



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:07 PM UTC

PDB ID : 8IQD / pdb_00008iqd
Title : Crystal structure of AsfvPrimPol N-terminal Prim/Pol domain in complex with Mn²⁺ and dCTP
Authors : Shao, Z.W.; Gan, J.H.
Deposited on : 2023-03-16
Resolution : 2.39 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

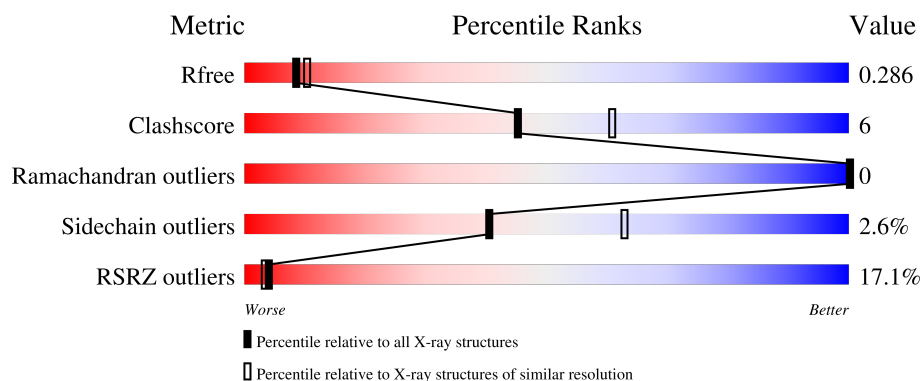
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	254	9% 73% 14% . 12%
1	B	254	10% 78% 12% 10%
1	C	254	21% 86% 11% .
1	D	254	23% 77% 18% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6931 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 Putative primase C962R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1653	1061	278	307	7			
1	B	229	Total	C	N	O	S	0	0	0
			1701	1087	292	315	7			
1	C	247	Total	C	N	O	S	0	0	0
			1753	1115	301	330	7			
1	D	244	Total	C	N	O	S	0	0	0
			1711	1089	295	320	7			

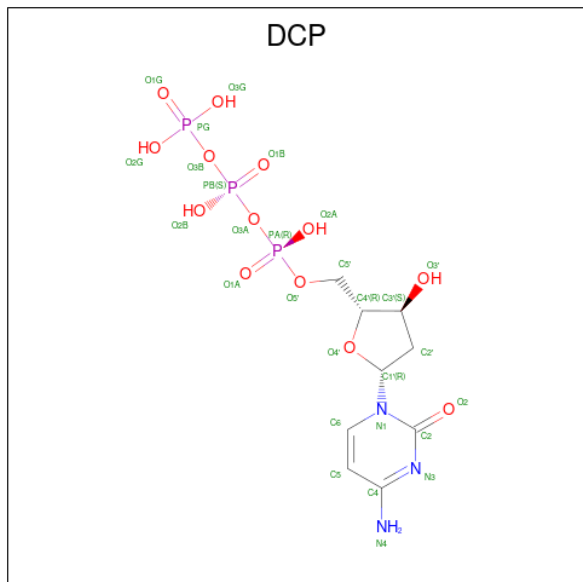
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP A0A0C5B022
A	20	SER	-	expression tag	UNP A0A0C5B022
B	19	GLY	-	expression tag	UNP A0A0C5B022
B	20	SER	-	expression tag	UNP A0A0C5B022
C	19	GLY	-	expression tag	UNP A0A0C5B022
C	20	SER	-	expression tag	UNP A0A0C5B022
D	19	GLY	-	expression tag	UNP A0A0C5B022
D	20	SER	-	expression tag	UNP A0A0C5B022

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	4	Total	Mn	0	0
			4	4		
2	C	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		

- Molecule 3 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: $\text{C}_9\text{H}_{16}\text{N}_3\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 28	C 9	N 3	O 13 P 3	0	0
3	B	1	Total 28	C 9	N 3	O 13 P 3	0	0
3	C	1	Total 9	O 7	P 2		0	0
3	D	1	Total 13	O 10	P 3		0	0

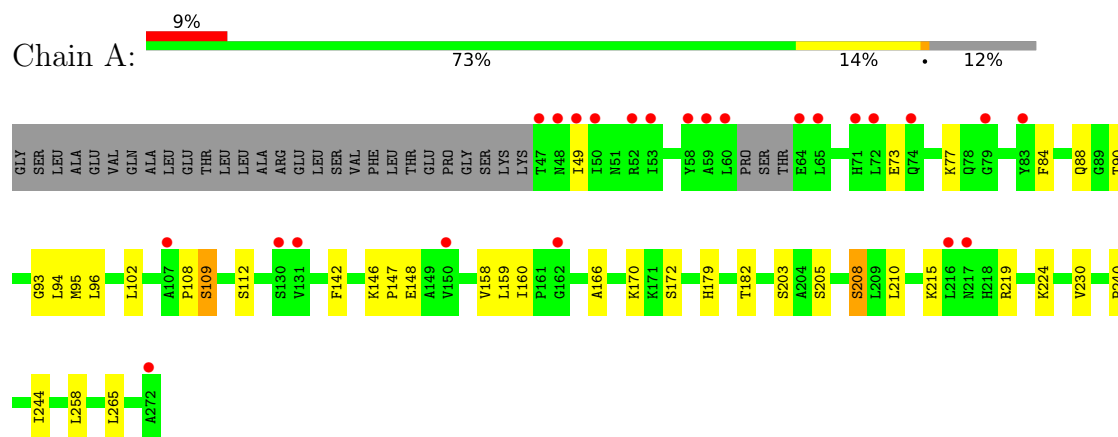
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	5	Total O 5 5	0	0
4	C	3	Total O 3 3	0	0
4	D	2	Total O 2 2	0	0

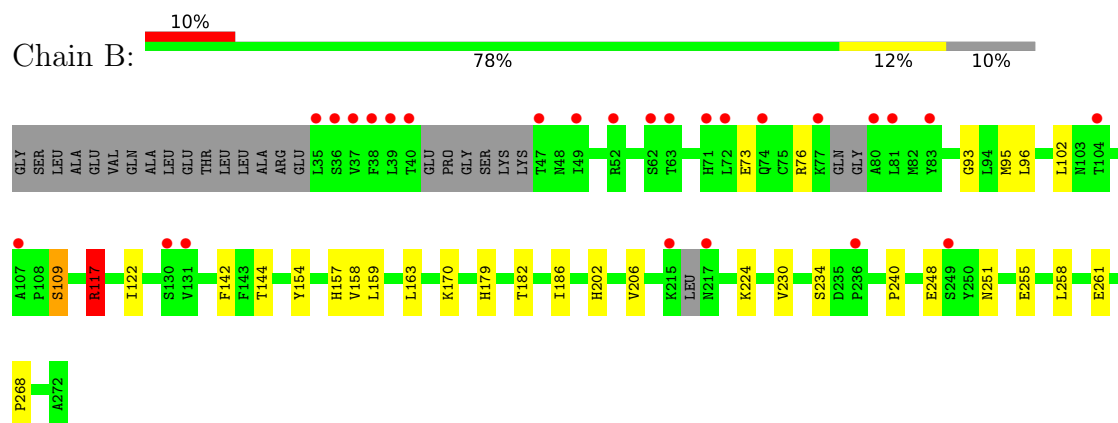
3 Residue-property plots

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.

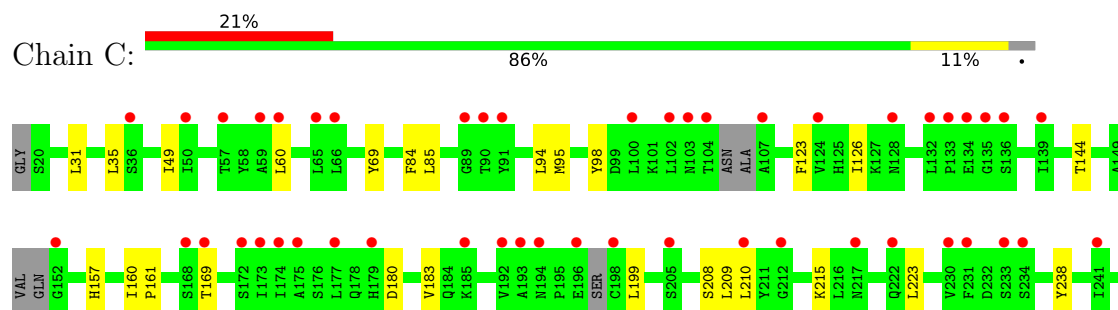
• Molecule 1: Putative primase C962R

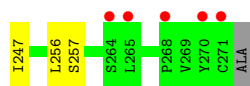


• Molecule 1: Putative primase C962R

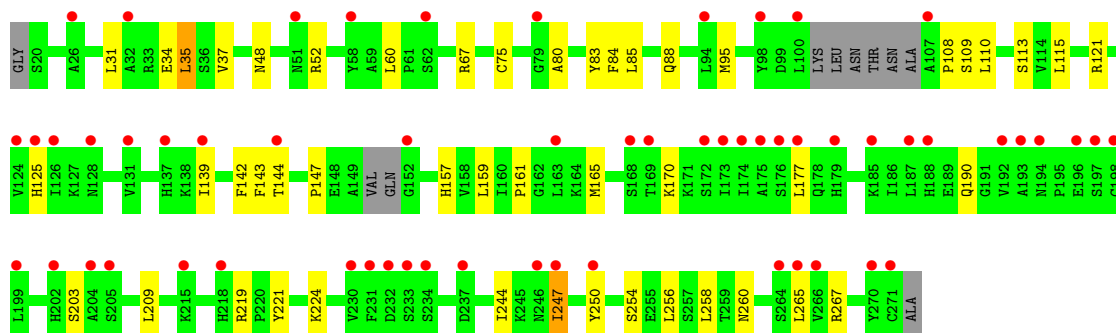
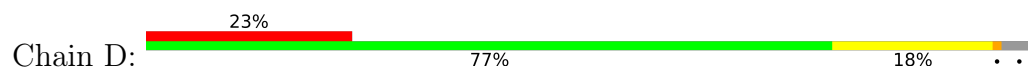


• Molecule 1: Putative primase C962R





● Molecule 1: Putative primase C962R



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	209.16Å 42.81Å 128.21Å 90.00° 125.04° 90.00°	Depositor
Resolution (Å)	85.62 – 2.39 85.62 – 2.39	Depositor EDS
% Data completeness (in resolution range)	97.0 (85.62-2.39) 97.0 (85.62-2.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.19.1_4122: ???)	Depositor
R, R_{free}	0.241 , 0.283 0.244 , 0.286	Depositor DCC
R_{free} test set	1798 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6931	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 70.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8572e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DCP, MN

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	0.16	0/1691	0.33	0/2300
1	B	0.15	0/1738	0.31	0/2361
1	C	0.14	0/1789	0.32	0/2432
1	D	0.16	0/1746	0.34	0/2376
All	All	0.15	0/6964	0.32	0/9469

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	117	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	1653	0	1561	20	0
1	B	1701	0	1589	19	0
1	C	1753	0	1545	17	0
1	D	1711	0	1506	24	0
2	A	3	0	0	0	0
2	B	4	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	28	0	12	1	0
3	B	28	0	12	1	0
3	C	9	0	0	2	0
3	D	13	0	0	0	0
4	A	14	0	0	0	0
4	B	5	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
All	All	6931	0	6225	78	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 6.

All (78) 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:D:95:MET:HB2	1:D:258:LEU:HD11	1.70	0.73
1:A:102:LEU:HD21	1:A:108:PRO:HD3	1.82	0.60
1:A:142:PHE:HB2	1:A:159:LEU:HB2	1.84	0.58
1:A:93:GLY:O	1:A:170:LYS:NZ	2.36	0.58
1:D:31:LEU:HD11	1:D:84:PHE:HZ	1.69	0.57
1:C:31:LEU:HA	1:C:35:LEU:HB2	1.87	0.57
1:D:165:MET:HE3	1:D:170:LYS:HA	1.87	0.56
1:C:157:HIS:NE2	3:C:303:DCP:O1G	2.35	0.55
1:B:142:PHE:HB2	1:B:159:LEU:HB2	1.88	0.54
1:A:109:SER:O	1:A:224:LYS:NZ	2.41	0.53
1:A:95:MET:HE2	1:A:208:SER:HB2	1.91	0.53
1:B:95:MET:HB2	1:B:258:LEU:HD11	1.90	0.53
1:C:223:LEU:HD21	1:C:247:ILE:HD13	1.91	0.53
1:A:146:LYS:HD3	1:A:148:GLU:O	2.10	0.52
1:C:180:ASP:HB3	1:C:183:VAL:HB	1.93	0.50
1:A:49:ILE:HD12	1:A:210:LEU:HD11	1.93	0.50
1:B:122:ILE:HD13	1:B:158:VAL:HG11	1.93	0.50
1:A:147:PRO:HG2	1:A:219:ARG:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:GLN:NE2	1:D:203:SER:O	2.42	0.50
1:C:210:LEU:HD23	1:C:257:SER:HB2	1.94	0.50
1:B:102:LEU:HD11	1:B:154:TYR:HB2	1.93	0.49
1:A:95:MET:HB2	1:A:258:LEU:HD11	1.95	0.49
1:A:230:VAL:O	1:A:240:PRO:HD2	2.12	0.49
1:C:215:LYS:NZ	3:C:303:DCP:O3A	2.43	0.49
1:D:144:THR:OG1	1:D:157:HIS:HB2	2.13	0.48
1:B:93:GLY:O	1:B:170:LYS:NZ	2.39	0.48
1:A:182:THR:OG1	1:B:179:HIS:ND1	2.34	0.48
1:A:73:GLU:HG3	1:A:77:LYS:HE2	1.96	0.48
1:B:248:GLU:H	1:B:248:GLU:CD	2.21	0.48
1:C:85:LEU:HG	1:C:209:LEU:HD23	1.95	0.48
1:D:244:ILE:HB	1:D:247:ILE:HD12	1.96	0.47
1:D:147:PRO:HG2	1:D:219:ARG:HB3	1.97	0.47
1:C:69:TYR:CE1	1:C:210:LEU:HD22	2.49	0.47
1:C:123:PHE:HA	1:C:126:ILE:HB	1.96	0.47
1:B:109:SER:O	1:B:224:LYS:NZ	2.46	0.46
1:D:125:HIS:CD2	1:D:177:LEU:HA	2.50	0.46
1:D:161:PRO:HG3	1:D:256:LEU:HA	1.98	0.46
1:D:144:THR:HB	1:D:221:TYR:HB3	1.97	0.45
1:C:98:TYR:CE1	1:C:199:LEU:HD13	2.52	0.45
1:D:267:ARG:HA	1:D:267:ARG:HE	1.81	0.45
1:A:88:GLN:NE2	1:A:203:SER:O	2.47	0.45
1:D:110:LEU:O	1:D:224:LYS:NZ	2.50	0.45
1:D:34:GLU:OE1	1:D:67:ARG:NH2	2.48	0.45
1:B:230:VAL:O	1:B:240:PRO:HD2	2.17	0.45
1:D:52:ARG:HB3	1:D:83:TYR:HB3	2.00	0.44
1:D:142:PHE:HB2	1:D:159:LEU:HB2	2.00	0.44
1:C:161:PRO:HG3	1:C:256:LEU:HA	1.99	0.44
1:D:115:LEU:HD22	1:D:143:PHE:CD2	2.53	0.44
1:B:202:HIS:O	1:B:206:VAL:HG13	2.18	0.44
1:A:244:ILE:HD13	1:A:265:LEU:HD21	1.99	0.44
1:B:144:THR:OG1	1:B:157:HIS:HB2	2.18	0.44
1:A:215:LYS:HG2	3:A:304:DCP:C5	2.48	0.44
1:A:84:PHE:HB3	1:A:210:LEU:HD12	2.00	0.43
1:D:254:SER:OG	1:D:260:ASN:ND2	2.51	0.43
1:D:85:LEU:HG	1:D:209:LEU:HD23	2.01	0.43
1:A:94:LEU:HD23	1:A:160:ILE:HD13	2.00	0.43
1:C:144:THR:OG1	1:C:157:HIS:HB2	2.19	0.43
1:A:96:LEU:HB2	1:A:158:VAL:HB	2.01	0.43
1:C:49:ILE:HG13	1:C:60:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ASN:O	1:B:255:GLU:HG2	2.19	0.42
1:A:90:THR:O	1:A:166:ALA:HA	2.20	0.42
1:D:75:CYS:HB3	1:D:80:ALA:HB3	2.01	0.42
1:D:48:ASN:ND2	1:D:60:LEU:O	2.52	0.42
1:B:96:LEU:HB2	1:B:158:VAL:HB	2.02	0.42
1:C:94:LEU:HD23	1:C:160:ILE:HD13	2.02	0.42
1:D:31:LEU:HA	1:D:35:LEU:HB2	2.02	0.41
3:B:305:DCP:H6	3:B:305:DCP:H2'1	1.73	0.41
1:C:31:LEU:HD11	1:C:84:PHE:HZ	1.85	0.41
1:D:250:TYR:CE2	1:D:265:LEU:HB2	2.55	0.41
1:C:31:LEU:HD23	1:C:35:LEU:HD12	2.02	0.41
1:D:121:ARG:HA	1:D:121:ARG:HD2	1.79	0.41
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.80	0.41
1:D:108:PRO:HB3	1:D:190:GLN:O	2.21	0.41
1:B:117:ARG:NE	1:B:186:ILE:HD11	2.35	0.41
1:B:73:GLU:CD	1:B:76:ARG:HH21	2.28	0.41
1:B:261:GLU:HA	1:B:268:PRO:HG3	2.03	0.41
1:A:179:HIS:ND1	1:B:182:THR:OG1	2.48	0.40
1:B:117:ARG:HG2	1:C:238:TYR:CZ	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	219/254 (86%)	216 (99%)	3 (1%)	0	100	100
1	B	221/254 (87%)	220 (100%)	1 (0%)	0	100	100
1	C	239/254 (94%)	237 (99%)	2 (1%)	0	100	100
1	D	238/254 (94%)	234 (98%)	4 (2%)	0	100	100
All	All	917/1016 (90%)	907 (99%)	10 (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	A	168/225 (75%)	163 (97%)	5 (3%)	36	58
1	B	171/225 (76%)	168 (98%)	3 (2%)	51	73
1	C	162/225 (72%)	159 (98%)	3 (2%)	50	71
1	D	155/225 (69%)	149 (96%)	6 (4%)	28	48
All	All	656/900 (73%)	639 (97%)	17 (3%)	40	63

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	SER
1	A	112	SER
1	A	172	SER
1	A	205	SER
1	A	208	SER
1	B	109	SER
1	B	117	ARG
1	B	234	SER
1	C	95	MET
1	C	169	THR
1	C	208	SER
1	D	35	LEU
1	D	37	VAL
1	D	109	SER
1	D	113	SER
1	D	139	ILE
1	D	247	ILE

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	242	HIS
1	C	120	HIS
1	C	222	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 15 ligands modelled in this entry, 11 are 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	DCP	B	305	2	28,29,29	0.99	1 (3%)	41,45,45	1.16	4 (9%)
3	DCP	C	303	2	6,8,29	0.97	0	12,13,45	0.91	0
3	DCP	D	303	2	10,12,29	1.15	0	17,20,45	0.85	0
3	DCP	A	304	2	28,29,29	1.05	3 (10%)	41,45,45	1.24	5 (12%)

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	DCP	B	305	2	-	14/22/34/34	0/2/2/2
3	DCP	C	303	2	-	0/6/6/34	-
3	DCP	D	303	2	-	3/12/12/34	-
3	DCP	A	304	2	-	13/22/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	304	DCP	C4-N3	2.22	1.39	1.34
3	A	304	DCP	PB-O3B	2.20	1.61	1.59
3	A	304	DCP	PA-O3A	2.14	1.61	1.59
3	B	305	DCP	PA-O3A	2.01	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	305	DCP	O4'-C1'-N1	3.58	114.22	107.86
3	A	304	DCP	N4-C4-N3	2.97	123.23	117.91
3	A	304	DCP	O4'-C1'-N1	2.82	112.86	107.86
3	B	305	DCP	O2-C2-N3	-2.75	117.99	122.33
3	A	304	DCP	O2-C2-N3	-2.67	118.11	122.33
3	A	304	DCP	C1'-N1-C2	2.66	122.39	117.83
3	A	304	DCP	C5-C4-N3	-2.43	117.22	121.32
3	B	305	DCP	O2B-PB-O3B	2.04	112.78	107.27
3	B	305	DCP	O2G-PG-O3B	2.02	111.42	104.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	304	DCP	O4'-C1'-N1-C2
3	A	304	DCP	O4'-C1'-N1-C6
3	A	304	DCP	O4'-C4'-C5'-O5'
3	B	305	DCP	O4'-C1'-N1-C2
3	B	305	DCP	C3'-C4'-C5'-O5'
3	B	305	DCP	O4'-C4'-C5'-O5'
3	B	305	DCP	C5'-O5'-PA-O1A
3	B	305	DCP	C5'-O5'-PA-O2A
3	D	303	DCP	PB-O3B-PG-O2G
3	B	305	DCP	O4'-C1'-N1-C6
3	A	304	DCP	C3'-C4'-C5'-O5'

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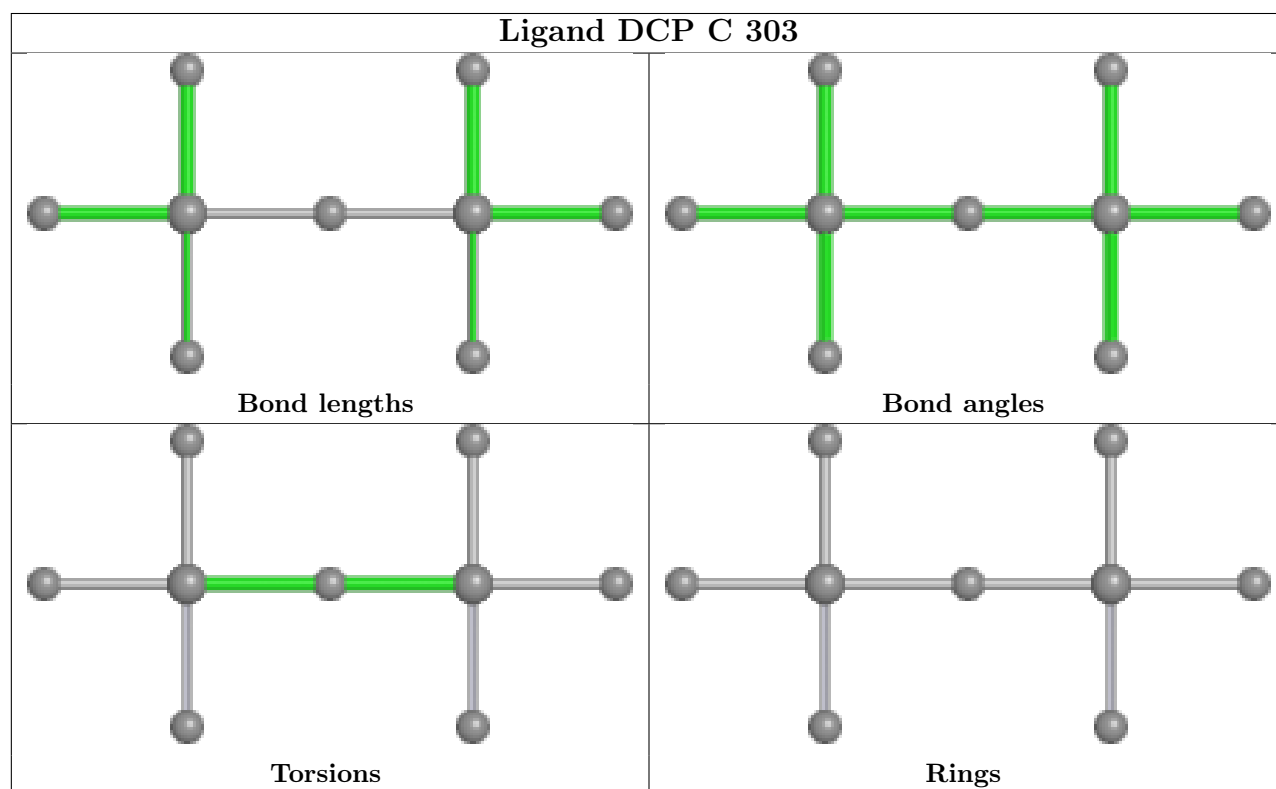
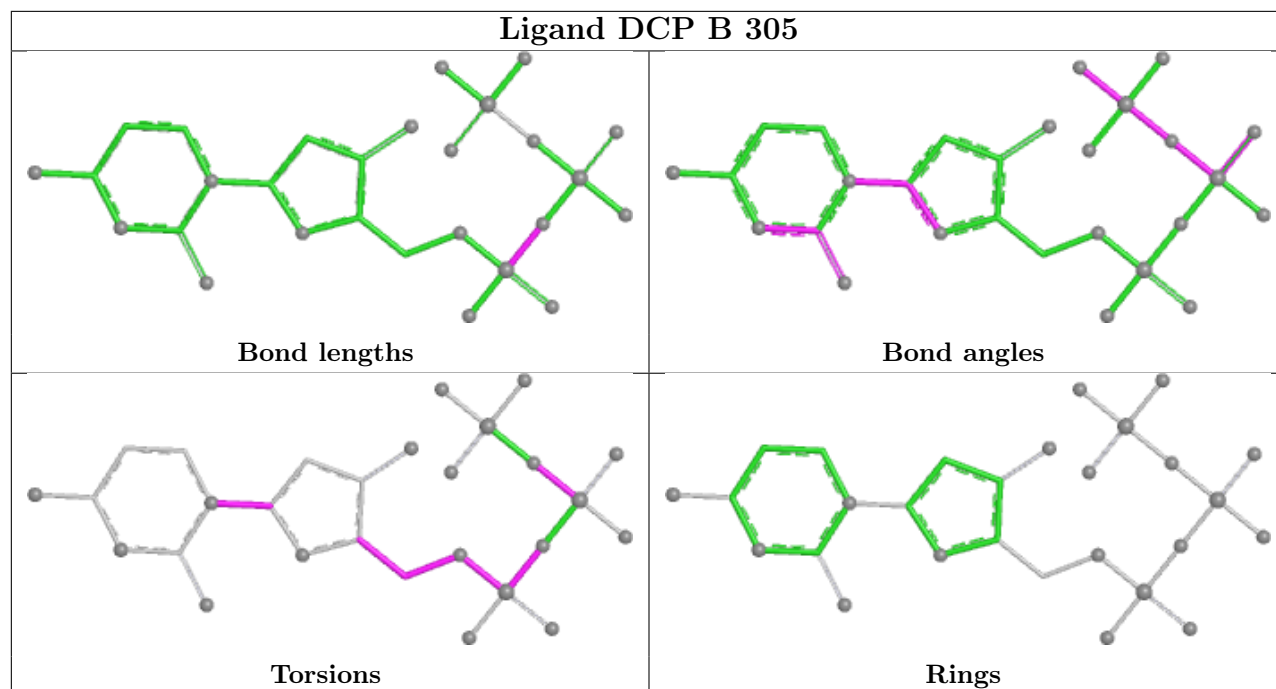
Mol	Chain	Res	Type	Atoms
3	B	305	DCP	C2'-C1'-N1-C6
3	D	303	DCP	PA-O3A-PB-O1B
3	A	304	DCP	C2'-C1'-N1-C6
3	A	304	DCP	PB-O3A-PA-O1A
3	B	305	DCP	PB-O3A-PA-O2A
3	B	305	DCP	C2'-C1'-N1-C2
3	A	304	DCP	C5'-O5'-PA-O1A
3	A	304	DCP	C5'-O5'-PA-O2A
3	A	304	DCP	C5'-O5'-PA-O3A
3	B	305	DCP	C5'-O5'-PA-O3A
3	B	305	DCP	C4'-C5'-O5'-PA
3	A	304	DCP	C4'-C5'-O5'-PA
3	D	303	DCP	PB-O3B-PG-O1G
3	A	304	DCP	PG-O3B-PB-O2B
3	B	305	DCP	PB-O3A-PA-O1A
3	B	305	DCP	PG-O3B-PB-O1B
3	B	305	DCP	PG-O3B-PB-O2B
3	A	304	DCP	C2'-C1'-N1-C2
3	A	304	DCP	PB-O3A-PA-O2A

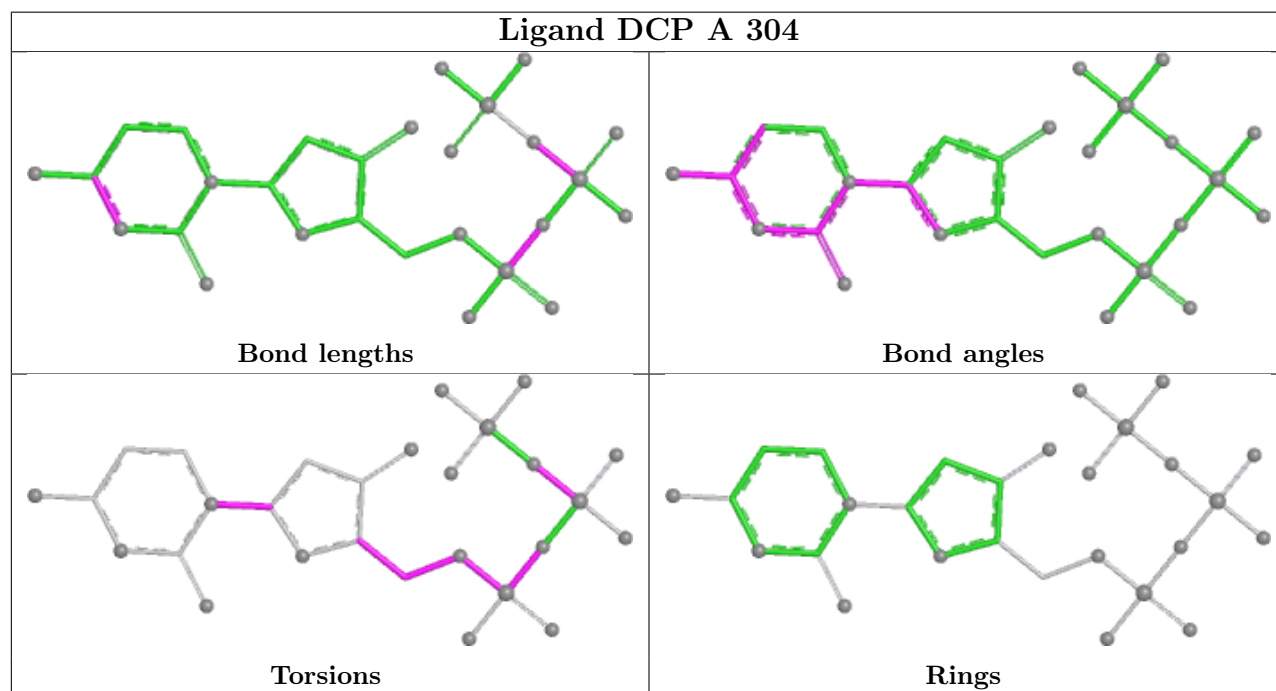
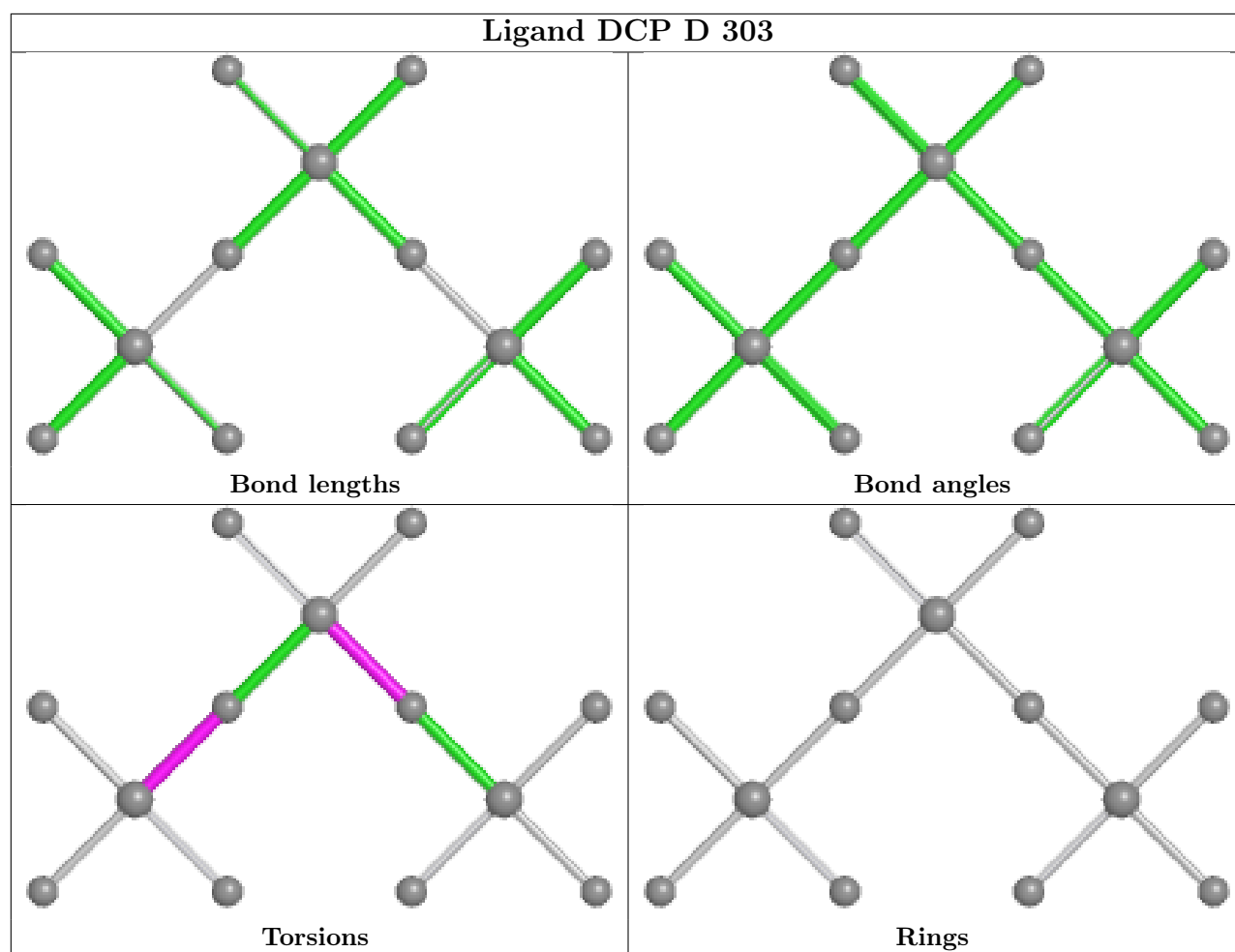
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	305	DCP	1	0
3	C	303	DCP	2	0
3	A	304	DCP	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	223/254 (87%)	0.80	24 (10%) 11 8	29, 43, 65, 73	0
1	B	229/254 (90%)	0.92	26 (11%) 10 7	29, 46, 77, 89	0
1	C	247/254 (97%)	1.34	53 (21%) 2 2	43, 62, 81, 95	0
1	D	244/254 (96%)	1.45	58 (23%) 2 1	42, 62, 82, 90	0
All	All	943/1016 (92%)	1.14	161 (17%) 4 3	29, 56, 80, 95	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	168	SER	6.0
1	B	40	THR	4.8
1	D	271	CYS	4.1
1	D	168	SER	4.0
1	D	270	TYR	4.0
1	D	139	ILE	3.9
1	D	192	VAL	3.9
1	D	199	LEU	3.9
1	D	264	SER	3.8
1	B	217	ASN	3.7
1	A	47	THR	3.6
1	C	90	THR	3.6
1	C	104	THR	3.6
1	C	234	SER	3.6
1	C	264	SER	3.6
1	D	174	ILE	3.6
1	A	53	ILE	3.5
1	C	133	PRO	3.5
1	C	265	LEU	3.5
1	C	103	ASN	3.4
1	B	130	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	177	LEU	3.4
1	D	100	LEU	3.4
1	B	215	LYS	3.3
1	A	216	LEU	3.3
1	B	35	LEU	3.3
1	B	37	VAL	3.3
1	A	272	ALA	3.3
1	C	132	LEU	3.3
1	B	71	HIS	3.2
1	D	124	VAL	3.2
1	C	271	CYS	3.2
1	D	187	LEU	3.2
1	D	152	GLY	3.2
1	D	265	LEU	3.2
1	B	47	THR	3.1
1	B	72	LEU	3.1
1	B	49	ILE	3.1
1	A	83	TYR	3.1
1	D	205	SER	3.1
1	A	79	GLY	3.1
1	D	237	ASP	3.1
1	A	60	LEU	3.1
1	D	32	ALA	3.0
1	D	234	SER	3.0
1	B	38	PHE	3.0
1	A	130	SER	3.0
1	D	233	SER	3.0
1	B	39	LEU	2.9
1	C	134	GLU	2.9
1	C	192	VAL	2.9
1	C	152	GLY	2.9
1	C	102	LEU	2.9
1	D	107	ALA	2.9
1	D	193	ALA	2.9
1	C	36	SER	2.9
1	D	232	ASP	2.9
1	A	71	HIS	2.8
1	B	52	ARG	2.8
1	C	173	ILE	2.8
1	C	198	CYS	2.8
1	A	74	GLN	2.8
1	D	246	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	72	LEU	2.8
1	B	107	ALA	2.8
1	C	210	LEU	2.7
1	A	217	ASN	2.7
1	C	174	ILE	2.7
1	C	230	VAL	2.7
1	C	57	THR	2.7
1	B	81	LEU	2.7
1	D	188	HIS	2.7
1	B	62	SER	2.7
1	C	91	TYR	2.6
1	C	135	GLY	2.6
1	D	204	ALA	2.6
1	A	48	ASN	2.6
1	D	231	PHE	2.6
1	A	58	TYR	2.6
1	C	177	LEU	2.6
1	B	80	ALA	2.6
1	D	250	TYR	2.6
1	C	270	TYR	2.6
1	C	89	GLY	2.5
1	C	212	GLY	2.5
1	C	268	PRO	2.5
1	B	74	GLN	2.5
1	B	36	SER	2.5
1	A	52	ARG	2.5
1	D	79	GLY	2.5
1	D	137	HIS	2.5
1	A	64	GLU	2.5
1	A	50	ILE	2.5
1	D	194	ASN	2.5
1	D	179	HIS	2.5
1	C	172	SER	2.4
1	D	172	SER	2.4
1	C	66	LEU	2.4
1	D	218	HIS	2.4
1	A	107	ALA	2.4
1	A	162	GLY	2.4
1	D	175	ALA	2.4
1	D	94	LEU	2.4
1	D	98	TYR	2.4
1	C	169	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	124	VAL	2.4
1	C	128	ASN	2.3
1	C	185	LYS	2.3
1	B	104	THR	2.3
1	C	136	SER	2.3
1	D	198	CYS	2.3
1	B	63	THR	2.3
1	C	217	ASN	2.3
1	C	205	SER	2.3
1	D	176	SER	2.3
1	C	179	HIS	2.3
1	D	202	HIS	2.3
1	C	50	ILE	2.3
1	B	131	VAL	2.3
1	C	231	PHE	2.3
1	B	249	SER	2.3
1	C	196	GLU	2.3
1	D	128	ASN	2.2
1	D	125	HIS	2.2
1	D	197	SER	2.2
1	C	139	ILE	2.2
1	C	194	ASN	2.2
1	D	185	LYS	2.2
1	A	65	LEU	2.2
1	C	65	LEU	2.2
1	A	150	VAL	2.2
1	C	233	SER	2.2
1	B	83	TYR	2.2
1	D	131	VAL	2.2
1	D	58	TYR	2.1
1	D	173	ILE	2.1
1	D	51	ASN	2.1
1	D	266	VAL	2.1
1	B	77	LYS	2.1
1	C	59	ALA	2.1
1	A	49	ILE	2.1
1	D	126	ILE	2.1
1	D	247	ILE	2.1
1	D	26	ALA	2.1
1	D	62	SER	2.1
1	D	144	THR	2.1
1	D	215	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	163	LEU	2.1
1	D	230	VAL	2.1
1	C	193	ALA	2.1
1	C	241	ILE	2.1
1	B	236	PRO	2.1
1	D	169	THR	2.0
1	C	107	ALA	2.0
1	C	222	GLN	2.0
1	C	60	LEU	2.0
1	A	131	VAL	2.0
1	D	196	GLU	2.0
1	A	59	ALA	2.0
1	C	175	ALA	2.0
1	C	100	LEU	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
2	MN	B	304	1/1	0.70	0.13	98,98,98,98	0
3	DCP	D	303	13/28	0.82	0.12	73,79,91,97	0
3	DCP	C	303	9/28	0.84	0.12	53,62,70,70	0
3	DCP	B	305	28/28	0.85	0.13	50,62,73,75	0
3	DCP	A	304	28/28	0.88	0.14	42,54,66,67	0
2	MN	C	301	1/1	0.94	0.06	77,77,77,77	0
2	MN	D	301	1/1	0.94	0.06	83,83,83,83	0
2	MN	B	302	1/1	0.97	0.05	61,61,61,61	0
2	MN	D	302	1/1	0.97	0.04	76,76,76,76	0

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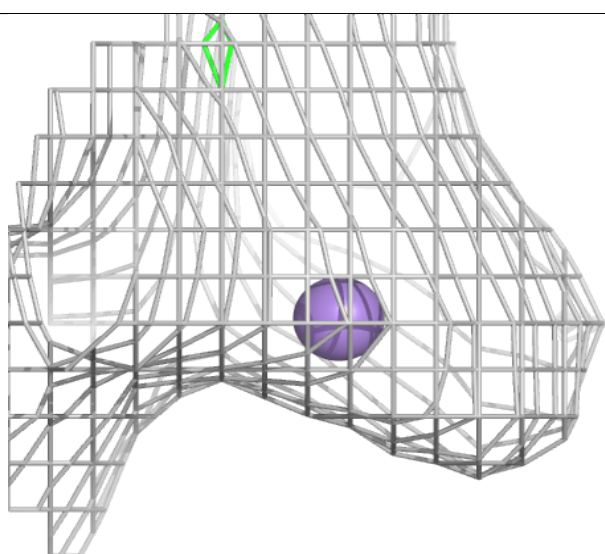
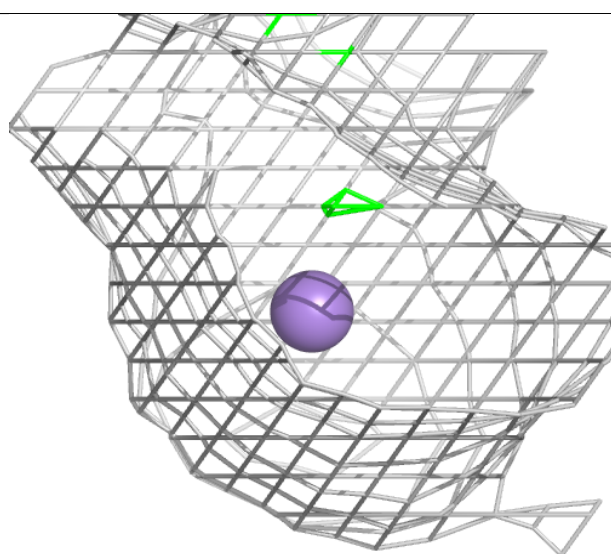
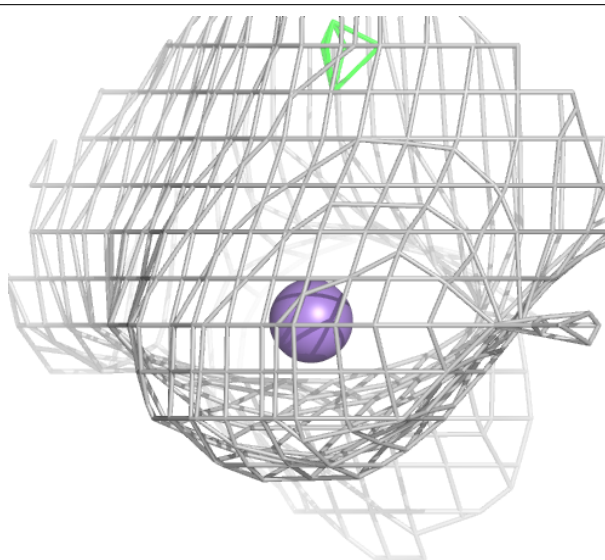
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	C	302	1/1	0.97	0.05	67,67,67,67	0
2	MN	A	302	1/1	0.98	0.07	65,65,65,65	0
2	MN	B	301	1/1	0.98	0.04	48,48,48,48	0
2	MN	B	303	1/1	0.99	0.05	53,53,53,53	0
2	MN	A	303	1/1	0.99	0.04	43,43,43,43	0
2	MN	A	301	1/1	1.00	0.02	43,43,43,43	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.

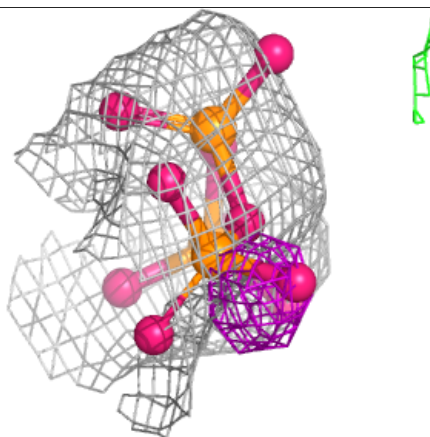
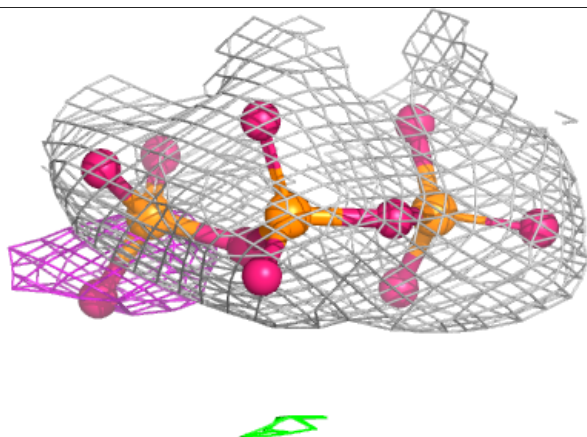
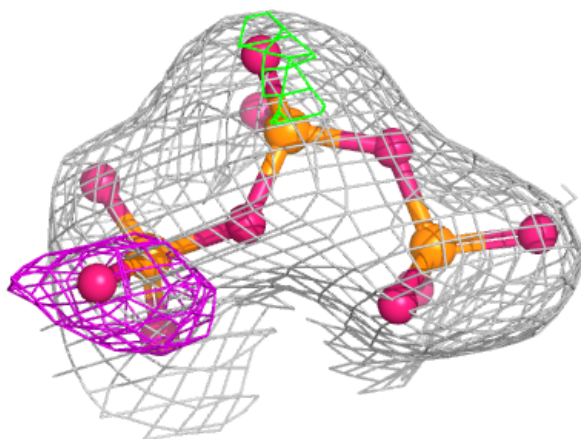
Electron density around MN B 304:

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

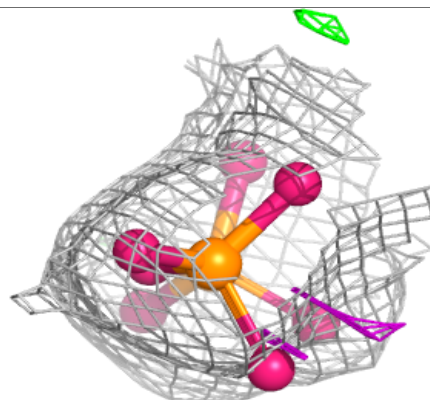
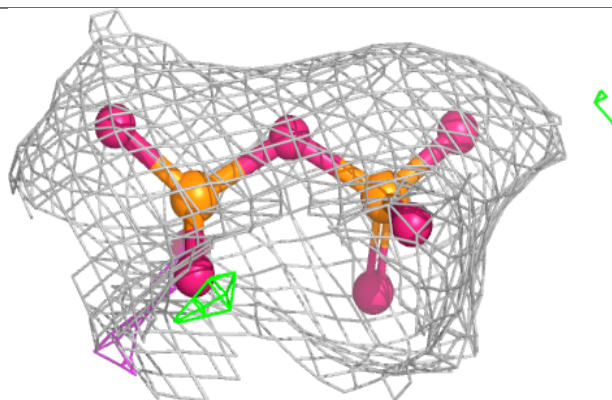
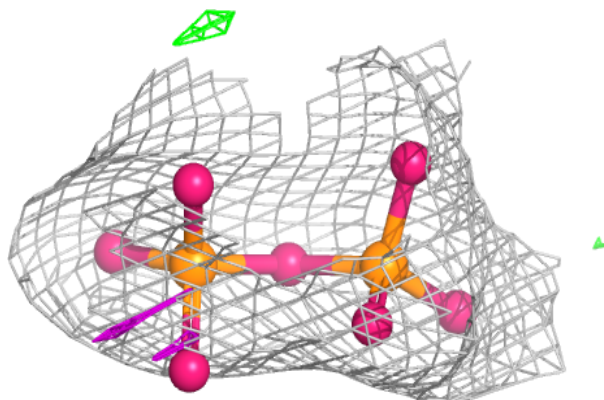


Electron density around DCP D 303:

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and green (positive)

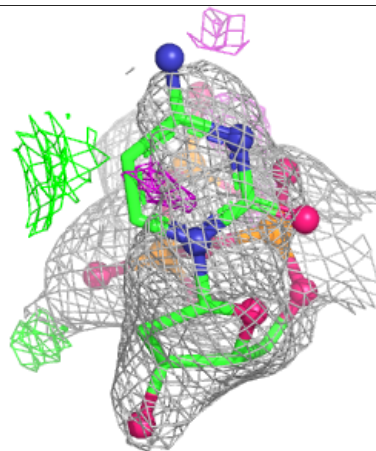
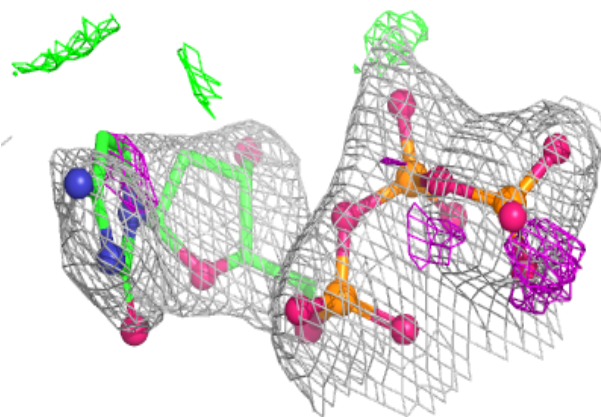
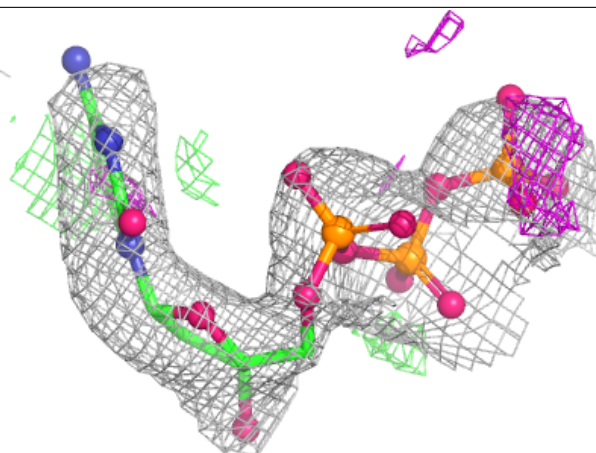
**Electron density around DCP C 303:**

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and green (positive)



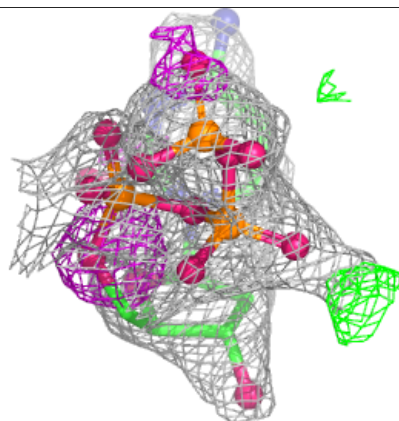
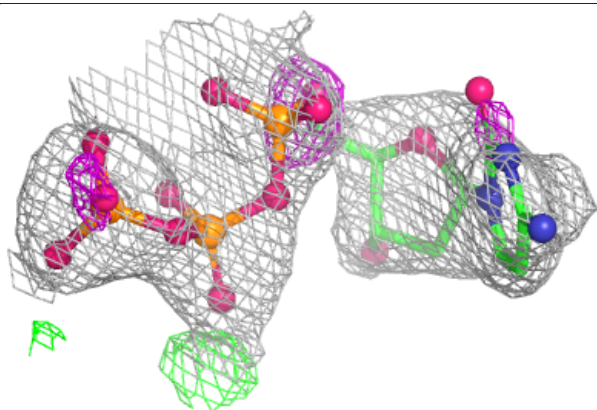
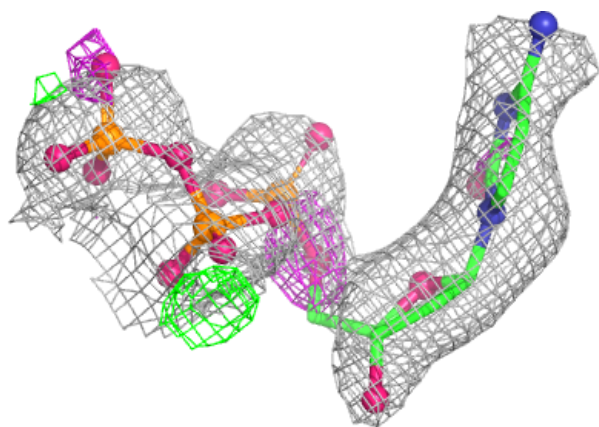
Electron density around DCP B 305:

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



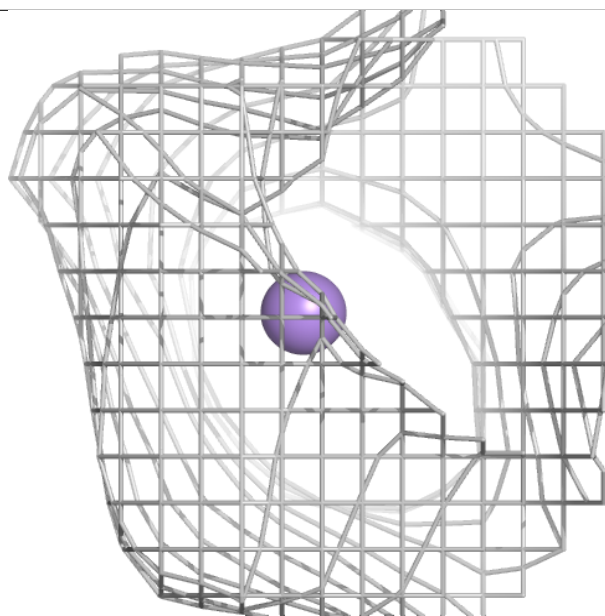
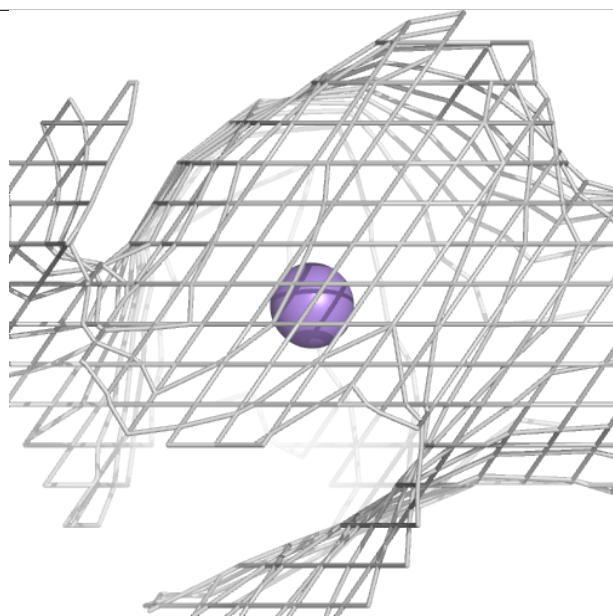
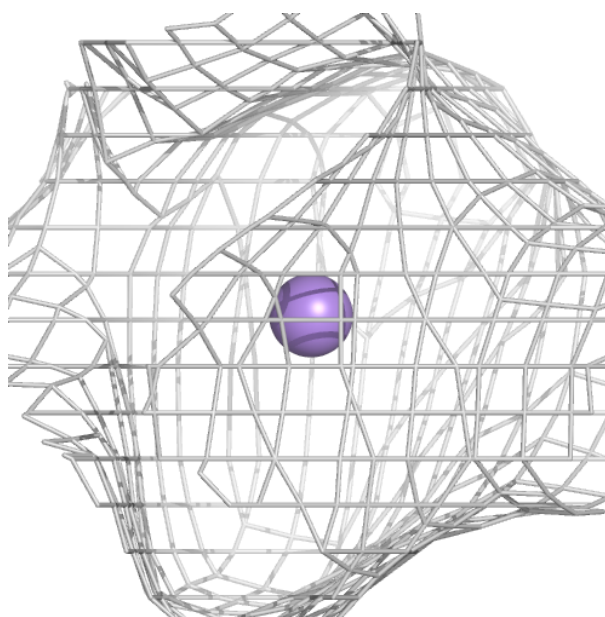
Electron density around DCP A 304:

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and green (positive)



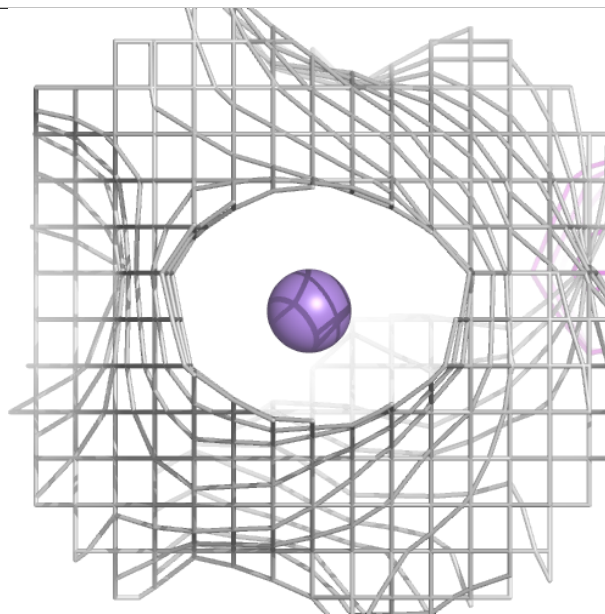
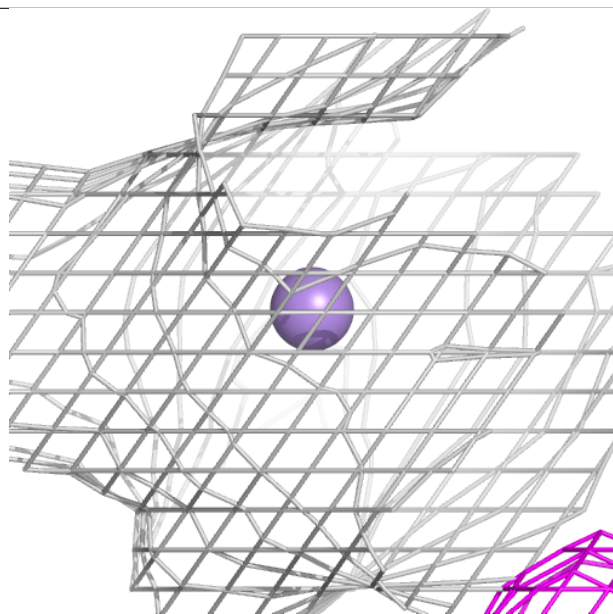
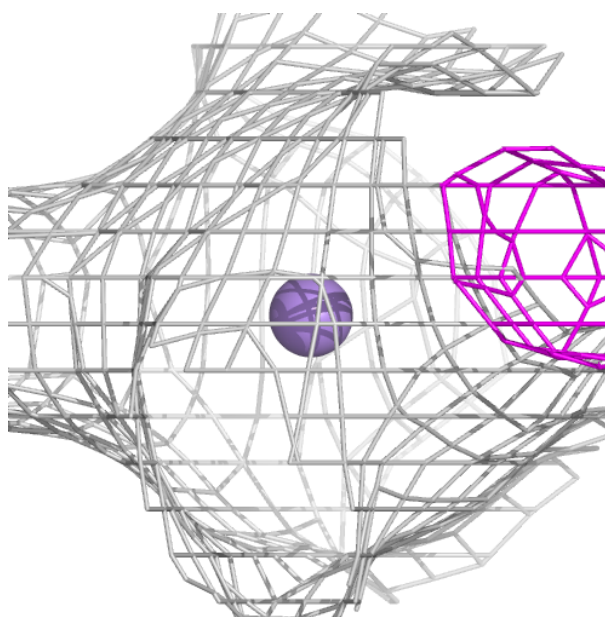
Electron density around MN C 301:

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and green (positive)



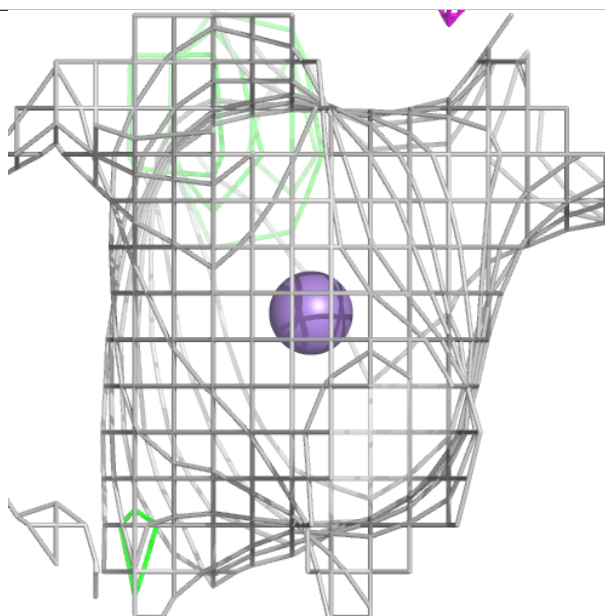
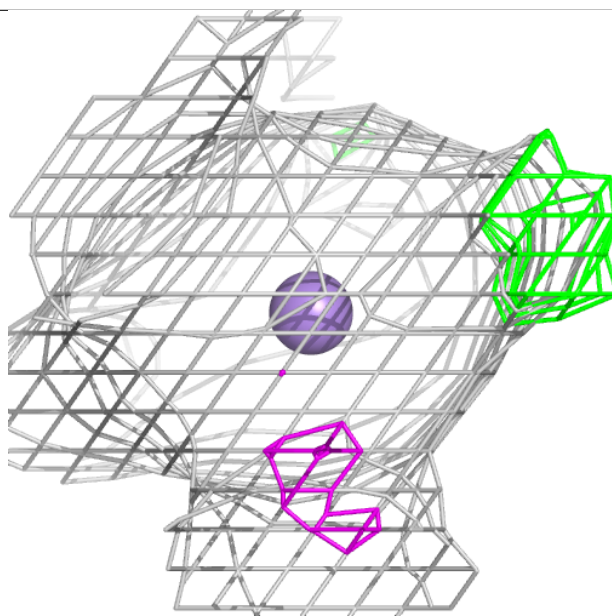
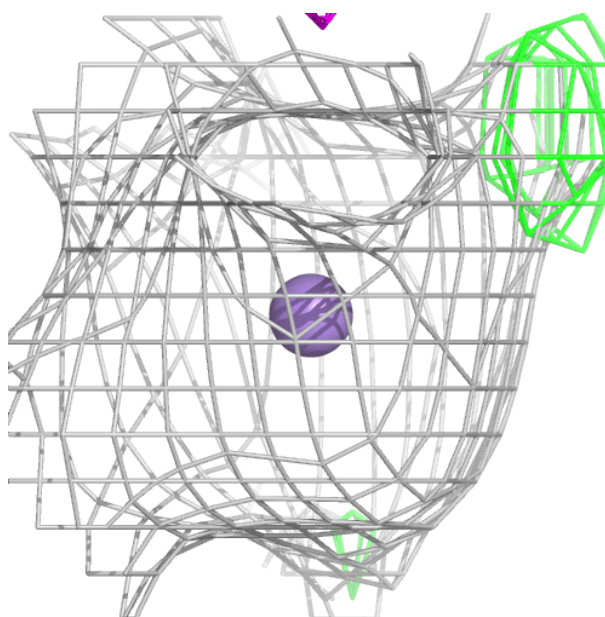
Electron density around MN D 301:

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



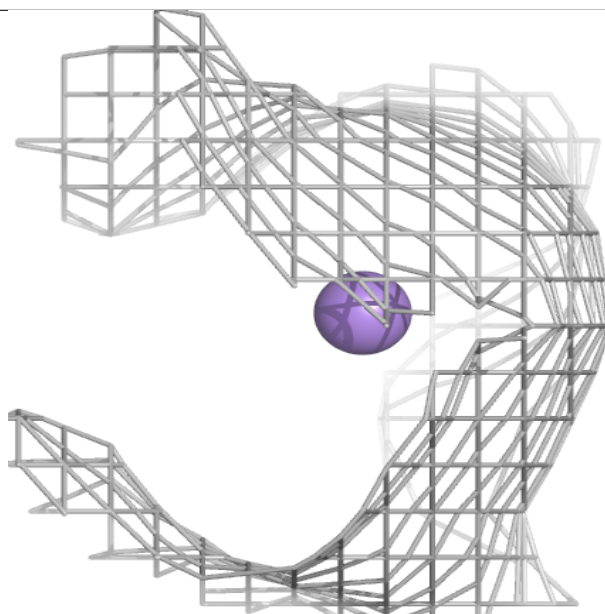
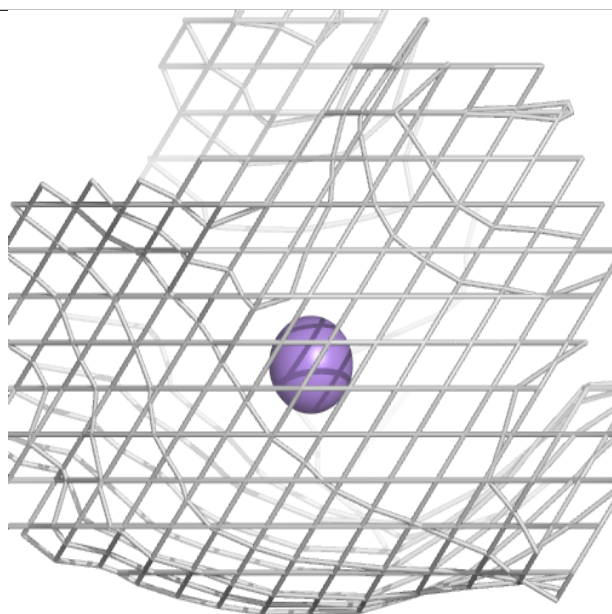
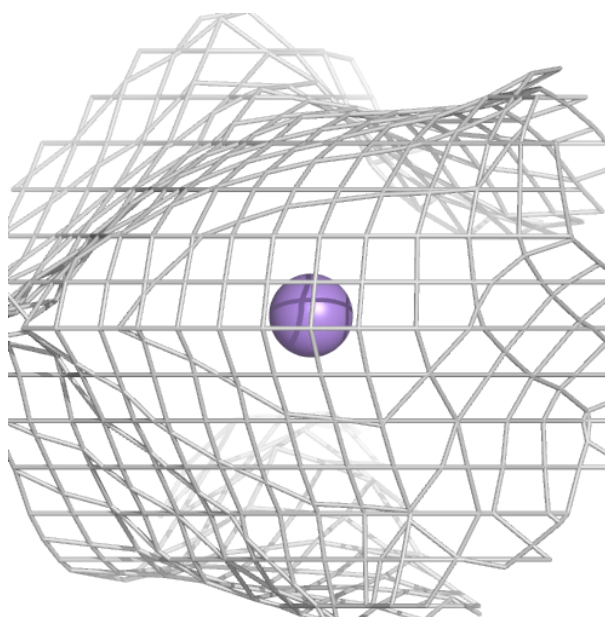
Electron density around MN B 302:

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



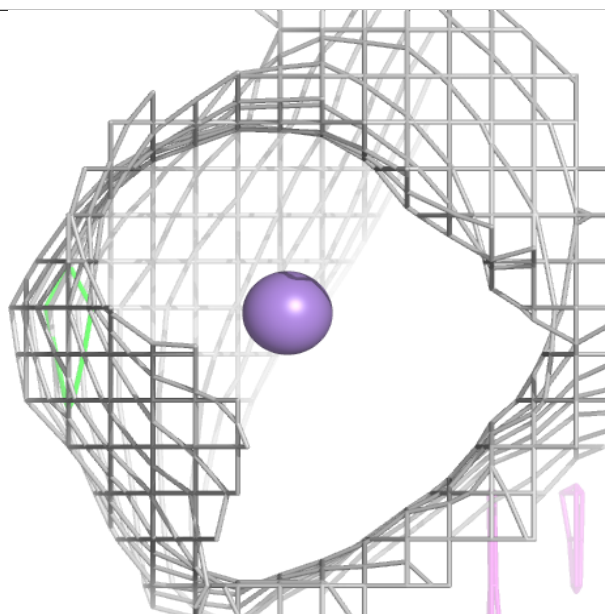
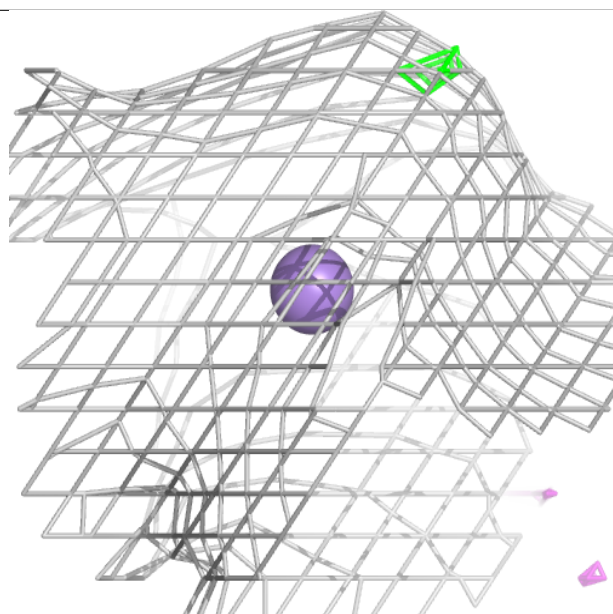
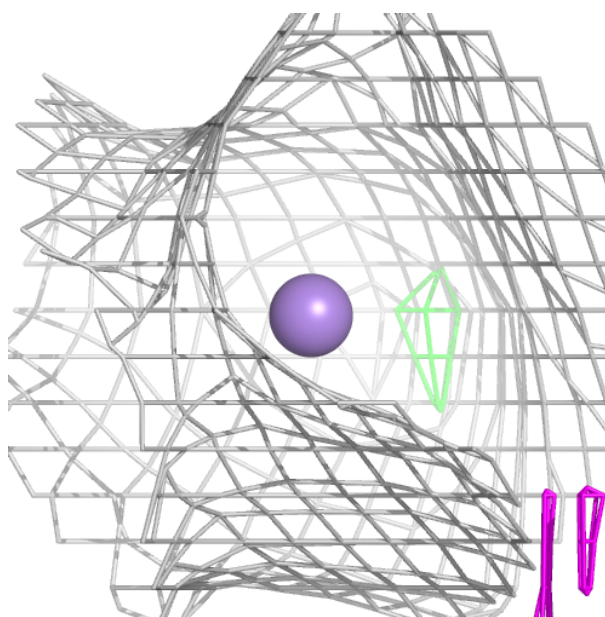
Electron density around MN D 302:

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



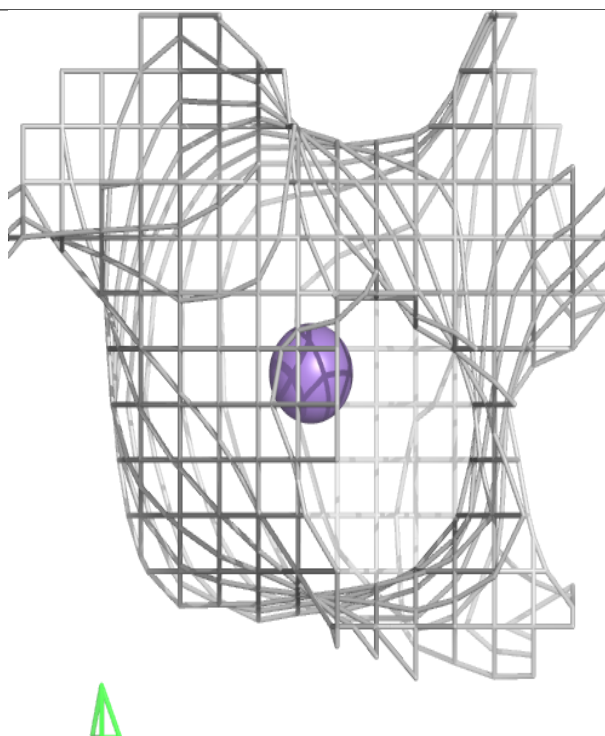
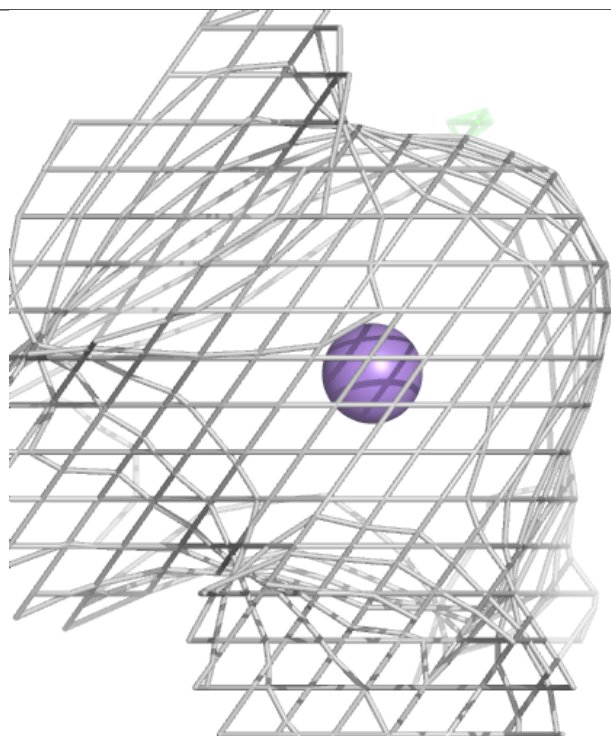
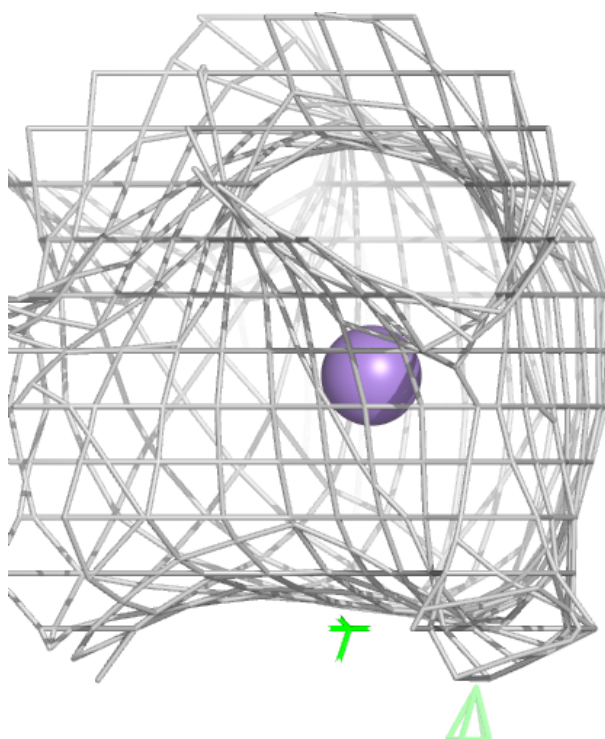
Electron density around MN C 302:

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



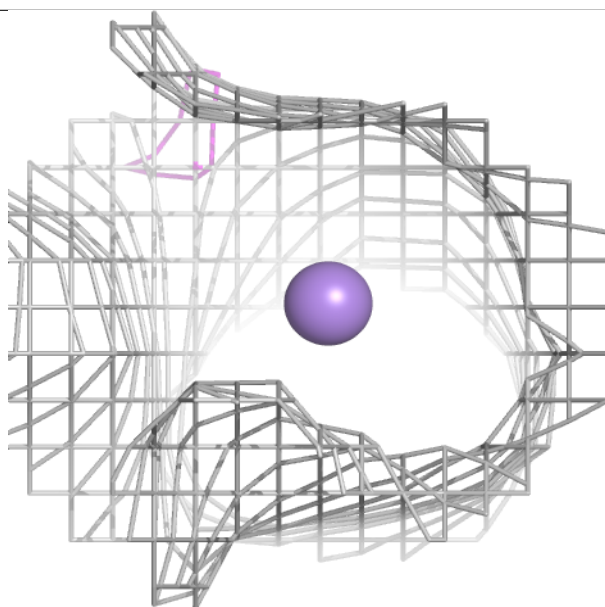
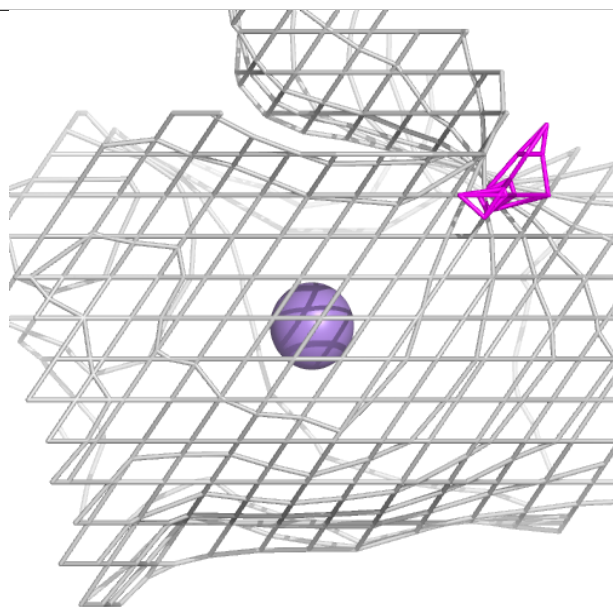
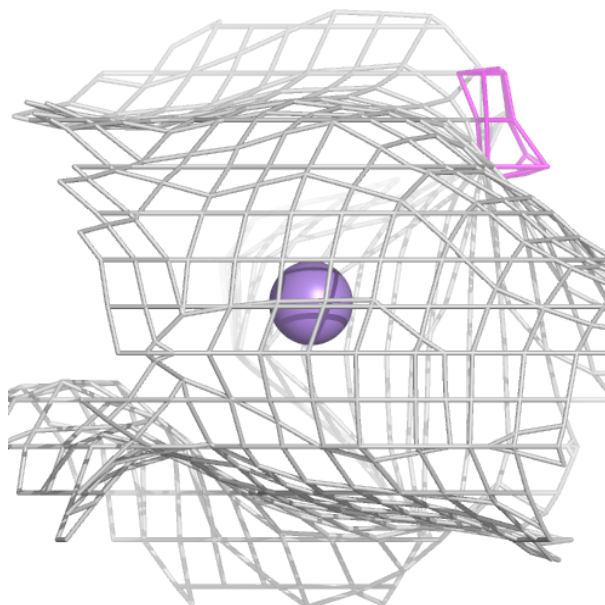
Electron density around MN A 302:

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



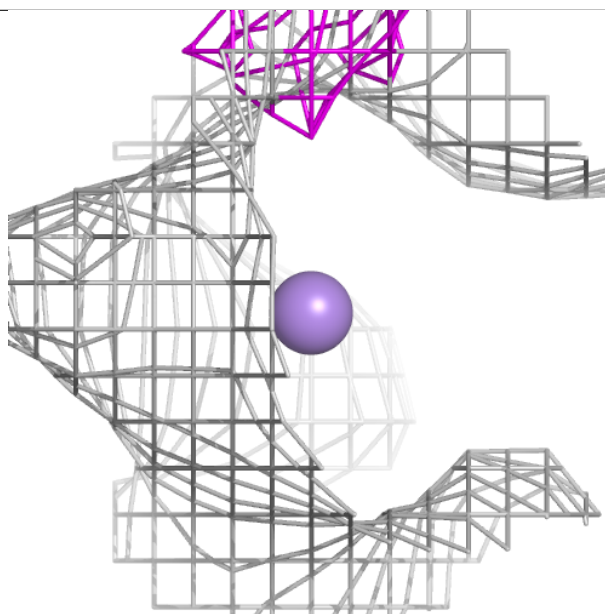
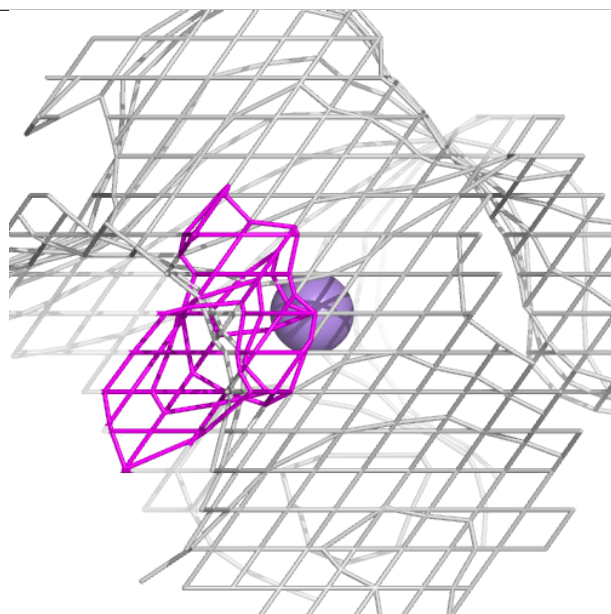
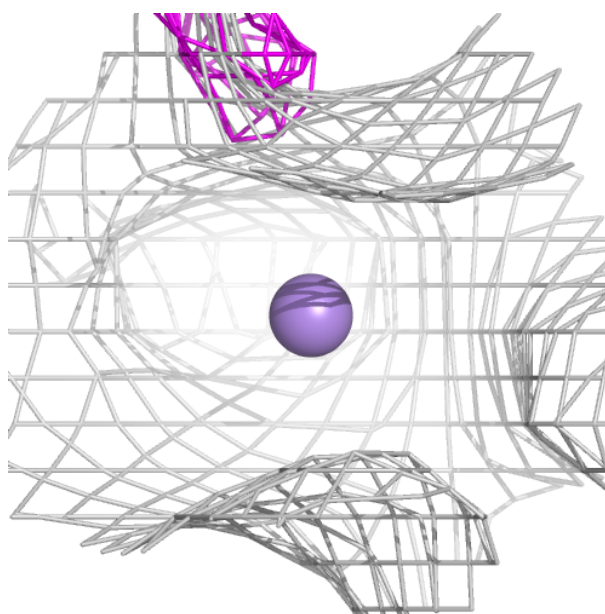
Electron density around MN B 301:

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



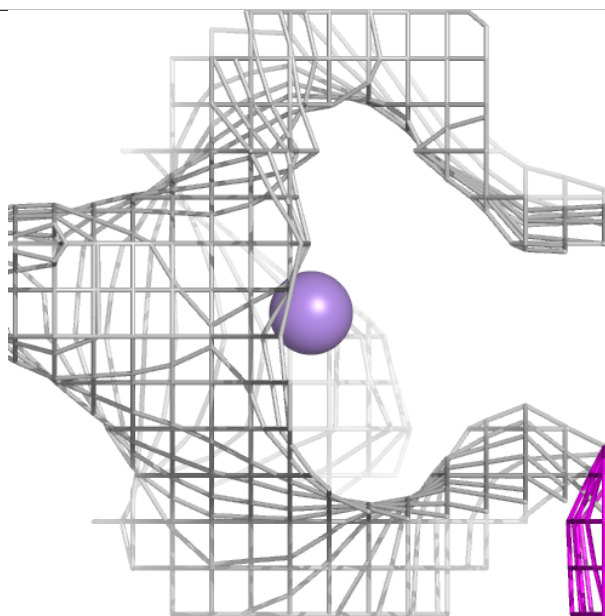
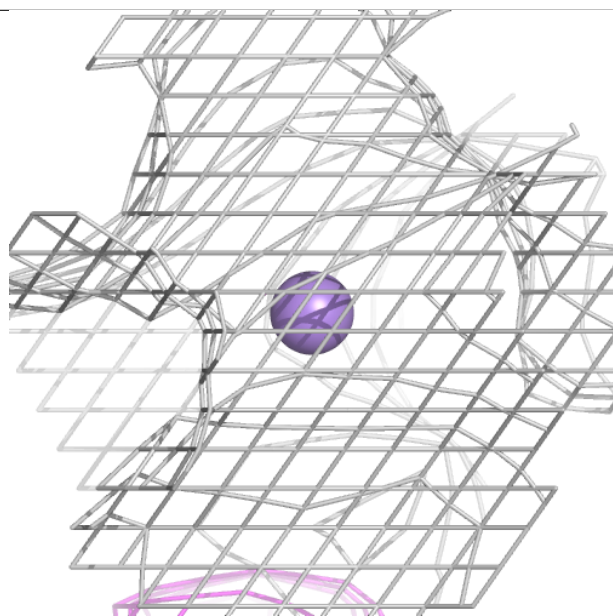
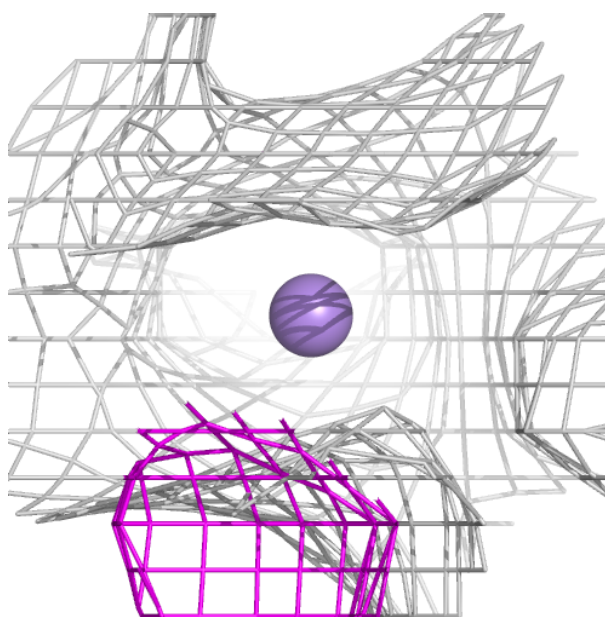
Electron density around MN B 303:

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



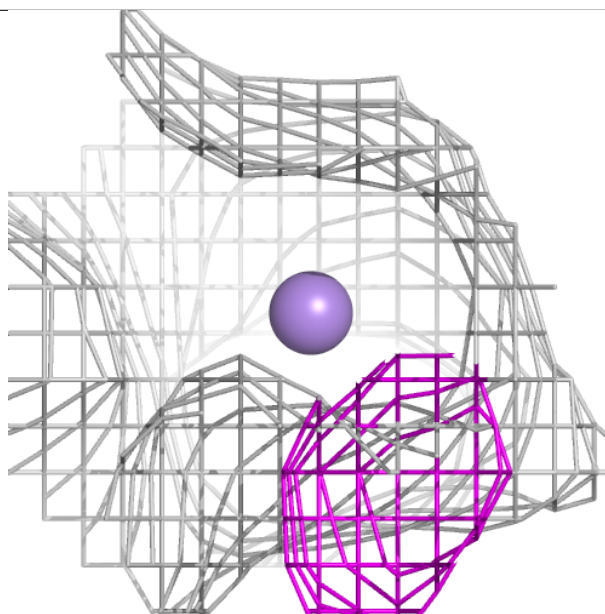
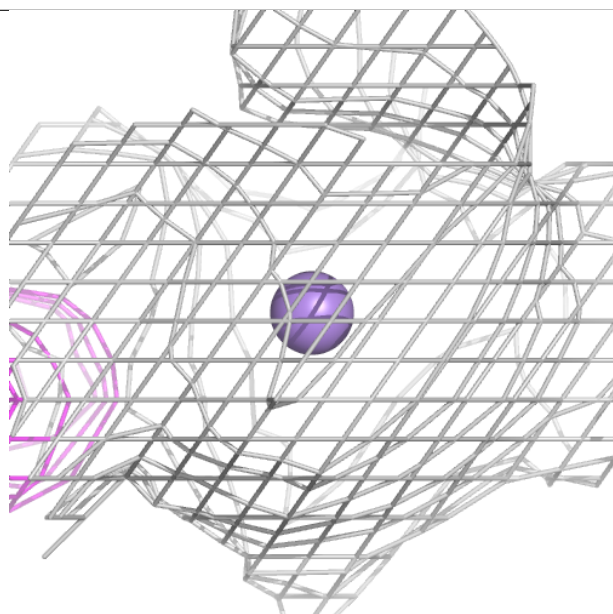
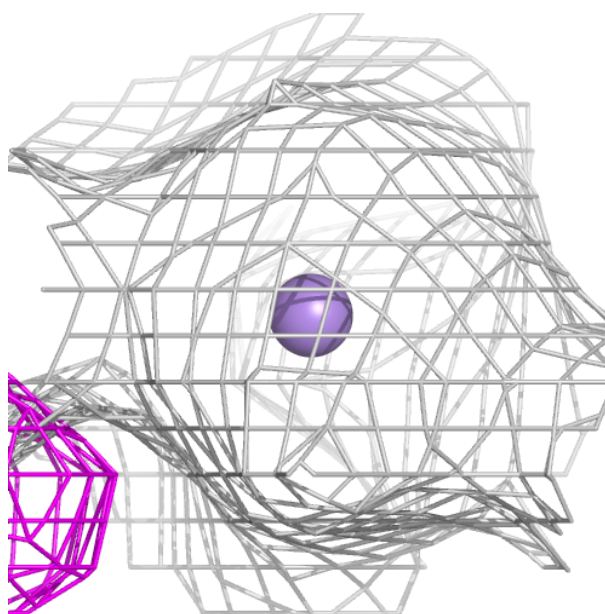
Electron density around MN A 303:

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



Electron density around MN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.