



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 20, 2026 – 04:16 pm BST

PDB ID : 9SQG / pdb_00009sqg
Title : PaMurU in complex with Mn²⁺ and UDPNAM (uridine diphosphate N-acetyl muramic acid)
Authors : Jimenez-Faraco, E.; Hermoso, J.A.
Deposited on : 2025-09-22
Resolution : 1.85 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.4, CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

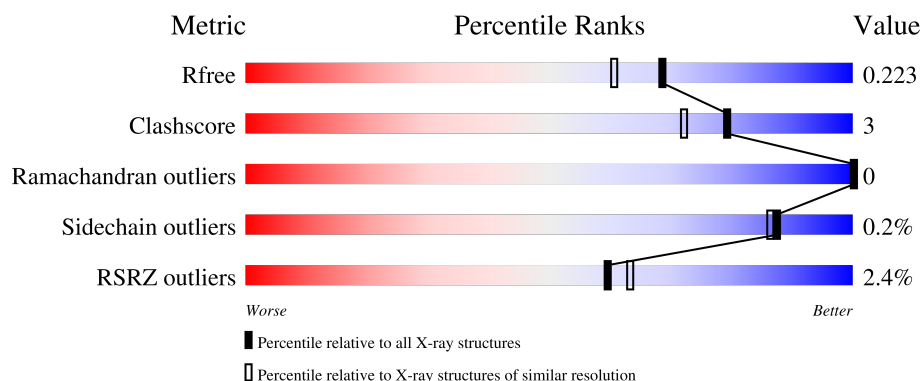
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

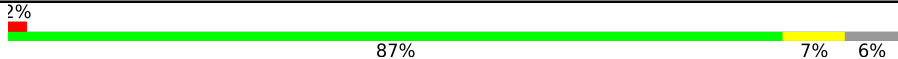
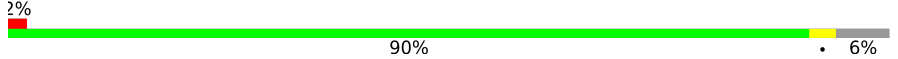
The reported resolution of this entry is 1.85 Å.

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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	239	
1	B	239	
1	C	239	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	302	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5621 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 N-acetylmuramate alpha-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	224	Total	C	N	O	S	0	0	0
			1709	1080	314	311	4			
1	A	225	Total	C	N	O	S	0	0	0
			1715	1083	315	313	4			
1	B	223	Total	C	N	O	S	0	0	0
			1704	1077	313	310	4			

There are 45 discrepancies between the modelled and reference sequences:

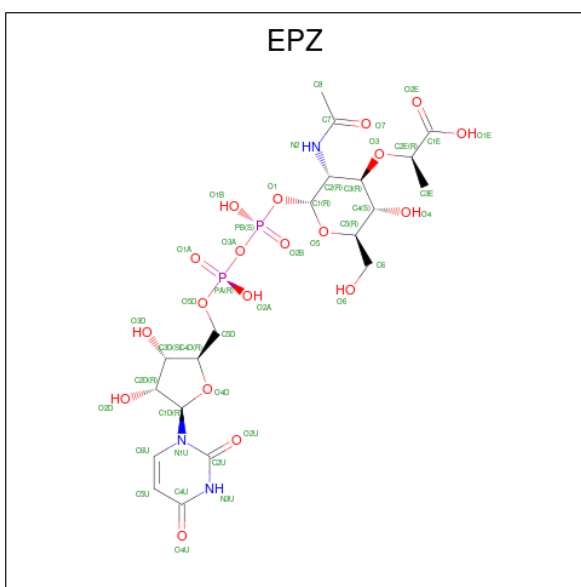
Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	MET	-	initiating methionine	UNP Q9I5U0
C	-13	HIS	-	expression tag	UNP Q9I5U0
C	-12	HIS	-	expression tag	UNP Q9I5U0
C	-11	HIS	-	expression tag	UNP Q9I5U0
C	-10	HIS	-	expression tag	UNP Q9I5U0
C	-9	HIS	-	expression tag	UNP Q9I5U0
C	-8	HIS	-	expression tag	UNP Q9I5U0
C	-7	GLU	-	expression tag	UNP Q9I5U0
C	-6	PHE	-	expression tag	UNP Q9I5U0
C	-5	SER	-	expression tag	UNP Q9I5U0
C	-4	GLN	-	expression tag	UNP Q9I5U0
C	-3	GLN	-	expression tag	UNP Q9I5U0
C	-2	ASP	-	expression tag	UNP Q9I5U0
C	-1	SER	-	expression tag	UNP Q9I5U0
C	0	ASP	-	expression tag	UNP Q9I5U0
A	-14	MET	-	initiating methionine	UNP Q9I5U0
A	-13	HIS	-	expression tag	UNP Q9I5U0
A	-12	HIS	-	expression tag	UNP Q9I5U0
A	-11	HIS	-	expression tag	UNP Q9I5U0
A	-10	HIS	-	expression tag	UNP Q9I5U0
A	-9	HIS	-	expression tag	UNP Q9I5U0
A	-8	HIS	-	expression tag	UNP Q9I5U0
A	-7	GLU	-	expression tag	UNP Q9I5U0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	PHE	-	expression tag	UNP Q9I5U0
A	-5	SER	-	expression tag	UNP Q9I5U0
A	-4	GLN	-	expression tag	UNP Q9I5U0
A	-3	GLN	-	expression tag	UNP Q9I5U0
A	-2	ASP	-	expression tag	UNP Q9I5U0
A	-1	SER	-	expression tag	UNP Q9I5U0
A	0	ASP	-	expression tag	UNP Q9I5U0
B	-14	MET	-	initiating methionine	UNP Q9I5U0
B	-13	HIS	-	expression tag	UNP Q9I5U0
B	-12	HIS	-	expression tag	UNP Q9I5U0
B	-11	HIS	-	expression tag	UNP Q9I5U0
B	-10	HIS	-	expression tag	UNP Q9I5U0
B	-9	HIS	-	expression tag	UNP Q9I5U0
B	-8	HIS	-	expression tag	UNP Q9I5U0
B	-7	GLU	-	expression tag	UNP Q9I5U0
B	-6	PHE	-	expression tag	UNP Q9I5U0
B	-5	SER	-	expression tag	UNP Q9I5U0
B	-4	GLN	-	expression tag	UNP Q9I5U0
B	-3	GLN	-	expression tag	UNP Q9I5U0
B	-2	ASP	-	expression tag	UNP Q9I5U0
B	-1	SER	-	expression tag	UNP Q9I5U0
B	0	ASP	-	expression tag	UNP Q9I5U0

- Molecule 2 is (2R)-2-[[[(2R,3R,4R,5S,6R)-3-(acetylamino)-2-[[[(S)-[[[(R)-[[[(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]oxy}-5-hydroxy-6-(hydroxymethyl)tetrahydro-2H-pyran-4-yl]oxy}propanoic acid (CCD ID: EPZ) (formula: C₂₀H₃₁N₃O₁₉P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
2	A	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
2	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

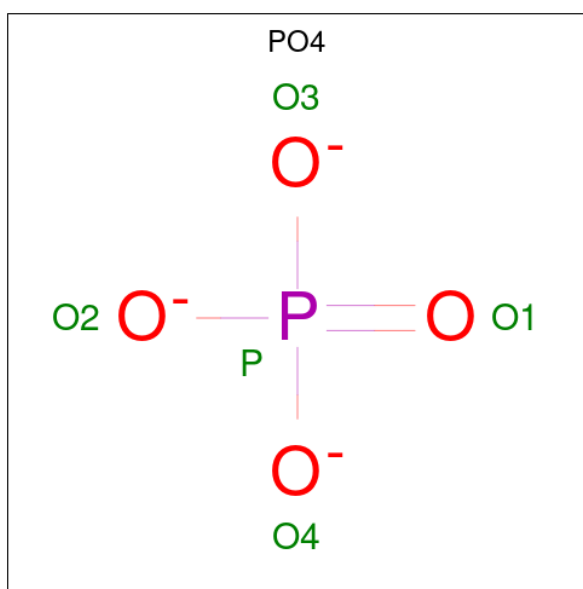
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Mn	0	0
			2	2		
4	A	2	Total	Mn	0	0
			2	2		
4	B	2	Total	Mn	0	0
			2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	116	Total	O	0	0
			116	116		
7	A	112	Total	O	0	0
			112	112		
7	B	107	Total	O	0	0
			107	107		

- Molecule 1: N-acetylmuramate alpha-1-phosphate uridylyltransferase



MET	H1S	H1S	H1S	H1S	H1S	H1S	H1S	GLU	PHE	SER	GLN	ASP	S-1	I5	G9	R13	T18	T21	P22	K23	E61	R69	E84	T86	R116	L117	H118	A155	G156	A183	P184	R187	G197	V207	R212	H223	A1A
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MET	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLU	PHE	SER	GLN	GLN	ASP	SER	DO	M14	R15	T18	L19	H20	T21	H53	P78	G97	R116	D144	E154	ALA	G156	G157	N158	R187	V205	D206	V207	H210	E211	R212	V216	H223	ALA
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.78Å 51.78Å 72.54Å 90.62° 90.67° 102.60°	Depositor
Resolution (Å)	72.53 – 1.85 72.53 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (72.53-1.85) 96.3 (72.53-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.177 , 0.215 0.187 , 0.223	Depositor DCC
R_{free} test set	2936 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.005 for k,h,-l 0.013 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5621	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.97% 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: GOL, MN, PO4, CL, EPZ

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	0.60	0/1757	1.03	2/2386 (0.1%)
1	B	0.62	0/1745	1.00	2/2368 (0.1%)
1	C	0.63	0/1751	1.05	1/2378 (0.0%)
All	All	0.62	0/5253	1.03	5/7132 (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	3
1	B	0	2
1	C	0	1
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	GLU	N-CA-CB	5.52	118.24	110.12
1	B	158	ASN	CA-CB-CG	-5.35	107.25	112.60
1	A	61	GLU	CB-CA-C	-5.33	101.94	110.79
1	A	116	ARG	CB-CA-C	-5.12	99.60	110.31
1	B	116	ARG	CB-CA-C	-5.04	99.88	110.17

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	ARG	Sidechain
1	A	212	ARG	Sidechain
1	A	69	ARG	Sidechain
1	B	187	ARG	Sidechain
1	C	212	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	1715	0	1685	12	0
1	B	1704	0	1674	11	0
1	C	1709	0	1680	5	0
2	A	44	0	28	0	0
2	B	44	0	28	0	0
2	C	44	0	28	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	6	0	8	6	0
5	B	6	0	8	0	0
6	B	5	0	0	0	0
7	A	112	0	0	1	0
7	B	107	0	0	2	0
7	C	116	0	0	2	0
All	All	5621	0	5139	28	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 3.

The worst 5 of 28 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:C:203:GLN:HG3	7:C:512:HOH:O	1.46	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLU:OE2	5:A:302:GOL:H11	1.68	0.93
1:A:13:ARG:NH1	7:A:401:HOH:O	2.26	0.67
1:B:154:GLU:O	1:B:156:GLY:N	2.33	0.62
1:A:85:THR:CG2	5:A:302:GOL:H12	2.30	0.61

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	223/239 (93%)	219 (98%)	4 (2%)	0	100	100
1	B	219/239 (92%)	212 (97%)	7 (3%)	0	100	100
1	C	222/239 (93%)	216 (97%)	6 (3%)	0	100	100
All	All	664/717 (93%)	647 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	170/183 (93%)	170 (100%)	0	100	100
1	B	169/183 (92%)	168 (99%)	1 (1%)	78	73
1	C	169/183 (92%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	508/549 (92%)	507 (100%)	1 (0%)	87	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	ARG

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	59	GLN
1	A	223	HIS
1	B	118	HIS
1	B	210	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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
5	GOL	A	302	-	5,5,5	0.07	0	5,5,5	0.44	0
2	EPZ	B	303	4	43,46,46	0.88	2 (4%)	60,69,69	1.14	6 (10%)
5	GOL	B	304	4	5,5,5	0.14	0	5,5,5	0.41	0
2	EPZ	A	301	4	43,46,46	0.80	0	60,69,69	1.02	5 (8%)
2	EPZ	C	301	4	43,46,46	1.06	4 (9%)	60,69,69	1.27	8 (13%)
6	PO4	B	302	4	4,4,4	1.28	1 (25%)	6,6,6	0.45	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
5	GOL	A	302	-	-	4/4/4/4	-
2	EPZ	B	303	4	-	2/34/71/71	0/3/3/3
5	GOL	B	304	4	-	4/4/4/4	-
2	EPZ	A	301	4	-	2/34/71/71	0/3/3/3
2	EPZ	C	301	4	-	4/34/71/71	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	EPZ	C2E-C1E	2.64	1.56	1.52
2	C	301	EPZ	PB-O1B	2.29	1.66	1.55
2	B	303	EPZ	PA-O1A	-2.29	1.42	1.50
6	B	302	PO4	P-O1	2.27	1.56	1.50
2	C	301	EPZ	C1-C2	2.21	1.56	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	EPZ	O3A-PB-O1	-3.32	95.79	102.48
2	C	301	EPZ	O1B-PB-O1	3.11	119.06	106.78
2	C	301	EPZ	O4D-C4D-C5D	-2.84	100.03	109.37
2	B	303	EPZ	O4D-C4D-C5D	-2.74	100.36	109.37
2	C	301	EPZ	C1-C2-N2	2.71	115.67	111.00

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	EPZ	C1-O1-PB-O1B
5	A	302	GOL	O1-C1-C2-C3
5	B	304	GOL	C1-C2-C3-O3
5	A	302	GOL	O1-C1-C2-O2
5	A	302	GOL	C1-C2-C3-O3

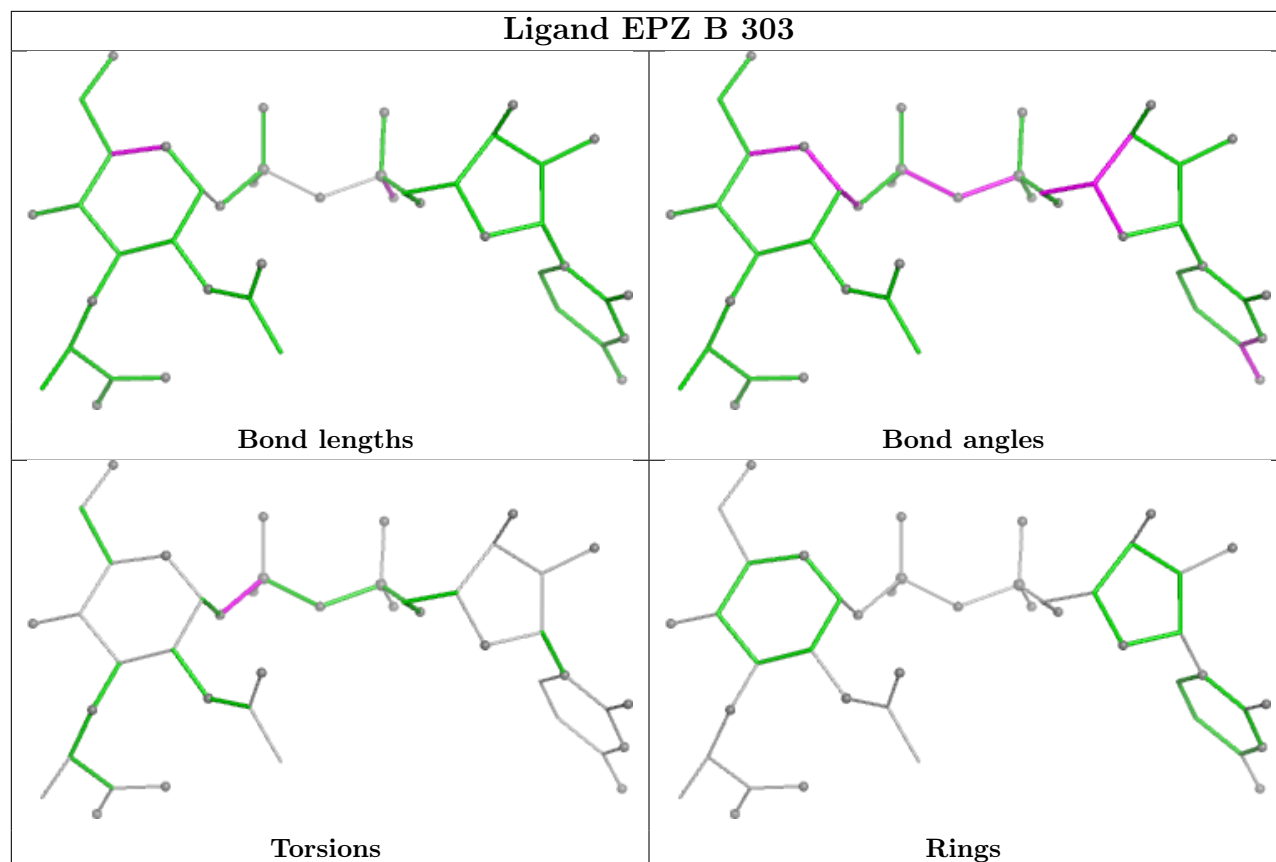
There are no ring outliers.

1 monomer is involved in 6 short contacts:

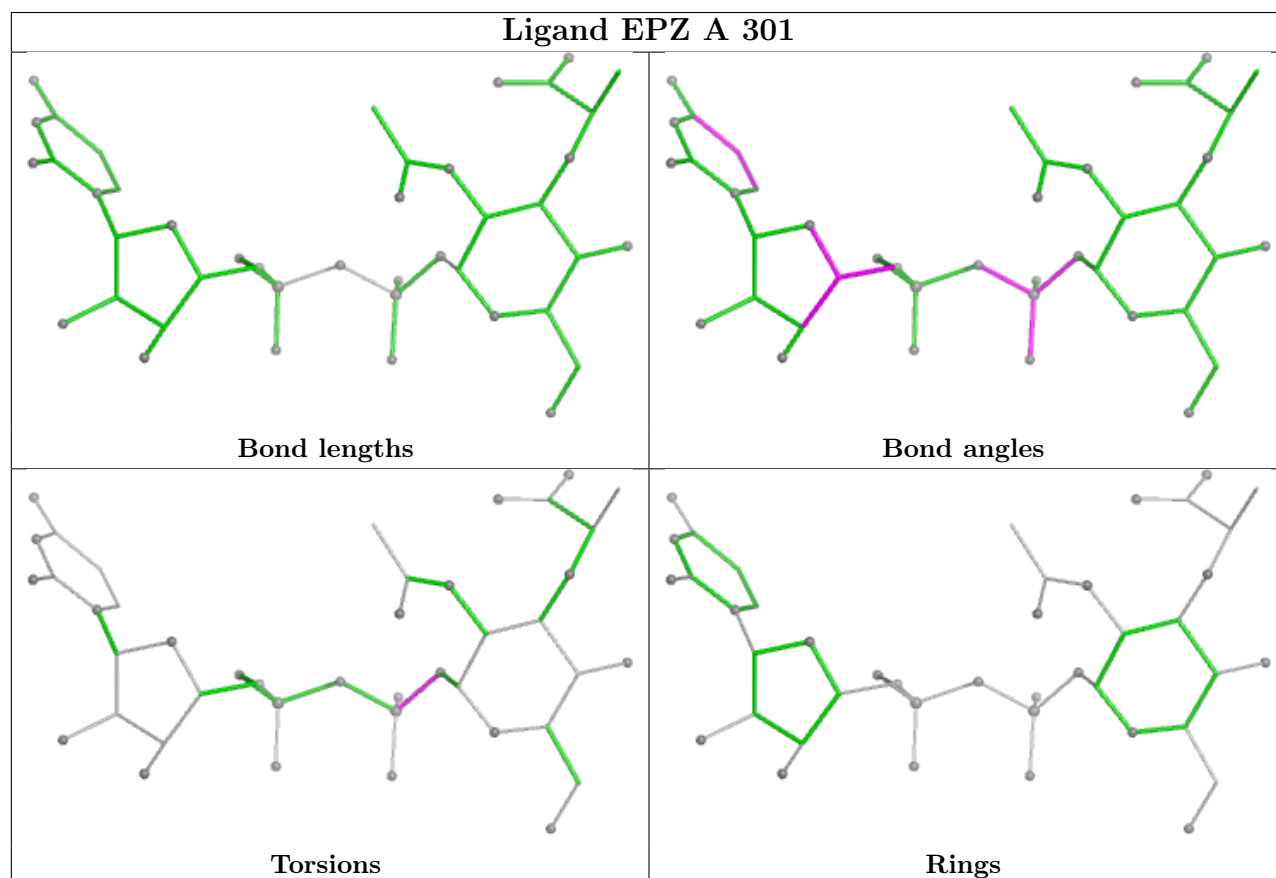
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	302	GOL	6	0

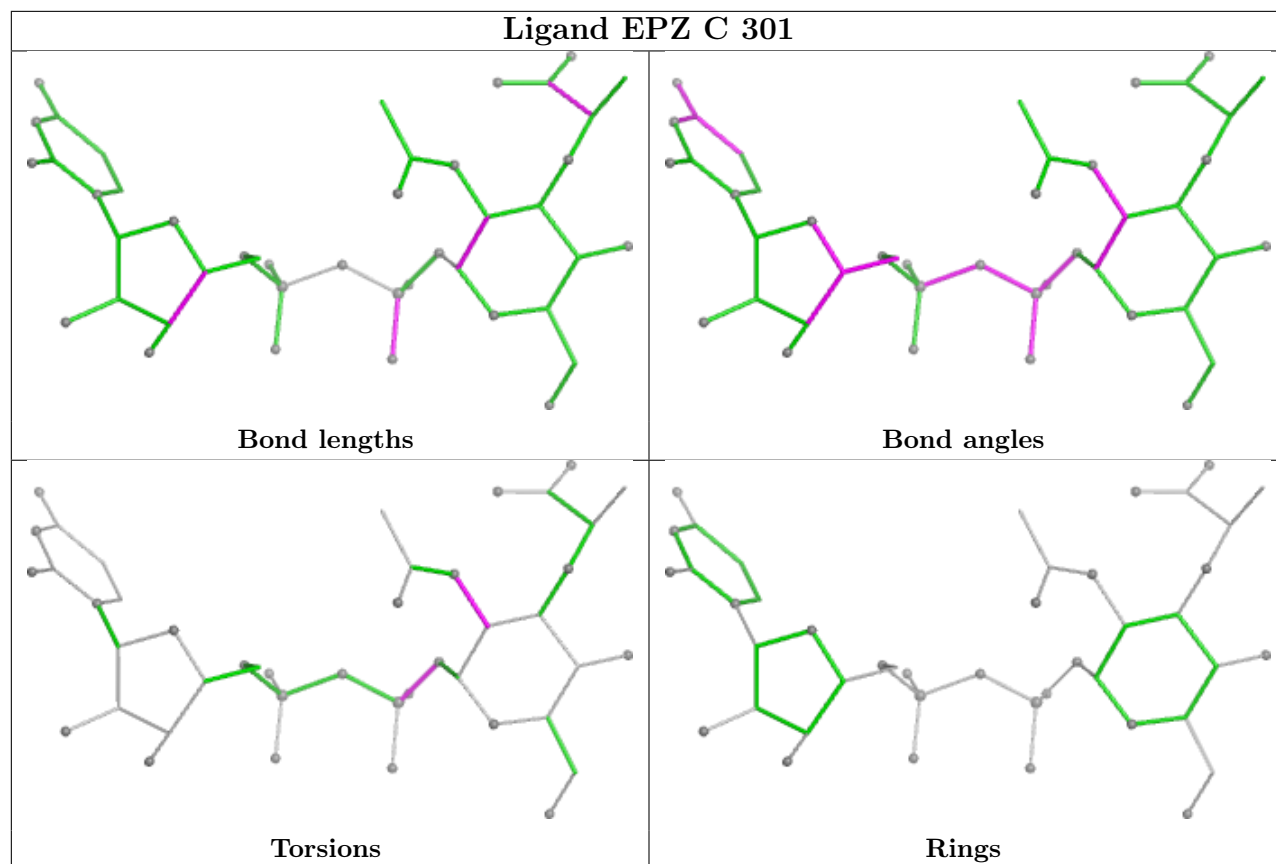
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

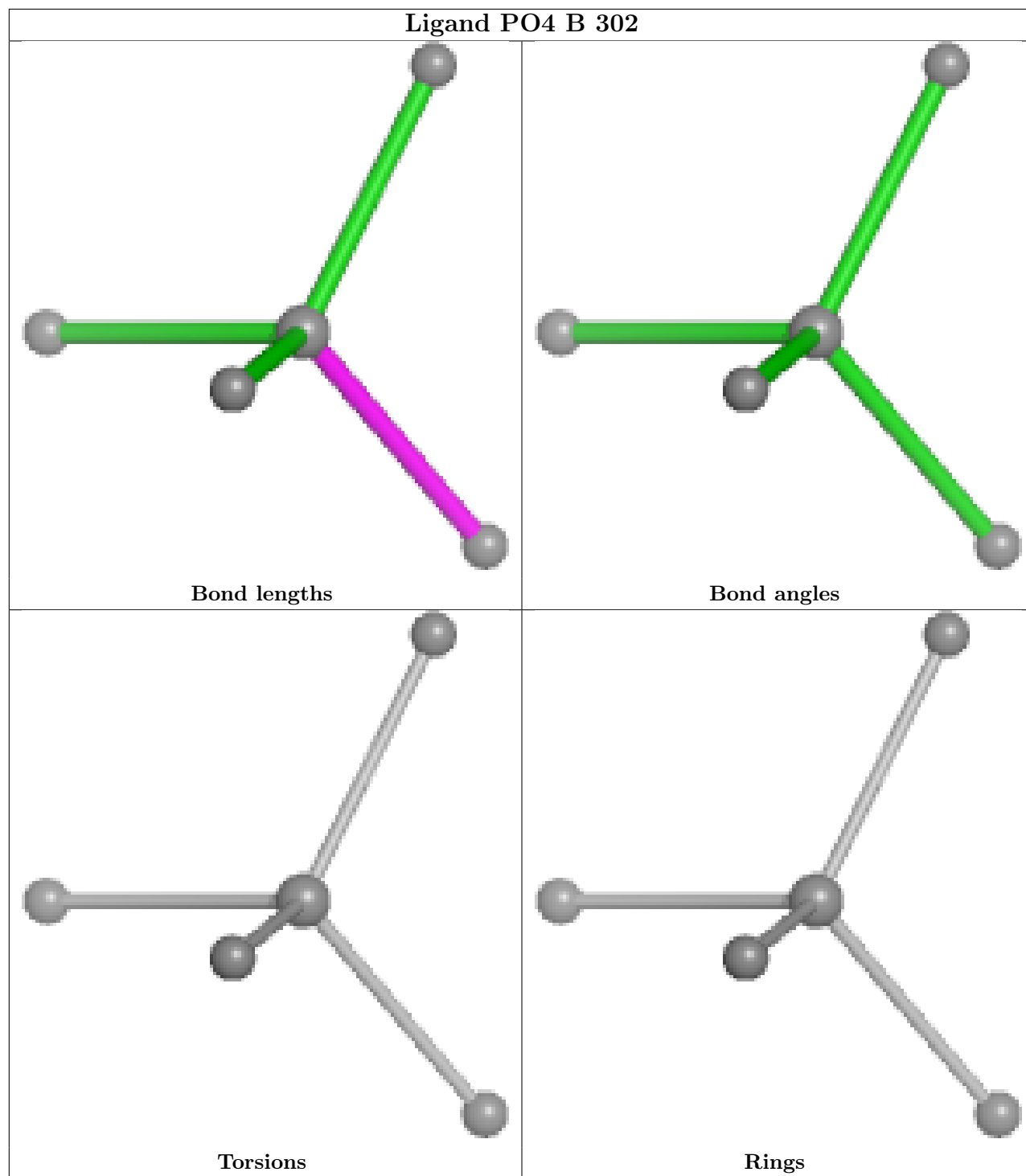
Ligand EPZ B 303



Ligand EPZ A 301







5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	225/239 (94%)	0.30	5 (2%) 62 66	24, 32, 56, 101	0
1	B	223/239 (93%)	0.22	7 (3%) 51 55	24, 32, 52, 94	0
1	C	224/239 (93%)	0.16	4 (1%) 67 71	22, 31, 50, 74	0
All	All	672/717 (93%)	0.23	16 (2%) 59 63	22, 32, 54, 101	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	ALA	5.5
1	A	156	GLY	3.5
1	B	156	GLY	3.5
1	A	118	HIS	3.4
1	A	-1	SER	3.0

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](#)

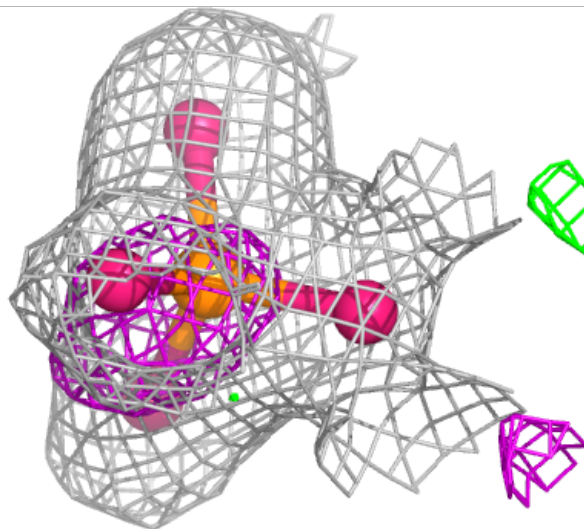
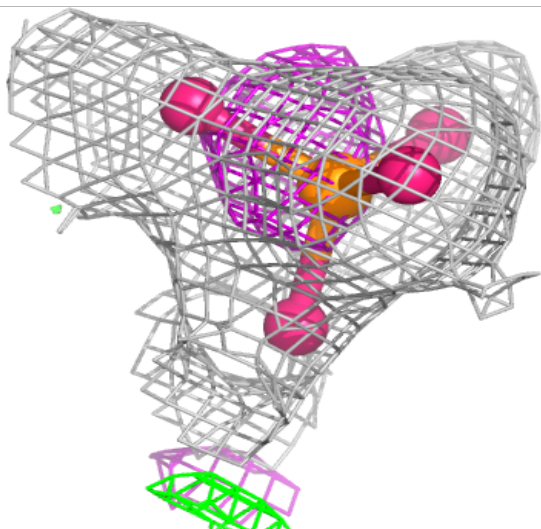
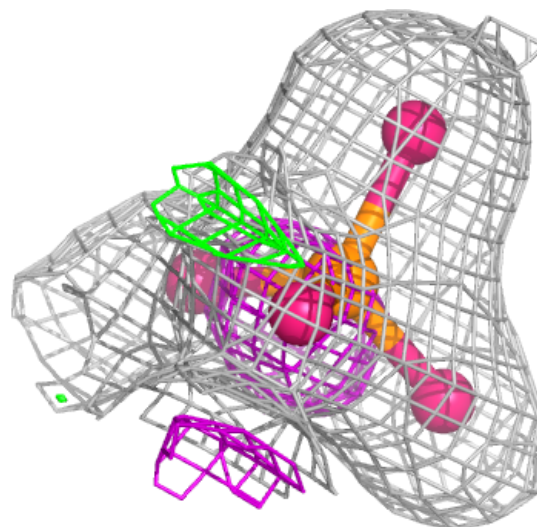
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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
6	PO4	B	302	5/5	0.87	0.12	30,44,51,55	0
5	GOL	B	304	6/6	0.91	0.12	33,46,49,56	0
5	GOL	A	302	6/6	0.91	0.11	33,44,49,51	0
4	MN	C	304	1/1	0.93	0.11	75,75,75,75	0
4	MN	A	305	1/1	0.94	0.12	64,64,64,64	0
2	EPZ	B	303	44/44	0.96	0.07	24,27,34,38	0
2	EPZ	C	301	44/44	0.96	0.07	24,28,36,39	0
2	EPZ	A	301	44/44	0.96	0.07	25,29,35,43	0
3	CL	C	302	1/1	0.97	0.08	39,39,39,39	0
3	CL	A	303	1/1	0.98	0.10	36,36,36,36	0
3	CL	B	301	1/1	0.98	0.06	32,32,32,32	0
4	MN	B	306	1/1	0.98	0.11	50,50,50,50	0
4	MN	C	303	1/1	0.99	0.05	30,30,30,30	0
4	MN	B	305	1/1	0.99	0.03	28,28,28,28	0
4	MN	A	304	1/1	0.99	0.04	29,29,29,29	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.

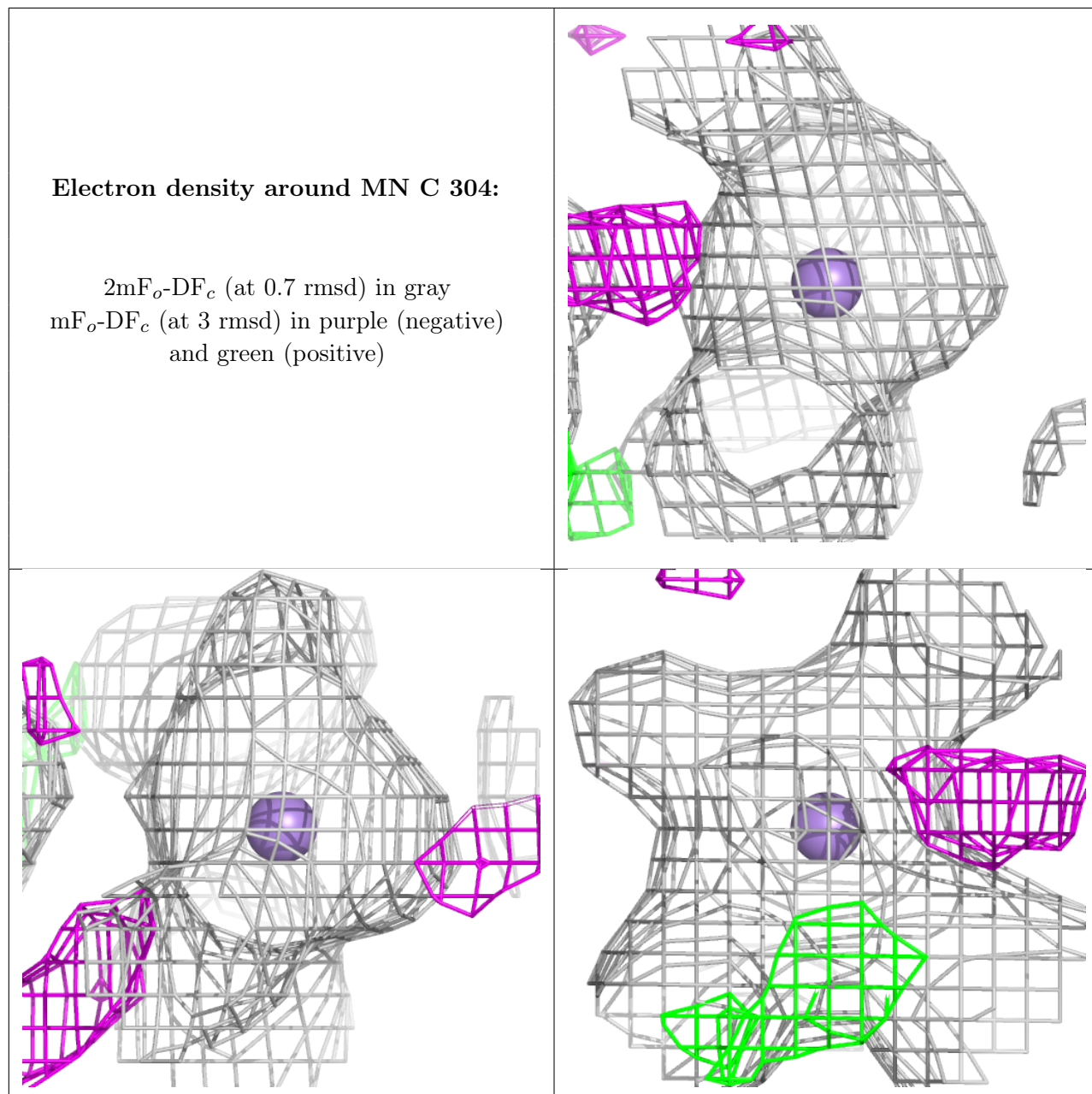
Electron density around PO4 B 302:

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



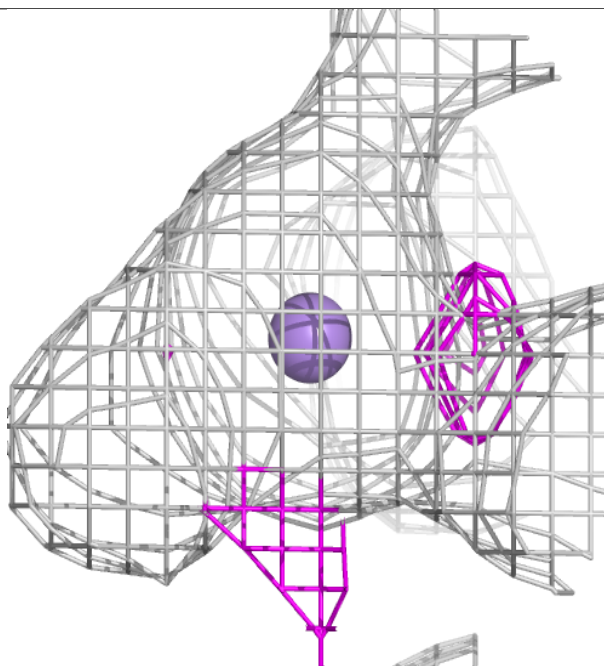
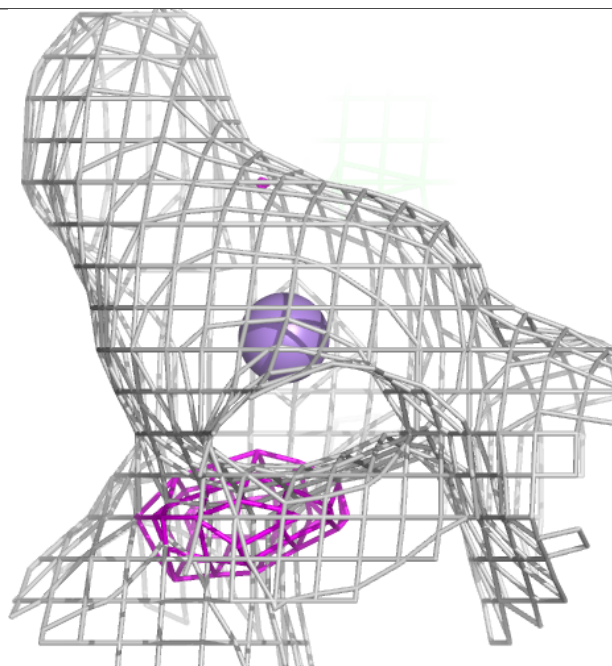
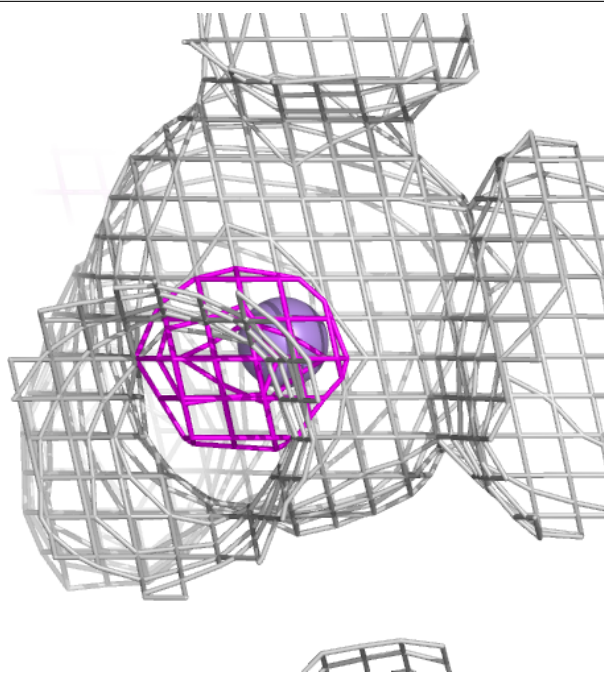
Electron density around MN C 304:

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



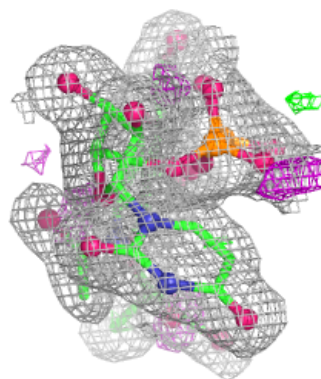
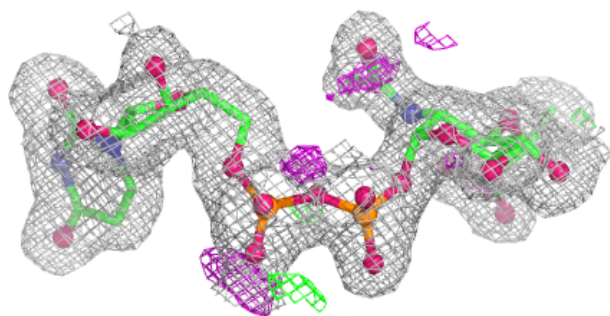
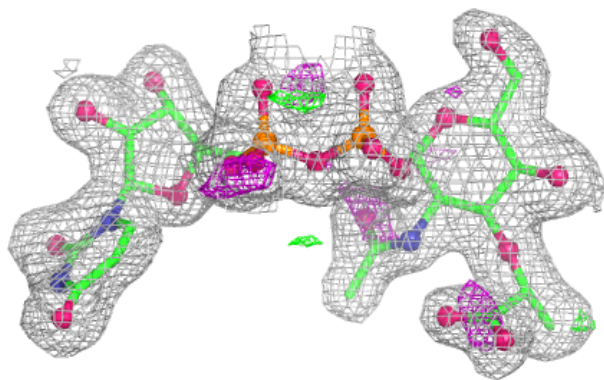
Electron density around MN A 305:

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

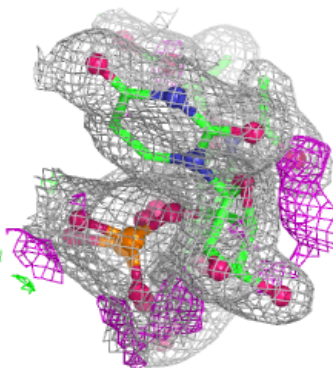
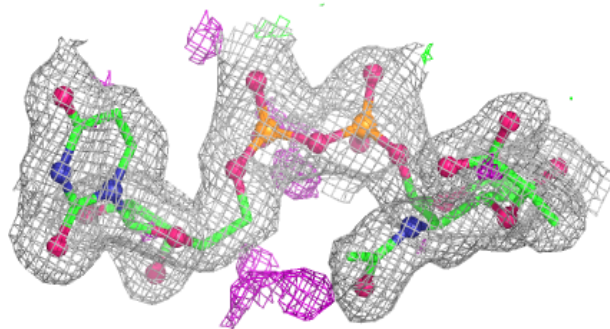
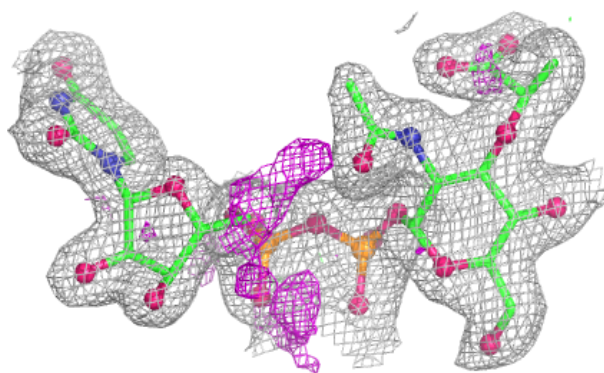


Electron density around EPZ B 303:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

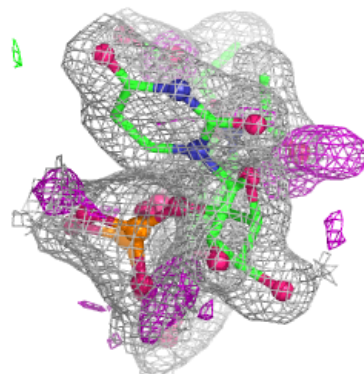
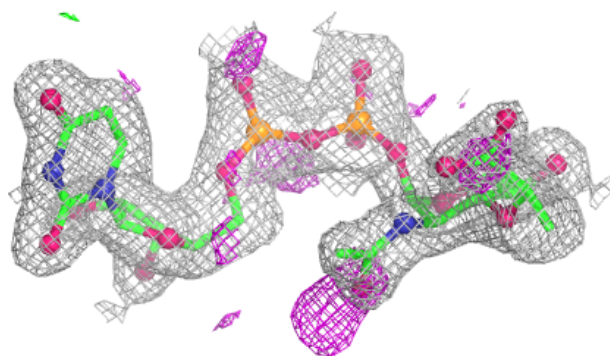
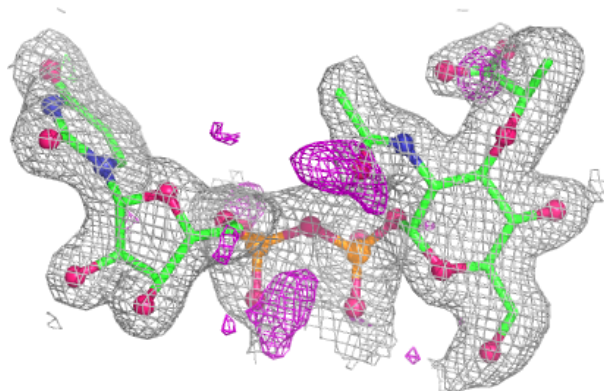
**Electron density around EPZ C 301:**

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



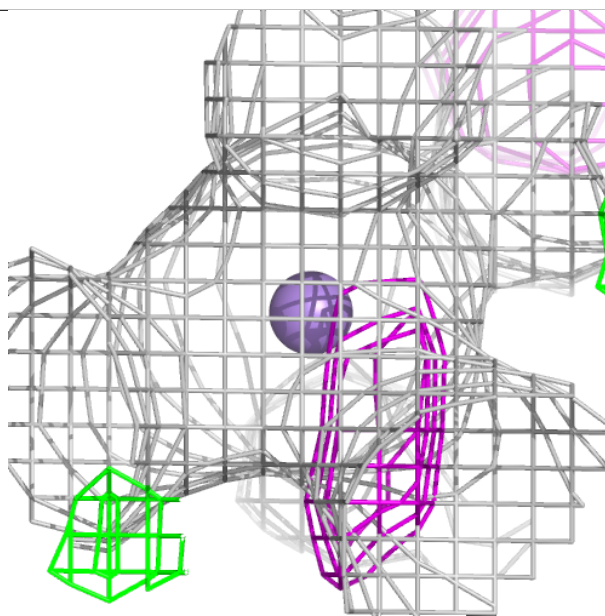
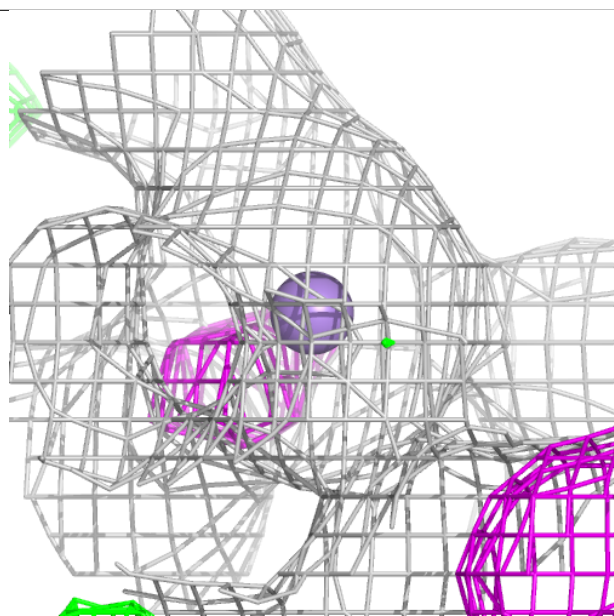
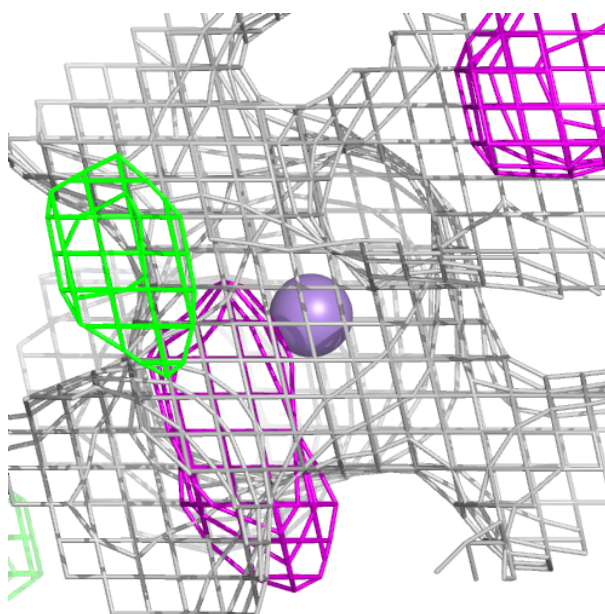
Electron density around EPZ A 301:

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



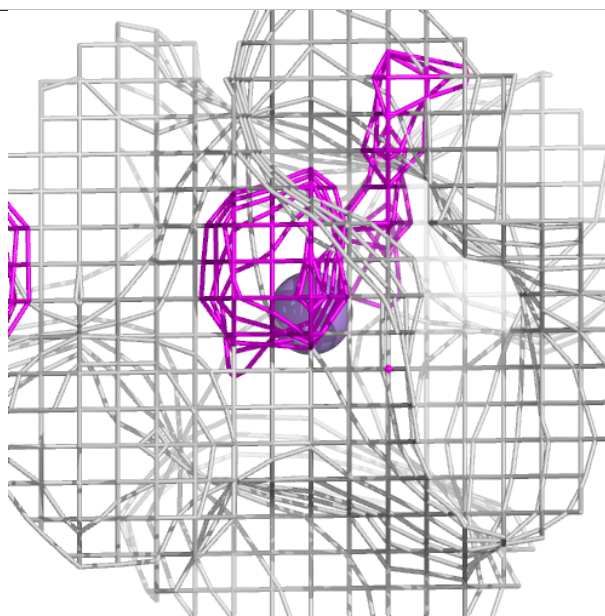
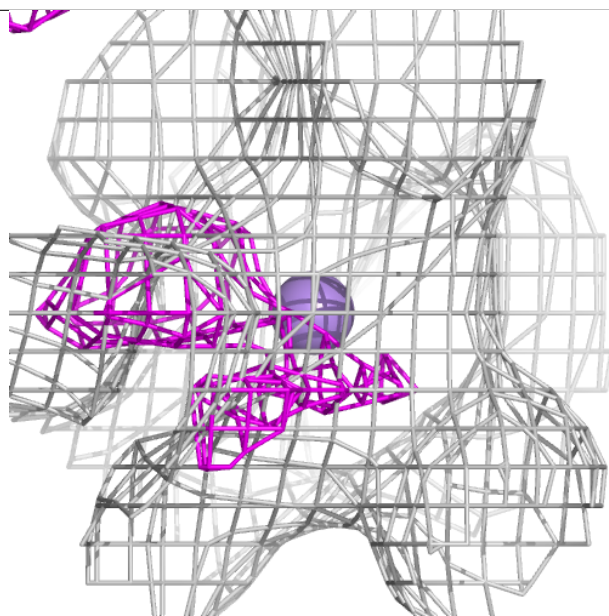
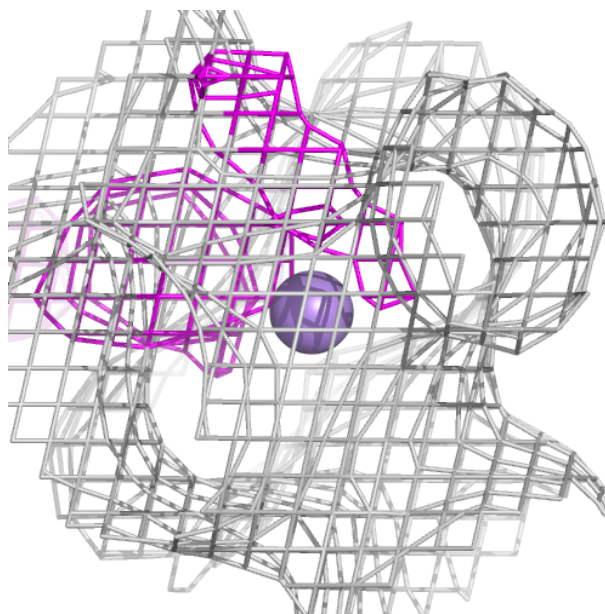
Electron density around MN B 306:

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



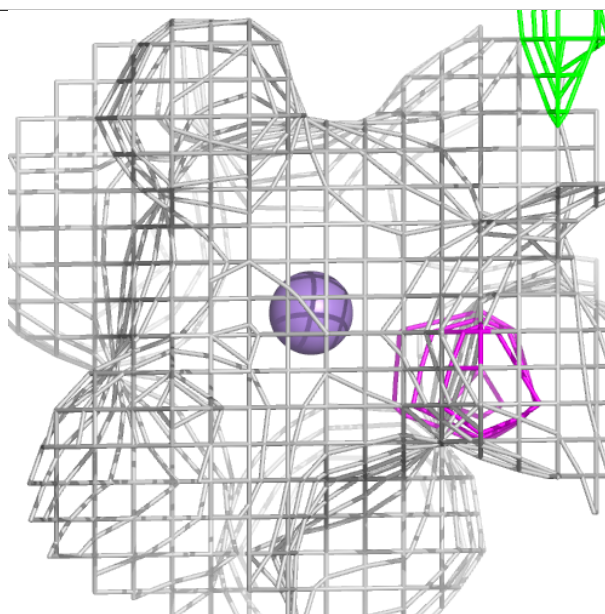
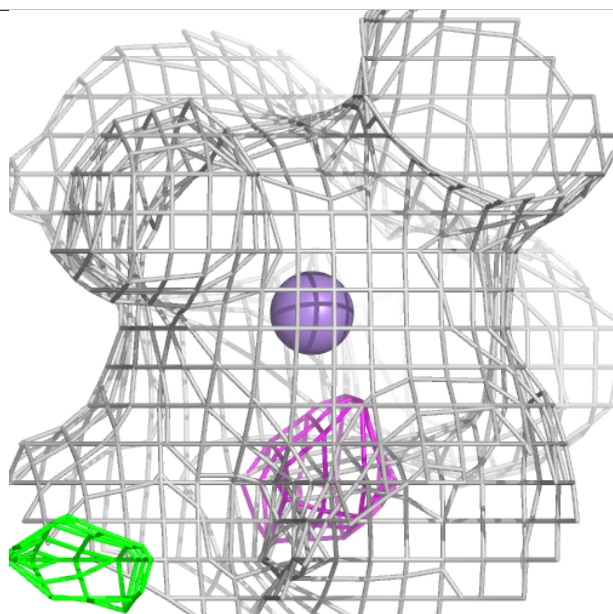
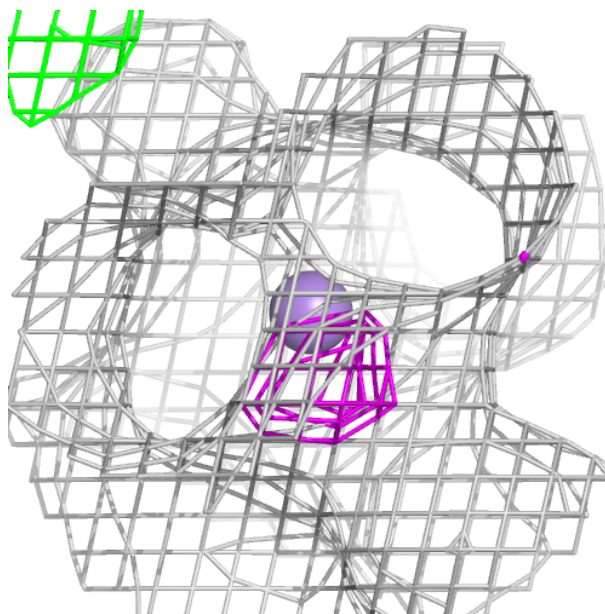
Electron density around MN C 303:

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



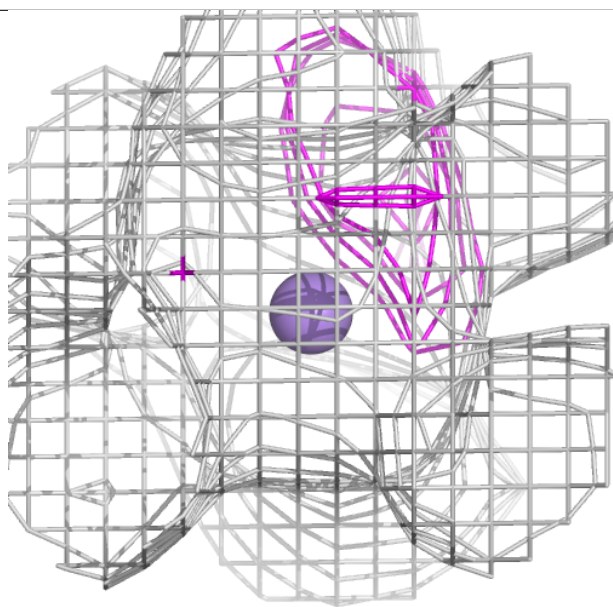
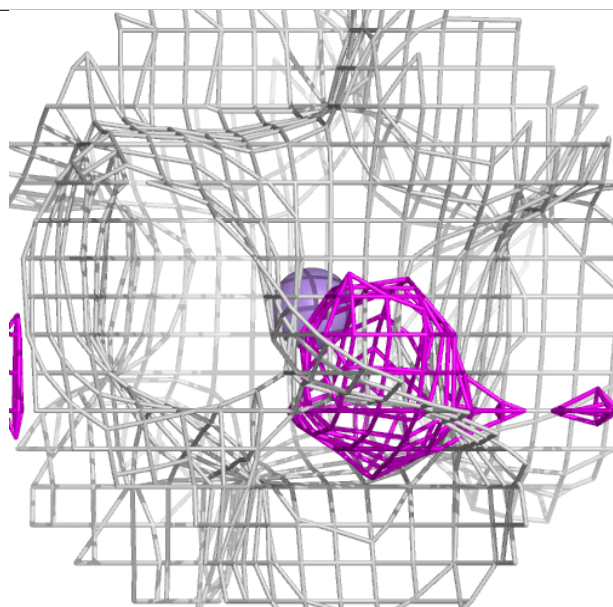
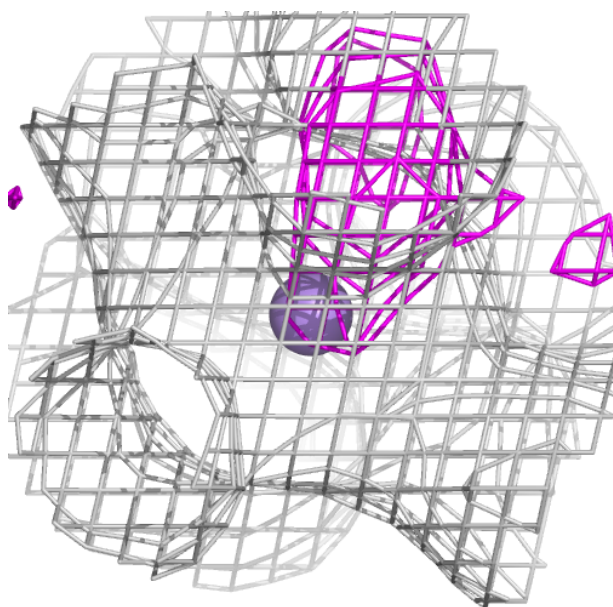
Electron density around MN B 305:

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



Electron density around MN A 304:

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.