



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 1, 2025 – 10:42 AM JST

PDB ID : 8YL2 / pdb_00008yl2
Title : Crystal Structure of Homo Tetrameric RagA-like small GTPase from Asgard
Lokiarchaeota (LokiRagO) in complex with GTP
Authors : Alsheikh, F.B.; Robinson, R.C.
Deposited on : 2024-03-05
Resolution : 2.20 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:

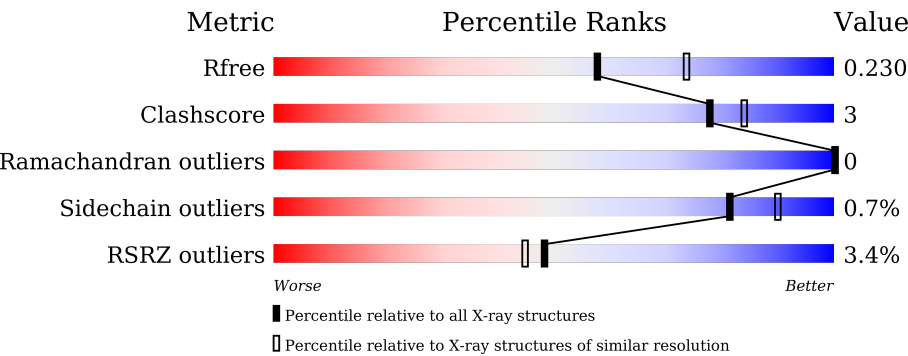
MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

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 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	342	<div><div>%</div><div>78%7%14%</div></div>
1	B	342	<div><div>3%</div><div>77%7%16%</div></div>
1	C	342	<div><div>4%</div><div>74%8%17%</div></div>
1	D	342	<div><div>4%</div><div>78%6%16%</div></div>
1	E	342	<div><div>2%</div><div>80%6%14%</div></div>
1	F	342	<div><div>2%</div><div>77%7%16%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	342	<div><div></div><div>3%</div><div>77%</div><div>6%</div><div>•</div><div>16%</div></div>
1	H	342	<div><div></div><div>4%</div><div>80%</div><div>5%</div><div>14%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19749 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 GTP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	1	0
			2419	1560	393	460	6			
1	B	288	Total	C	N	O	S	0	1	0
			2377	1535	383	453	6			
1	C	284	Total	C	N	O	S	0	1	0
			2347	1518	378	445	6			
1	D	288	Total	C	N	O	S	0	1	0
			2377	1535	383	453	6			
1	E	293	Total	C	N	O	S	0	1	0
			2419	1560	393	460	6			
1	F	288	Total	C	N	O	S	0	1	0
			2377	1535	383	453	6			
1	G	288	Total	C	N	O	S	0	1	0
			2377	1535	383	453	6			
1	H	293	Total	C	N	O	S	0	1	0
			2419	1560	393	460	6			

There are 16 discrepancies between the modelled and reference sequences:

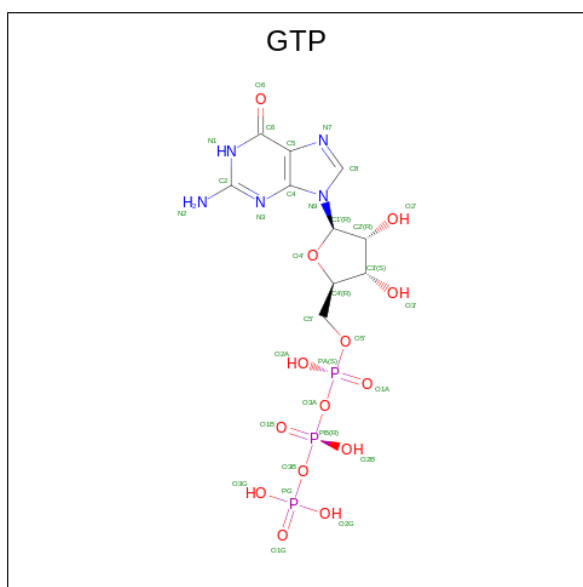
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A5B9DBS5
A	1	PRO	-	expression tag	UNP A0A5B9DBS5
B	0	GLY	-	expression tag	UNP A0A5B9DBS5
B	1	PRO	-	expression tag	UNP A0A5B9DBS5
C	0	GLY	-	expression tag	UNP A0A5B9DBS5
C	1	PRO	-	expression tag	UNP A0A5B9DBS5
D	0	GLY	-	expression tag	UNP A0A5B9DBS5
D	1	PRO	-	expression tag	UNP A0A5B9DBS5
E	0	GLY	-	expression tag	UNP A0A5B9DBS5
E	1	PRO	-	expression tag	UNP A0A5B9DBS5
F	0	GLY	-	expression tag	UNP A0A5B9DBS5
F	1	PRO	-	expression tag	UNP A0A5B9DBS5
G	0	GLY	-	expression tag	UNP A0A5B9DBS5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	PRO	-	expression tag	UNP A0A5B9DBS5
H	0	GLY	-	expression tag	UNP A0A5B9DBS5
H	1	PRO	-	expression tag	UNP A0A5B9DBS5

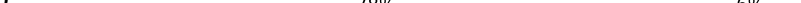
- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).

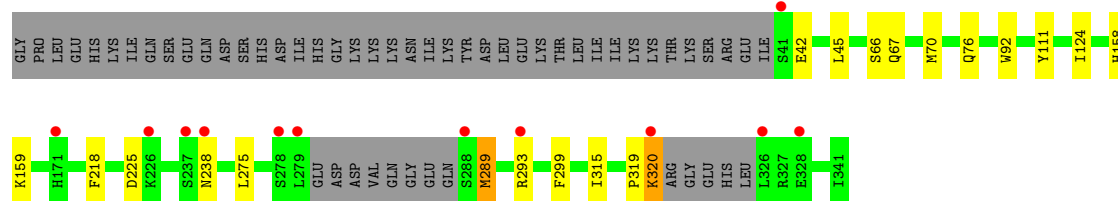


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total 1 Mg 1	0	0
3	B	1	Total 1 Mg 1	0	0
3	C	1	Total 1 Mg 1	0	0
3	D	1	Total 1 Mg 1	0	0
3	E	1	Total 1 Mg 1	0	0
3	F	1	Total 1 Mg 1	0	0
3	G	1	Total 1 Mg 1	0	0
3	H	1	Total 1 Mg 1	0	0

- Molecule 4 is water.

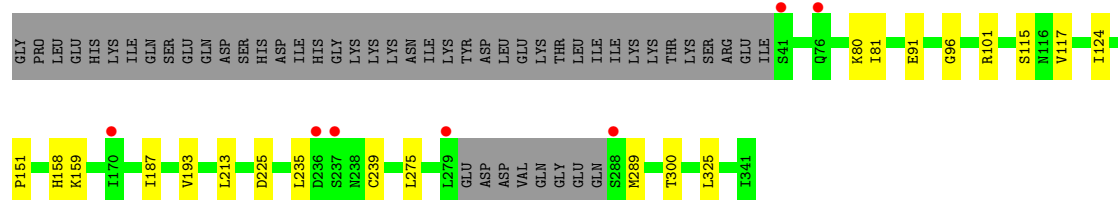
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	77	Total 77 O 77	0	0
4	B	48	Total 48 O 48	0	0
4	C	55	Total 55 O 55	0	0
4	D	37	Total 37 O 37	0	0
4	E	33	Total 33 O 33	0	0
4	F	50	Total 50 O 50	0	0
4	G	44	Total 44 O 44	0	0
4	H	29	Total 29 O 29	0	0

Chain D:  4% 78% 6% 16%

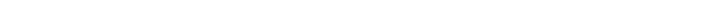


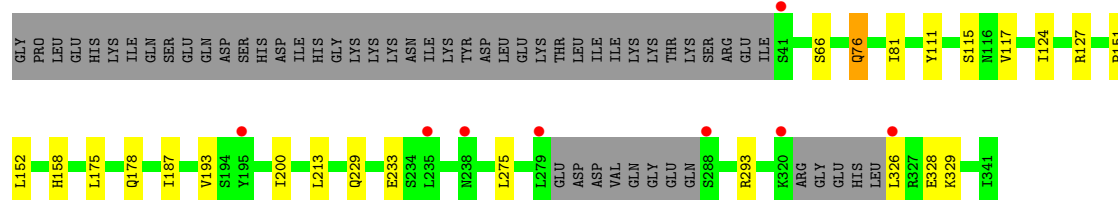
- Molecule 1: GTP-binding protein

Chain E:

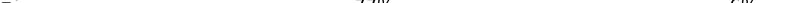


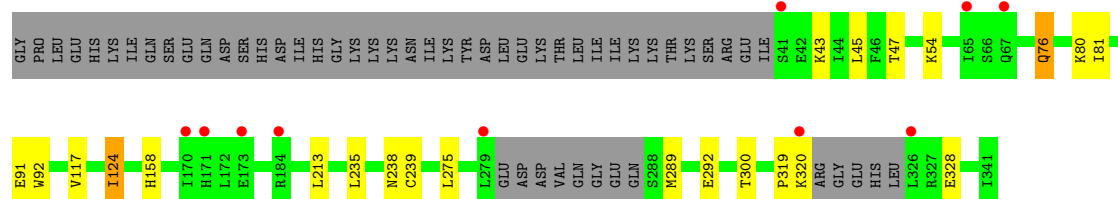
- Molecule 1: GTP-binding protein

Chain F:  2% 77% 7% 16%




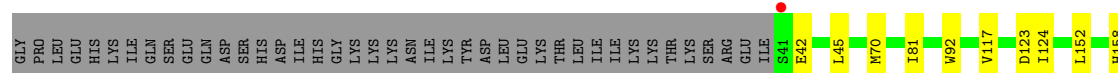
- Molecule 1: GTP-binding protein

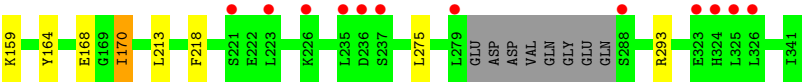
Chain G:  3% 77% 6% 16%



- Molecule 1: GTP-binding protein

Chain H: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.76Å 97.18Å 145.74Å 90.00° 104.28° 90.00°	Depositor
Resolution (Å)	27.25 – 2.20 27.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (27.25-2.20) 99.9 (27.25-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.202 , 0.230 0.205 , 0.230	Depositor DCC
R_{free} test set	8271 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19749	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 37.23 % 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 4.4242e-04. 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: GTP, MG

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	0/2463	0.30	0/3313
1	B	0.20	0/2419	0.33	0/3253
1	C	0.28	0/2388	0.38	1/3209 (0.0%)
1	D	0.18	0/2419	0.31	0/3253
1	E	0.13	0/2463	0.30	0/3313
1	F	0.22	0/2419	0.32	0/3253
1	G	0.22	0/2419	0.32	0/3253
1	H	0.13	0/2463	0.26	0/3313
All	All	0.20	0/19453	0.31	1/26160 (0.0%)

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	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ALA	N-CA-C	5.05	116.19	108.52

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	127	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	2419	0	2439	16	0
1	B	2377	0	2398	16	0
1	C	2347	0	2371	18	0
1	D	2377	0	2398	14	0
1	E	2419	0	2439	13	0
1	F	2377	0	2398	16	0
1	G	2377	0	2398	15	0
1	H	2419	0	2439	12	0
2	A	32	0	12	1	0
2	B	32	0	12	0	0
2	C	32	0	12	0	0
2	D	32	0	12	1	0
2	E	32	0	12	1	0
2	F	32	0	12	1	0
2	G	32	0	12	0	0
2	H	32	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	77	0	0	1	0
4	B	48	0	0	0	0
4	C	55	0	0	0	0
4	D	37	0	0	0	0
4	E	33	0	0	0	0
4	F	50	0	0	1	0
4	G	44	0	0	0	0
4	H	29	0	0	0	0
All	All	19749	0	19376	105	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 105 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:326:LEU:CD2	1:C:328:GLU:OE1	2.35	0.75
1:C:326:LEU:HD23	1:C:328:GLU:OE1	1.92	0.70
1:D:76:GLN:NE2	1:D:111:TYR:OH	2.25	0.69
1:A:87:ASN:ND2	4:A:501:HOH:O	2.24	0.67
1:C:117:VAL:HG22	1:C:152:LEU:HB3	1.76	0.67

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	290/342 (85%)	282 (97%)	8 (3%)	0	100	100
1	B	283/342 (83%)	276 (98%)	7 (2%)	0	100	100
1	C	277/342 (81%)	273 (99%)	4 (1%)	0	100	100
1	D	283/342 (83%)	276 (98%)	7 (2%)	0	100	100
1	E	290/342 (85%)	283 (98%)	7 (2%)	0	100	100
1	F	283/342 (83%)	277 (98%)	6 (2%)	0	100	100
1	G	283/342 (83%)	276 (98%)	7 (2%)	0	100	100
1	H	290/342 (85%)	284 (98%)	6 (2%)	0	100	100
All	All	2279/2736 (83%)	2227 (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	275/320 (86%)	274 (100%)	1 (0%)	89	95
1	B	271/320 (85%)	268 (99%)	3 (1%)	70	82
1	C	267/320 (83%)	264 (99%)	3 (1%)	70	82
1	D	271/320 (85%)	268 (99%)	3 (1%)	70	82
1	E	275/320 (86%)	274 (100%)	1 (0%)	89	95
1	F	271/320 (85%)	269 (99%)	2 (1%)	81	90
1	G	271/320 (85%)	269 (99%)	2 (1%)	81	90
1	H	275/320 (86%)	274 (100%)	1 (0%)	89	95
All	All	2176/2560 (85%)	2160 (99%)	16 (1%)	81	90

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	124	ILE
1	G	76	GLN
1	D	289	MET
1	F	329	LYS
1	D	225	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	276	ASN
1	G	97	GLN
1	G	51	ASN
1	G	197	ASN
1	B	276	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 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$
2	GTP	C	401	3	26,34,34	1.13	2 (7%)	32,54,54	1.52	6 (18%)
2	GTP	D	401	3	26,34,34	1.12	2 (7%)	32,54,54	1.46	6 (18%)
2	GTP	F	401	3	26,34,34	1.12	2 (7%)	32,54,54	1.54	6 (18%)
2	GTP	B	401	3	26,34,34	1.13	2 (7%)	32,54,54	1.49	6 (18%)
2	GTP	E	401	3	26,34,34	1.14	2 (7%)	32,54,54	1.50	6 (18%)
2	GTP	H	401	3	26,34,34	1.12	2 (7%)	32,54,54	1.53	6 (18%)
2	GTP	G	401	3	26,34,34	1.12	1 (3%)	32,54,54	1.53	6 (18%)
2	GTP	A	401	3	26,34,34	1.14	2 (7%)	32,54,54	1.46	6 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	C	401	3	-	4/18/38/38	0/3/3/3
2	GTP	D	401	3	-	3/18/38/38	0/3/3/3
2	GTP	F	401	3	-	6/18/38/38	0/3/3/3
2	GTP	B	401	3	-	7/18/38/38	0/3/3/3
2	GTP	E	401	3	-	5/18/38/38	0/3/3/3
2	GTP	H	401	3	-	6/18/38/38	0/3/3/3
2	GTP	G	401	3	-	5/18/38/38	0/3/3/3
2	GTP	A	401	3	-	7/18/38/38	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	GTP	C5-C6	-4.08	1.39	1.47
2	G	401	GTP	C5-C6	-4.06	1.39	1.47
2	A	401	GTP	C5-C6	-4.06	1.39	1.47
2	C	401	GTP	C5-C6	-4.04	1.39	1.47
2	B	401	GTP	C5-C6	-4.04	1.39	1.47

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	GTP	PB-O3B-PG	-3.73	120.03	132.83
2	E	401	GTP	PB-O3B-PG	-3.64	120.33	132.83
2	H	401	GTP	PB-O3B-PG	-3.61	120.44	132.83
2	C	401	GTP	PB-O3B-PG	-3.48	120.89	132.83
2	B	401	GTP	PB-O3B-PG	-3.48	120.89	132.83

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GTP	C5'-O5'-PA-O3A
2	B	401	GTP	C5'-O5'-PA-O3A
2	B	401	GTP	C5'-O5'-PA-O2A
2	C	401	GTP	C5'-O5'-PA-O3A
2	E	401	GTP	C5'-O5'-PA-O3A

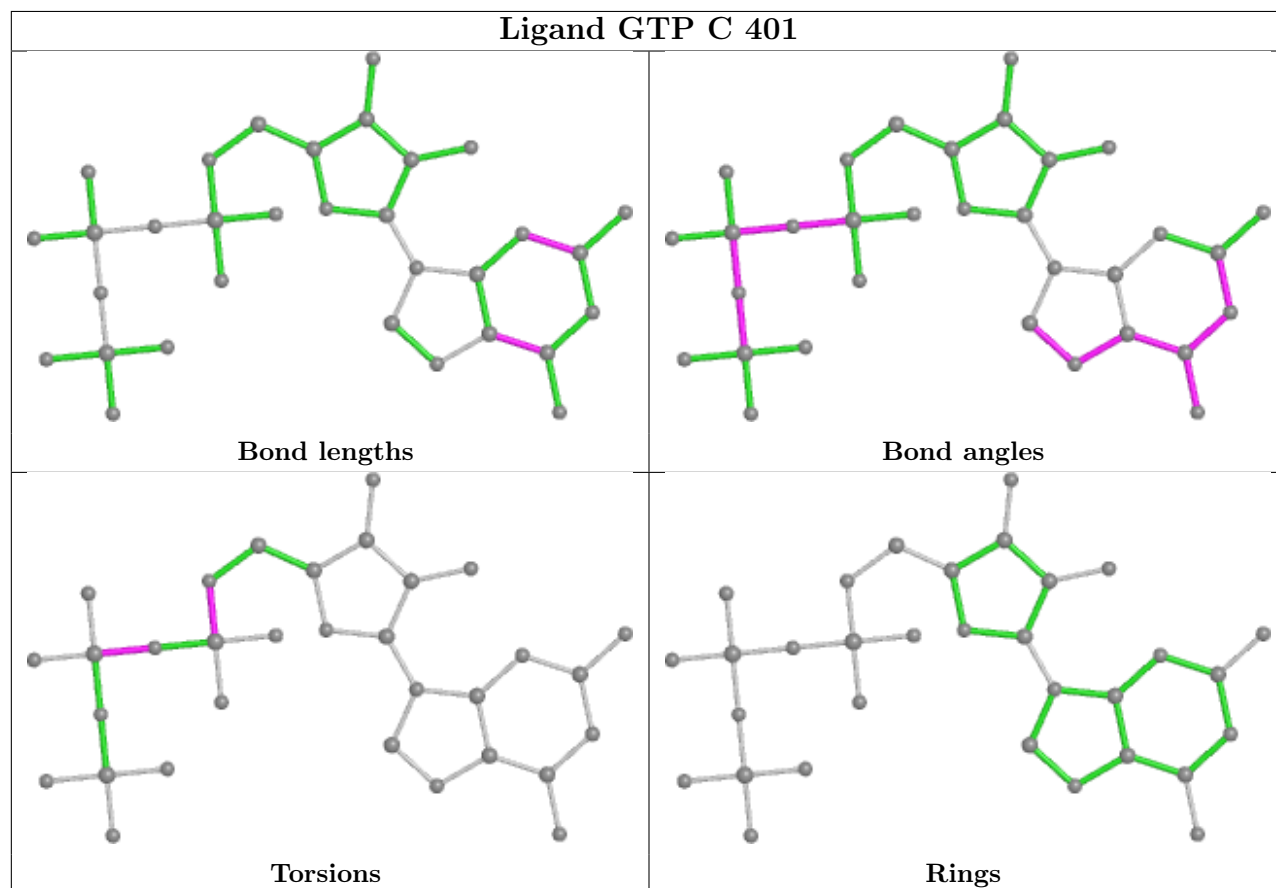
There are no ring outliers.

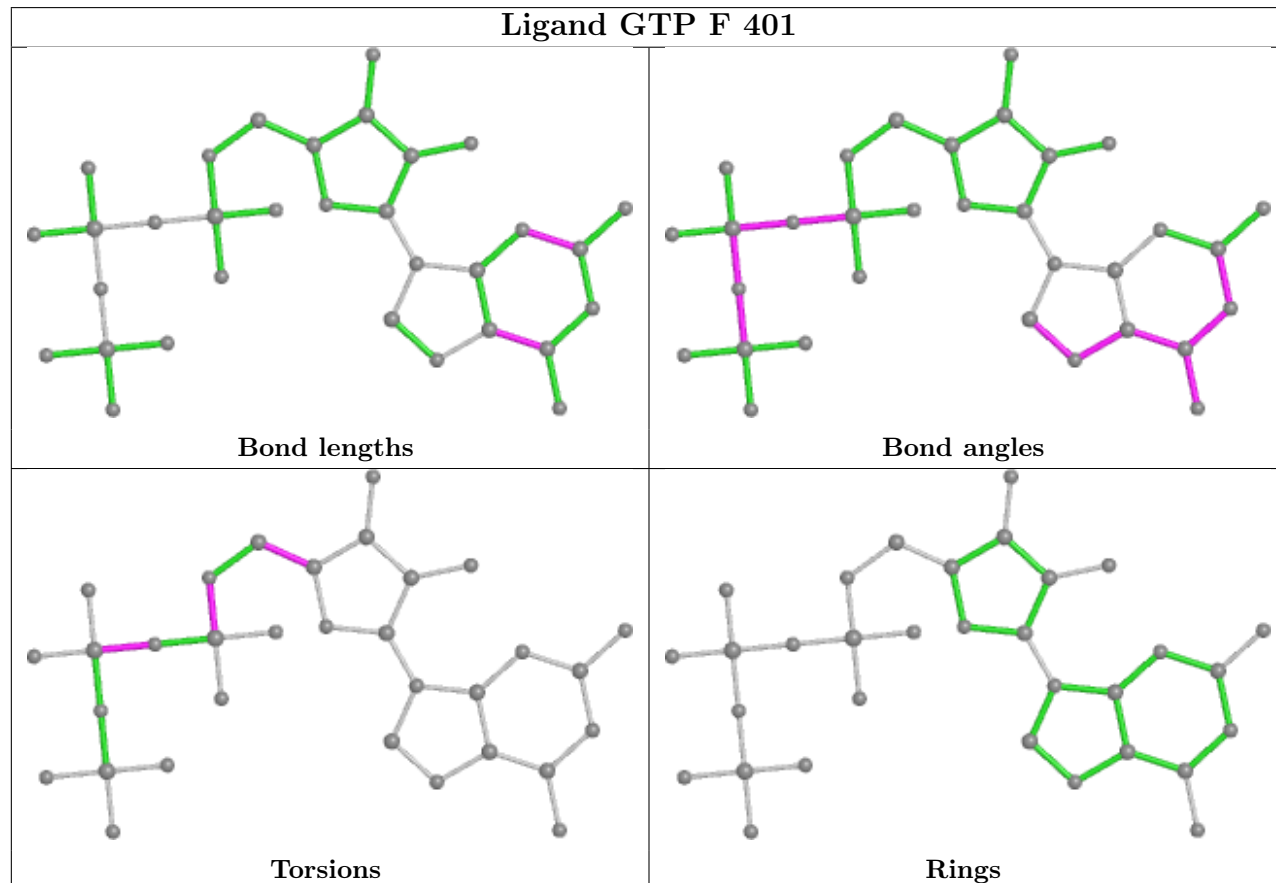
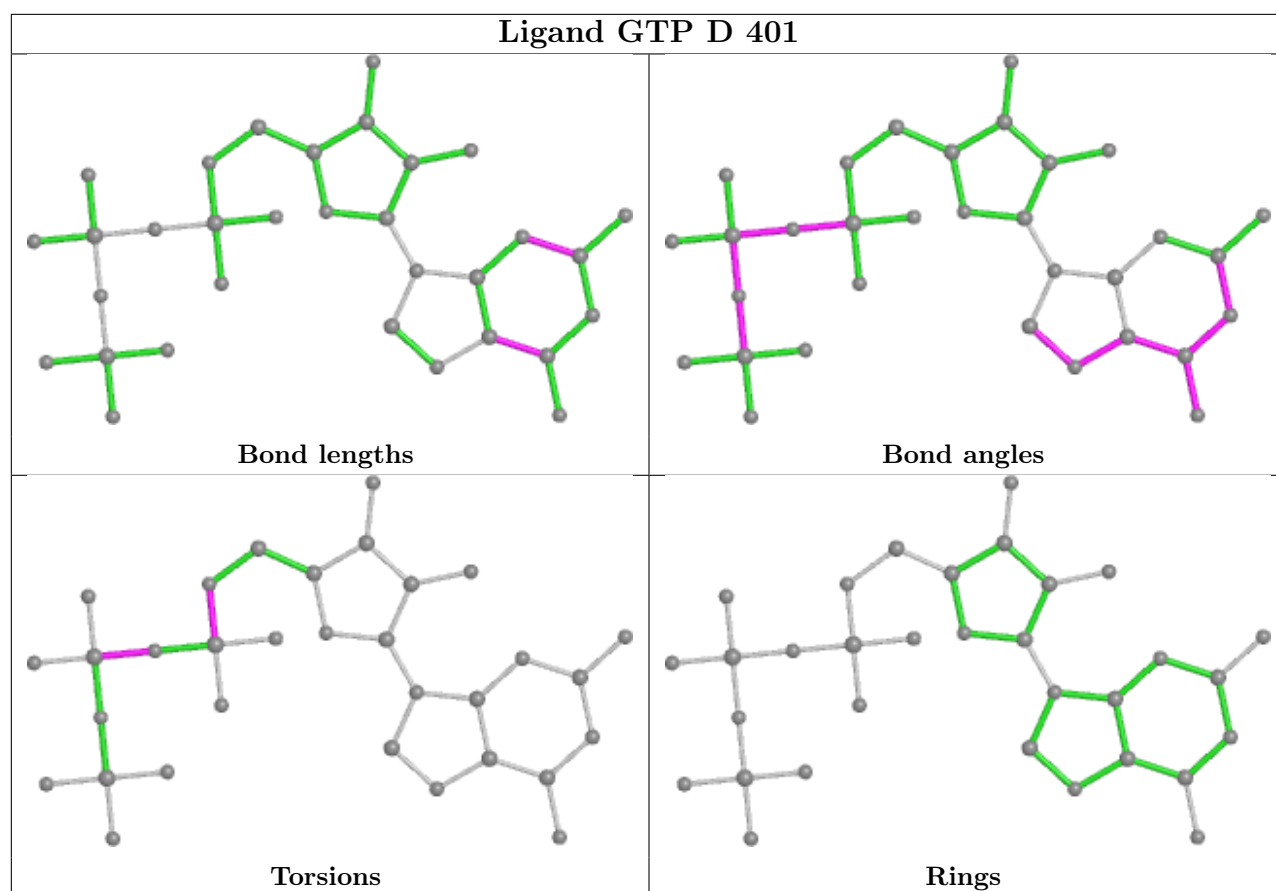
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	GTP	1	0
2	F	401	GTP	1	0
2	E	401	GTP	1	0
2	A	401	GTP	1	0

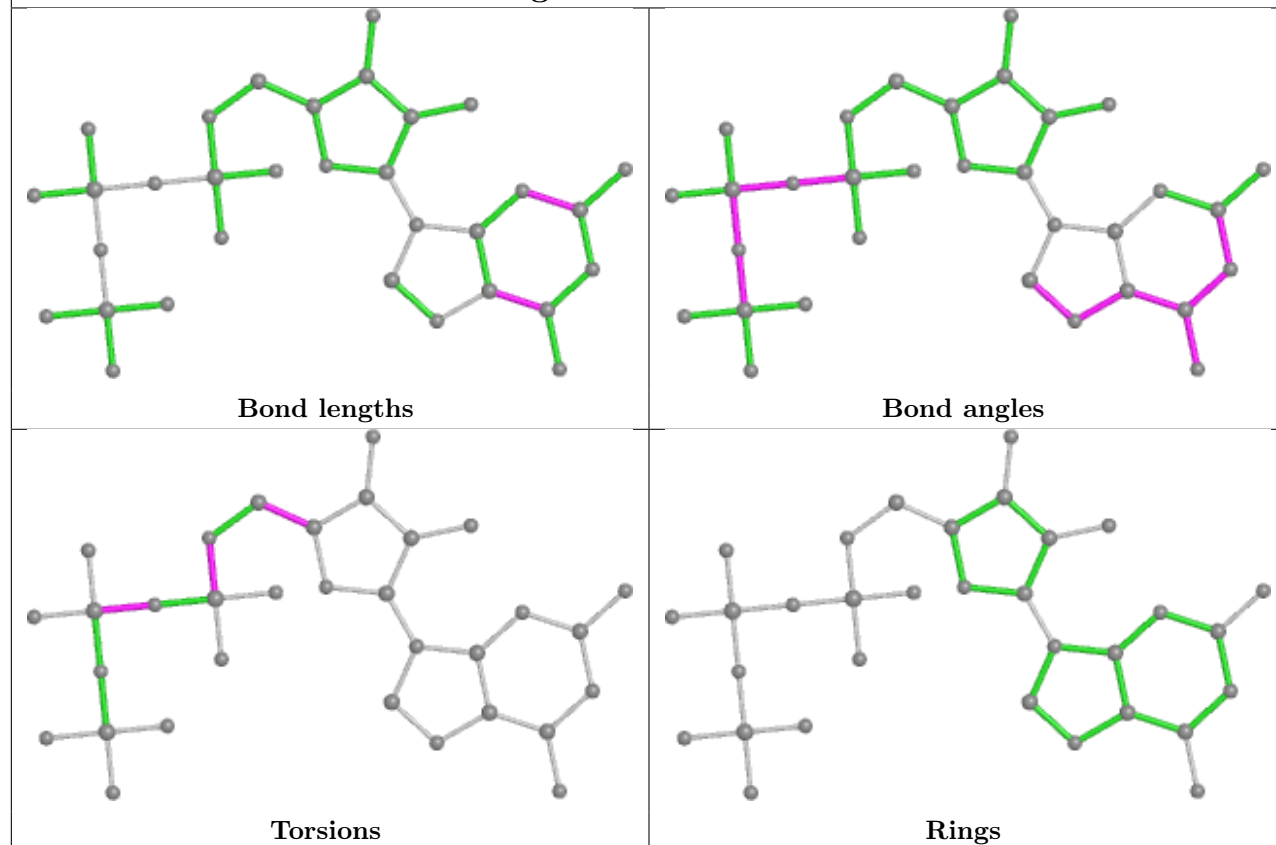
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

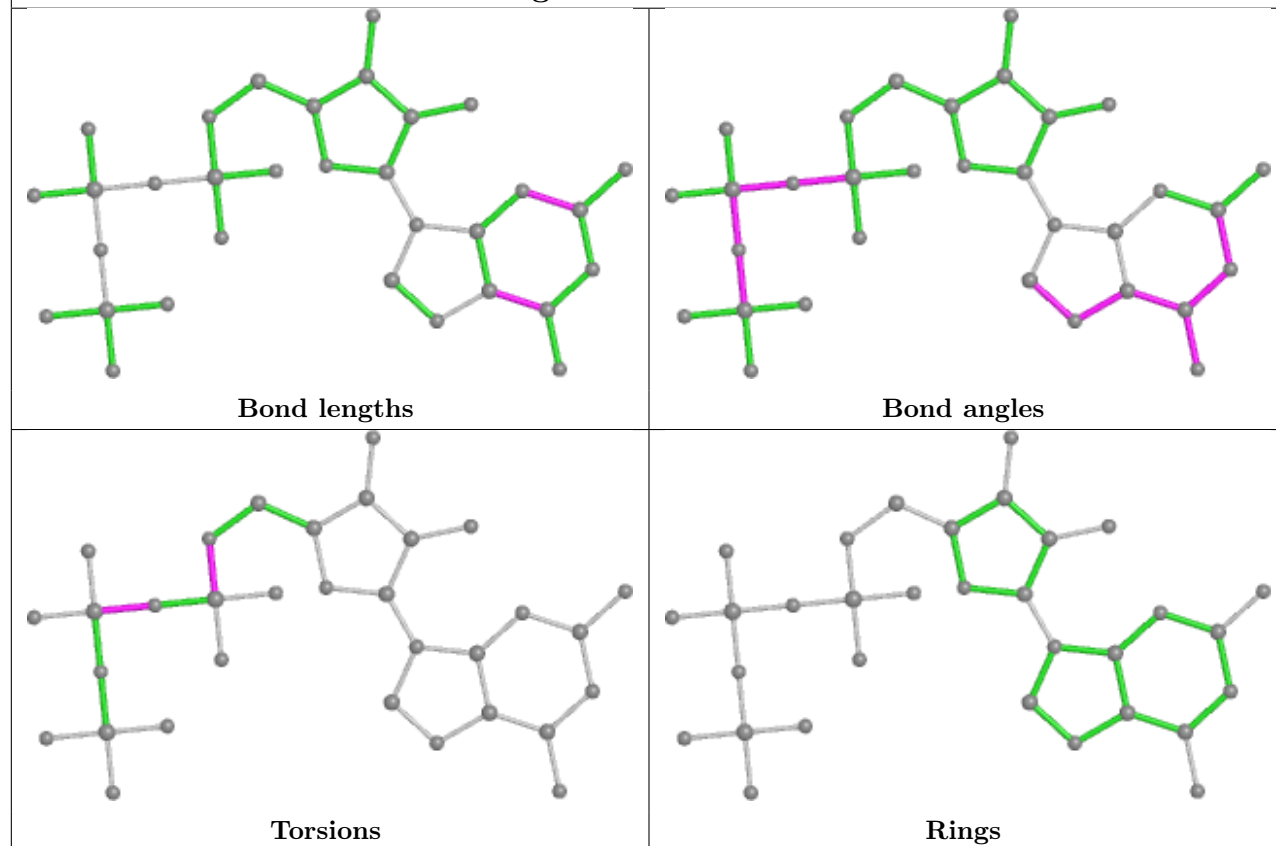


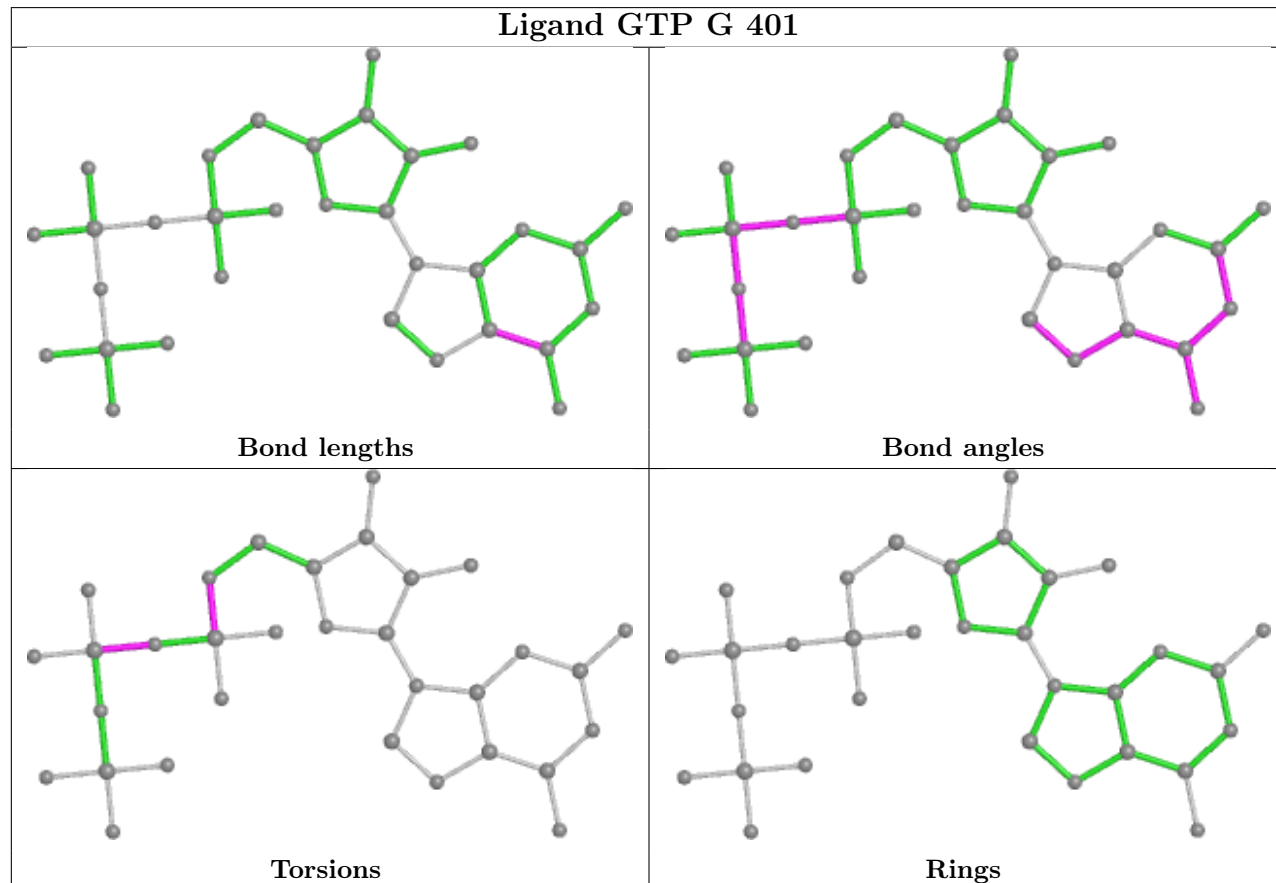
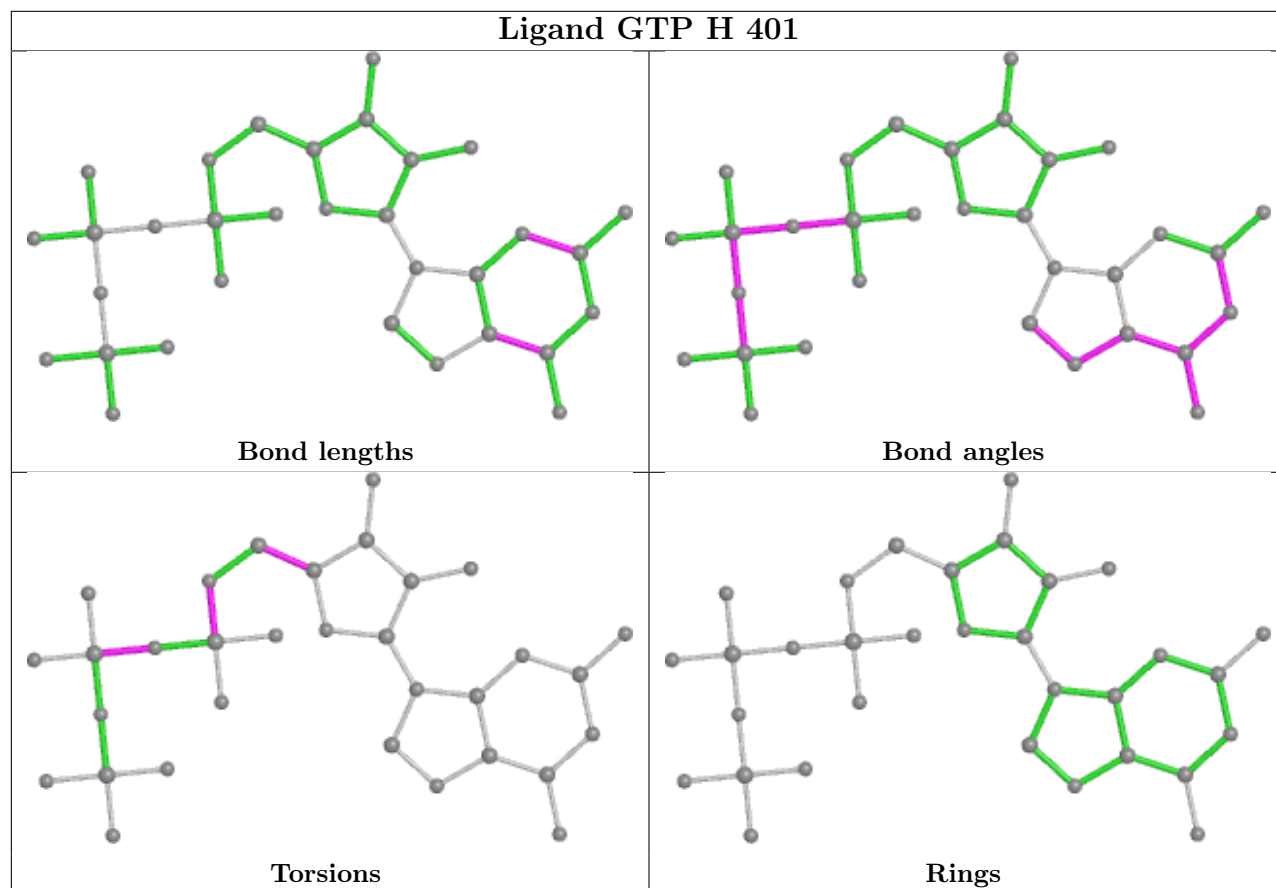


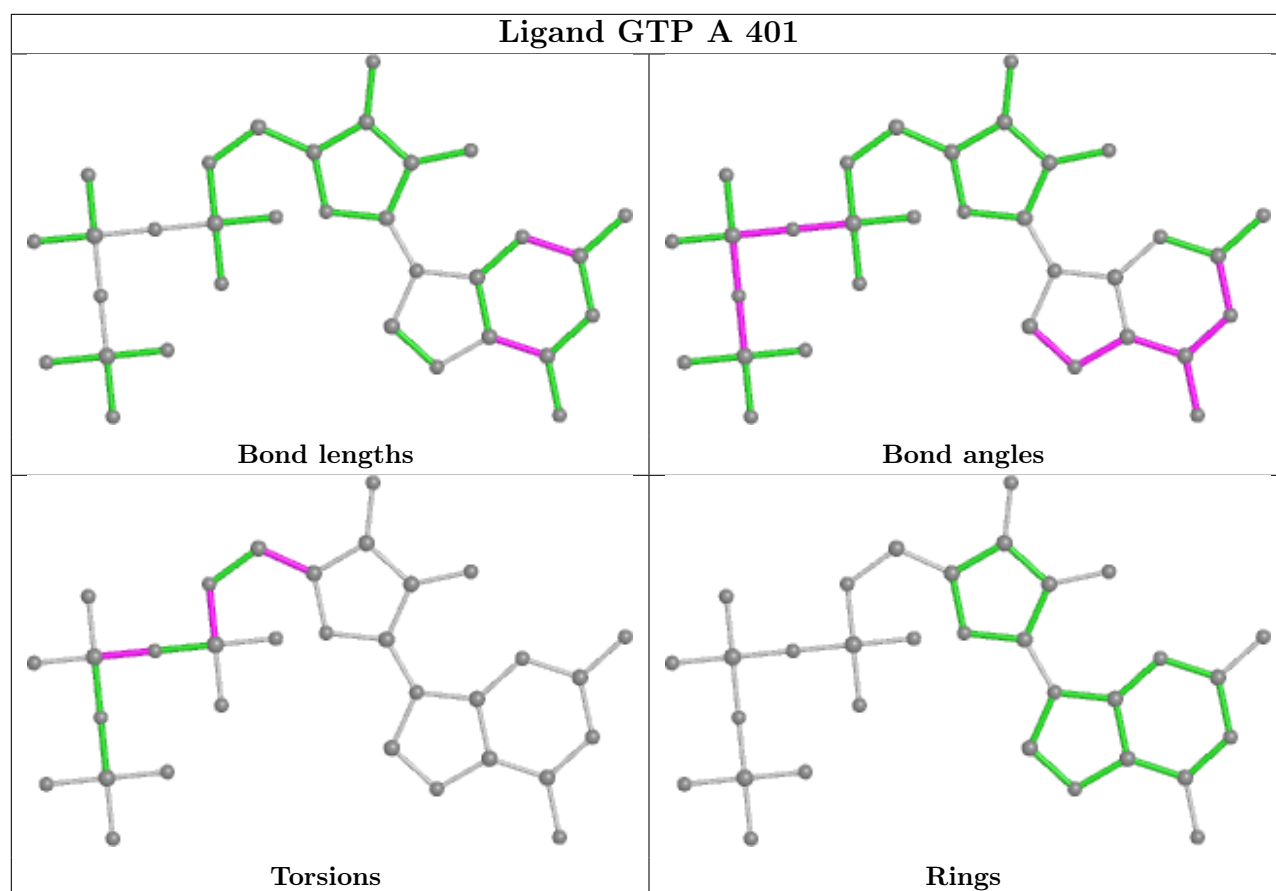
Ligand GTP B 401



Ligand GTP E 401







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	293/342 (85%)	-0.41	5 (1%) 69 65	13, 30, 56, 82	1 (0%)
1	B	288/342 (84%)	-0.23	9 (3%) 51 48	17, 34, 60, 95	1 (0%)
1	C	284/342 (83%)	-0.24	14 (4%) 36 33	12, 32, 64, 95	1 (0%)
1	D	288/342 (84%)	-0.04	12 (4%) 41 37	18, 40, 75, 113	1 (0%)
1	E	293/342 (85%)	-0.21	7 (2%) 59 56	17, 38, 65, 81	1 (0%)
1	F	288/342 (84%)	-0.11	8 (2%) 55 52	18, 39, 72, 116	1 (0%)
1	G	288/342 (84%)	-0.30	10 (3%) 47 44	14, 33, 62, 106	1 (0%)
1	H	293/342 (85%)	0.14	13 (4%) 39 36	25, 49, 84, 118	1 (0%)
All	All	2315/2736 (84%)	-0.18	78 (3%) 48 45	12, 37, 71, 118	8 (0%)

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	238	ASN	4.8
1	D	326	LEU	4.7
1	H	237	SER	4.4
1	C	293	ARG	4.3
1	B	326	LEU	4.3

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

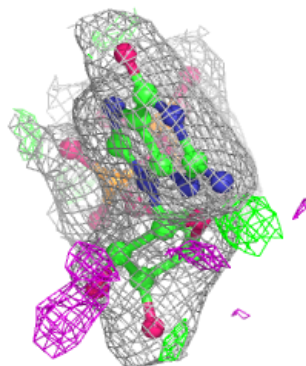
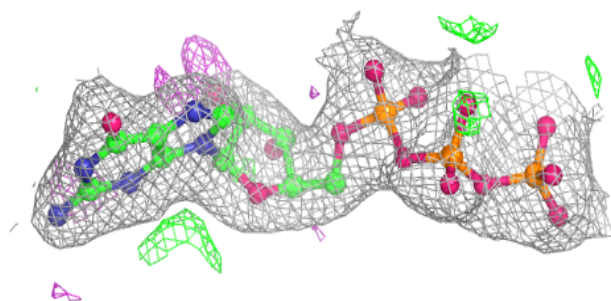
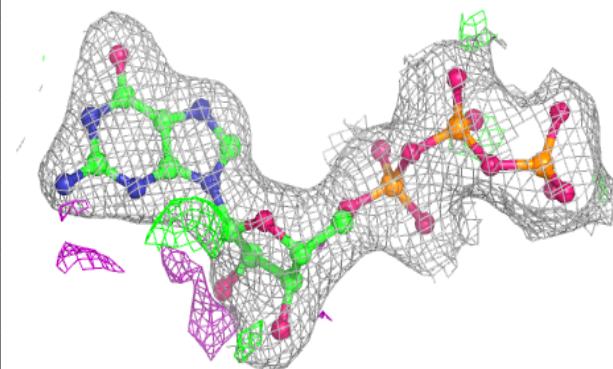
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GTP	H	401	32/32	0.96	0.06	20,26,35,37	0
2	GTP	D	401	32/32	0.97	0.06	13,20,28,31	0
2	GTP	A	401	32/32	0.97	0.05	8,16,25,30	0
2	GTP	B	401	32/32	0.98	0.05	14,22,29,36	0
2	GTP	E	401	32/32	0.98	0.04	14,19,32,37	0
2	GTP	F	401	32/32	0.98	0.05	19,24,33,39	0
2	GTP	G	401	32/32	0.98	0.04	11,18,22,25	0
2	GTP	C	401	32/32	0.98	0.04	9,15,20,25	0
3	MG	H	402	1/1	0.98	0.07	28,28,28,28	0
3	MG	C	402	1/1	0.99	0.03	15,15,15,15	0
3	MG	E	402	1/1	0.99	0.05	28,28,28,28	0
3	MG	F	402	1/1	0.99	0.01	27,27,27,27	0
3	MG	G	402	1/1	0.99	0.03	19,19,19,19	0
3	MG	A	402	1/1	0.99	0.03	23,23,23,23	0
3	MG	B	402	1/1	1.00	0.02	24,24,24,24	0
3	MG	D	402	1/1	1.00	0.05	23,23,23,23	0

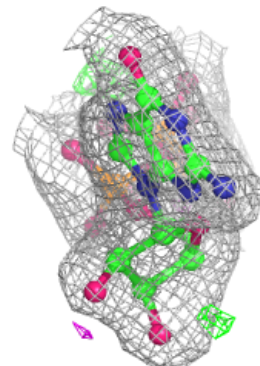
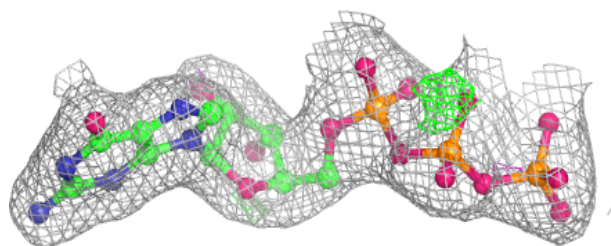
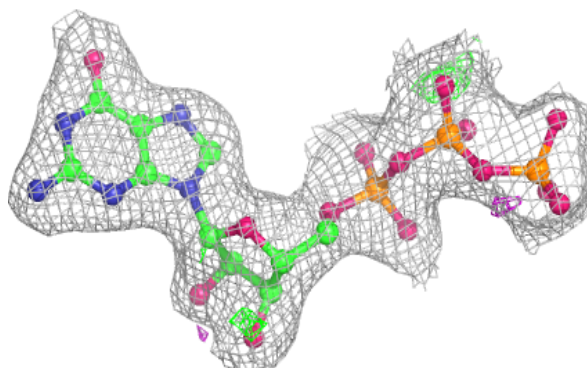
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GTP H 401:

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

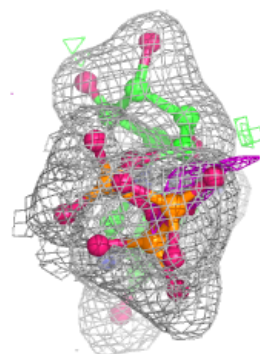
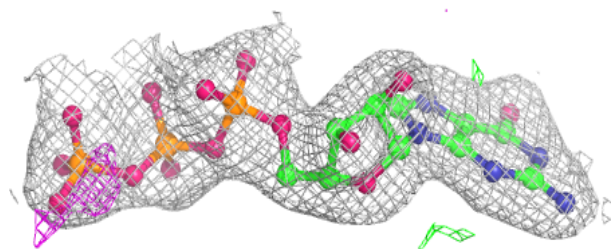
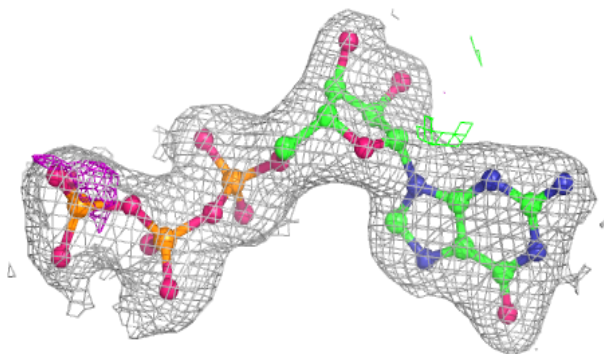
**Electron density around GTP D 401:**

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

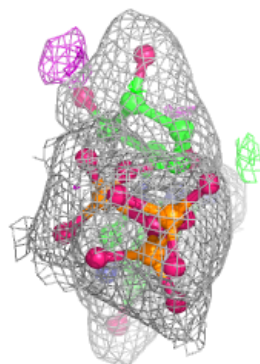
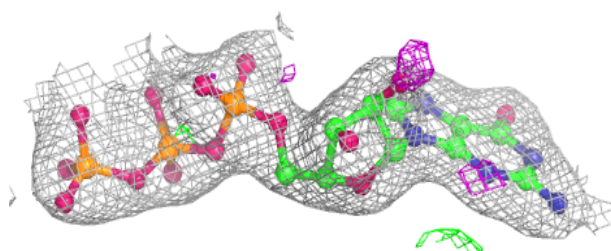
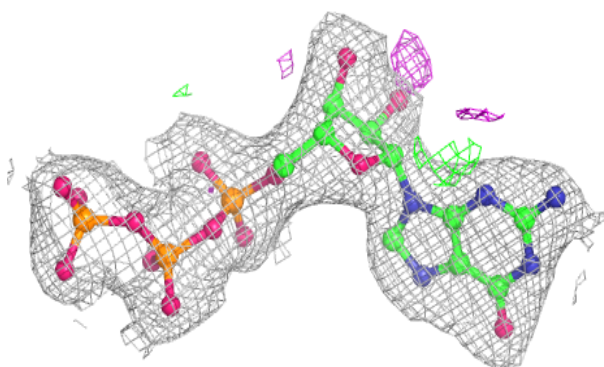


Electron density around GTP A 401:

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

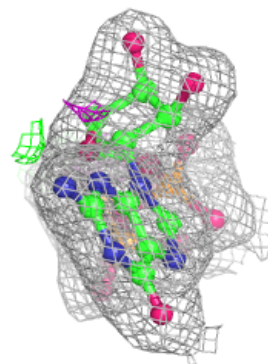
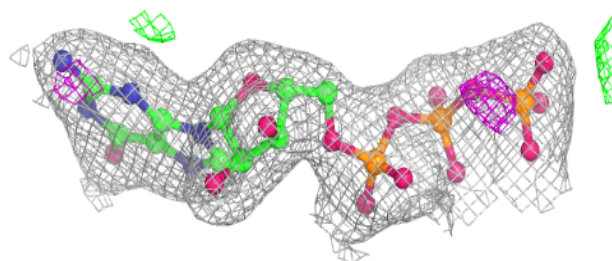
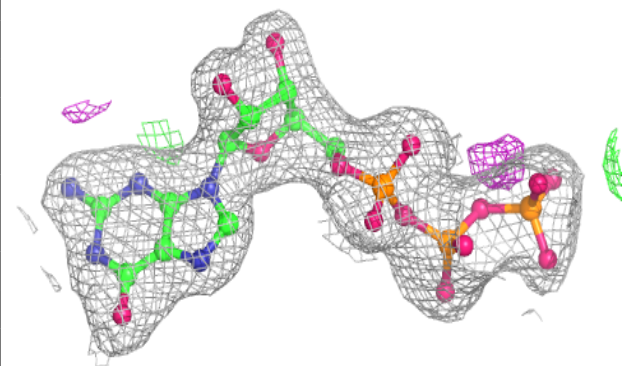
**Electron density around GTP B 401:**

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

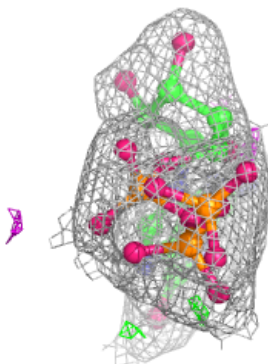
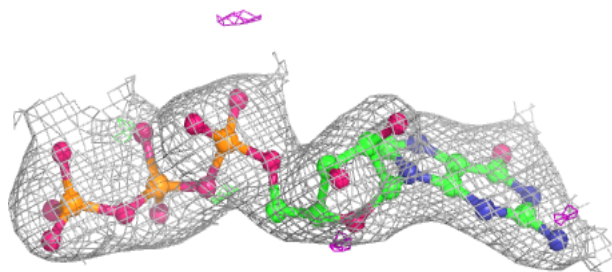
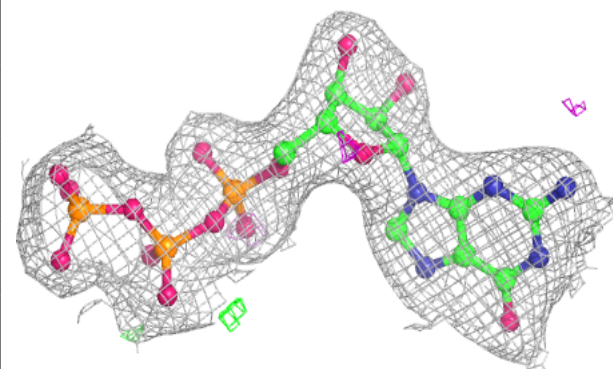


Electron density around GTP E 401:

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

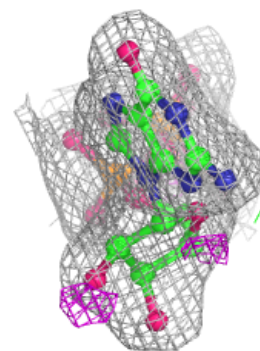
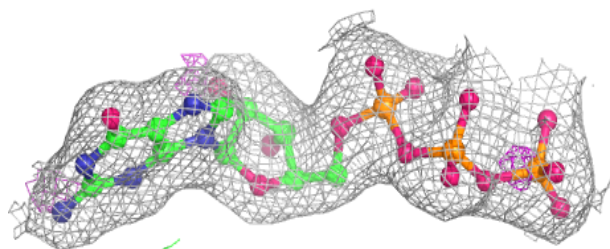
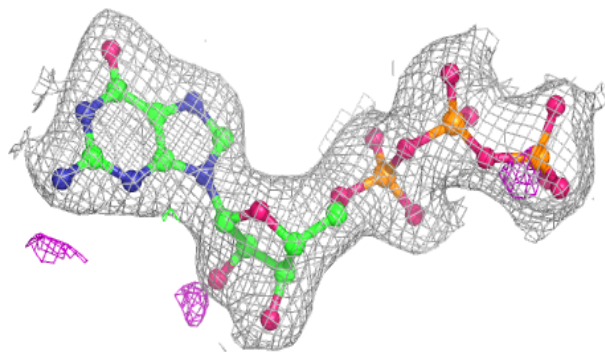
**Electron density around GTP F 401:**

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

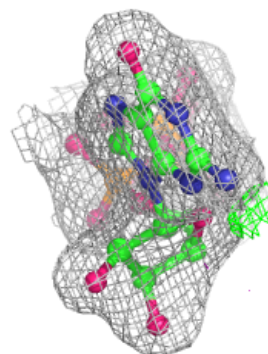
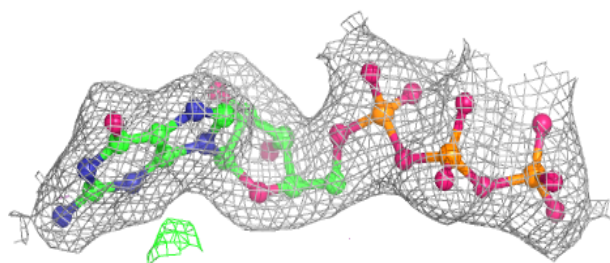
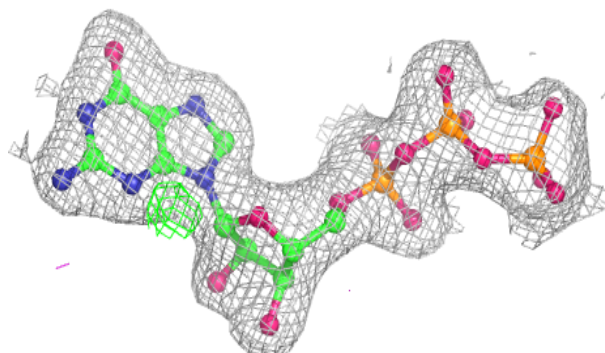


Electron density around GTP G 401:

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

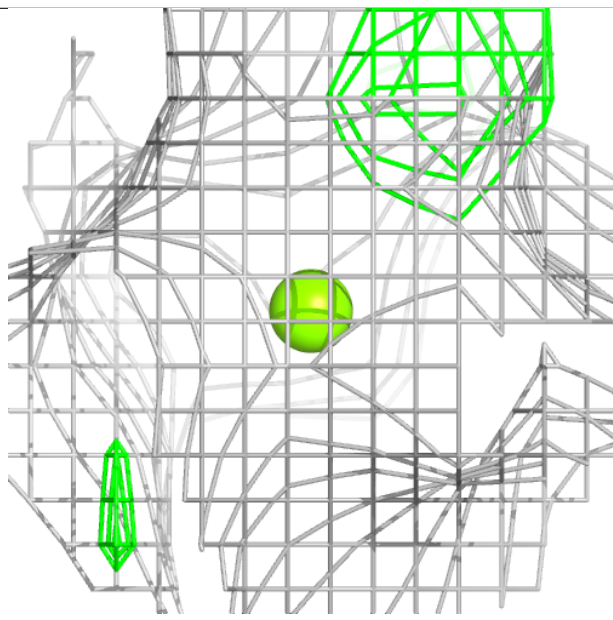
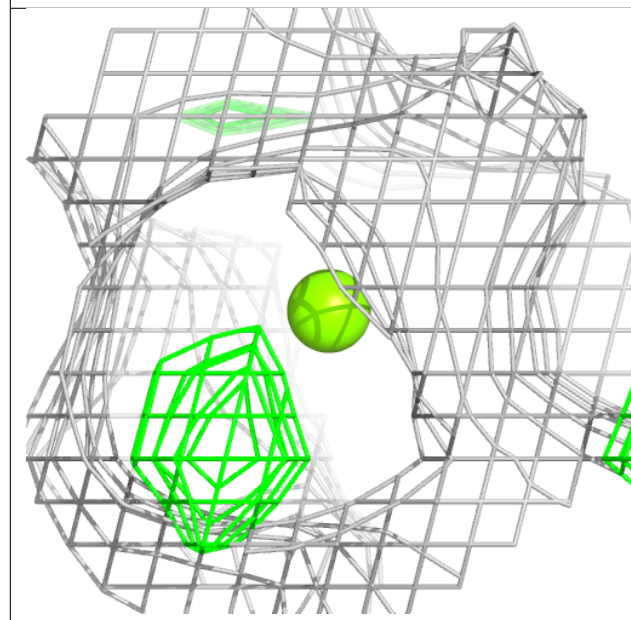
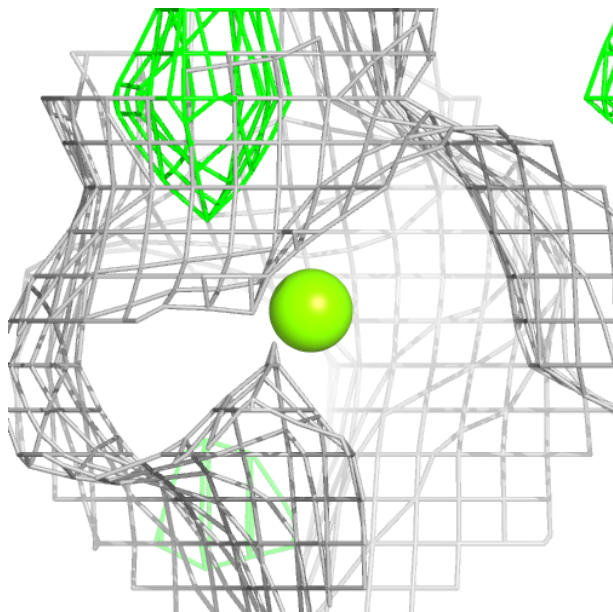
**Electron density around GTP C 401:**

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



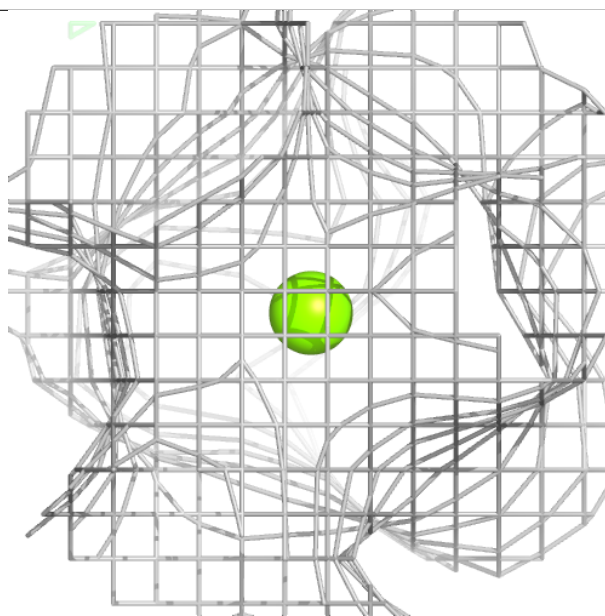
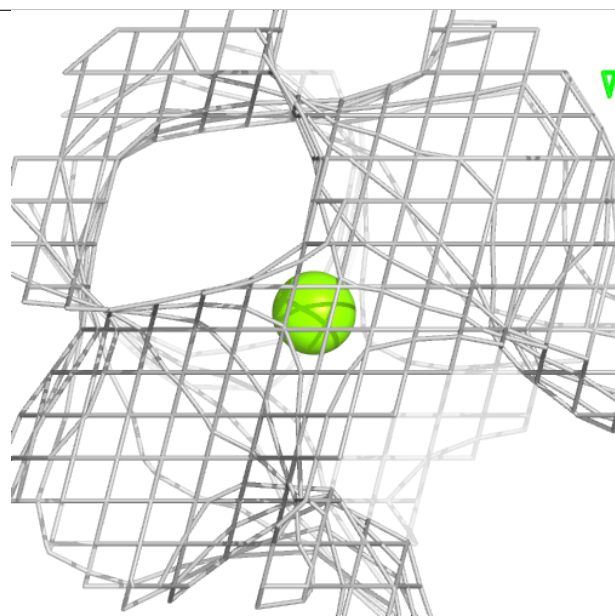
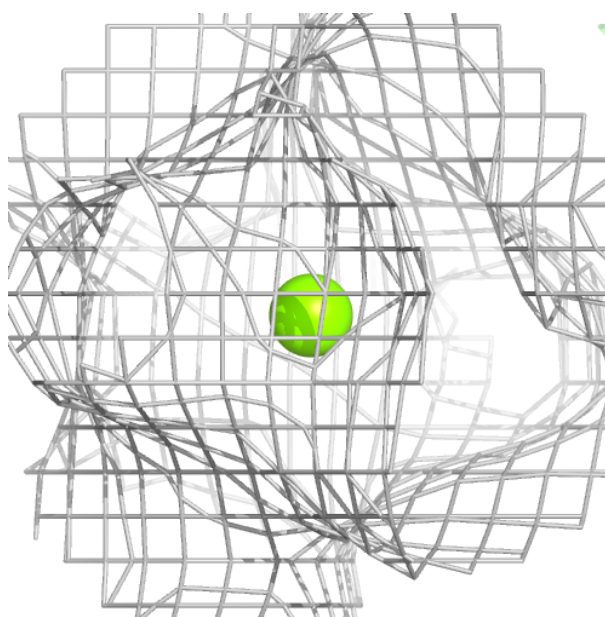
Electron density around MG H 402:

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



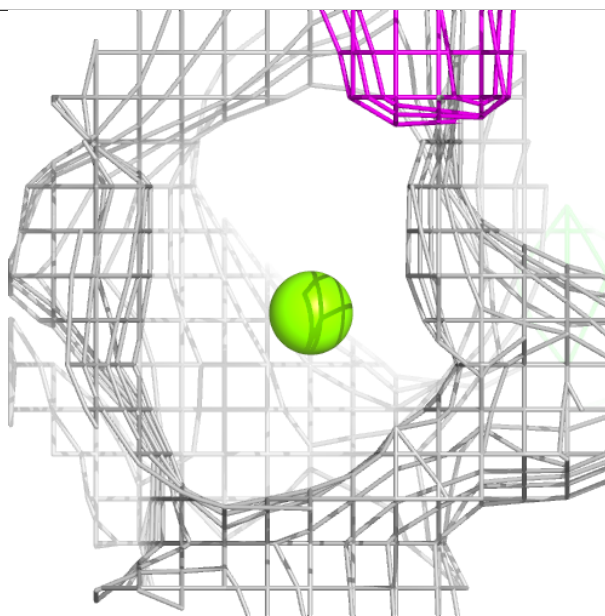
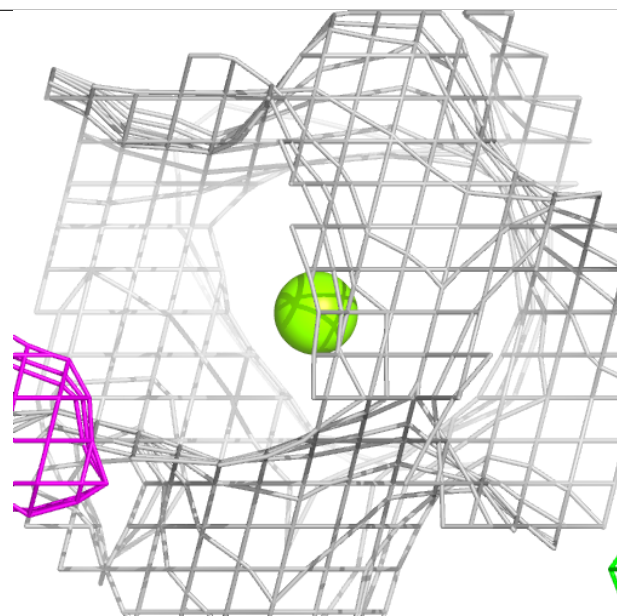
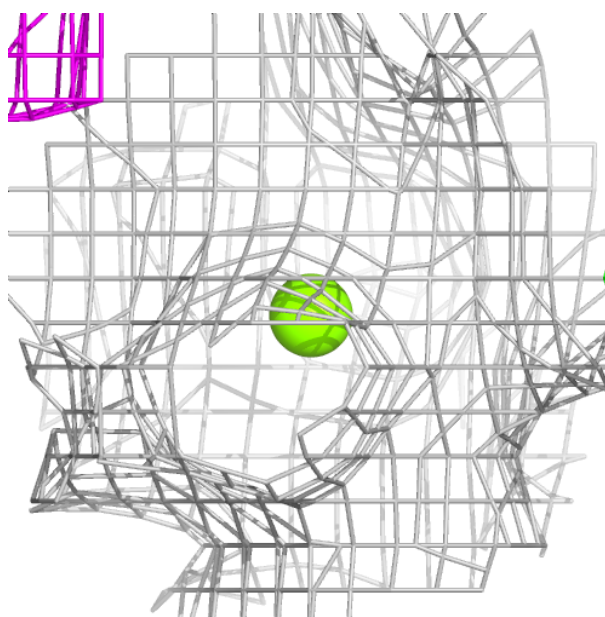
Electron density around MG C 402:

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



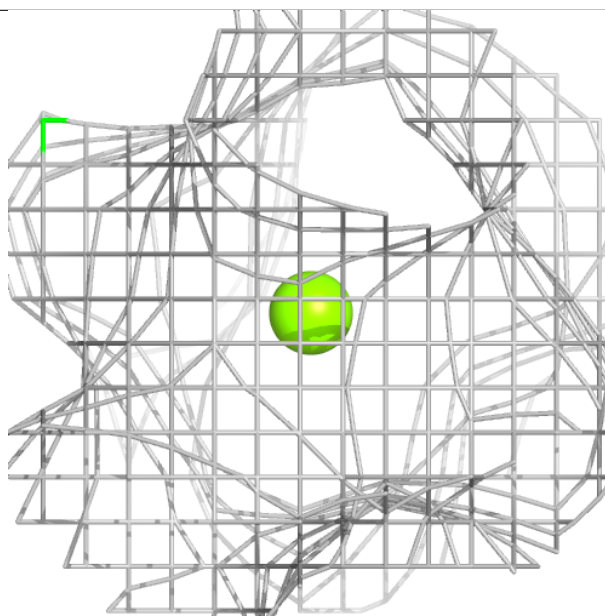
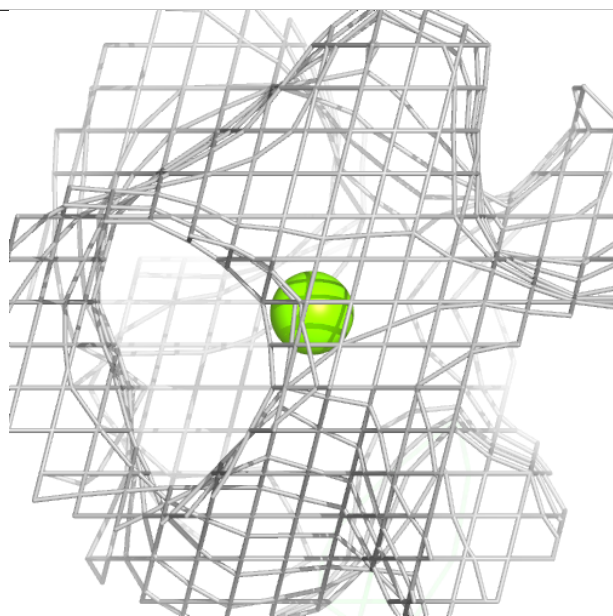
Electron density around MG E 402:

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



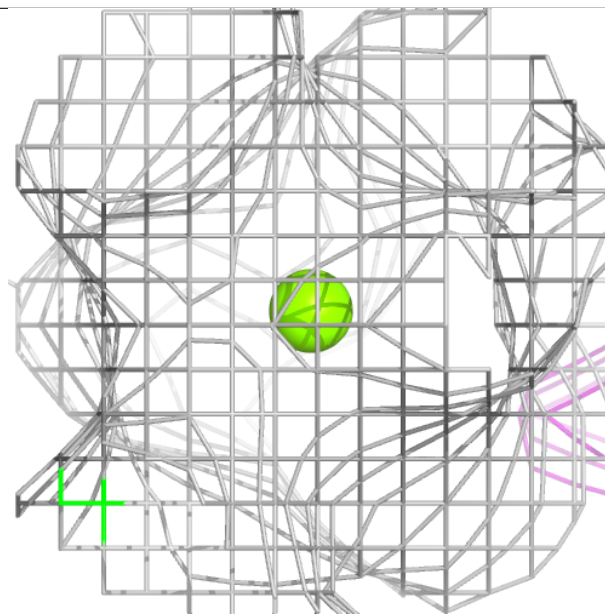
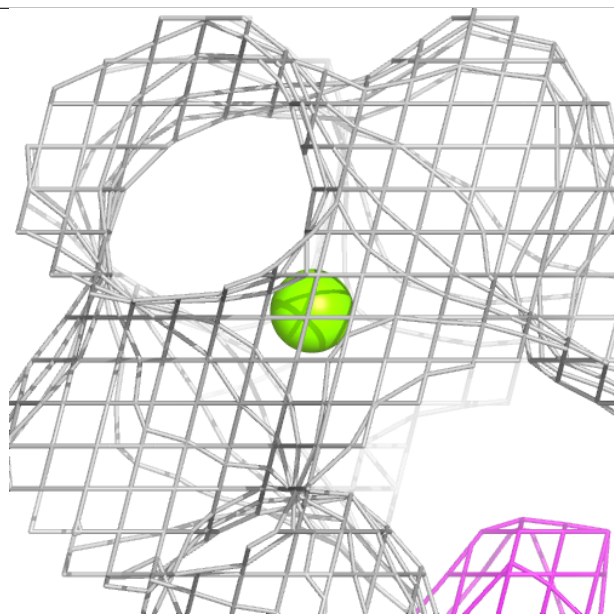
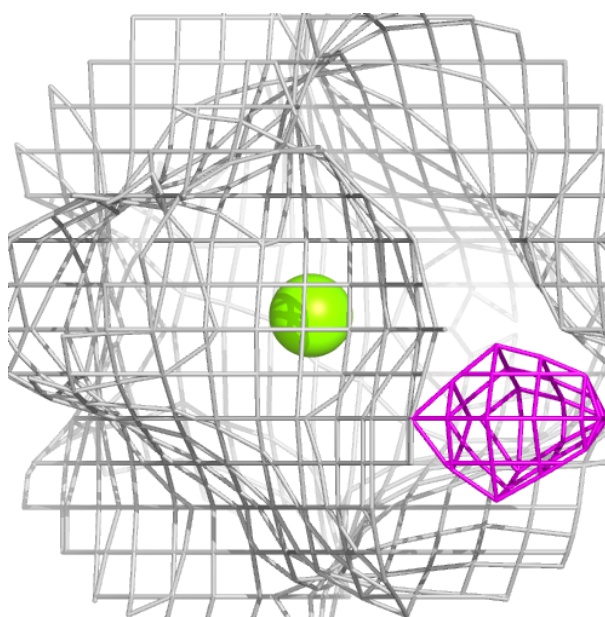
Electron density around MG F 402:

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



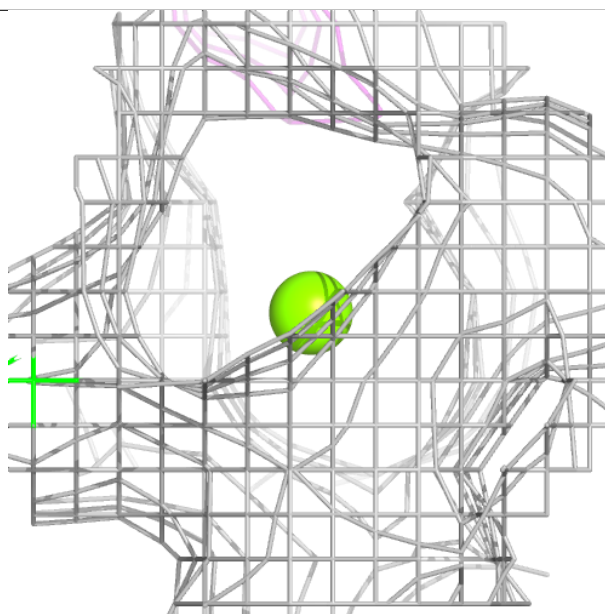
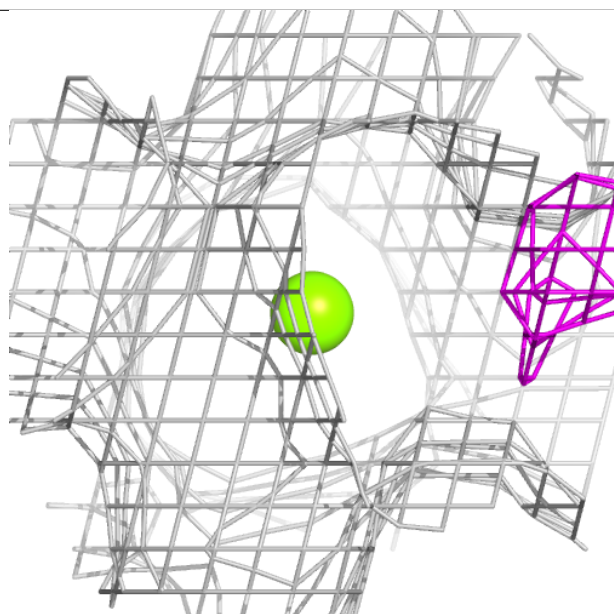
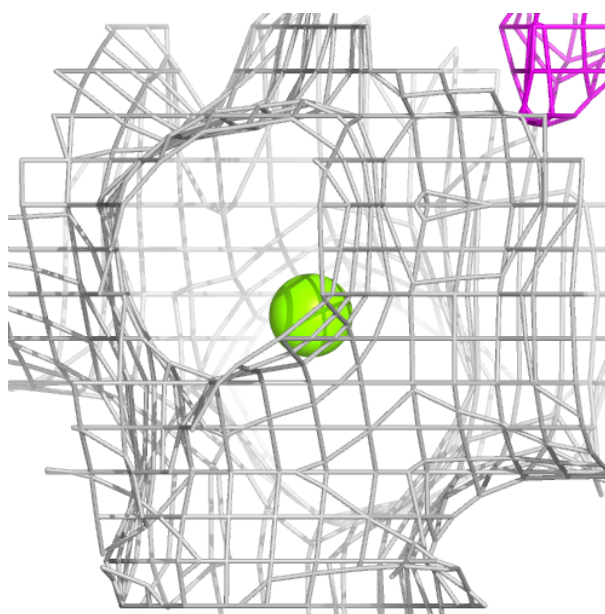
Electron density around MG G 402:

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and green (positive)



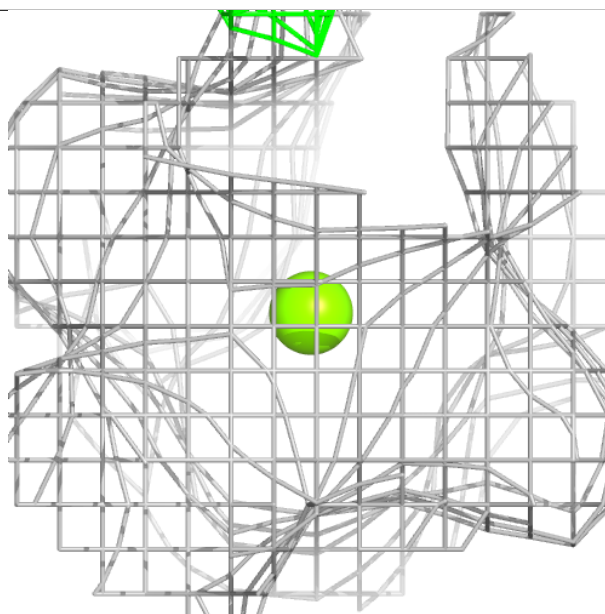
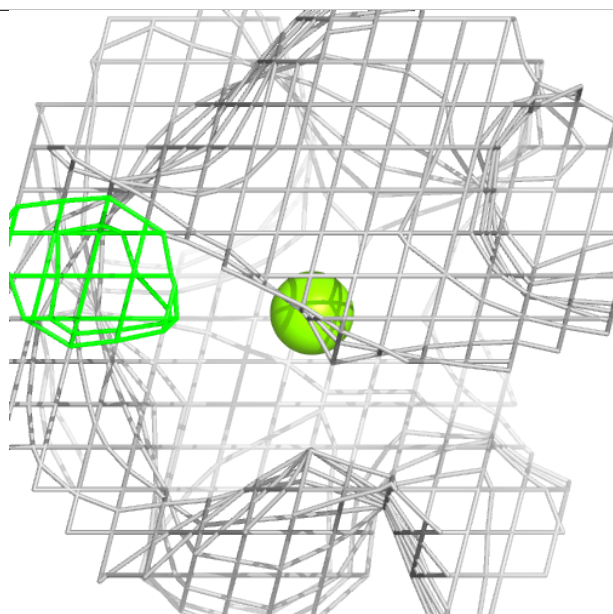
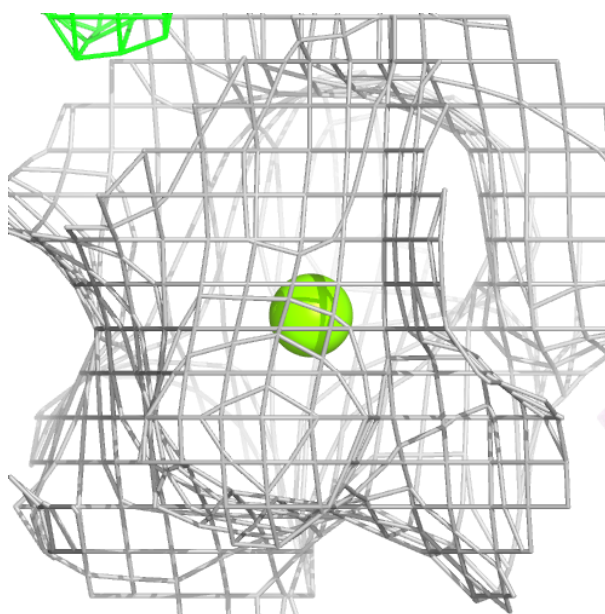
Electron density around MG A 402:

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and green (positive)



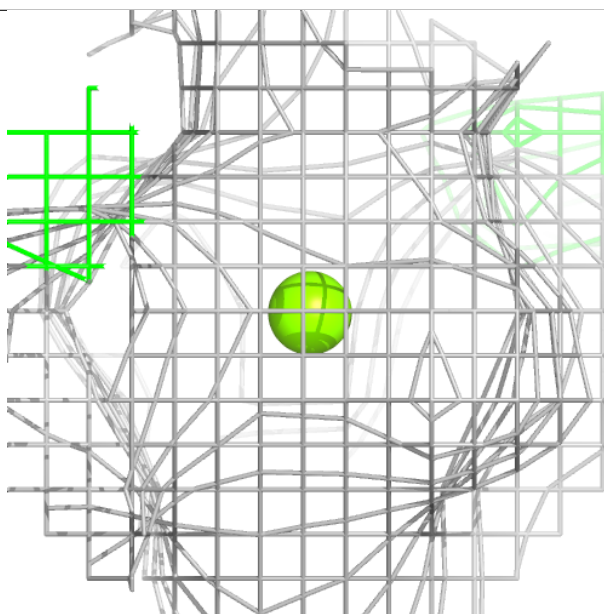
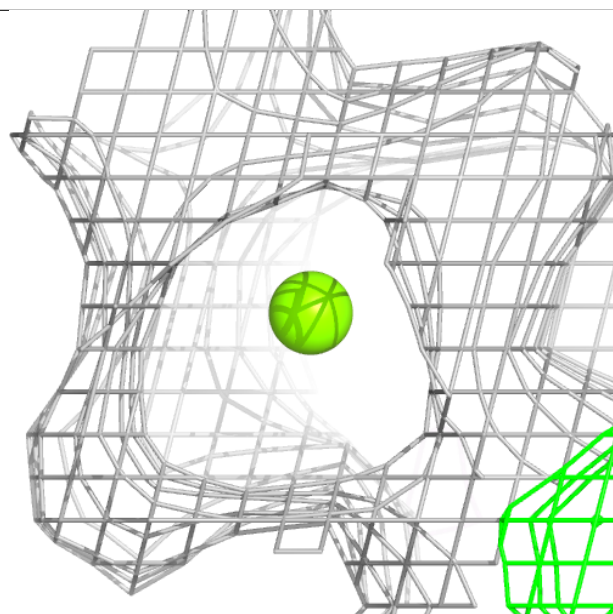
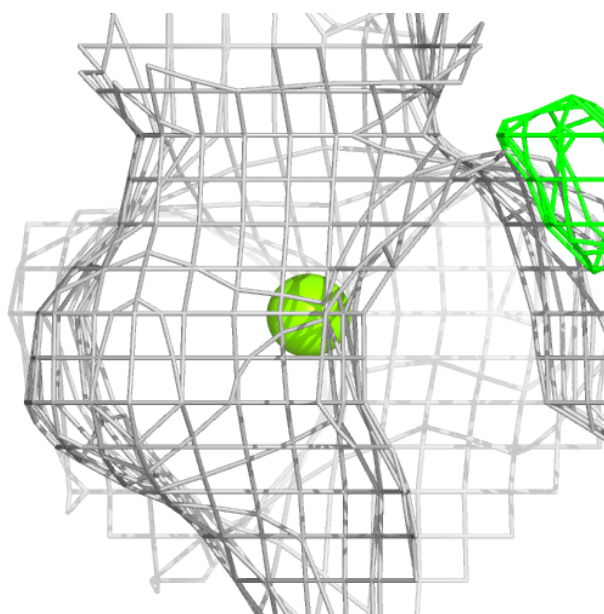
Electron density around MG B 402:

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



Electron density around MG D 402:

$2mF_o-DF_c$ (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.