wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2026 – 12:11 AM JST

PDB ID	:	20ZY / pdb_000020zy
Title	:	Crystal Structure of Helicobacter pylori Urease Accessory Protein UreE(1-158) and UreG in complex with GMPPNP and nickel
Authors	:	Chan, C.L.; Wong, K.B.
Deposited on	:	2025-12-04
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

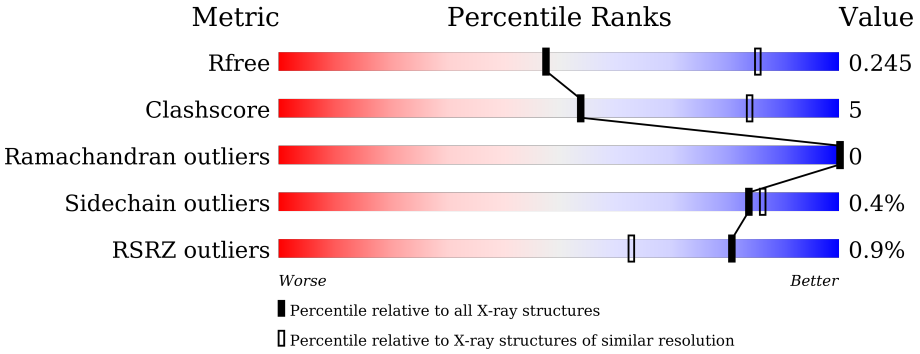
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 <=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	202	88% 11%
1	B	202	77% 23%
1	E	202	% 88% 12%
1	F	202	81% 18%
1	I	202	2% 89% 10%
1	J	202	86% 13%

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Mol	Chain	Length	Quality of chain
1	M	202	%, 85%, 15%
1	N	202	86%, 14%
2	C	158	88%, 10%
2	D	158	2%, 78%, 14%, 8%
2	G	158	%, 89%, 9%
2	H	158	%, 79%, 13%, 8%
2	K	158	%, 92%, 6%
2	L	158	2%, 81%, 11%, 8%
2	O	158	%, 89%, 9%
2	P	158	2%, 78%, 15%, 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21796 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 Urease accessory protein UreG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	1503	948	255	289	11	0	0	0
1	B	201	1513	953	256	293	11	0	0	0
1	E	201	1490	941	253	285	11	0	0	0
1	F	201	1513	953	256	293	11	0	0	0
1	I	201	1498	945	253	289	11	0	0	0
1	J	201	1513	953	256	293	11	0	0	0
1	M	201	1503	948	255	289	11	0	0	0
1	N	201	1513	953	256	293	11	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP Q09066
A	-1	ALA	-	expression tag	UNP Q09066
A	0	ALA	-	expression tag	UNP Q09066
A	1	ALA	-	expression tag	UNP Q09066
B	-2	MET	-	initiating methionine	UNP Q09066
B	-1	ALA	-	expression tag	UNP Q09066
B	0	ALA	-	expression tag	UNP Q09066
B	1	ALA	-	expression tag	UNP Q09066
E	-2	MET	-	initiating methionine	UNP Q09066
E	-1	ALA	-	expression tag	UNP Q09066
E	0	ALA	-	expression tag	UNP Q09066
E	1	ALA	-	expression tag	UNP Q09066
F	-2	MET	-	initiating methionine	UNP Q09066

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	ALA	-	expression tag	UNP Q09066
F	0	ALA	-	expression tag	UNP Q09066
F	1	ALA	-	expression tag	UNP Q09066
I	-2	MET	-	initiating methionine	UNP Q09066
I	-1	ALA	-	expression tag	UNP Q09066
I	0	ALA	-	expression tag	UNP Q09066
I	1	ALA	-	expression tag	UNP Q09066
J	-2	MET	-	initiating methionine	UNP Q09066
J	-1	ALA	-	expression tag	UNP Q09066
J	0	ALA	-	expression tag	UNP Q09066
J	1	ALA	-	expression tag	UNP Q09066
M	-2	MET	-	initiating methionine	UNP Q09066
M	-1	ALA	-	expression tag	UNP Q09066
M	0	ALA	-	expression tag	UNP Q09066
M	1	ALA	-	expression tag	UNP Q09066
N	-2	MET	-	initiating methionine	UNP Q09066
N	-1	ALA	-	expression tag	UNP Q09066
N	0	ALA	-	expression tag	UNP Q09066
N	1	ALA	-	expression tag	UNP Q09066

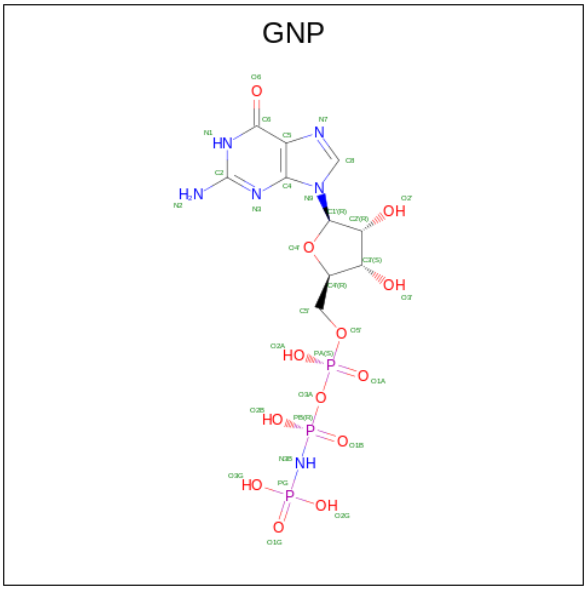
- Molecule 2 is a protein called Urease accessory protein UreE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	155	1206	774	207	223	2	0	0	0
			Total	C	N	O	S			
2	D	146	1159	743	203	212	1	0	0	0
			Total	C	N	O	S			
2	G	155	1203	773	206	222	2	0	0	0
			Total	C	N	O	S			
2	H	146	1160	744	203	212	1	0	0	0
			Total	C	N	O	S			
2	K	155	1206	774	207	223	2	0	0	0
			Total	C	N	O	S			
2	L	146	1159	743	203	212	1	0	0	0
			Total	C	N	O	S			
2	O	155	1206	774	207	223	2	0	0	0
			Total	C	N	O	S			
2	P	146	1164	746	203	214	1	0	0	0

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ni 1	0	0
3	B	2	Total 2	Ni 2	0	0
3	E	1	Total 1	Ni 1	0	0
3	F	2	Total 2	Ni 2	0	0
3	I	1	Total 1	Ni 1	0	0
3	J	2	Total 2	Ni 2	0	0
3	M	1	Total 1	Ni 1	0	0
3	N	2	Total 2	Ni 2	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	B	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	E	1	Total 32	C 10	N 6	O 13	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	F	1	32	10	6	13	3	0	0
4	I	1	32	10	6	13	3	0	0
4	J	1	32	10	6	13	3	0	0
4	M	1	32	10	6	13	3	0	0
4	N	1	32	10	6	13	3	0	0

- Molecule 5 is water.

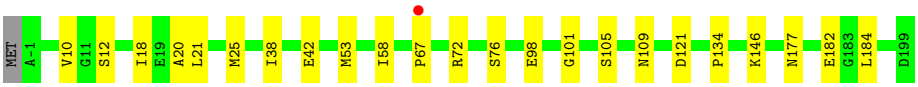
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	1	1	1	0	0
5	B	2	2	2	0	0
5	C	1	1	1	0	0
5	E	1	1	1	0	0
5	F	2	2	2	0	0
5	G	2	2	2	0	0
5	I	1	1	1	0	0
5	J	2	2	2	0	0
5	K	1	1	1	0	0
5	L	1	1	1	0	0
5	M	1	1	1	0	0
5	N	2	2	2	0	0
5	O	2	2	2	0	0

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.

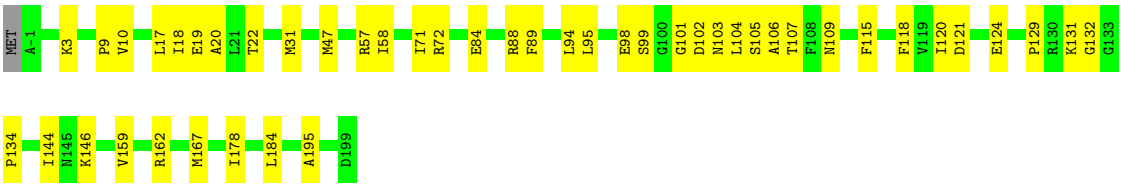
• Molecule 1: Urease accessory protein UreG

Chain A:



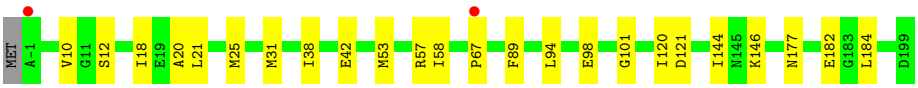
• Molecule 1: Urease accessory protein UreG

Chain B:



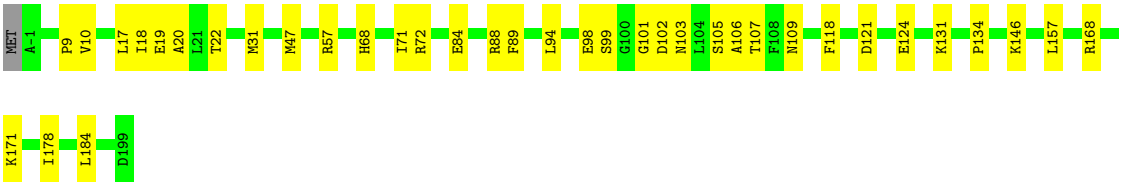
• Molecule 1: Urease accessory protein UreG

Chain E:



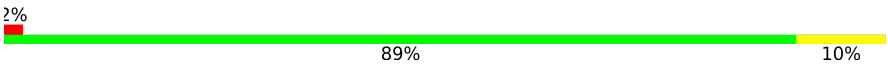
• Molecule 1: Urease accessory protein UreG

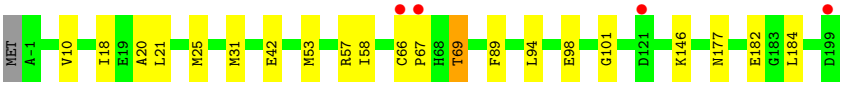
Chain F:



• Molecule 1: Urease accessory protein UreG

Chain I:



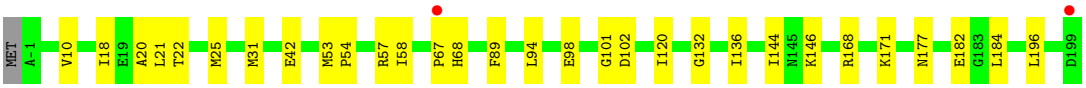


• Molecule 1: Urease accessory protein UreG

Chain J: 86% 13%

• Molecule 1: Urease accessory protein UreG

Chain M: % 85% 15%



• Molecule 1: Urease accessory protein UreG

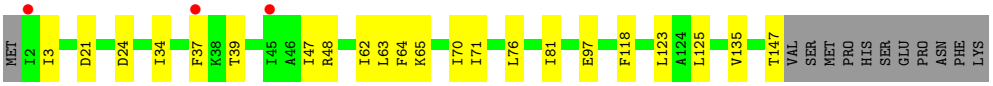
Chain N: 86% 14%

• Molecule 2: Urease accessory protein UreE

Chain C: 88% 10%

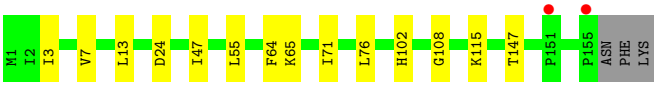
• Molecule 2: Urease accessory protein UreE

Chain D: 2% 78% 14% 8%



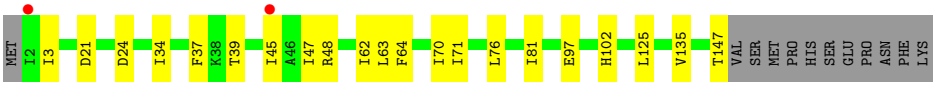
• Molecule 2: Urease accessory protein UreE

Chain G: % 89% 9%



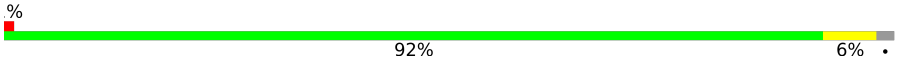
• Molecule 2: Urease accessory protein UreE

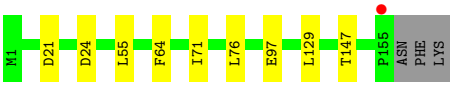
Chain H: % 79% 13% 8%



• Molecule 2: Urease accessory protein UreE

Chain K:





• Molecule 2: Urease accessory protein UreE

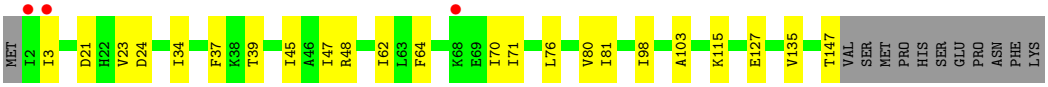
Chain L:

• Molecule 2: Urease accessory protein UreE

Chain O:

• Molecule 2: Urease accessory protein UreE

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.17Å 166.60Å 154.02Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	44.15 – 3.10 44.15 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (44.15-3.10) 97.9 (44.15-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.209 , 0.245 0.209 , 0.245	Depositor DCC
R_{free} test set	3189 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	72.8	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.070 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21796	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NI, GNP

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	0.10	0/1526	0.28	0/2065
1	B	0.10	0/1536	0.28	0/2077
1	E	0.10	0/1512	0.27	0/2047
1	F	0.10	0/1536	0.27	0/2077
1	I	0.10	0/1520	0.27	0/2057
1	J	0.10	0/1536	0.28	0/2077
1	M	0.11	0/1526	0.27	0/2065
1	N	0.10	0/1536	0.27	0/2077
2	C	0.09	0/1227	0.26	0/1659
2	D	0.10	0/1177	0.28	0/1585
2	G	0.09	0/1224	0.26	0/1655
2	H	0.10	0/1178	0.28	0/1587
2	K	0.09	0/1227	0.26	0/1659
2	L	0.10	0/1177	0.28	0/1585
2	O	0.09	0/1227	0.26	0/1659
2	P	0.11	0/1182	0.29	0/1592
All	All	0.10	0/21847	0.27	0/29523

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 (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	1503	0	1492	15	0
1	B	1513	0	1507	26	0
1	E	1490	0	1479	15	0
1	F	1513	0	1508	23	0
1	I	1498	0	1487	13	0
1	J	1513	0	1507	20	0
1	M	1503	0	1492	20	0
1	N	1513	0	1507	16	0
2	C	1206	0	1214	9	0
2	D	1159	0	1188	13	0
2	G	1203	0	1210	9	0
2	H	1160	0	1189	14	0
2	K	1206	0	1214	5	0
2	L	1159	0	1188	12	0
2	O	1206	0	1214	10	0
2	P	1164	0	1193	13	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	M	1	0	0	0	0
3	N	2	0	0	0	0
4	A	32	0	13	1	0
4	B	32	0	13	1	0
4	E	32	0	13	1	0
4	F	32	0	13	1	0
4	I	32	0	13	1	0
4	J	32	0	13	1	0
4	M	32	0	13	1	0
4	N	32	0	13	1	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0
5	I	1	0	0	0	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	2	0	0	0	0
5	O	2	0	0	0	0
All	All	21796	0	21693	214	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 5.

The worst 5 of 214 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:J:10:VAL:HG22	1:J:101:GLY:HA3	1.66	0.78
1:N:10:VAL:HG22	1:N:101:GLY:HA3	1.67	0.76
1:B:10:VAL:HG22	1:B:101:GLY:HA3	1.68	0.75
1:F:10:VAL:HG22	1:F:101:GLY:HA3	1.71	0.73
1:I:10:VAL:HG22	1:I:101:GLY:HA3	1.70	0.72

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	199/202 (98%)	195 (98%)	4 (2%)	0	100	100
1	B	199/202 (98%)	195 (98%)	4 (2%)	0	100	100
1	E	199/202 (98%)	195 (98%)	4 (2%)	0	100	100
1	F	199/202 (98%)	195 (98%)	4 (2%)	0	100	100
1	I	199/202 (98%)	195 (98%)	4 (2%)	0	100	100
1	J	199/202 (98%)	194 (98%)	5 (2%)	0	100	100
1	M	199/202 (98%)	195 (98%)	4 (2%)	0	100	100
1	N	199/202 (98%)	196 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	153/158 (97%)	152 (99%)	1 (1%)	0	100	100
2	D	144/158 (91%)	140 (97%)	4 (3%)	0	100	100
2	G	153/158 (97%)	152 (99%)	1 (1%)	0	100	100
2	H	144/158 (91%)	140 (97%)	4 (3%)	0	100	100
2	K	153/158 (97%)	152 (99%)	1 (1%)	0	100	100
2	L	144/158 (91%)	140 (97%)	4 (3%)	0	100	100
2	O	153/158 (97%)	152 (99%)	1 (1%)	0	100	100
2	P	144/158 (91%)	140 (97%)	4 (3%)	0	100	100
All	All	2780/2880 (96%)	2728 (98%)	52 (2%)	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	157/167 (94%)	157 (100%)	0	100	100
1	B	160/167 (96%)	159 (99%)	1 (1%)	78	83
1	E	154/167 (92%)	154 (100%)	0	100	100
1	F	160/167 (96%)	159 (99%)	1 (1%)	78	83
1	I	156/167 (93%)	155 (99%)	1 (1%)	78	83
1	J	160/167 (96%)	159 (99%)	1 (1%)	78	83
1	M	157/167 (94%)	157 (100%)	0	100	100
1	N	160/167 (96%)	159 (99%)	1 (1%)	78	83
2	C	128/141 (91%)	128 (100%)	0	100	100
2	D	124/141 (88%)	123 (99%)	1 (1%)	73	81
2	G	127/141 (90%)	127 (100%)	0	100	100
2	H	124/141 (88%)	123 (99%)	1 (1%)	73	81
2	K	128/141 (91%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	124/141 (88%)	123 (99%)	1 (1%)	73	81
2	O	128/141 (91%)	128 (100%)	0	100	100
2	P	125/141 (89%)	123 (98%)	2 (2%)	55	75
All	All	2272/2464 (92%)	2262 (100%)	10 (0%)	84	86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	107	THR
2	P	127	GLU
2	P	147	THR
2	H	147	THR
1	I	69	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	59	GLN
1	N	194	ASN
2	K	74	ASN
1	M	50	ASN
2	O	41	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 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GNP	M	202	3	33,34,34	2.22	5 (15%)	46,54,54	1.47	3 (6%)
4	GNP	F	203	3	33,34,34	2.20	5 (15%)	46,54,54	1.48	6 (13%)
4	GNP	N	203	3	33,34,34	2.26	5 (15%)	46,54,54	1.45	3 (6%)
4	GNP	B	203	3	33,34,34	2.23	5 (15%)	46,54,54	1.45	4 (8%)
4	GNP	J	203	3	33,34,34	2.20	5 (15%)	46,54,54	1.48	3 (6%)
4	GNP	E	202	3	33,34,34	2.20	5 (15%)	46,54,54	1.44	3 (6%)
4	GNP	A	202	3	33,34,34	2.20	6 (18%)	46,54,54	1.45	3 (6%)
4	GNP	I	202	3	33,34,34	2.21	5 (15%)	46,54,54	1.48	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
4	GNP	M	202	3	-	3/18/38/38	0/3/3/3
4	GNP	F	203	3	-	2/18/38/38	0/3/3/3
4	GNP	N	203	3	-	2/18/38/38	0/3/3/3
4	GNP	B	203	3	-	2/18/38/38	0/3/3/3
4	GNP	J	203	3	-	2/18/38/38	0/3/3/3
4	GNP	E	202	3	-	3/18/38/38	0/3/3/3
4	GNP	A	202	3	-	3/18/38/38	0/3/3/3
4	GNP	I	202	3	-	3/18/38/38	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	203	GNP	PB-O3A	8.26	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	203	GNP	PB-O3A	8.07	1.69	1.59
4	I	202	GNP	PB-O3A	7.95	1.69	1.59
4	M	202	GNP	PB-O3A	7.95	1.69	1.59
4	E	202	GNP	PB-O3A	7.92	1.69	1.59

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	203	GNP	O1G-PG-N3B	-7.44	100.82	111.77
4	M	202	GNP	O1G-PG-N3B	-7.22	101.14	111.77
4	I	202	GNP	O1G-PG-N3B	-7.22	101.14	111.77
4	N	203	GNP	O1G-PG-N3B	-7.19	101.18	111.77
4	B	203	GNP	O1G-PG-N3B	-7.14	101.26	111.77

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	202	GNP	PB-N3B-PG-O1G
4	A	202	GNP	PG-N3B-PB-O1B
4	A	202	GNP	PG-N3B-PB-O3A
4	B	203	GNP	PG-N3B-PB-O1B
4	E	202	GNP	PB-N3B-PG-O1G

There are no ring outliers.

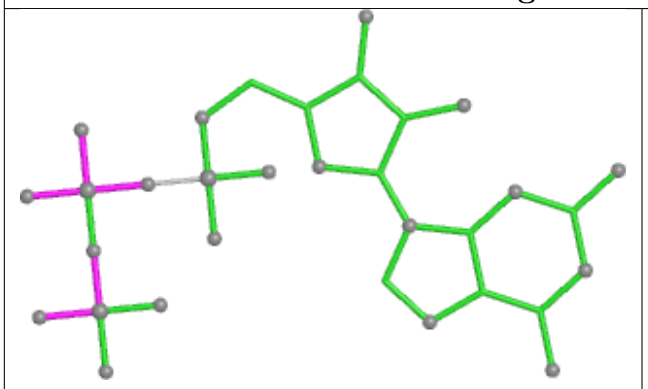
8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	202	GNP	1	0
4	F	203	GNP	1	0
4	N	203	GNP	1	0
4	B	203	GNP	1	0
4	J	203	GNP	1	0
4	E	202	GNP	1	0
4	A	202	GNP	1	0
4	I	202	GNP	1	0

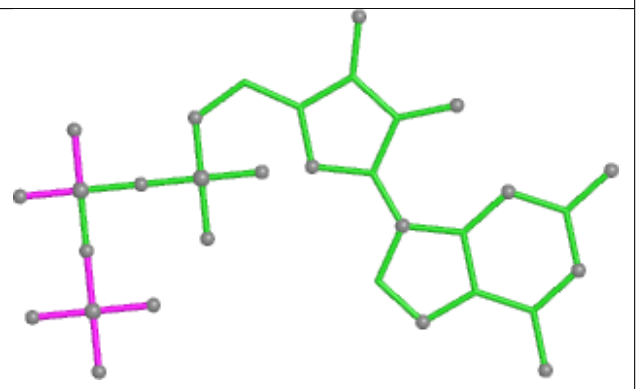
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

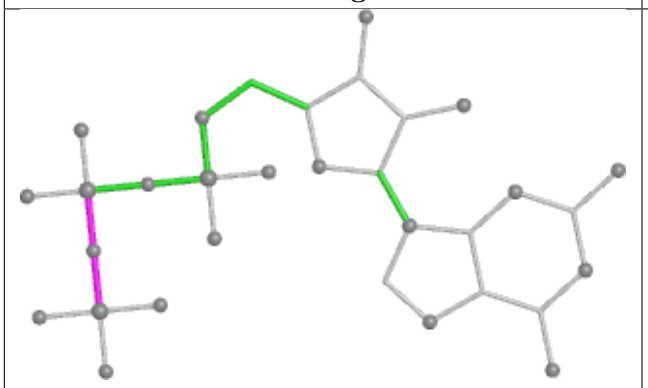
Ligand GNP M 202



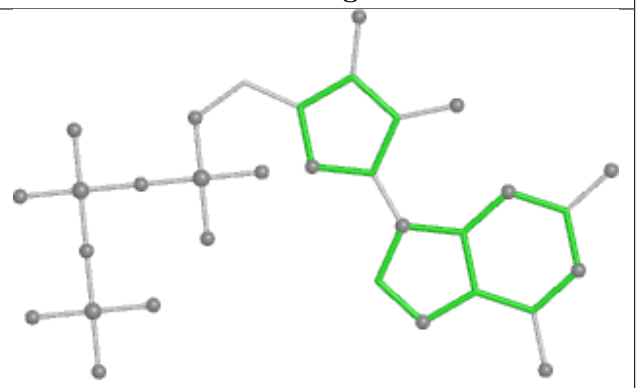
Bond lengths



Bond angles

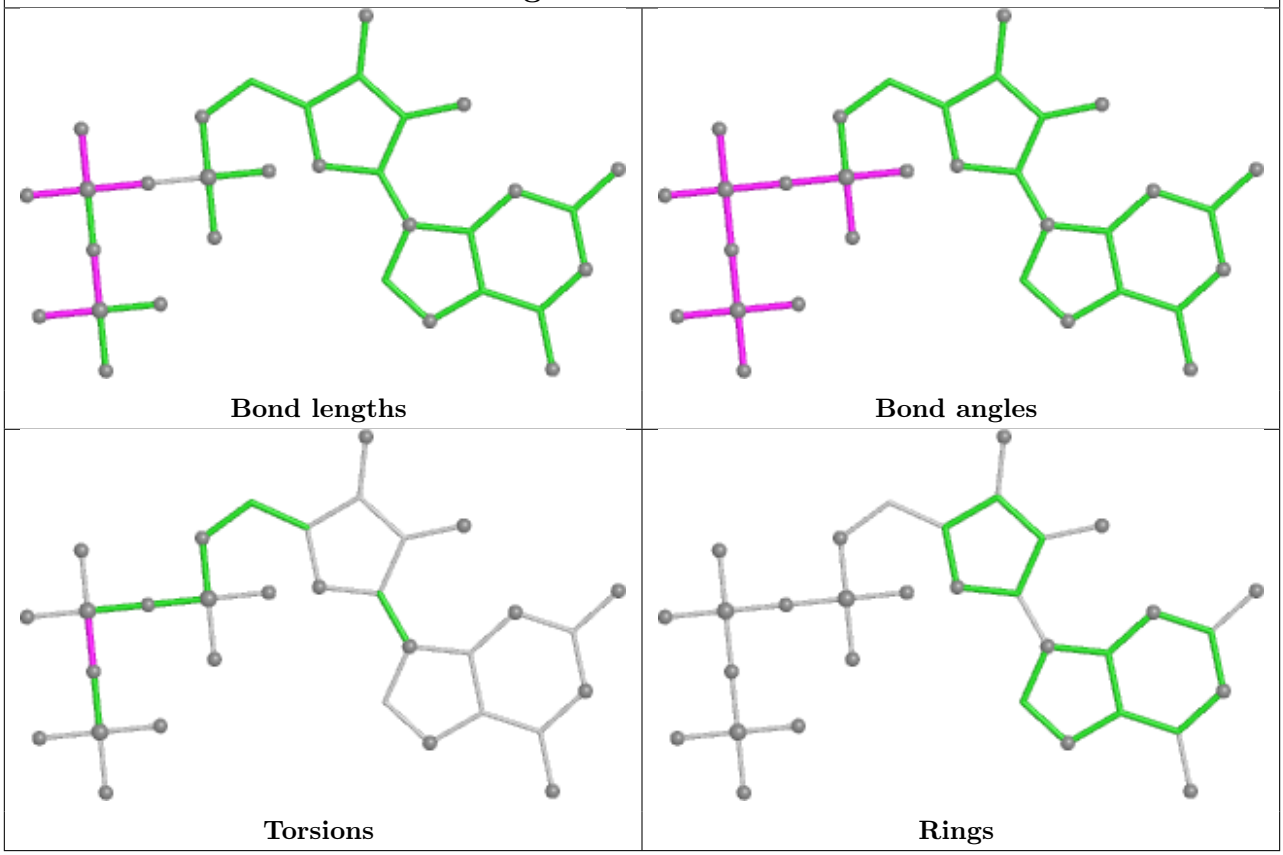


Torsions

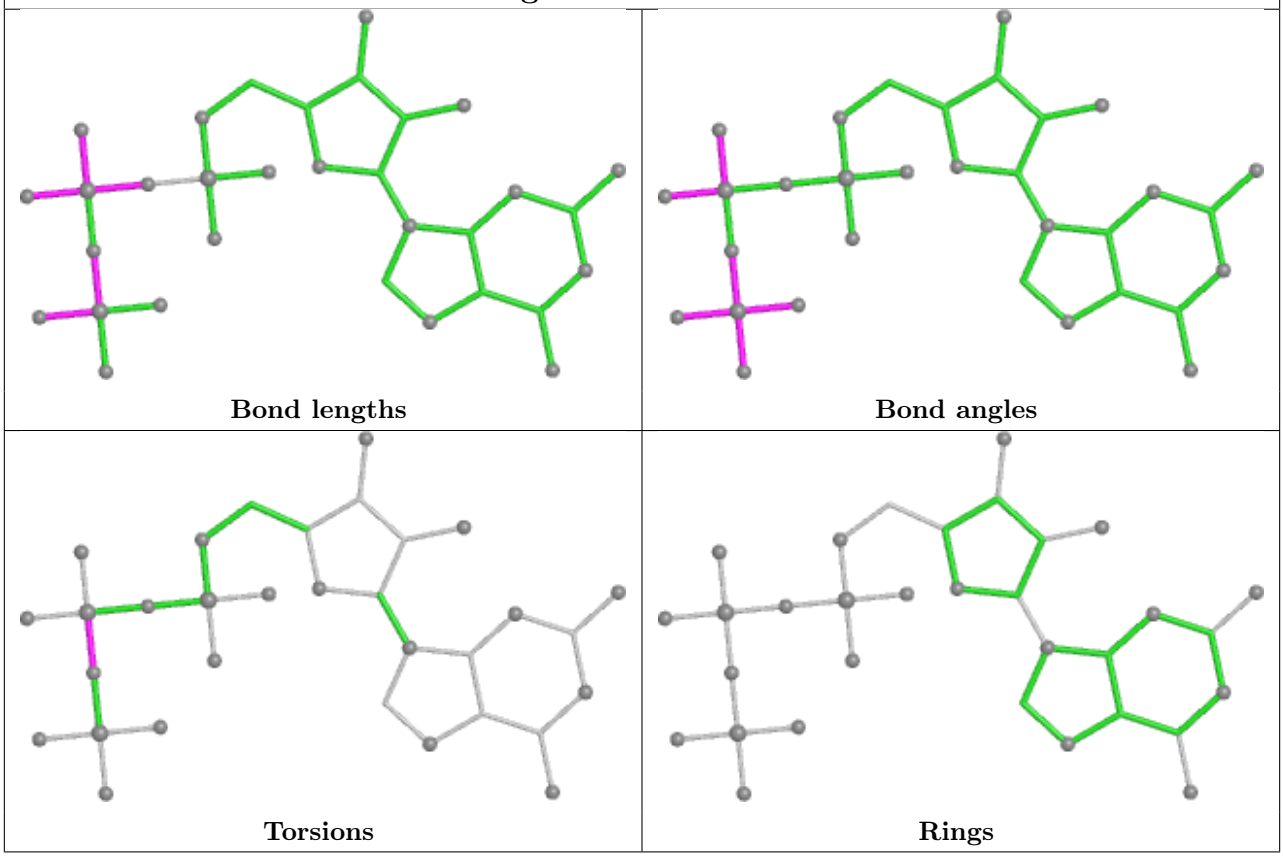


Rings

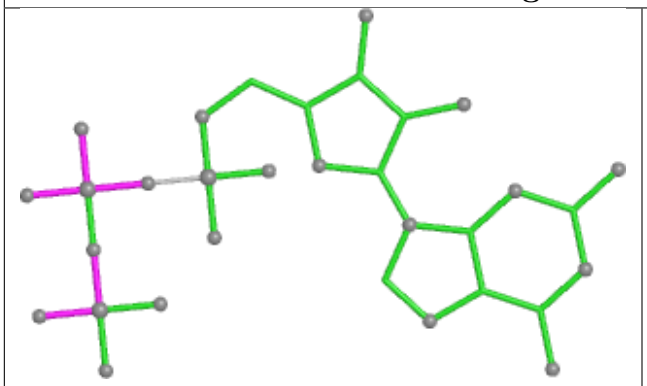
Ligand GNP F 203



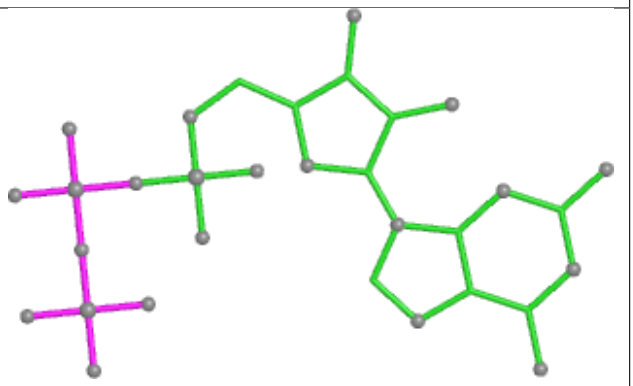
Ligand GNP N 203



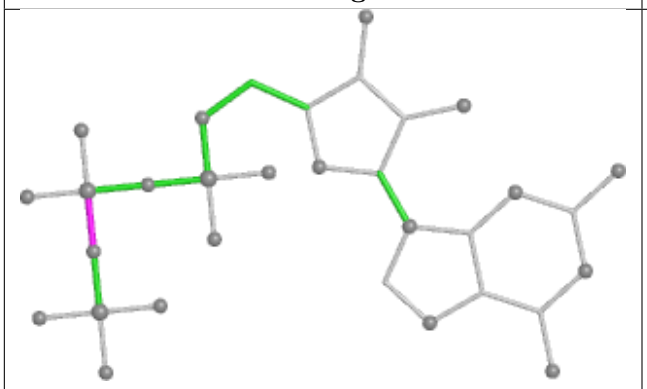
Ligand GNP B 203



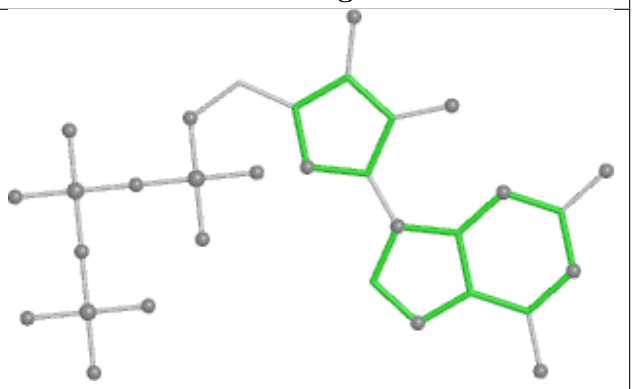
Bond lengths



Bond angles

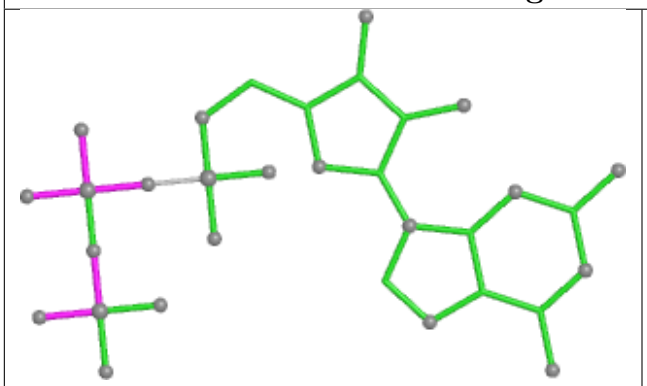


Torsions

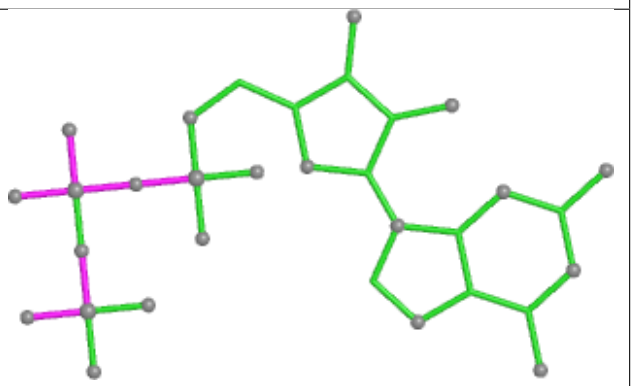


Rings

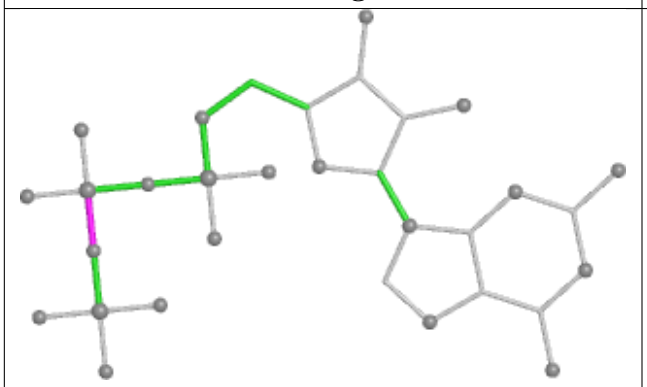
Ligand GNP J 203



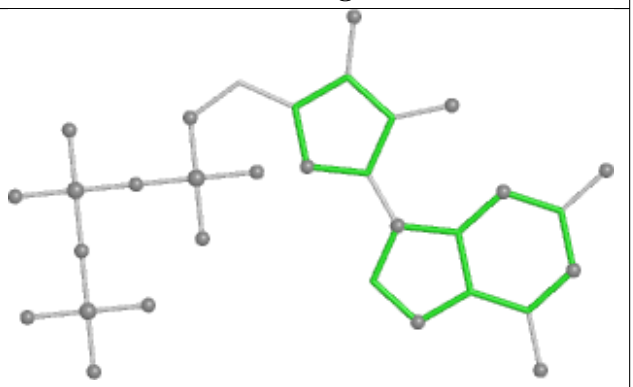
Bond lengths



Bond angles

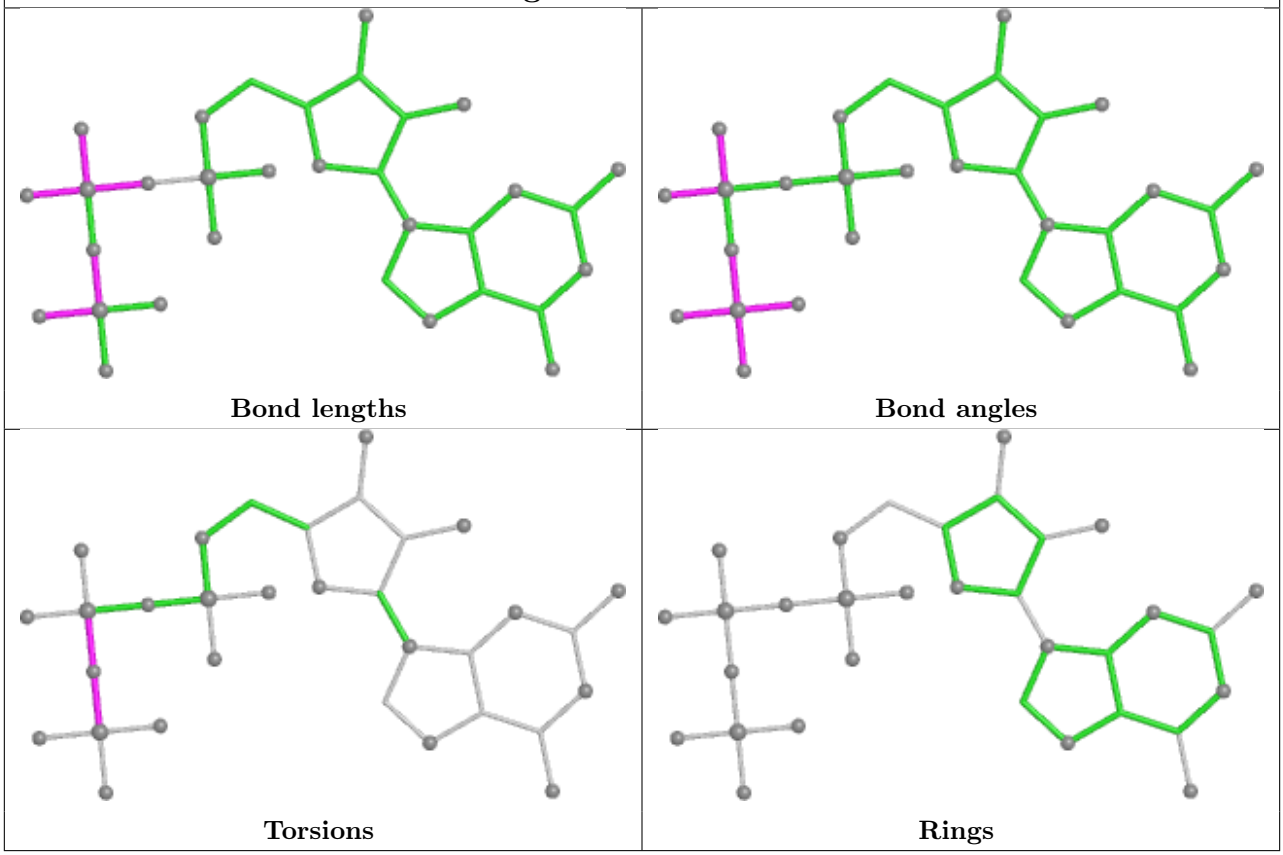


Torsions

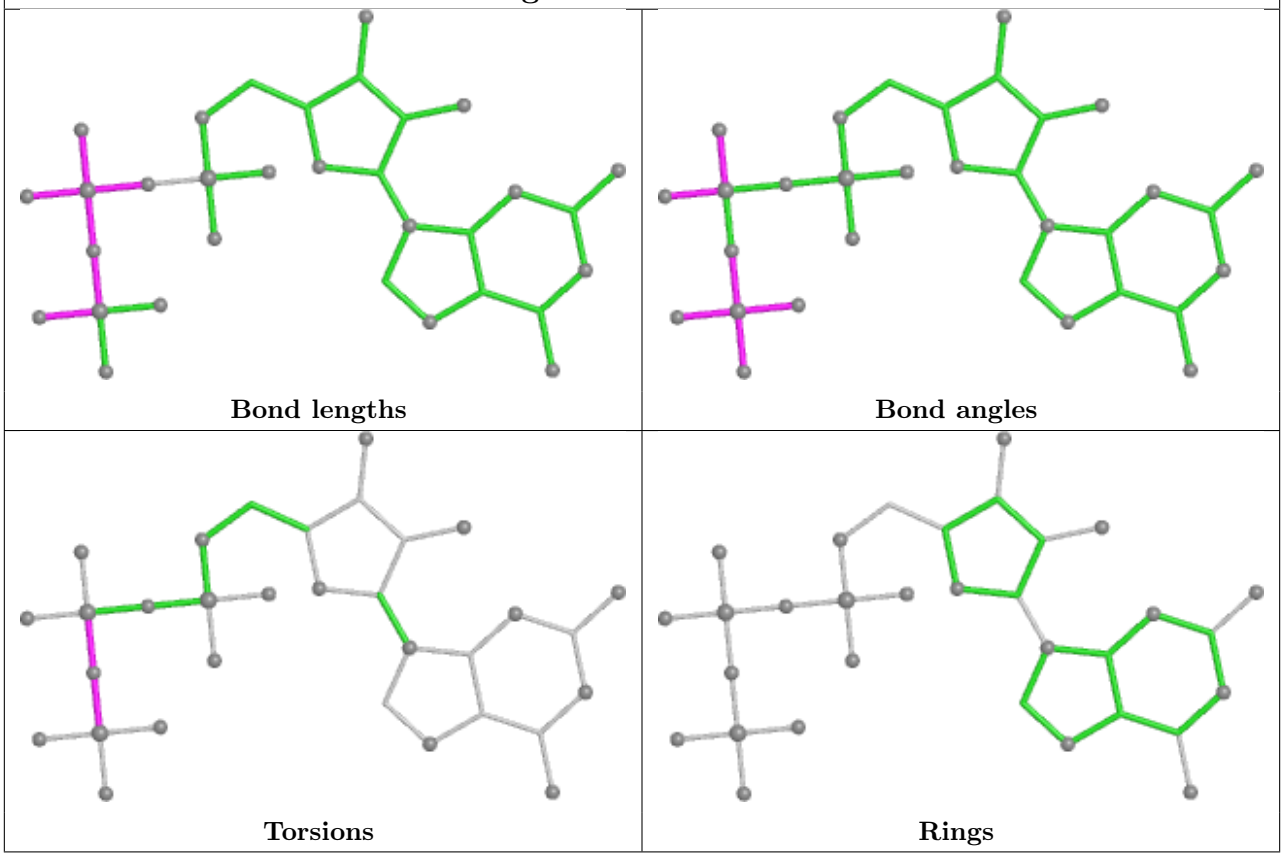


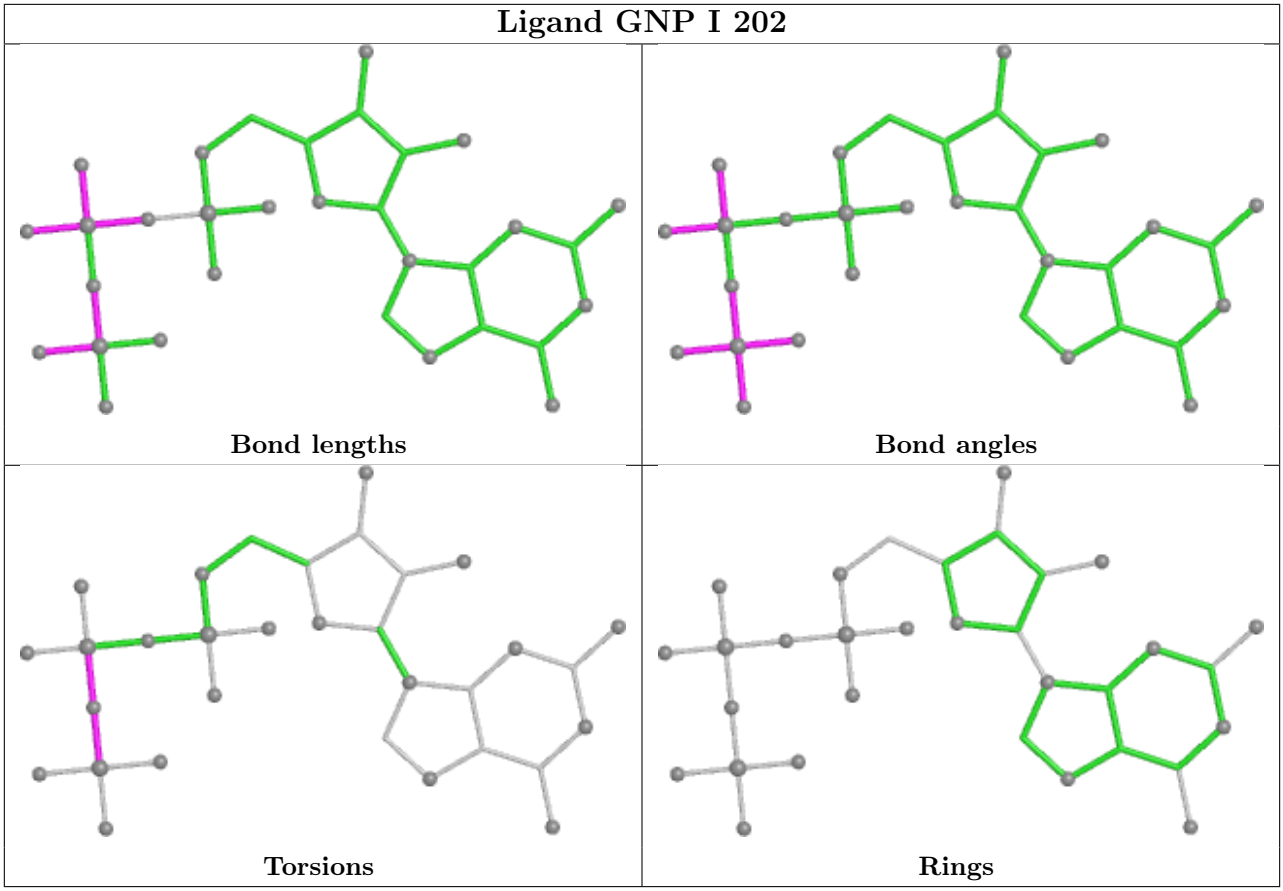
Rings

Ligand GNP E 202



Ligand GNP A 202





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 (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	201/202 (99%)	-0.05	1 (0%) 87 73	48, 69, 88, 100	0
1	B	201/202 (99%)	-0.15	0 100 100	46, 64, 88, 108	0
1	E	201/202 (99%)	-0.04	2 (0%) 79 61	53, 75, 94, 114	0
1	F	201/202 (99%)	0.05	0 100 100	57, 77, 102, 120	0
1	I	201/202 (99%)	0.14	4 (1%) 65 44	56, 77, 99, 119	0
1	J	201/202 (99%)	-0.12	0 100 100	44, 62, 81, 114	0
1	M	201/202 (99%)	0.08	2 (0%) 79 61	51, 73, 95, 117	0
1	N	201/202 (99%)	-0.01	0 100 100	48, 66, 85, 128	0
2	C	155/158 (98%)	-0.07	0 100 100	46, 70, 117, 131	0
2	D	146/158 (92%)	-0.07	3 (2%) 63 42	45, 75, 122, 133	0
2	G	155/158 (98%)	-0.02	2 (1%) 75 56	52, 76, 111, 139	0
2	H	146/158 (92%)	0.20	2 (1%) 73 53	48, 100, 141, 147	0
2	K	155/158 (98%)	-0.03	1 (0%) 85 70	48, 75, 130, 145	0
2	L	146/158 (92%)	0.14	3 (2%) 63 42	48, 96, 154, 163	0
2	O	155/158 (98%)	-0.06	1 (0%) 85 70	45, 70, 117, 126	0
2	P	146/158 (92%)	0.22	3 (2%) 63 42	45, 81, 137, 145	0
All	All	2812/2880 (97%)	0.01	24 (0%) 81 63	44, 72, 126, 163	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	67	PRO	3.8
1	M	67	PRO	3.6
2	K	155	PRO	3.1
2	P	2	ILE	3.1
2	H	2	ILE	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)

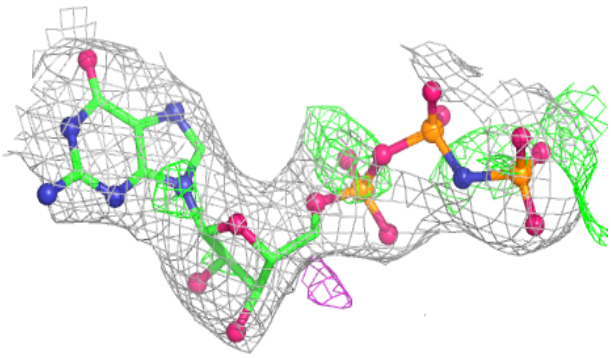
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

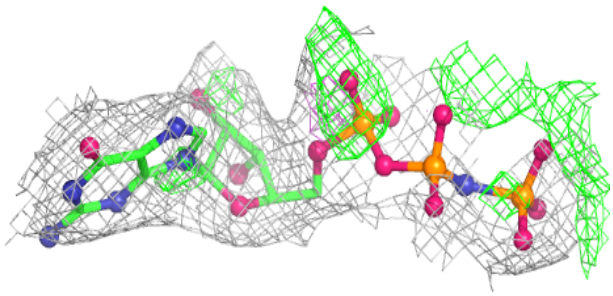
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GNP	M	202	32/32	0.90	0.13	87,90,93,94	0
4	GNP	I	202	32/32	0.93	0.11	91,94,97,98	0
4	GNP	A	202	32/32	0.93	0.12	82,85,88,89	0
4	GNP	E	202	32/32	0.94	0.12	84,87,89,91	0
4	GNP	F	203	32/32	0.95	0.10	86,90,94,97	0
4	GNP	B	203	32/32	0.95	0.09	79,83,87,91	0
4	GNP	J	203	32/32	0.95	0.10	74,78,82,85	0
3	NI	M	201	1/1	0.95	0.14	107,107,107,107	0
4	GNP	N	203	32/32	0.95	0.10	79,82,86,90	0
3	NI	I	201	1/1	0.96	0.10	118,118,118,118	0
3	NI	B	202	1/1	0.96	0.08	94,94,94,94	0
3	NI	F	202	1/1	0.97	0.09	120,120,120,120	0
3	NI	E	201	1/1	0.97	0.10	118,118,118,118	0
3	NI	J	202	1/1	0.97	0.08	100,100,100,100	0
3	NI	F	201	1/1	0.97	0.08	91,91,91,91	0
3	NI	N	202	1/1	0.98	0.08	94,94,94,94	0
3	NI	B	201	1/1	0.98	0.10	86,86,86,86	0
3	NI	A	201	1/1	0.98	0.13	102,102,102,102	0
3	NI	J	201	1/1	0.99	0.10	86,86,86,86	0
3	NI	N	201	1/1	1.00	0.07	87,87,87,87	0

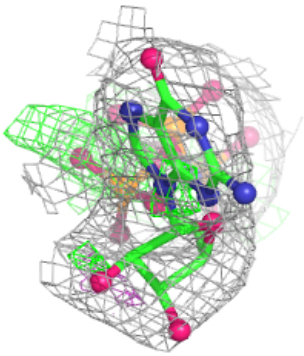
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNP M 202:

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

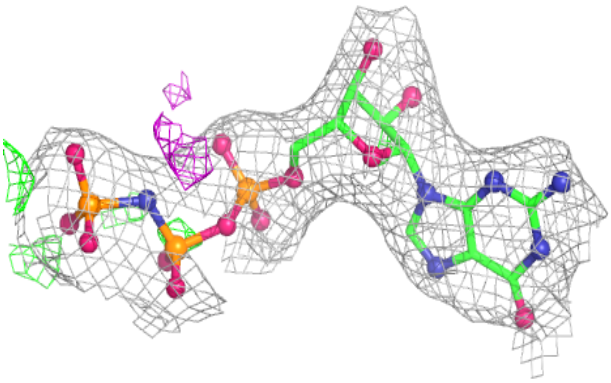


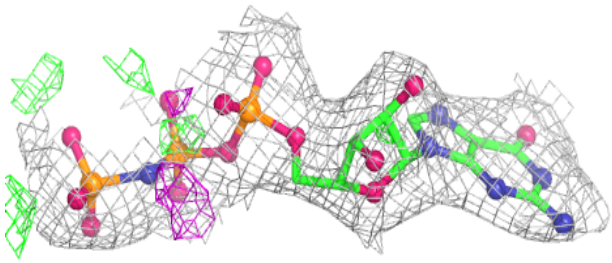


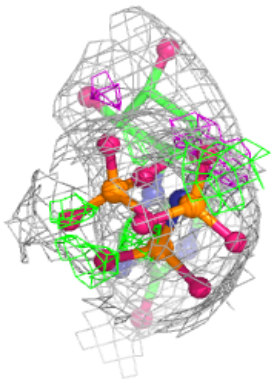


Electron density around GNP I 202:

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

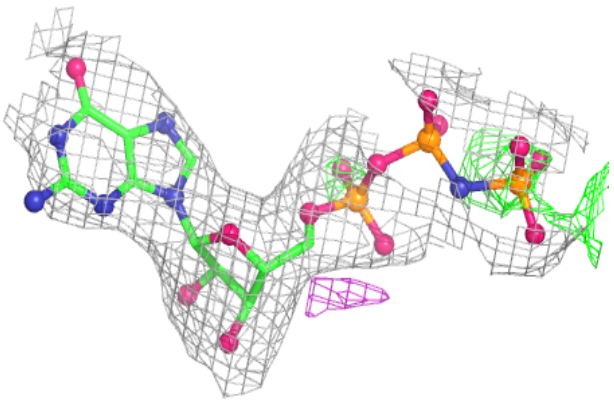


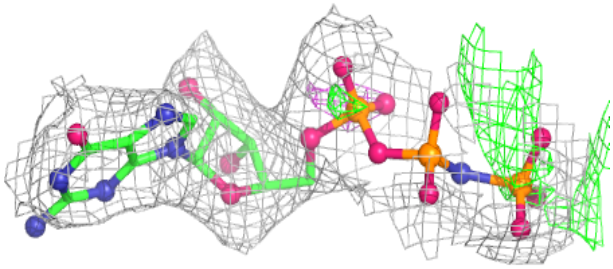


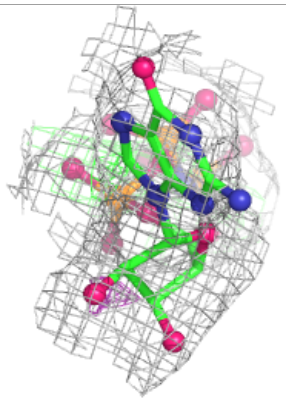


Electron density around GNP A 202:

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

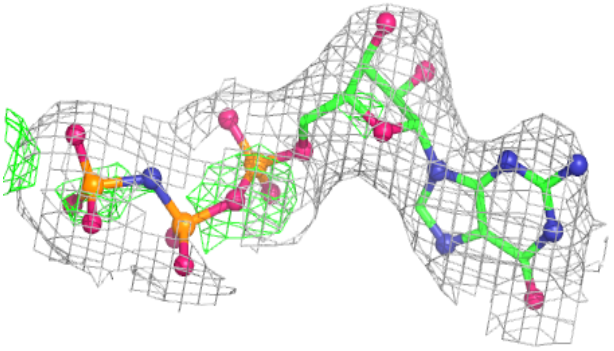


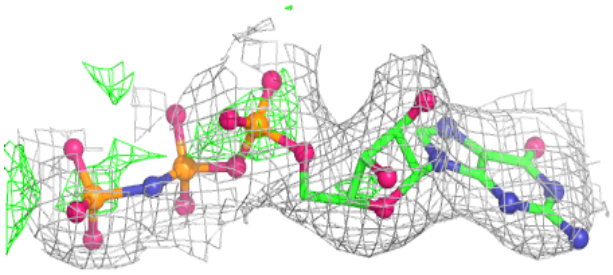


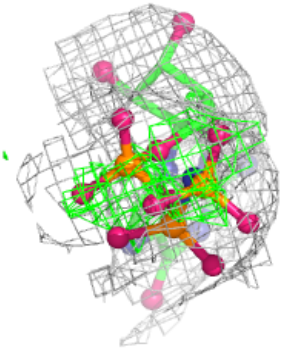


Electron density around GNP E 202:

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

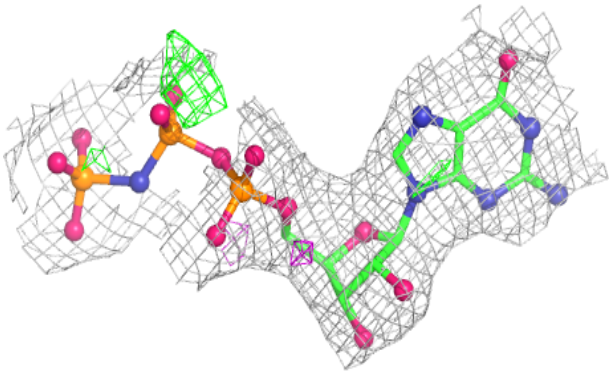


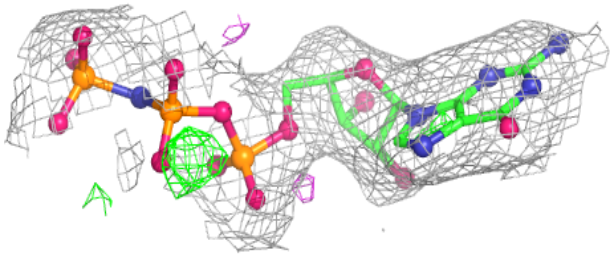


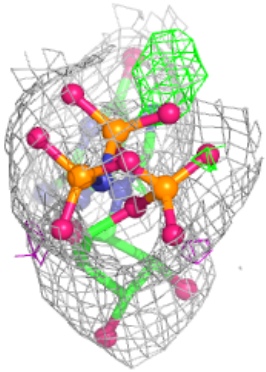


Electron density around GNP F 203:

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

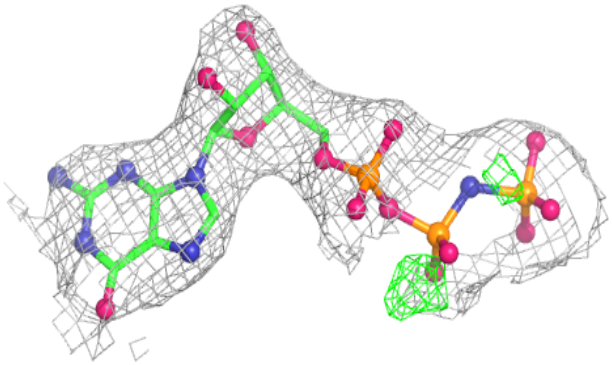


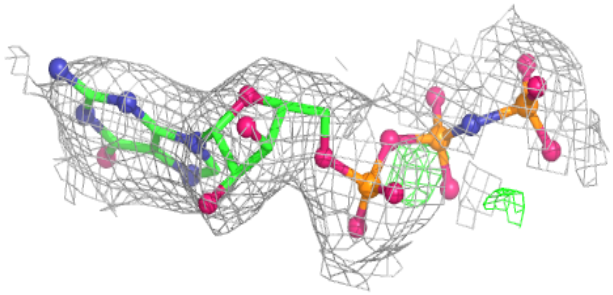


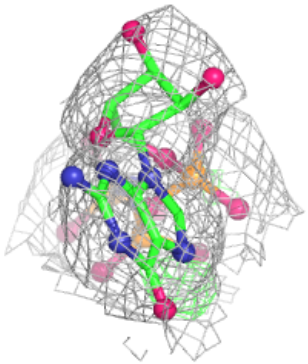


Electron density around GNP B 203:

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

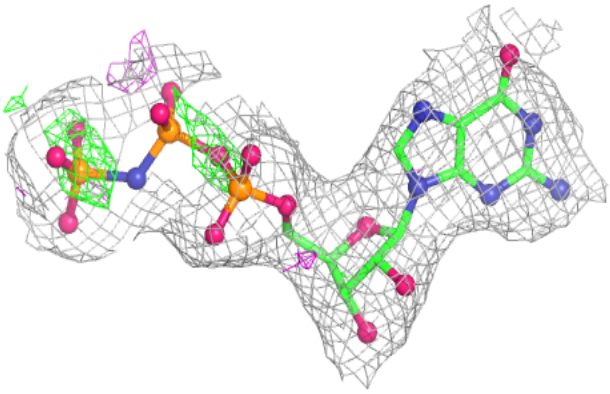


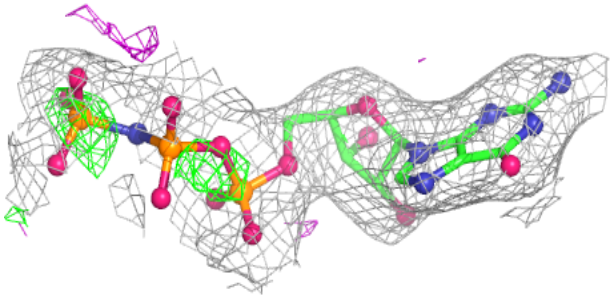


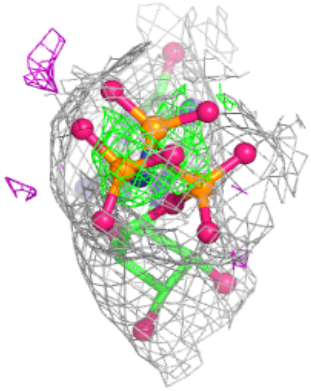


Electron density around GNP J 203:

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

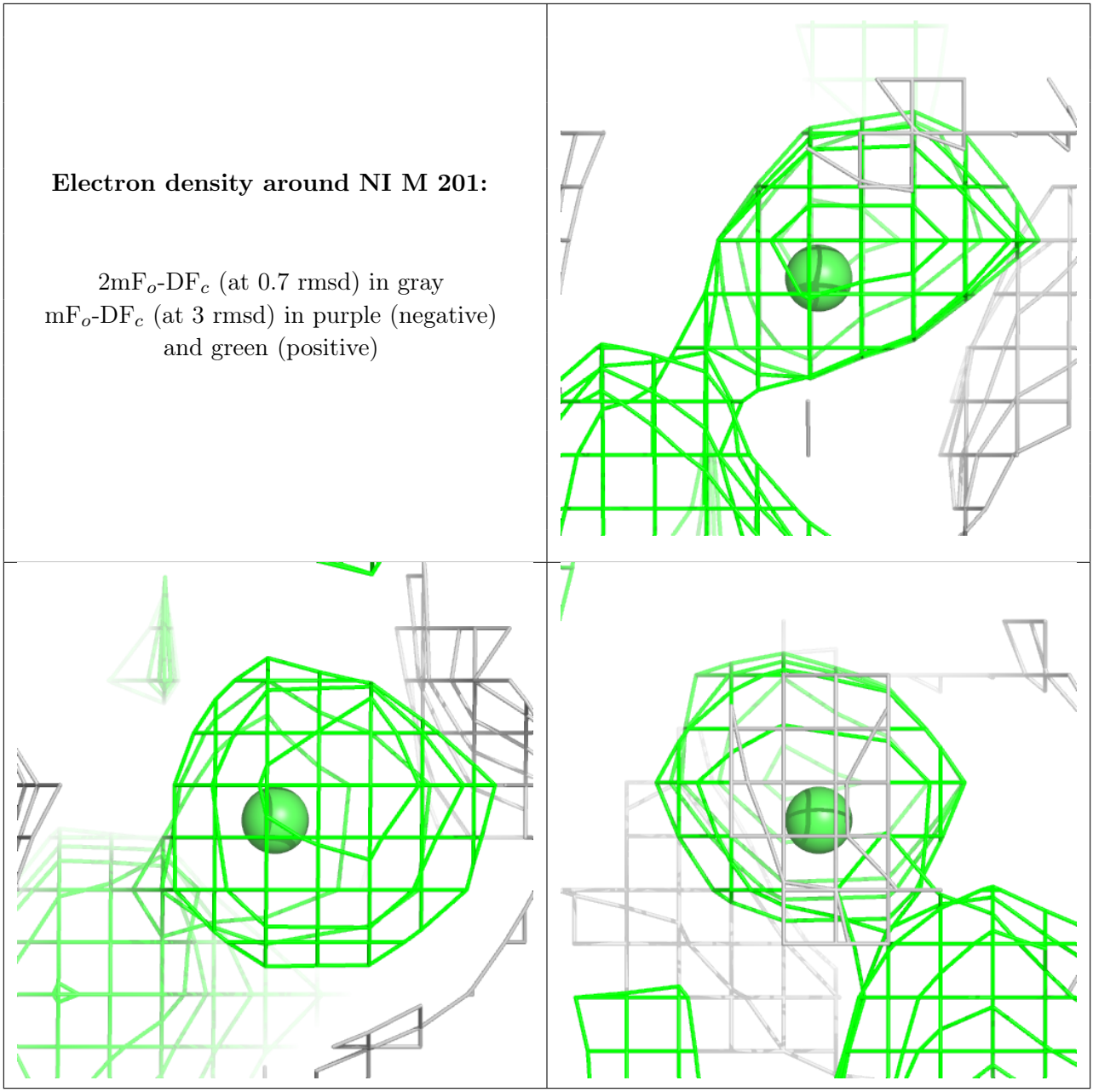






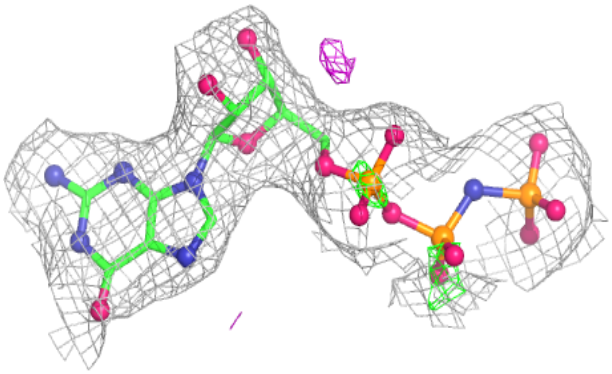
Electron density around NI M 201:

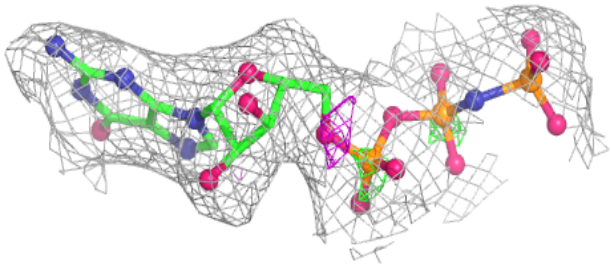
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

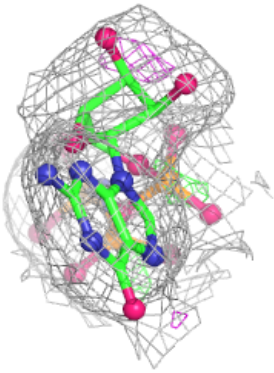


Electron density around GNP N 203:

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

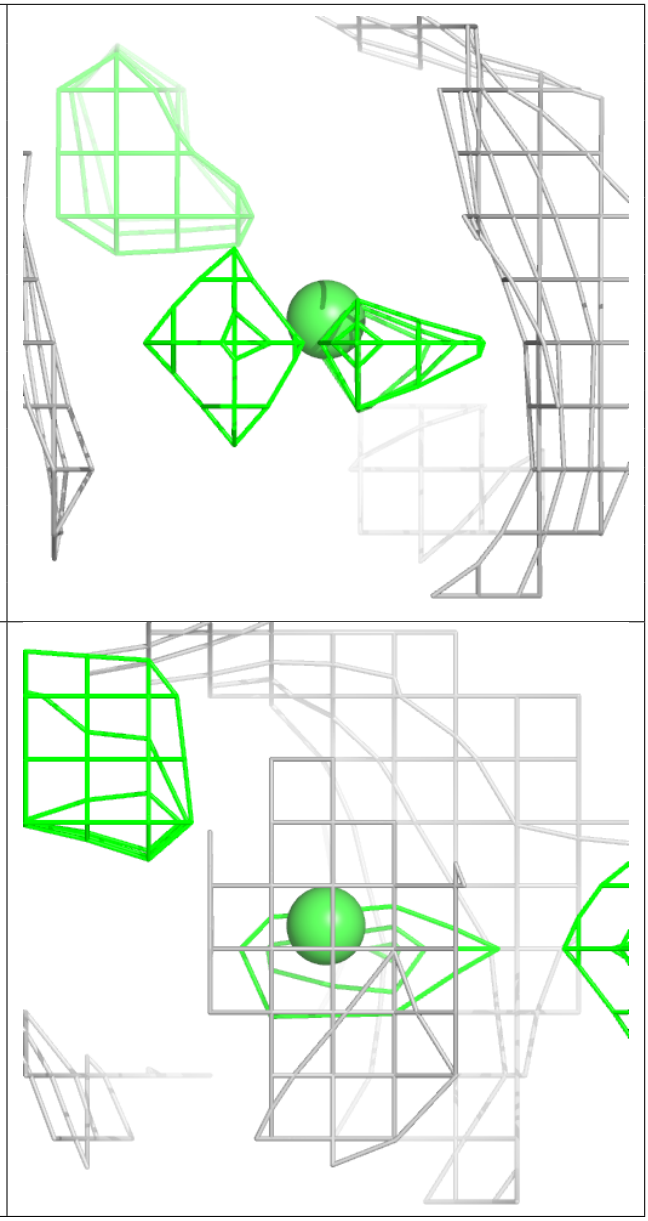






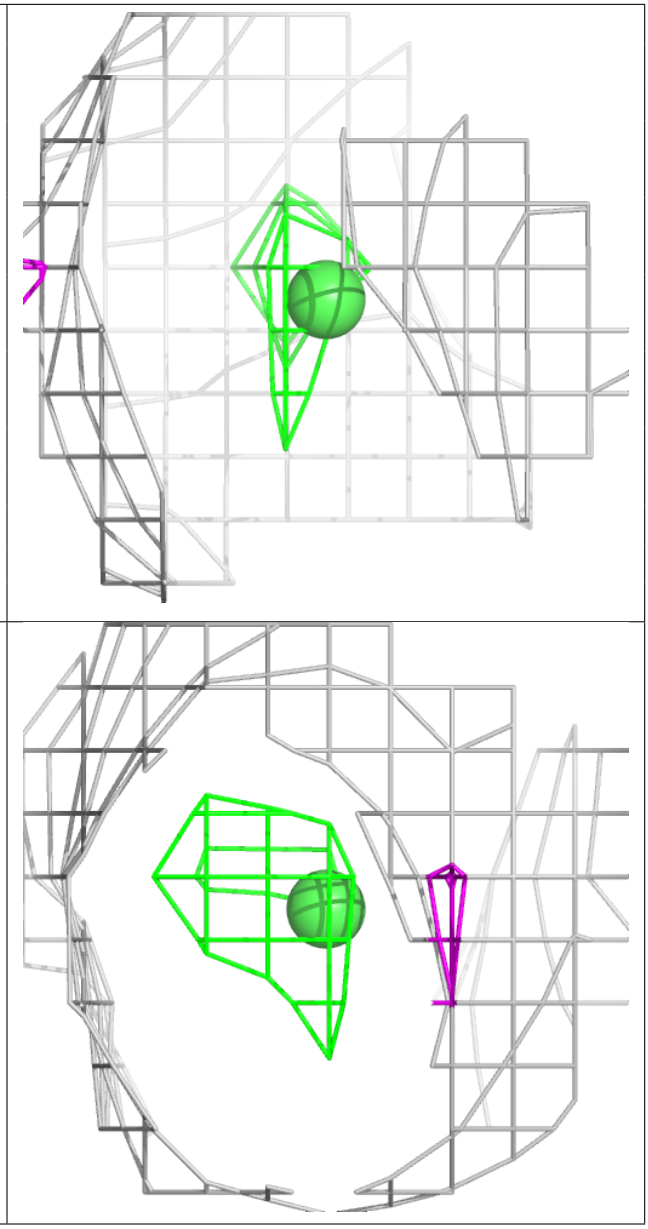
Electron density around NI I 201:

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



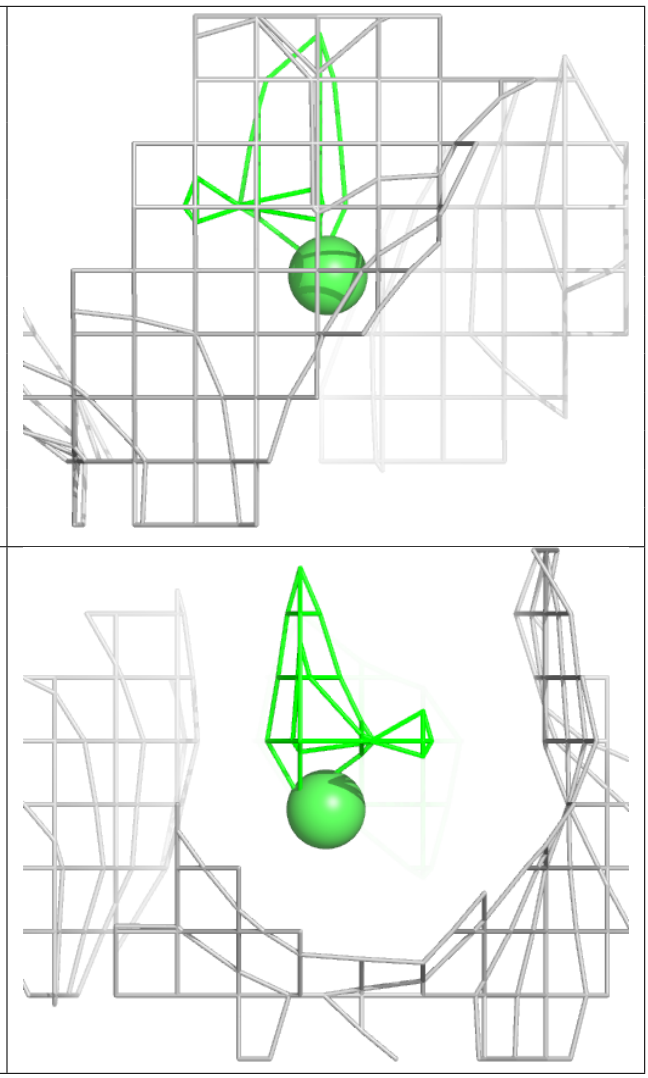
Electron density around NI B 202:

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



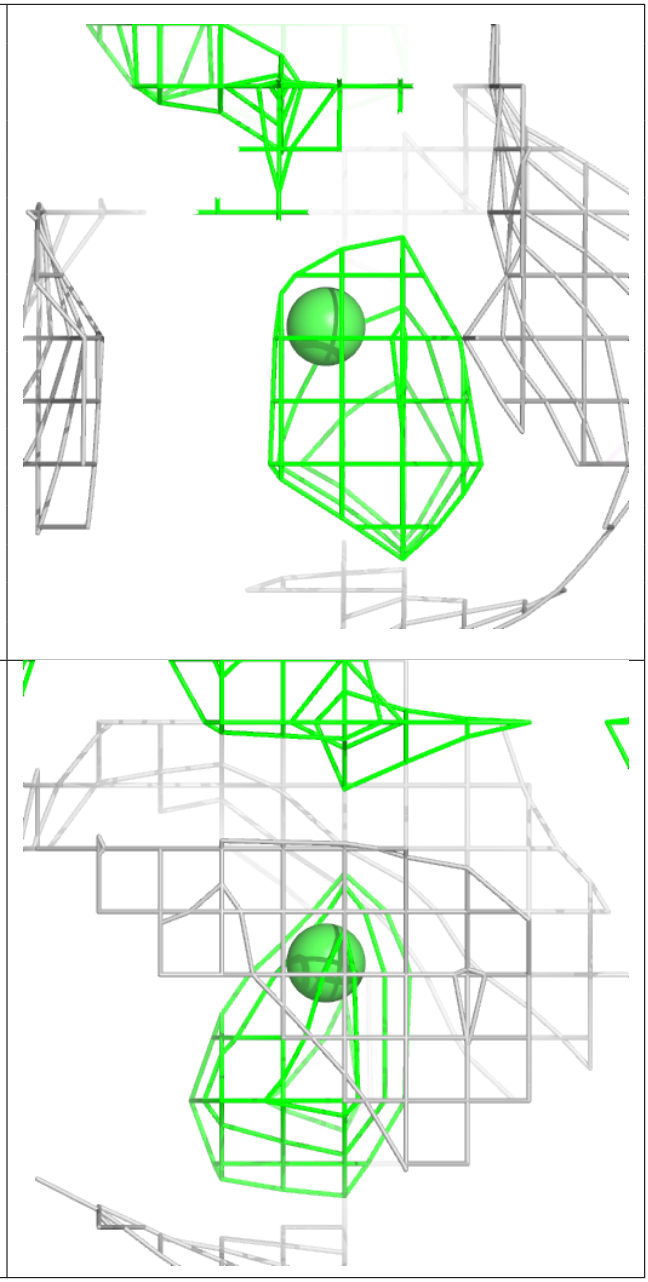
Electron density around NI F 202:

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



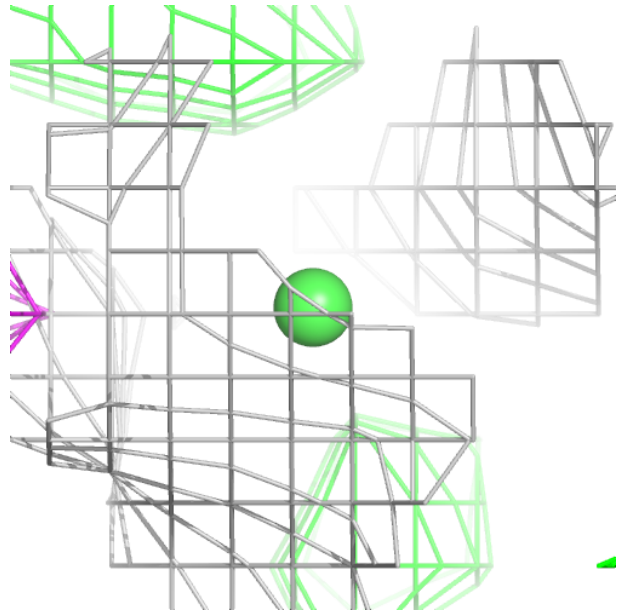
Electron density around NI E 201:

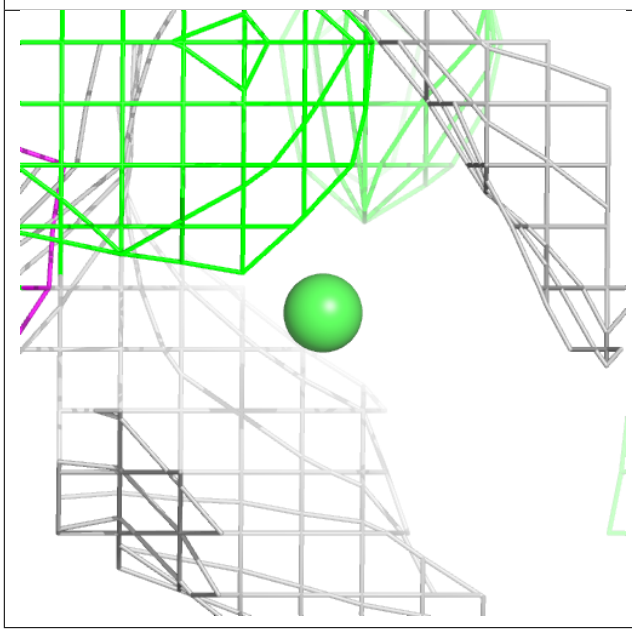
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

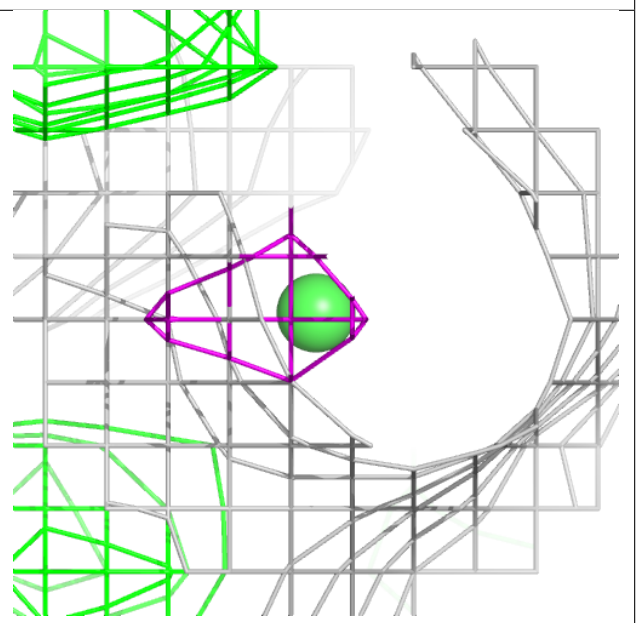


Electron density around NI J 202:

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

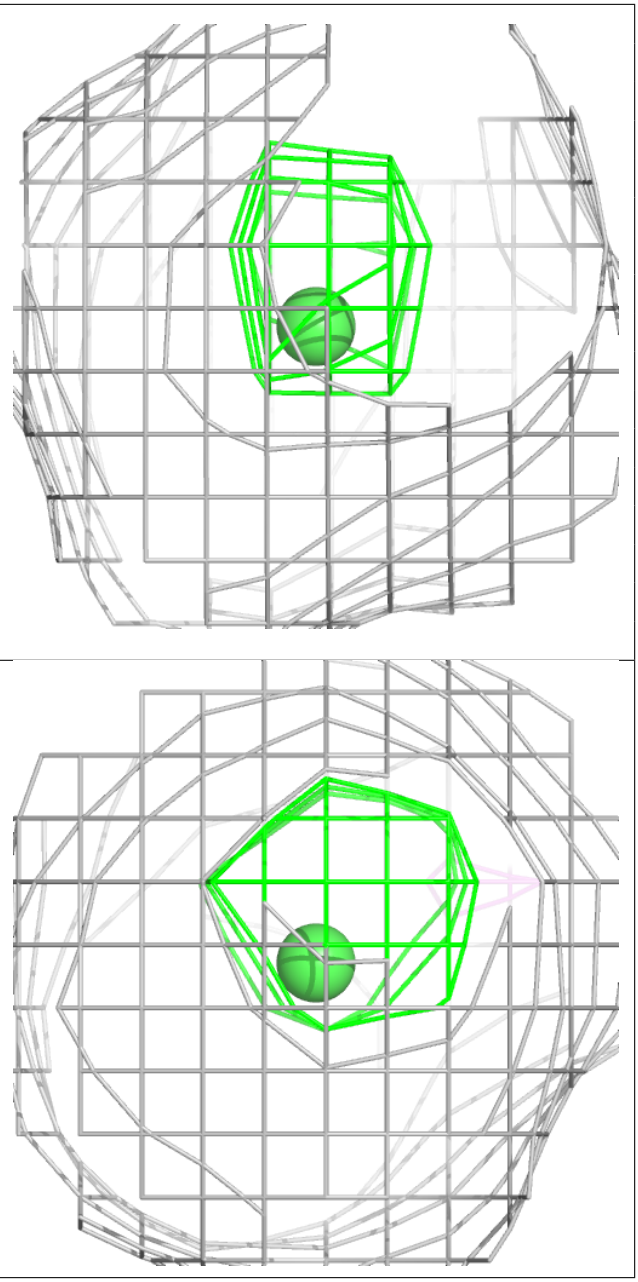






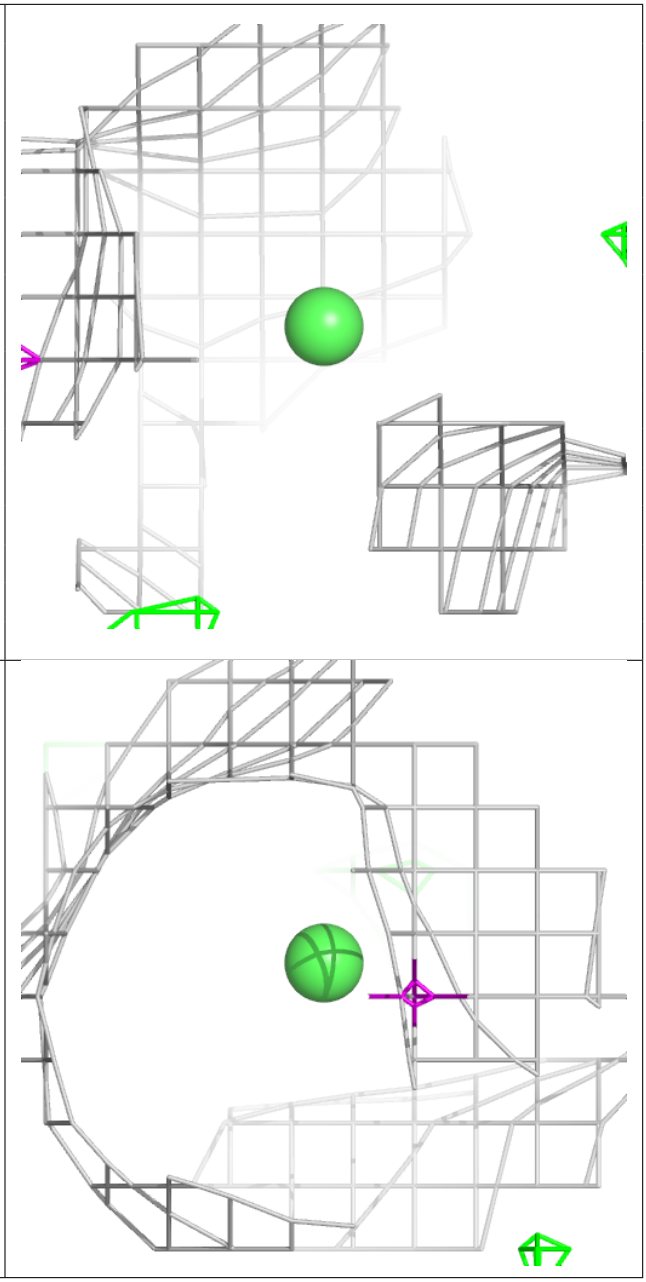
Electron density around NI F 201:

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



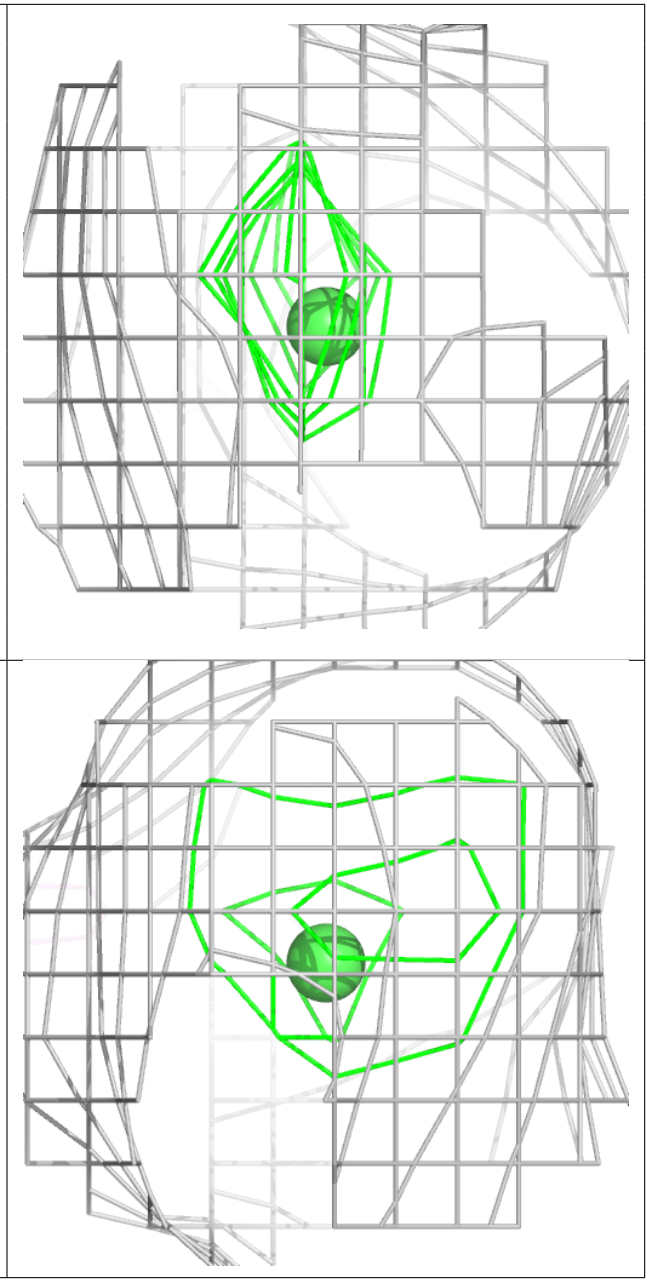
Electron density around NI N 202:

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



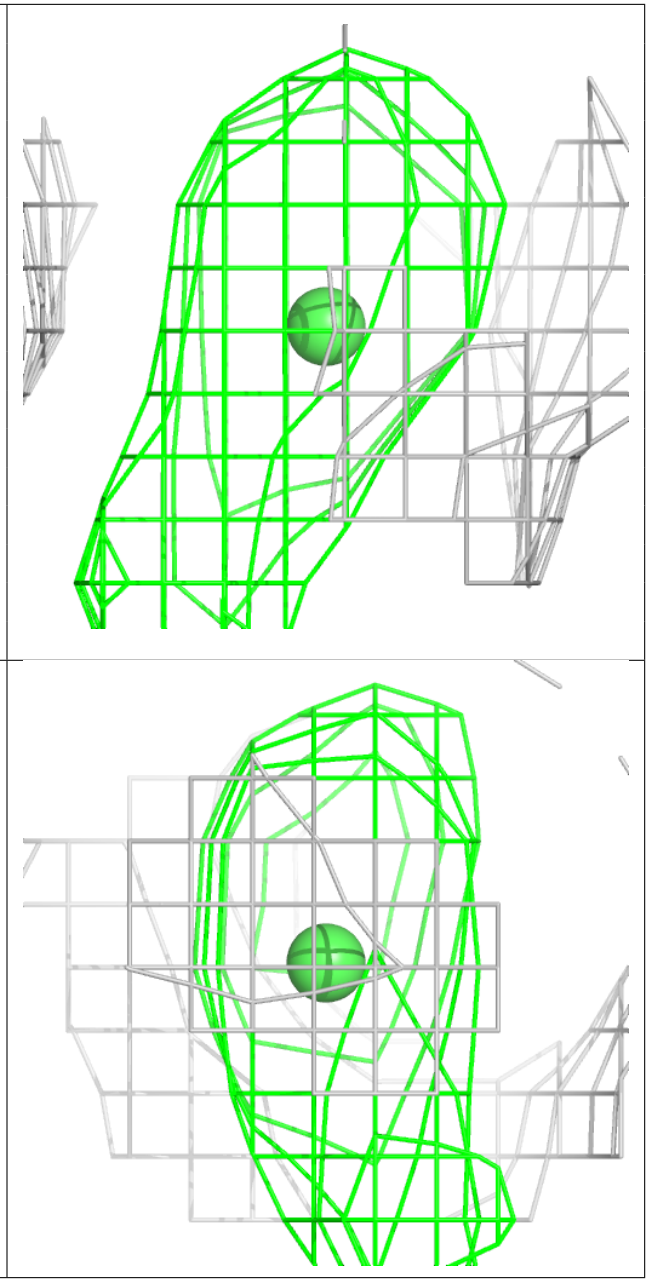
Electron density around NI B 201:

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



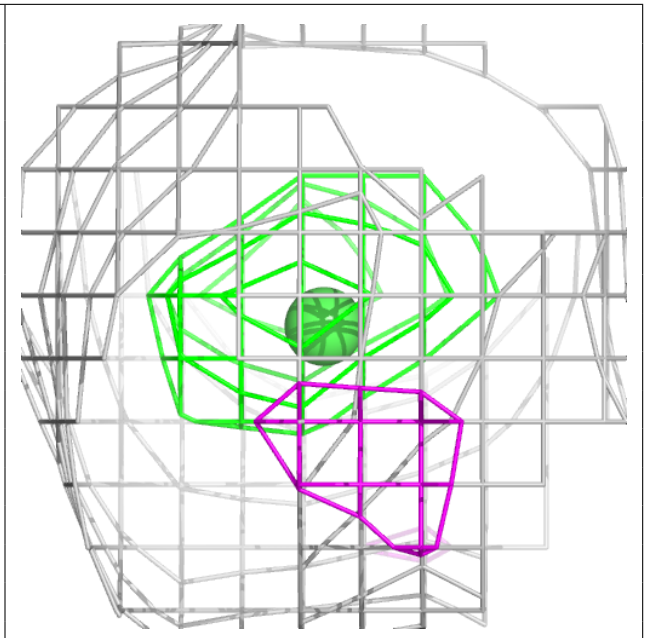
Electron density around NI A 201:

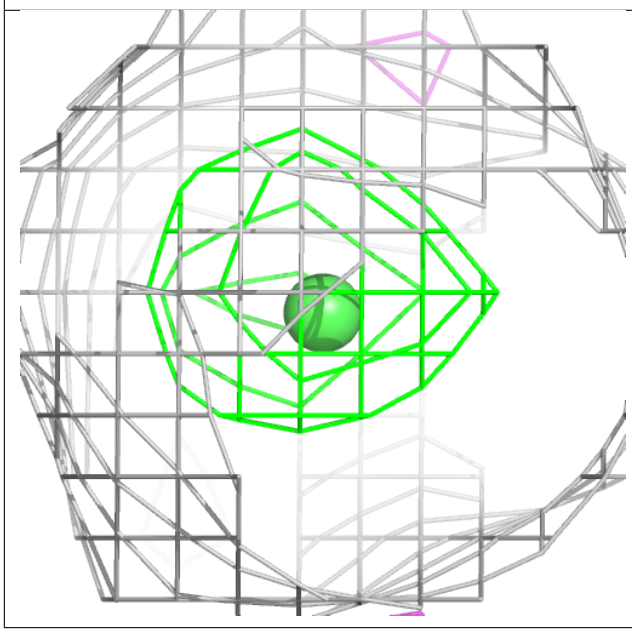
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

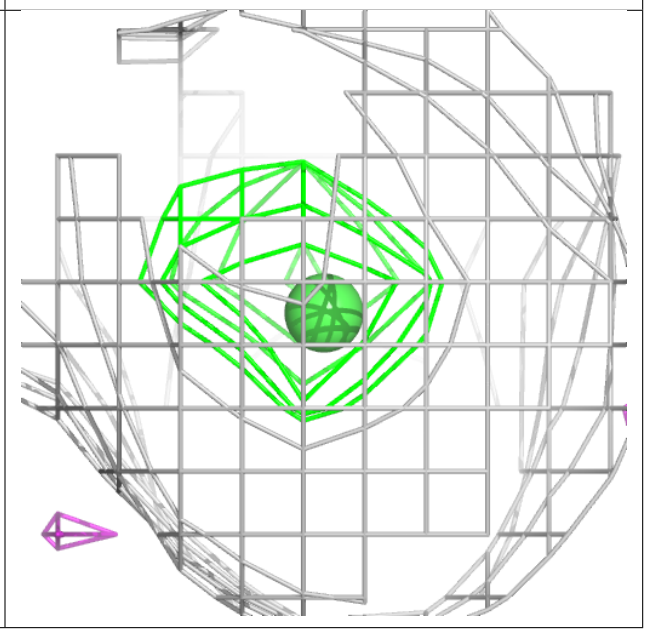


Electron density around NI J 201:

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

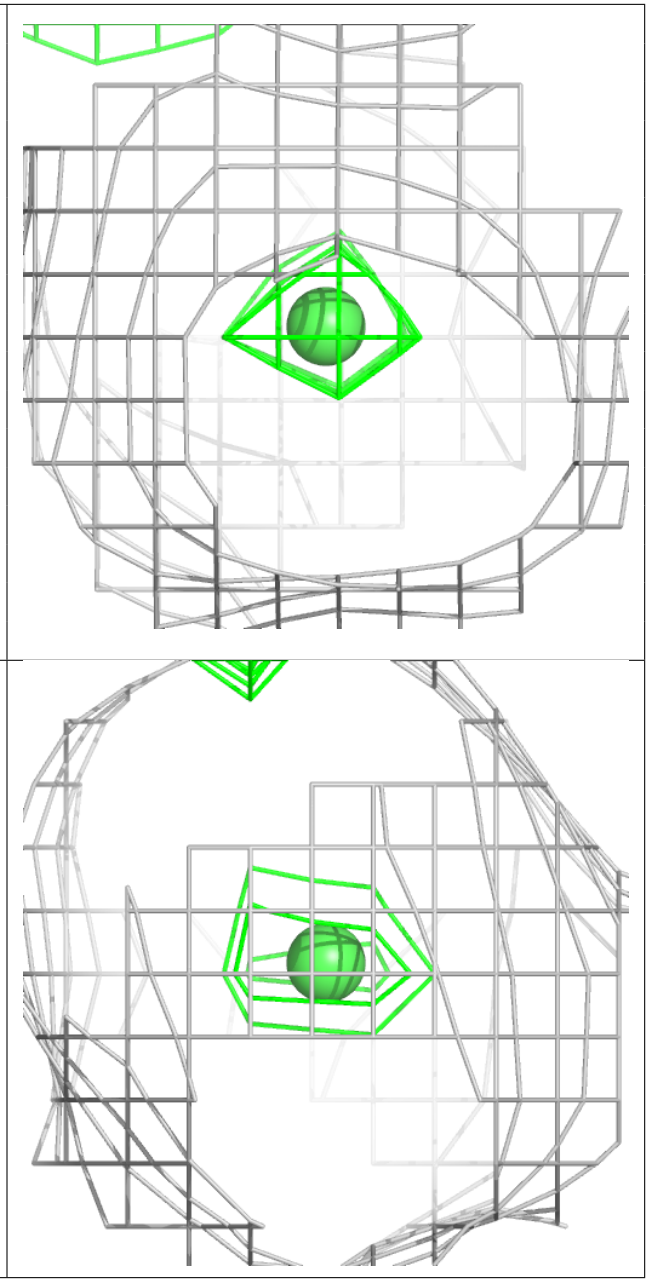






Electron density around NI N 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.