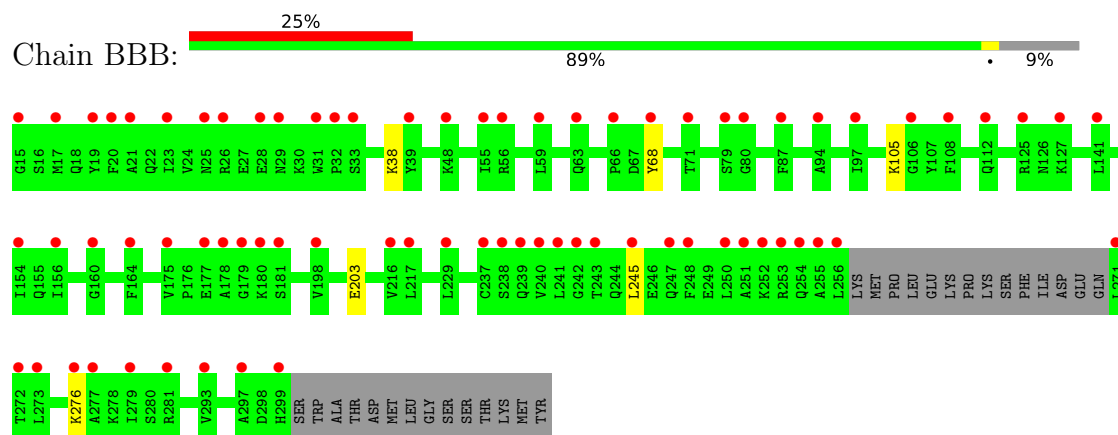
3 Residue-property plots [i](#)

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: YeGT glycosyltransferase



- Molecule 1: YeGT glycosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.13Å 114.55Å 69.38Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	47.13 – 1.12 47.13 – 1.12	Depositor EDS
% Data completeness (in resolution range)	76.6 (47.13-1.12) 80.1 (47.13-1.12)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.12Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.153 , 0.169 (Not available) , 0.190	Depositor DCC
R_{free} test set	11268 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.763	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.108 for h,-k,-l	Xtriage
Reported twinning fraction	0.534 for H, K, L 0.466 for -h,-k,l	Depositor
Outliers	0 of 223599 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5565	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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: CD, NA, UDP, MN, EDO, ACT

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	AAA	0.92	0/2361	1.21	1/3176 (0.0%)
1	BBB	0.92	0/2319	1.25	0/3122
All	All	0.92	0/4680	1.23	1/6298 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	152	ASP	CA-CB-CG	5.32	117.92	112.60

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	AAA	2306	0	2332	5	0
1	BBB	2252	0	2294	4	0
2	AAA	25	0	11	0	0
2	BBB	25	0	11	0	0
3	AAA	12	0	9	0	0
3	BBB	8	0	6	0	0
4	AAA	12	0	18	0	0
4	BBB	32	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AAA	10	0	0	0	0
5	BBB	7	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
7	AAA	2	0	0	0	0
7	BBB	1	0	0	0	0
8	AAA	428	0	0	2	0
8	BBB	443	0	0	2	0
All	All	5565	0	4727	9	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 (9) 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:AAA:152:ASP:OD2	8:AAA:501:HOH:O	2.08	0.70
1:AAA:105:LYS:NZ	8:AAA:502:HOH:O	2.25	0.70
1:BBB:105:LYS:NZ	8:BBB:503:HOH:O	2.38	0.56
1:BBB:245:LEU:HD22	1:BBB:276:LYS:HD2	1.92	0.51
1:BBB:203:GLU:HG3	8:BBB:608:HOH:O	2.12	0.49
1:AAA:38:LYS:HA	1:AAA:68:TYR:CE2	2.51	0.46
1:BBB:38:LYS:HA	1:BBB:68:TYR:CE2	2.52	0.44
1:AAA:79[A]:SER:OG	1:AAA:127[A]:LYS:NZ	2.52	0.41
1:AAA:150:ASP:HB3	1:AAA:152:ASP:OD1	2.21	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	AAA	285/299 (95%)	284 (100%)	1 (0%)	0	100	100
1	BBB	280/299 (94%)	277 (99%)	3 (1%)	0	100	100
All	All	565/598 (94%)	561 (99%)	4 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	AAA	250/258 (97%)	247 (99%)	3 (1%)	63	25
1	BBB	245/258 (95%)	245 (100%)	0	100	100
All	All	495/516 (96%)	492 (99%)	3 (1%)	84	51

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	96	LYS
1	AAA	284[A]	LYS
1	AAA	284[B]	LYS

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

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 40 ligands modelled in this entry, 22 are monoatomic - leaving 18 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	$\# Z > 2$
2	UDP	BBB	403	6,5	25,26,26	0.45	0	38,40,40	0.68	0
4	EDO	BBB	405	-	3,3,3	0.06	0	2,2,2	0.09	0
2	UDP	AAA	401	6,5	25,26,26	0.46	0	38,40,40	0.80	0
4	EDO	AAA	407	-	3,3,3	0.07	0	2,2,2	0.09	0
4	EDO	BBB	404[A]	5	3,3,3	0.06	0	2,2,2	0.03	0
4	EDO	BBB	407	-	3,3,3	0.06	0	2,2,2	0.20	0
4	EDO	BBB	410	-	3,3,3	0.09	0	2,2,2	0.25	0
4	EDO	AAA	404	-	3,3,3	0.07	0	2,2,2	0.08	0
4	EDO	BBB	408	-	3,3,3	0.06	0	2,2,2	0.12	0
3	ACT	AAA	406	-	3,3,3	0.99	0	3,3,3	0.84	0
4	EDO	BBB	406	-	3,3,3	0.06	0	2,2,2	0.13	0
3	ACT	AAA	402	-	3,3,3	1.01	0	3,3,3	0.85	0
3	ACT	BBB	401	5	3,3,3	1.15	0	3,3,3	0.72	0
4	EDO	AAA	405	-	3,3,3	0.06	0	2,2,2	0.16	0
4	EDO	BBB	404[B]	5	3,3,3	0.07	0	2,2,2	0.16	0
4	EDO	BBB	409	-	3,3,3	0.06	0	2,2,2	0.14	0
3	ACT	AAA	403	5	3,3,3	1.11	0	3,3,3	0.71	0
3	ACT	BBB	402	-	3,3,3	1.02	0	3,3,3	0.79	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
2	UDP	BBB	403	6,5	-	1/16/32/32	0/2/2/2
4	EDO	BBB	405	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	AAA	401	6,5	-	2/16/32/32	0/2/2/2
4	EDO	AAA	407	-	-	0/1/1/1	-
4	EDO	BBB	404[A]	5	-	1/1/1/1	-
4	EDO	BBB	407	-	-	1/1/1/1	-
4	EDO	BBB	410	-	-	1/1/1/1	-
4	EDO	AAA	404	-	-	1/1/1/1	-
4	EDO	BBB	408	-	-	0/1/1/1	-
4	EDO	BBB	406	-	-	1/1/1/1	-
4	EDO	AAA	405	-	-	0/1/1/1	-
4	EDO	BBB	404[B]	5	-	0/1/1/1	-
4	EDO	BBB	409	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

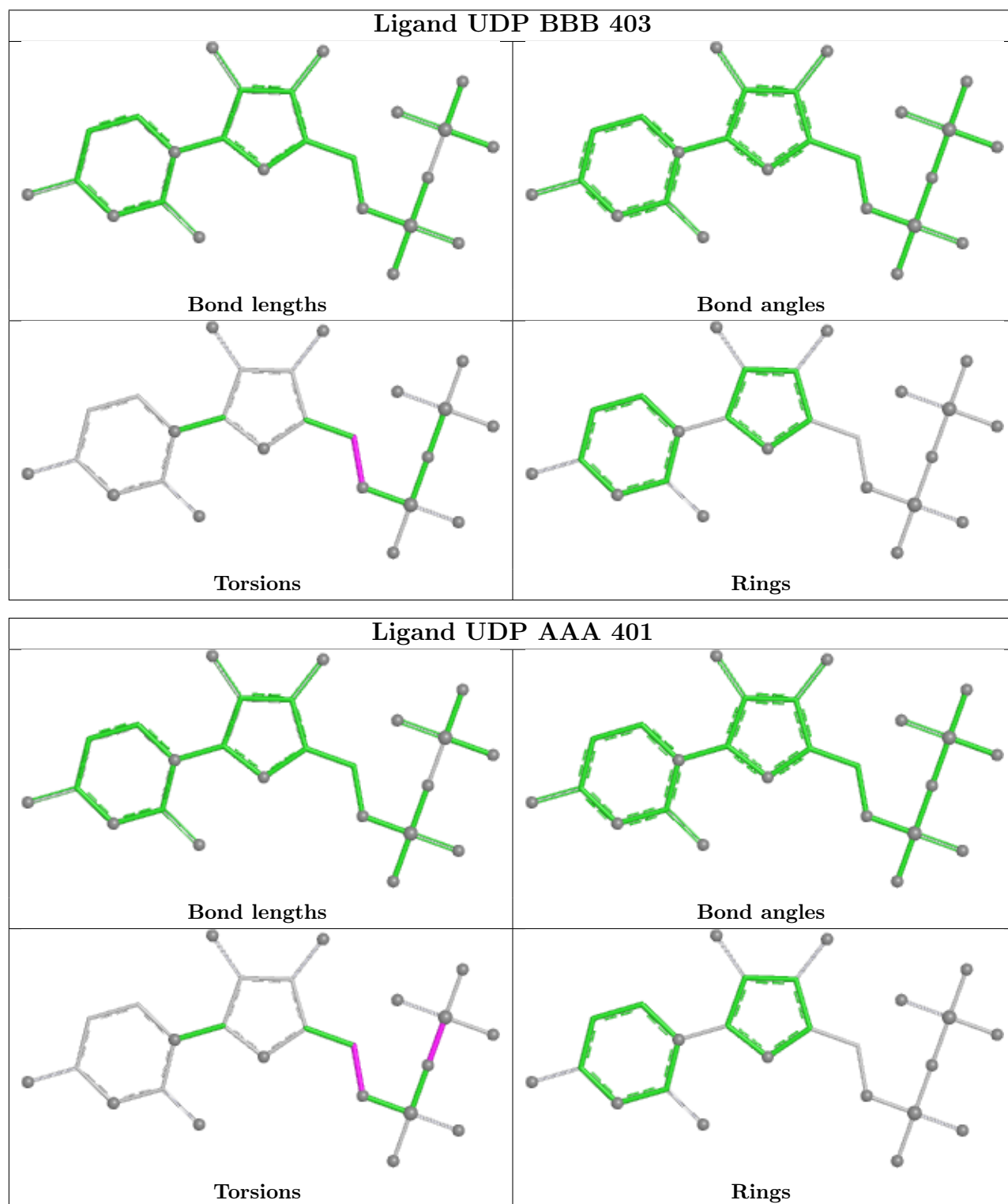
Mol	Chain	Res	Type	Atoms
4	BBB	410	EDO	O1-C1-C2-O2
2	AAA	401	UDP	PA-O3A-PB-O1B
4	BBB	406	EDO	O1-C1-C2-O2
4	BBB	404[A]	EDO	O1-C1-C2-O2
4	BBB	409	EDO	O1-C1-C2-O2
4	BBB	407	EDO	O1-C1-C2-O2
2	AAA	401	UDP	C4'-C5'-O5'-PA
2	BBB	403	UDP	C4'-C5'-O5'-PA
4	AAA	404	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	AAA	276/299 (92%)	1.27	55 (19%) 3 6	5, 15, 24, 35	19 (6%)
1	BBB	271/299 (90%)	1.54	74 (27%) 1 3	8, 16, 30, 40	18 (6%)
All	All	547/598 (91%)	1.40	129 (23%) 2 4	5, 16, 27, 40	37 (6%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	255	ALA	5.5
1	BBB	243	THR	5.5
1	BBB	48[A]	LYS	5.4
1	BBB	256	LEU	5.0
1	BBB	15	GLY	4.9
1	BBB	273	LEU	4.8
1	BBB	94	ALA	4.7
1	AAA	178	ALA	4.7
1	BBB	29	ASN	4.6
1	BBB	250	LEU	4.5
1	BBB	240	VAL	4.3
1	BBB	23[B]	ILE	4.3
1	AAA	268	ASP	4.3
1	AAA	284[A]	LYS	4.2
1	BBB	179	GLY	4.2
1	BBB	245	LEU	4.1
1	BBB	32	PRO	4.0
1	BBB	217	LEU	4.0
1	AAA	300	SER	4.0
1	BBB	254	GLN	3.9
1	BBB	279	ILE	3.9
1	BBB	271	LEU	3.8
1	BBB	248	PHE	3.7
1	BBB	251	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	BBB	97	ILE	3.7
1	BBB	21	ALA	3.6
1	BBB	178	ALA	3.6
1	AAA	79[A]	SER	3.5
1	BBB	253	ARG	3.4
1	AAA	273	LEU	3.4
1	AAA	237	CYS	3.4
1	AAA	216	VAL	3.4
1	AAA	269	GLU	3.4
1	AAA	125[A]	ARG	3.3
1	AAA	23	ILE	3.3
1	BBB	25	ASN	3.2
1	BBB	17	MET	3.2
1	AAA	25	ASN	3.2
1	AAA	29	ASN	3.2
1	AAA	235	GLY	3.2
1	BBB	66	PRO	3.2
1	BBB	239[A]	GLN	3.2
1	AAA	271	LEU	3.1
1	AAA	94	ALA	3.1
1	BBB	87	PHE	3.1
1	BBB	180	LYS	3.1
1	BBB	242	GLY	3.1
1	AAA	274[A]	GLN	3.0
1	AAA	297	ALA	3.0
1	AAA	177	GLU	3.0
1	BBB	80	GLY	3.0
1	AAA	181	SER	3.0
1	BBB	164	PHE	2.9
1	AAA	32[A]	PRO	2.9
1	BBB	241	LEU	2.9
1	AAA	253	ARG	2.9
1	BBB	19	TYR	2.9
1	AAA	56[A]	ARG	2.8
1	BBB	20	PHE	2.8
1	BBB	216	VAL	2.7
1	AAA	223	ASP	2.7
1	BBB	26	ARG	2.7
1	AAA	89	SER	2.7
1	AAA	180	LYS	2.7
1	AAA	87	PHE	2.7
1	BBB	156	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	AAA	243	THR	2.6
1	AAA	245	LEU	2.6
1	BBB	59	LEU	2.6
1	BBB	237	CYS	2.6
1	AAA	126	ASN	2.6
1	AAA	254	GLN	2.6
1	AAA	256	LEU	2.6
1	BBB	277	ALA	2.6
1	BBB	229[A]	LEU	2.5
1	BBB	33	SER	2.5
1	AAA	217	LEU	2.5
1	BBB	160	GLY	2.5
1	BBB	247	GLN	2.5
1	BBB	198	VAL	2.5
1	BBB	238	SER	2.5
1	BBB	39	TYR	2.5
1	AAA	257	LYS	2.5
1	BBB	272	THR	2.4
1	BBB	31	TRP	2.4
1	AAA	231	GLN	2.4
1	AAA	229[A]	LEU	2.4
1	AAA	250	LEU	2.4
1	BBB	141	LEU	2.4
1	AAA	270	GLN	2.4
1	BBB	79	SER	2.4
1	BBB	177	GLU	2.4
1	AAA	15	GLY	2.3
1	AAA	183	ALA	2.3
1	BBB	106	GLY	2.3
1	AAA	109	HIS	2.3
1	BBB	108	PHE	2.3
1	BBB	154	ILE	2.3
1	BBB	175	VAL	2.3
1	BBB	181	SER	2.3
1	BBB	63[A]	GLN	2.3
1	AAA	283	TYR	2.2
1	AAA	49	ASN	2.2
1	BBB	276	LYS	2.2
1	AAA	119	TYR	2.2
1	BBB	125	ARG	2.2
1	BBB	252	LYS	2.2
1	BBB	297	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	293	VAL	2.2
1	AAA	81	TYR	2.2
1	BBB	112[A]	GLN	2.2
1	AAA	272	THR	2.1
1	BBB	71	THR	2.1
1	AAA	154	ILE	2.1
1	BBB	55	ILE	2.1
1	BBB	281	ARG	2.1
1	BBB	28	GLU	2.1
1	AAA	57	LEU	2.1
1	BBB	299	HIS	2.1
1	AAA	191	ALA	2.1
1	AAA	78	ILE	2.0
1	AAA	189	ILE	2.0
1	AAA	233	ILE	2.0
1	BBB	56[A]	ARG	2.0
1	BBB	68	TYR	2.0
1	AAA	98[A]	THR	2.0
1	BBB	127[A]	LYS	2.0
1	AAA	248	PHE	2.0
1	AAA	179	GLY	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	EDO	AAA	405	4/4	0.62	0.21	35,36,37,39	0
4	EDO	BBB	410	4/4	0.67	0.21	26,26,27,30	0

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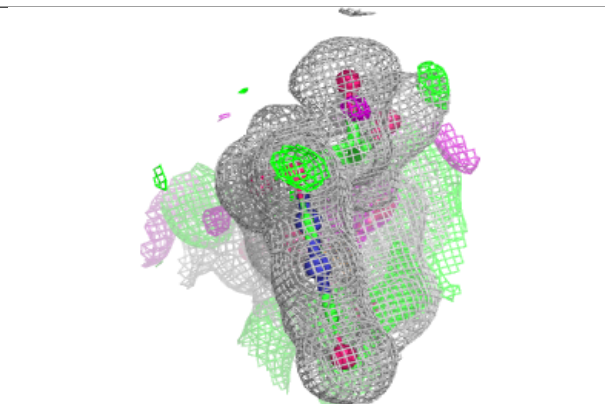
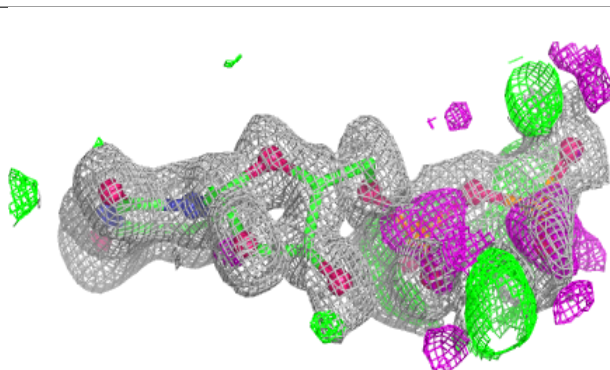
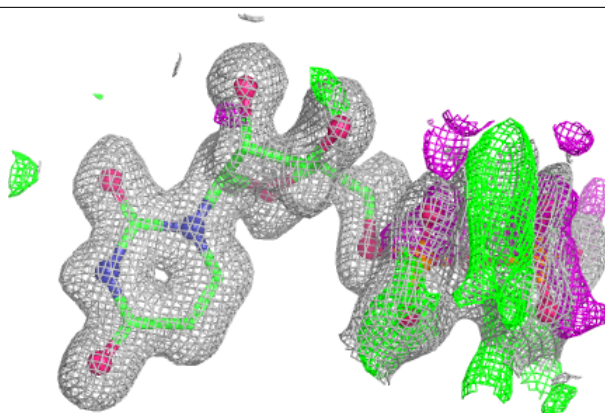
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	BBB	406	4/4	0.76	0.16	33,34,34,36	0
4	EDO	BBB	405	4/4	0.76	0.19	28,30,30,31	0
4	EDO	BBB	408	4/4	0.78	0.17	28,30,31,33	0
4	EDO	BBB	407	4/4	0.79	0.15	30,30,30,31	0
3	ACT	AAA	406	4/4	0.81	0.16	30,30,31,32	0
4	EDO	BBB	409	4/4	0.84	0.15	32,32,33,34	0
4	EDO	AAA	407	4/4	0.85	0.14	23,24,26,26	0
4	EDO	BBB	404[A]	4/4	0.89	0.11	17,17,18,18	4
4	EDO	BBB	404[B]	4/4	0.89	0.11	12,14,15,16	4
4	EDO	AAA	404	4/4	0.90	0.12	27,27,27,28	0
7	NA	AAA	420	1/1	0.90	0.15	41,41,41,41	0
5	CD	BBB	412	1/1	0.91	0.13	29,29,29,29	0
5	CD	AAA	409	1/1	0.92	0.12	26,26,26,26	0
2	UDP	BBB	403	25/25	0.92	0.10	10,12,19,23	0
3	ACT	AAA	403	4/4	0.92	0.11	16,17,17,19	0
3	ACT	BBB	402	4/4	0.93	0.09	15,15,16,16	0
2	UDP	AAA	401	25/25	0.95	0.08	10,12,18,21	0
3	ACT	AAA	402	4/4	0.95	0.10	17,17,17,18	0
3	ACT	BBB	401	4/4	0.95	0.09	16,16,17,18	0
5	CD	BBB	414	1/1	0.96	0.17	42,42,42,42	0
5	CD	AAA	416	1/1	0.97	0.23	36,36,36,36	1
5	CD	BBB	413	1/1	0.97	0.13	36,36,36,36	1
5	CD	AAA	414	1/1	0.98	0.09	28,28,28,28	0
5	CD	AAA	412	1/1	0.99	0.08	31,31,31,31	0
5	CD	AAA	415	1/1	0.99	0.05	13,13,13,13	1
5	CD	AAA	413	1/1	0.99	0.14	24,24,24,24	1
5	CD	BBB	415	1/1	0.99	0.17	24,24,24,24	1
5	CD	BBB	416	1/1	0.99	0.04	14,14,14,14	1
5	CD	BBB	417	1/1	0.99	0.05	22,22,22,22	1
5	CD	AAA	417	1/1	0.99	0.10	20,20,20,20	1
7	NA	BBB	419	1/1	0.99	0.04	13,13,13,13	0
5	CD	AAA	408	1/1	1.00	0.01	12,12,12,12	0
5	CD	AAA	410	1/1	1.00	0.01	13,13,13,13	0
6	MN	AAA	418	1/1	1.00	0.06	10,10,10,10	0
6	MN	BBB	418	1/1	1.00	0.07	11,11,11,11	0
7	NA	AAA	419	1/1	1.00	0.02	14,14,14,14	0
5	CD	AAA	411	1/1	1.00	0.01	15,15,15,15	0
5	CD	BBB	411	1/1	1.00	0.01	13,13,13,13	0

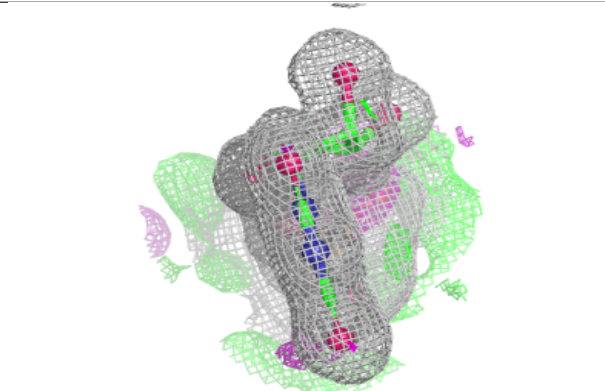
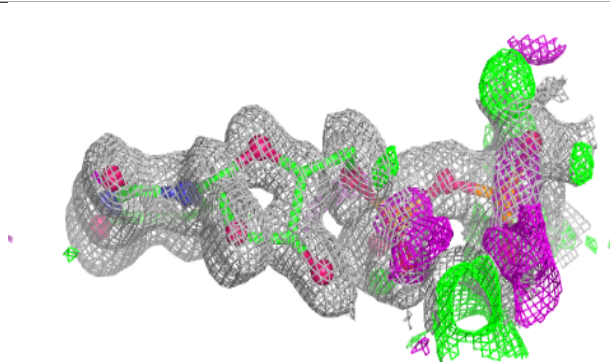
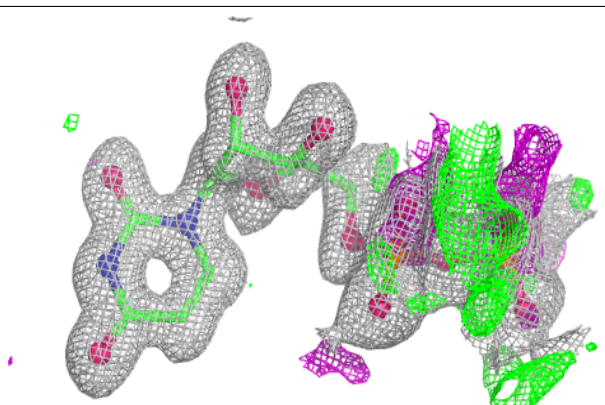
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP BBB 403:

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

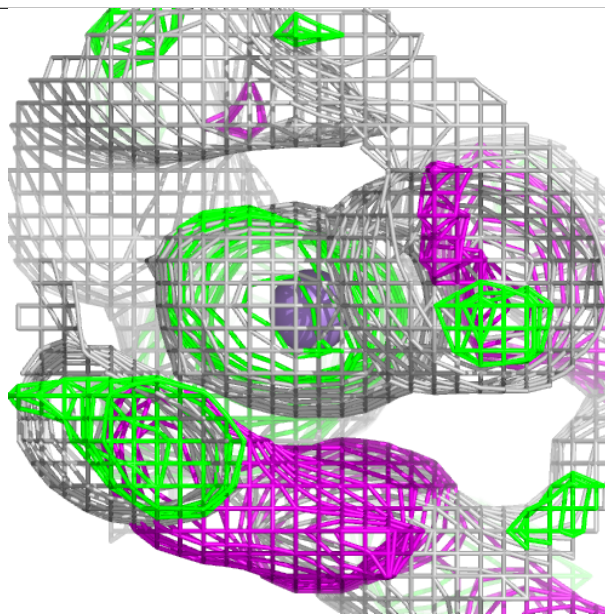
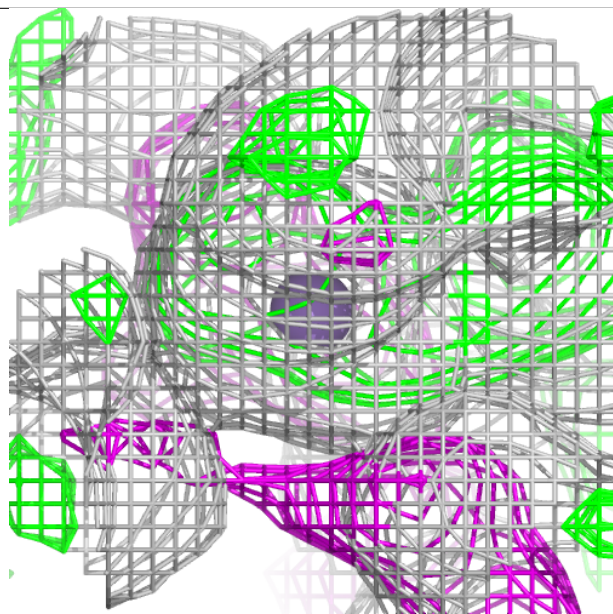
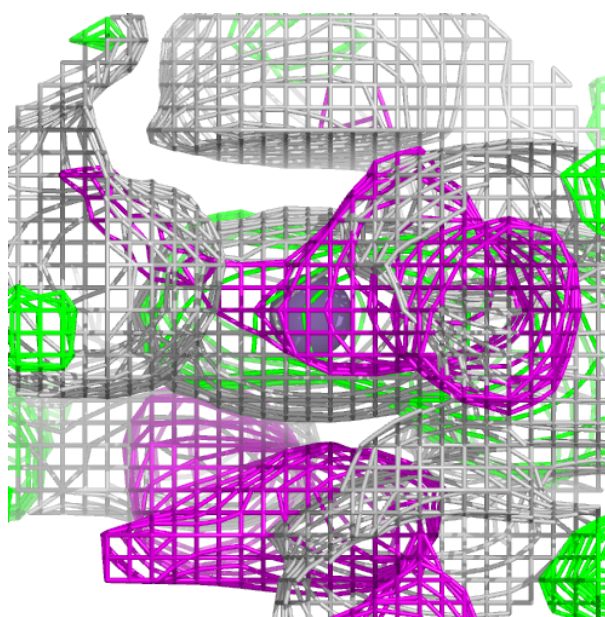
**Electron density around UDP AAA 401:**

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



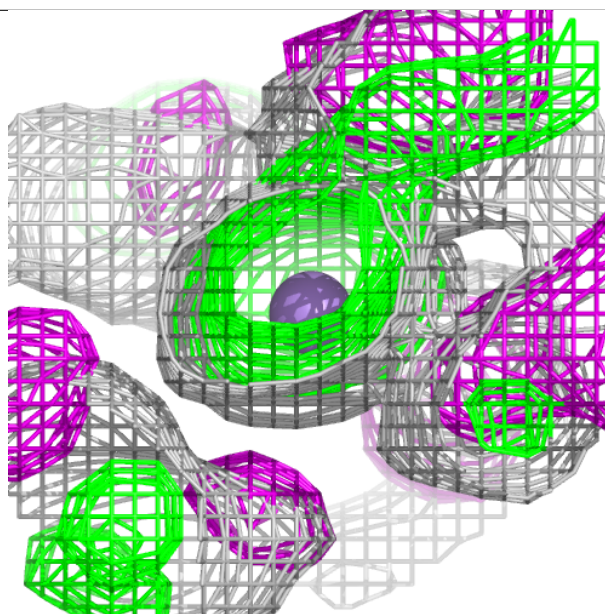
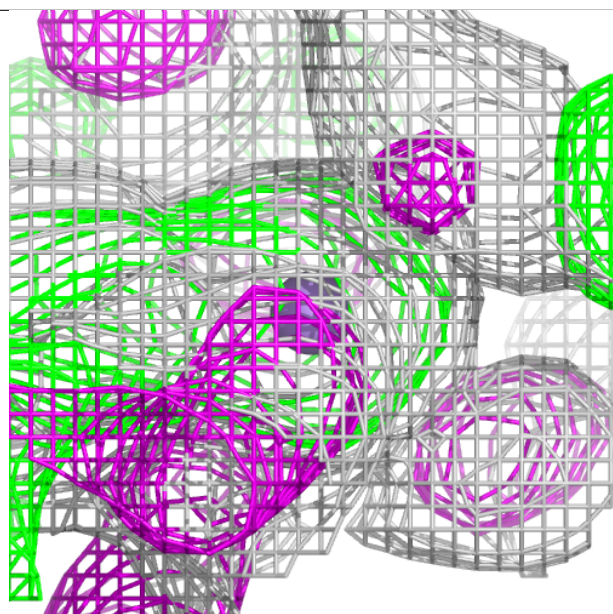
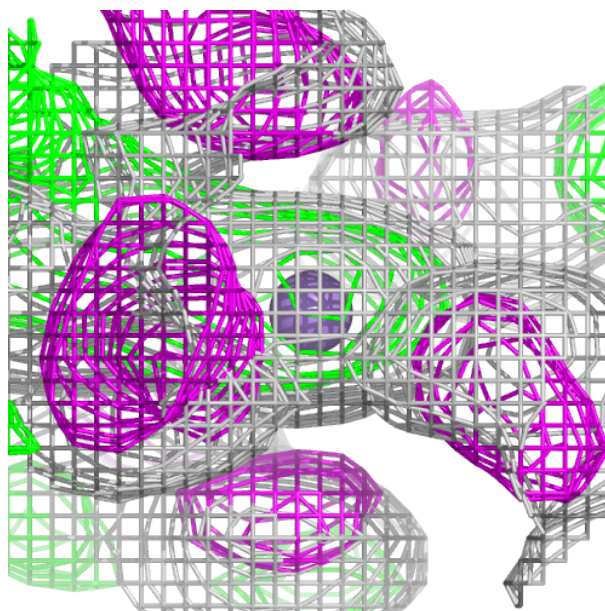
Electron density around MN AAA 418:

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



Electron density around MN BBB 418:

$2mF_o-DF_c$ (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.