Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 07:51 PM JST

PDB ID	:	7BOP
Title	:	Crystal Structure of Core-mannan synthase A (CmsA/Ktr4) from Aspergillus fumigatus, Mn/GDP-form
Authors	:	Hira, D.; Onoue, T.; Oka, T.
Deposited on	:	2020-03-19
Resolution	:	1.90 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:

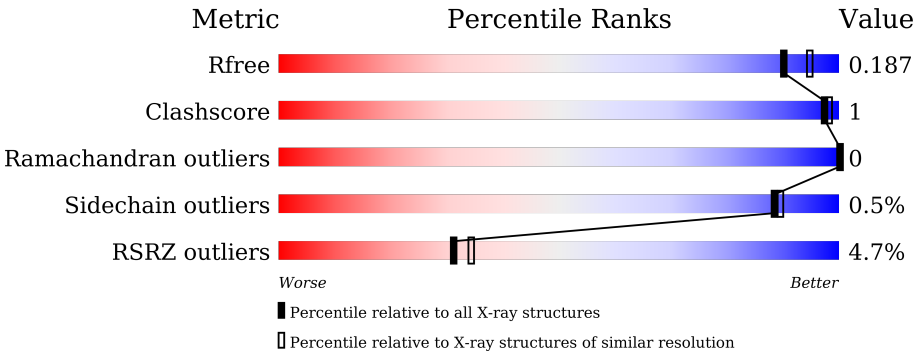
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	386	4% 91% • 5%
1	B	386	5% 91% • 5%
1	C	386	3% 93% • •
1	D	386	9% 92% • 5%
1	E	386	3% 94% • •
1	F	386	3% 94% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20839 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 Alpha-1,2-mannosyltransferase (Ktr4), putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	1	0
			3049	1962	510	560	17			
1	B	365	Total	C	N	O	S	0	2	0
			3057	1968	511	561	17			
1	C	372	Total	C	N	O	S	0	7	0
			3138	2016	528	577	17			
1	D	365	Total	C	N	O	S	0	7	0
			3082	1983	514	568	17			
1	E	372	Total	C	N	O	S	0	4	0
			3113	2000	521	575	17			
1	F	372	Total	C	N	O	S	0	5	0
			3125	2007	529	572	17			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP B0Y2F5
A	13	GLY	-	expression tag	UNP B0Y2F5
A	14	SER	-	expression tag	UNP B0Y2F5
A	15	SER	-	expression tag	UNP B0Y2F5
A	16	HIS	-	expression tag	UNP B0Y2F5
A	17	HIS	-	expression tag	UNP B0Y2F5
A	18	HIS	-	expression tag	UNP B0Y2F5
A	19	HIS	-	expression tag	UNP B0Y2F5
A	20	HIS	-	expression tag	UNP B0Y2F5
A	21	HIS	-	expression tag	UNP B0Y2F5
A	22	SER	-	expression tag	UNP B0Y2F5
A	23	SER	-	expression tag	UNP B0Y2F5
A	24	GLY	-	expression tag	UNP B0Y2F5
A	25	HIS	-	expression tag	UNP B0Y2F5
A	26	SER	-	expression tag	UNP B0Y2F5
B	12	MET	-	initiating methionine	UNP B0Y2F5
B	13	GLY	-	expression tag	UNP B0Y2F5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	14	SER	-	expression tag	UNP B0Y2F5
B	15	SER	-	expression tag	UNP B0Y2F5
B	16	HIS	-	expression tag	UNP B0Y2F5
B	17	HIS	-	expression tag	UNP B0Y2F5
B	18	HIS	-	expression tag	UNP B0Y2F5
B	19	HIS	-	expression tag	UNP B0Y2F5
B	20	HIS	-	expression tag	UNP B0Y2F5
B	21	HIS	-	expression tag	UNP B0Y2F5
B	22	SER	-	expression tag	UNP B0Y2F5
B	23	SER	-	expression tag	UNP B0Y2F5
B	24	GLY	-	expression tag	UNP B0Y2F5
B	25	HIS	-	expression tag	UNP B0Y2F5
B	26	SER	-	expression tag	UNP B0Y2F5
C	12	MET	-	initiating methionine	UNP B0Y2F5
C	13	GLY	-	expression tag	UNP B0Y2F5
C	14	SER	-	expression tag	UNP B0Y2F5
C	15	SER	-	expression tag	UNP B0Y2F5
C	16	HIS	-	expression tag	UNP B0Y2F5
C	17	HIS	-	expression tag	UNP B0Y2F5
C	18	HIS	-	expression tag	UNP B0Y2F5
C	19	HIS	-	expression tag	UNP B0Y2F5
C	20	HIS	-	expression tag	UNP B0Y2F5
C	21	HIS	-	expression tag	UNP B0Y2F5
C	22	SER	-	expression tag	UNP B0Y2F5
C	23	SER	-	expression tag	UNP B0Y2F5
C	24	GLY	-	expression tag	UNP B0Y2F5
C	25	HIS	-	expression tag	UNP B0Y2F5
C	26	SER	-	expression tag	UNP B0Y2F5
D	12	MET	-	initiating methionine	UNP B0Y2F5
D	13	GLY	-	expression tag	UNP B0Y2F5
D	14	SER	-	expression tag	UNP B0Y2F5
D	15	SER	-	expression tag	UNP B0Y2F5
D	16	HIS	-	expression tag	UNP B0Y2F5
D	17	HIS	-	expression tag	UNP B0Y2F5
D	18	HIS	-	expression tag	UNP B0Y2F5
D	19	HIS	-	expression tag	UNP B0Y2F5
D	20	HIS	-	expression tag	UNP B0Y2F5
D	21	HIS	-	expression tag	UNP B0Y2F5
D	22	SER	-	expression tag	UNP B0Y2F5
D	23	SER	-	expression tag	UNP B0Y2F5
D	24	GLY	-	expression tag	UNP B0Y2F5
D	25	HIS	-	expression tag	UNP B0Y2F5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	26	SER	-	expression tag	UNP B0Y2F5
E	12	MET	-	initiating methionine	UNP B0Y2F5
E	13	GLY	-	expression tag	UNP B0Y2F5
E	14	SER	-	expression tag	UNP B0Y2F5
E	15	SER	-	expression tag	UNP B0Y2F5
E	16	HIS	-	expression tag	UNP B0Y2F5
E	17	HIS	-	expression tag	UNP B0Y2F5
E	18	HIS	-	expression tag	UNP B0Y2F5
E	19	HIS	-	expression tag	UNP B0Y2F5
E	20	HIS	-	expression tag	UNP B0Y2F5
E	21	HIS	-	expression tag	UNP B0Y2F5
E	22	SER	-	expression tag	UNP B0Y2F5
E	23	SER	-	expression tag	UNP B0Y2F5
E	24	GLY	-	expression tag	UNP B0Y2F5
E	25	HIS	-	expression tag	UNP B0Y2F5
E	26	SER	-	expression tag	UNP B0Y2F5
F	12	MET	-	initiating methionine	UNP B0Y2F5
F	13	GLY	-	expression tag	UNP B0Y2F5
F	14	SER	-	expression tag	UNP B0Y2F5
F	15	SER	-	expression tag	UNP B0Y2F5
F	16	HIS	-	expression tag	UNP B0Y2F5
F	17	HIS	-	expression tag	UNP B0Y2F5
F	18	HIS	-	expression tag	UNP B0Y2F5
F	19	HIS	-	expression tag	UNP B0Y2F5
F	20	HIS	-	expression tag	UNP B0Y2F5
F	21	HIS	-	expression tag	UNP B0Y2F5
F	22	SER	-	expression tag	UNP B0Y2F5
F	23	SER	-	expression tag	UNP B0Y2F5
F	24	GLY	-	expression tag	UNP B0Y2F5
F	25	HIS	-	expression tag	UNP B0Y2F5
F	26	SER	-	expression tag	UNP B0Y2F5

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

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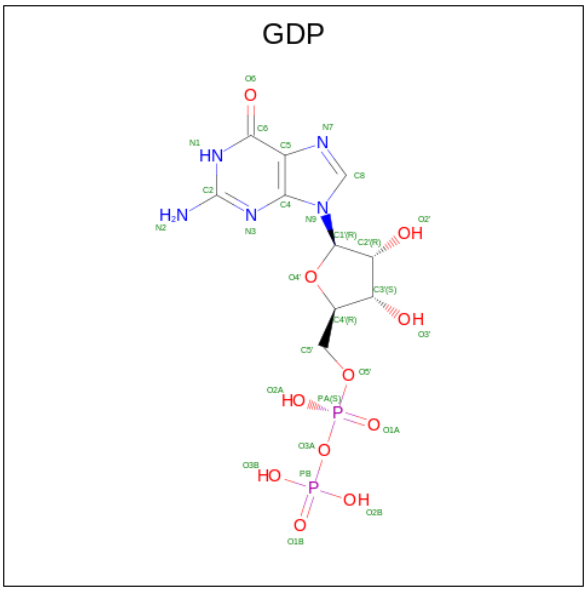
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

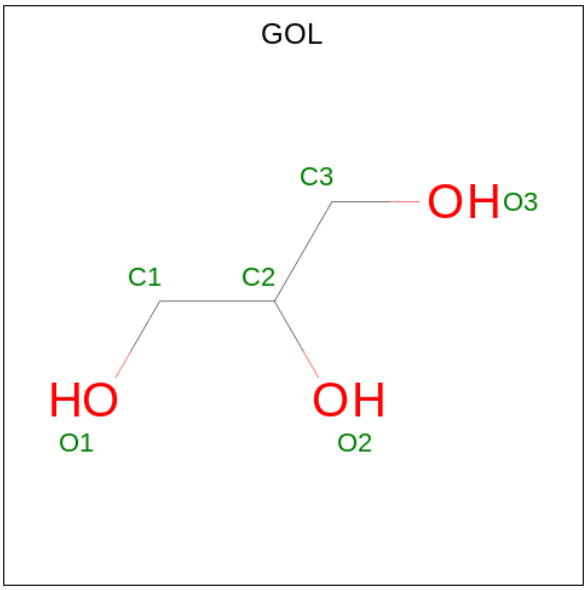


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 28 10 5 11 2	0	0
3	B	1	Total C N O P 28 10 5 11 2	0	0
3	C	1	Total C N O P 28 10 5 11 2	0	0
3	D	1	Total C N O P 28 10 5 11 2	0	0
3	E	1	Total C N O P 28 10 5 11 2	0	0
3	F	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0
4	B	2	Total Na 2 2	0	0
4	C	1	Total Na 1 1	0	0
4	D	2	Total Na 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

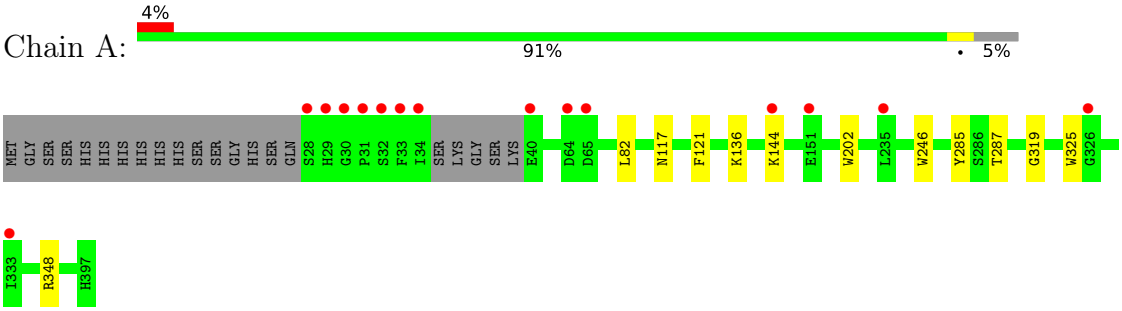
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	369	Total O 369 369	0	0
6	B	371	Total O 371 371	0	0
6	C	342	Total O 342 342	0	0
6	D	319	Total O 319 319	0	0
6	E	285	Total O 285 285	0	0
6	F	294	Total O 294 294	0	0

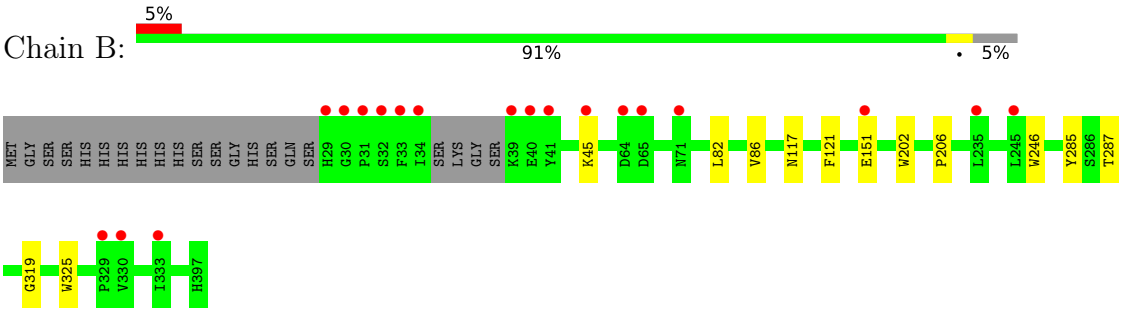
3 Residue-property plots (i)

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.

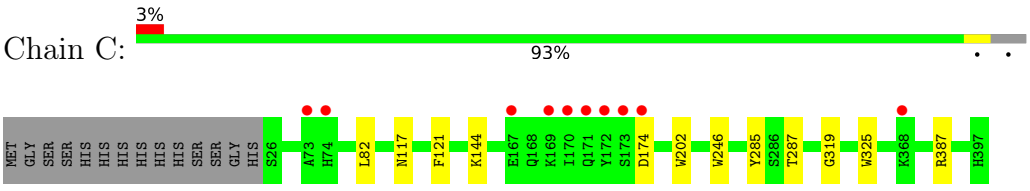
• Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative



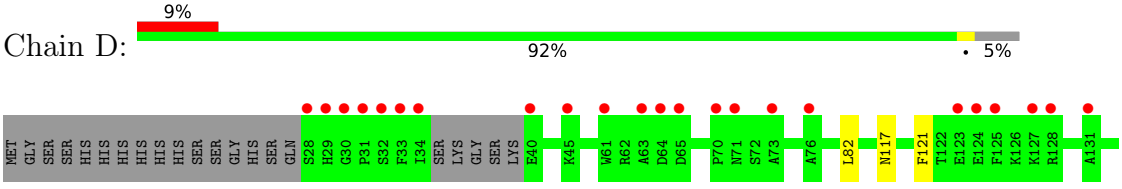
• Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative

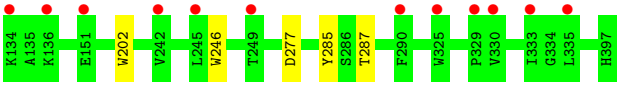


• Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative

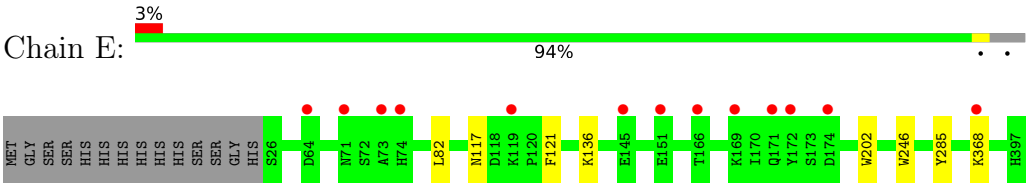


• Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative

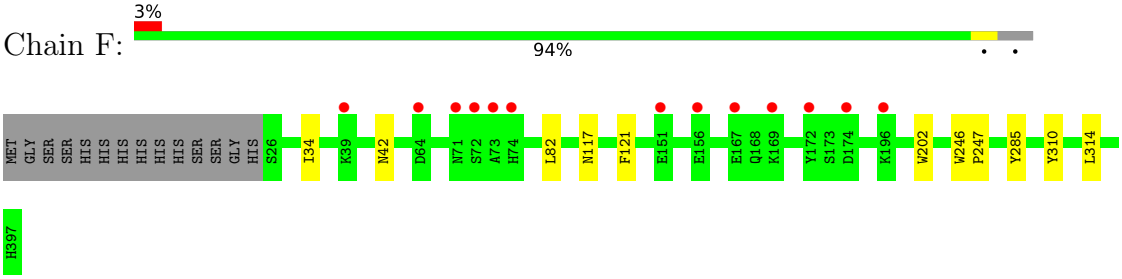




• Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative



• Molecule 1: Alpha-1,2-mannosyltransferase (Ktr4), putative



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	154.50Å 273.01Å 186.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.82 – 1.90 49.32 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.82-1.90) 99.9 (49.32-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.160 , 0.181 0.168 , 0.187	Depositor DCC
R_{free} test set	15120 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.009 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20839	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, GDP, GOL, NA

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	0.43	0/3162	0.64	2/4291 (0.0%)
1	B	0.43	0/3173	0.63	0/4305
1	C	0.42	0/3270	0.62	1/4433 (0.0%)
1	D	0.42	0/3213	0.61	0/4359
1	E	0.42	0/3236	0.61	0/4389
1	F	0.42	0/3251	0.60	0/4407
All	All	0.42	0/19305	0.62	3/26184 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	348	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	348	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	C	387	ARG	NE-CZ-NH2	-5.25	117.67	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3049	0	2812	5	0
1	B	3057	0	2824	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3138	0	2919	5	0
1	D	3082	0	2852	4	0
1	E	3113	0	2884	3	0
1	F	3125	0	2909	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	28	0	12	0	0
3	B	28	0	12	0	0
3	C	28	0	12	0	0
3	D	28	0	12	0	0
3	E	28	0	12	0	0
3	F	28	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	24	0	32	0	0
5	B	24	0	32	0	0
5	C	12	0	16	0	0
5	D	18	0	24	0	0
5	E	24	0	32	0	0
5	F	12	0	16	0	0
6	A	369	0	0	0	0
6	B	371	0	0	0	0
6	C	342	0	0	0	0
6	D	319	0	0	0	0
6	E	285	0	0	0	0
6	F	294	0	0	0	0
All	All	20839	0	17424	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (29) 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:82:LEU:HD23	1:D:202:TRP:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HD23	1:A:202:TRP:HB3	1.90	0.52
1:F:82:LEU:HD23	1:F:202:TRP:HB3	1.92	0.52
1:C:82:LEU:HD23	1:C:202:TRP:HB3	1.91	0.52
1:D:117:ASN:HB2	1:D:121:PHE:CZ	2.46	0.51
1:F:34:ILE:HG23	1:F:42:ASN:HB2	1.93	0.51
1:C:117:ASN:HB2	1:C:121:PHE:CZ	2.46	0.51
1:E:82:LEU:HD23	1:E:202:TRP:HB3	1.93	0.51
1:B:117:ASN:HB2	1:B:121:PHE:CZ	2.47	0.49
1:B:246:TRP:HB2	1:B:285:TYR:HB2	1.93	0.49
1:B:82:LEU:HD23	1:B:202:TRP:HB3	1.95	0.49
1:D:285:TYR:CE2	1:D:287:THR:HA	2.50	0.47
1:C:246:TRP:HB2	1:C:285:TYR:HB2	1.97	0.46
1:F:117:ASN:HB2	1:F:121:PHE:CZ	2.51	0.46
1:B:285:TYR:CE2	1:B:287:THR:HA	2.51	0.46
1:A:246:TRP:HB2	1:A:285:TYR:HB2	1.99	0.45
1:A:117:ASN:HB2	1:A:121:PHE:CZ	2.53	0.44
1:A:285:TYR:CE2	1:A:287:THR:HA	2.52	0.44
1:E:117:ASN:HB2	1:E:121:PHE:CZ	2.52	0.44
1:F:246:TRP:HB2	1:F:285:TYR:HB2	2.00	0.43
1:B:86:VAL:HG23	1:B:206:PRO:HG3	1.99	0.43
1:D:246:TRP:HB2	1:D:285:TYR:HB2	2.00	0.43
1:A:319:GLY:HA3	1:A:325:TRP:CZ2	2.56	0.41
1:F:310:TYR:CZ	1:F:314:LEU:HD11	2.56	0.41
1:F:246:TRP:HB3	1:F:247:PRO:HD3	2.03	0.41
1:C:319:GLY:HA3	1:C:325:TRP:CZ2	2.56	0.40
1:E:246:TRP:HB2	1:E:285:TYR:HB2	2.01	0.40
1:B:319:GLY:HA3	1:B:325:TRP:CZ2	2.57	0.40
1:C:285:TYR:CE2	1:C:287:THR:HA	2.56	0.40

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	362/386 (94%)	354 (98%)	8 (2%)	0	100	100
1	B	363/386 (94%)	356 (98%)	7 (2%)	0	100	100
1	C	377/386 (98%)	370 (98%)	7 (2%)	0	100	100
1	D	368/386 (95%)	361 (98%)	7 (2%)	0	100	100
1	E	374/386 (97%)	367 (98%)	7 (2%)	0	100	100
1	F	375/386 (97%)	365 (97%)	10 (3%)	0	100	100
All	All	2219/2316 (96%)	2173 (98%)	46 (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	323/340 (95%)	321 (99%)	2 (1%)	86	87
1	B	324/340 (95%)	322 (99%)	2 (1%)	86	87
1	C	335/340 (98%)	333 (99%)	2 (1%)	86	87
1	D	329/340 (97%)	327 (99%)	2 (1%)	86	87
1	E	332/340 (98%)	330 (99%)	2 (1%)	86	87
1	F	333/340 (98%)	333 (100%)	0	100	100
All	All	1976/2040 (97%)	1966 (100%)	10 (0%)	88	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LYS
1	A	144	LYS
1	B	45	LYS
1	B	151	GLU
1	C	144	LYS
1	C	174	ASP
1	D	277[A]	ASP

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Mol	Chain	Res	Type
1	D	277[B]	ASP
1	E	136	LYS
1	E	368	LYS

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

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 13 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	F	403	-	5,5,5	0.37	0	5,5,5	0.18	0
5	GOL	C	404	-	5,5,5	0.45	0	5,5,5	0.44	0
5	GOL	B	405	-	5,5,5	0.20	0	5,5,5	0.59	0
5	GOL	B	407	-	5,5,5	0.37	0	5,5,5	0.35	0
5	GOL	C	405	-	5,5,5	0.25	0	5,5,5	0.33	0
5	GOL	E	405	-	5,5,5	0.46	0	5,5,5	0.52	0
5	GOL	B	406	-	5,5,5	0.41	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GDP	A	402	2	24,30,30	0.75	0	30,47,47	1.30	4 (13%)
5	GOL	A	405	-	5,5,5	0.50	0	5,5,5	0.48	0
3	GDP	E	402	2	24,30,30	0.89	1 (4%)	30,47,47	1.35	5 (16%)
5	GOL	A	406	-	5,5,5	0.44	0	5,5,5	0.28	0
3	GDP	B	402	2	24,30,30	0.88	0	30,47,47	1.27	5 (16%)
5	GOL	B	408	-	5,5,5	0.25	0	5,5,5	0.33	0
5	GOL	A	408	-	5,5,5	0.43	0	5,5,5	0.25	0
5	GOL	E	406	-	5,5,5	0.32	0	5,5,5	0.39	0
5	GOL	E	404	-	5,5,5	0.31	0	5,5,5	0.30	0
5	GOL	E	403	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GDP	F	402	2	24,30,30	0.84	2 (8%)	30,47,47	1.25	5 (16%)
5	GOL	D	407	-	5,5,5	0.30	0	5,5,5	0.33	0
3	GDP	D	402	2	24,30,30	0.89	0	30,47,47	1.32	4 (13%)
5	GOL	D	405	-	5,5,5	0.34	0	5,5,5	0.28	0
3	GDP	C	402	2	24,30,30	0.83	0	30,47,47	1.34	5 (16%)
5	GOL	A	407	-	5,5,5	0.25	0	5,5,5	0.27	0
5	GOL	F	404	-	5,5,5	0.37	0	5,5,5	0.41	0
5	GOL	D	406	-	5,5,5	0.39	0	5,5,5	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	F	403	-	-	1/4/4/4	-
5	GOL	C	404	-	-	4/4/4/4	-
5	GOL	B	405	-	-	2/4/4/4	-
5	GOL	B	407	-	-	1/4/4/4	-
5	GOL	C	405	-	-	2/4/4/4	-
5	GOL	E	405	-	-	2/4/4/4	-
5	GOL	B	406	-	-	4/4/4/4	-
3	GDP	A	402	2	-	1/12/32/32	0/3/3/3
5	GOL	A	405	-	-	0/4/4/4	-
3	GDP	E	402	2	-	0/12/32/32	0/3/3/3
5	GOL	A	406	-	-	2/4/4/4	-
3	GDP	B	402	2	-	1/12/32/32	0/3/3/3
5	GOL	B	408	-	-	0/4/4/4	-
5	GOL	A	408	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	E	406	-	-	2/4/4/4	-
5	GOL	E	404	-	-	2/4/4/4	-
5	GOL	E	403	-	-	4/4/4/4	-
3	GDP	F	402	2	-	1/12/32/32	0/3/3/3
5	GOL	D	407	-	-	1/4/4/4	-
3	GDP	D	402	2	-	0/12/32/32	0/3/3/3
5	GOL	D	405	-	-	0/4/4/4	-
3	GDP	C	402	2	-	1/12/32/32	0/3/3/3
5	GOL	A	407	-	-	2/4/4/4	-
5	GOL	F	404	-	-	2/4/4/4	-
5	GOL	D	406	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	402	GDP	O4'-C1'	2.09	1.44	1.41
3	E	402	GDP	O4'-C1'	2.02	1.43	1.41
3	F	402	GDP	C6-N1	-2.00	1.34	1.37

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	GDP	C5-C6-N1	2.85	118.98	113.95
3	B	402	GDP	C5-C6-N1	2.79	118.89	113.95
3	F	402	GDP	C5-C6-N1	2.77	118.85	113.95
3	D	402	GDP	C5-C6-N1	2.74	118.80	113.95
3	F	402	GDP	PA-O3A-PB	-2.71	123.51	132.83
3	A	402	GDP	O6-C6-C5	-2.71	119.08	124.37
3	E	402	GDP	O6-C6-C5	-2.67	119.16	124.37
3	D	402	GDP	PA-O3A-PB	-2.65	123.72	132.83
3	B	402	GDP	O6-C6-C5	-2.55	119.39	124.37
3	C	402	GDP	C5-C6-N1	2.55	118.45	113.95
3	E	402	GDP	PA-O3A-PB	-2.53	124.14	132.83
3	E	402	GDP	O3B-PB-O2B	2.50	117.19	107.64
3	A	402	GDP	C8-N7-C5	2.48	107.71	102.99
3	E	402	GDP	C5-C6-N1	2.45	118.28	113.95
3	D	402	GDP	C8-N7-C5	2.44	107.64	102.99
3	B	402	GDP	C8-N7-C5	2.41	107.59	102.99
3	B	402	GDP	PA-O3A-PB	-2.41	124.55	132.83
3	E	402	GDP	C8-N7-C5	2.37	107.50	102.99
3	D	402	GDP	O6-C6-C5	-2.37	119.75	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	GDP	C8-N7-C5	2.36	107.50	102.99
3	C	402	GDP	O6-C6-C5	-2.30	119.87	124.37
3	C	402	GDP	PA-O3A-PB	-2.29	124.97	132.83
3	B	402	GDP	O2A-PA-O1A	2.16	122.91	112.24
3	F	402	GDP	C8-N7-C5	2.09	106.98	102.99
3	F	402	GDP	O6-C6-C5	-2.09	120.29	124.37
3	F	402	GDP	O2A-PA-O1A	2.05	122.38	112.24
3	A	402	GDP	PA-O3A-PB	-2.01	125.92	132.83
3	C	402	GDP	O3B-PB-O1B	2.00	118.52	110.68

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	407	GOL	O1-C1-C2-C3
5	B	405	GOL	C1-C2-C3-O3
5	B	406	GOL	C1-C2-C3-O3
5	C	404	GOL	O1-C1-C2-C3
5	C	404	GOL	C1-C2-C3-O3
5	C	405	GOL	O1-C1-C2-O2
5	C	405	GOL	O1-C1-C2-C3
5	E	405	GOL	C1-C2-C3-O3
5	E	406	GOL	C1-C2-C3-O3
5	A	406	GOL	O1-C1-C2-C3
5	A	408	GOL	O1-C1-C2-C3
5	B	406	GOL	O1-C1-C2-C3
5	E	403	GOL	O1-C1-C2-C3
5	E	403	GOL	C1-C2-C3-O3
5	E	404	GOL	O1-C1-C2-C3
5	F	403	GOL	C1-C2-C3-O3
5	F	404	GOL	C1-C2-C3-O3
5	A	406	GOL	O1-C1-C2-O2
5	A	407	GOL	O1-C1-C2-O2
5	A	408	GOL	O1-C1-C2-O2
5	B	405	GOL	O2-C2-C3-O3
5	B	406	GOL	O2-C2-C3-O3
5	E	404	GOL	O1-C1-C2-O2
5	E	406	GOL	O2-C2-C3-O3
5	F	404	GOL	O2-C2-C3-O3
5	C	404	GOL	O1-C1-C2-O2
5	C	404	GOL	O2-C2-C3-O3
5	E	405	GOL	O2-C2-C3-O3

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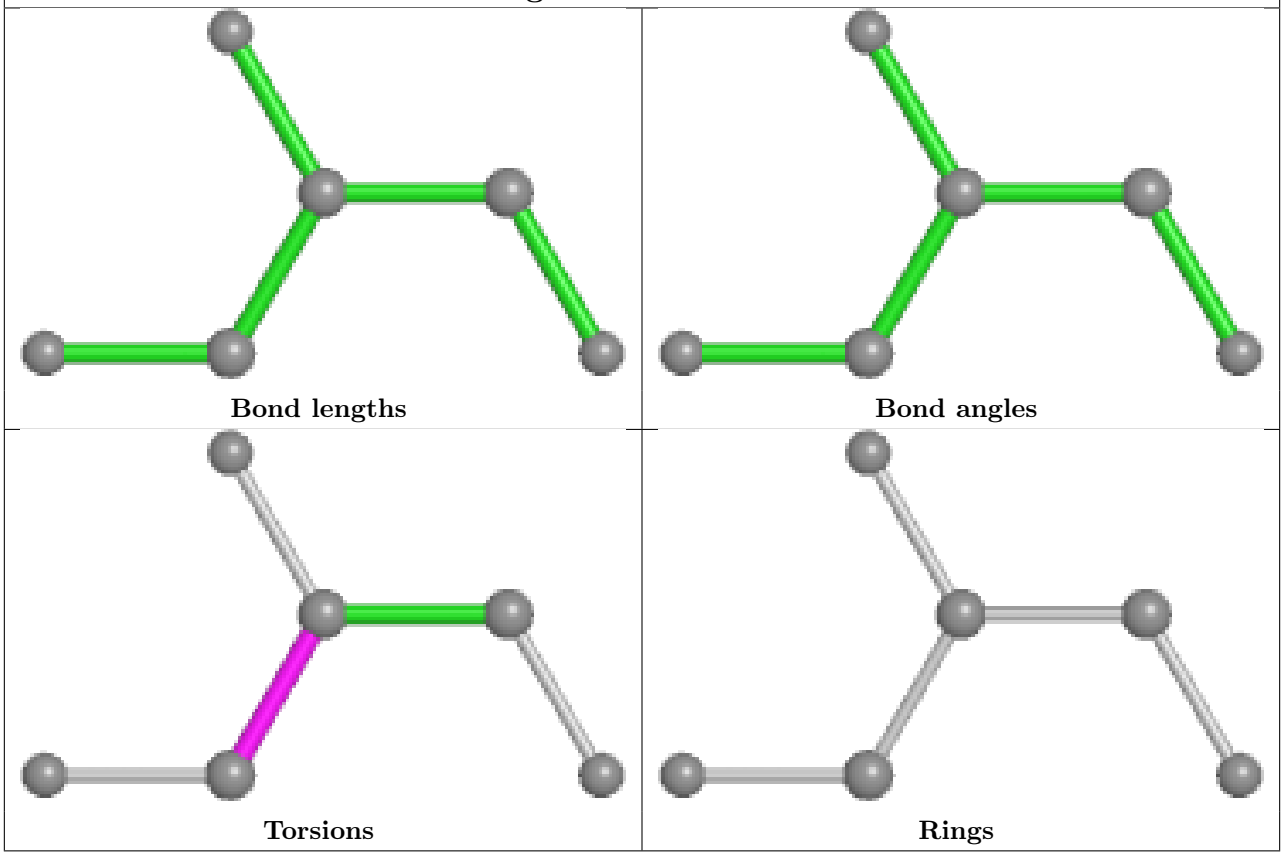
Mol	Chain	Res	Type	Atoms
5	B	406	GOL	O1-C1-C2-O2
5	E	403	GOL	O1-C1-C2-O2
5	E	403	GOL	O2-C2-C3-O3
3	A	402	GDP	PB-O3A-PA-O2A
3	C	402	GDP	PB-O3A-PA-O2A
3	B	402	GDP	PB-O3A-PA-O1A
3	F	402	GDP	PB-O3A-PA-O1A
5	B	407	GOL	O1-C1-C2-C3
5	D	407	GOL	C1-C2-C3-O3

There are no ring outliers.

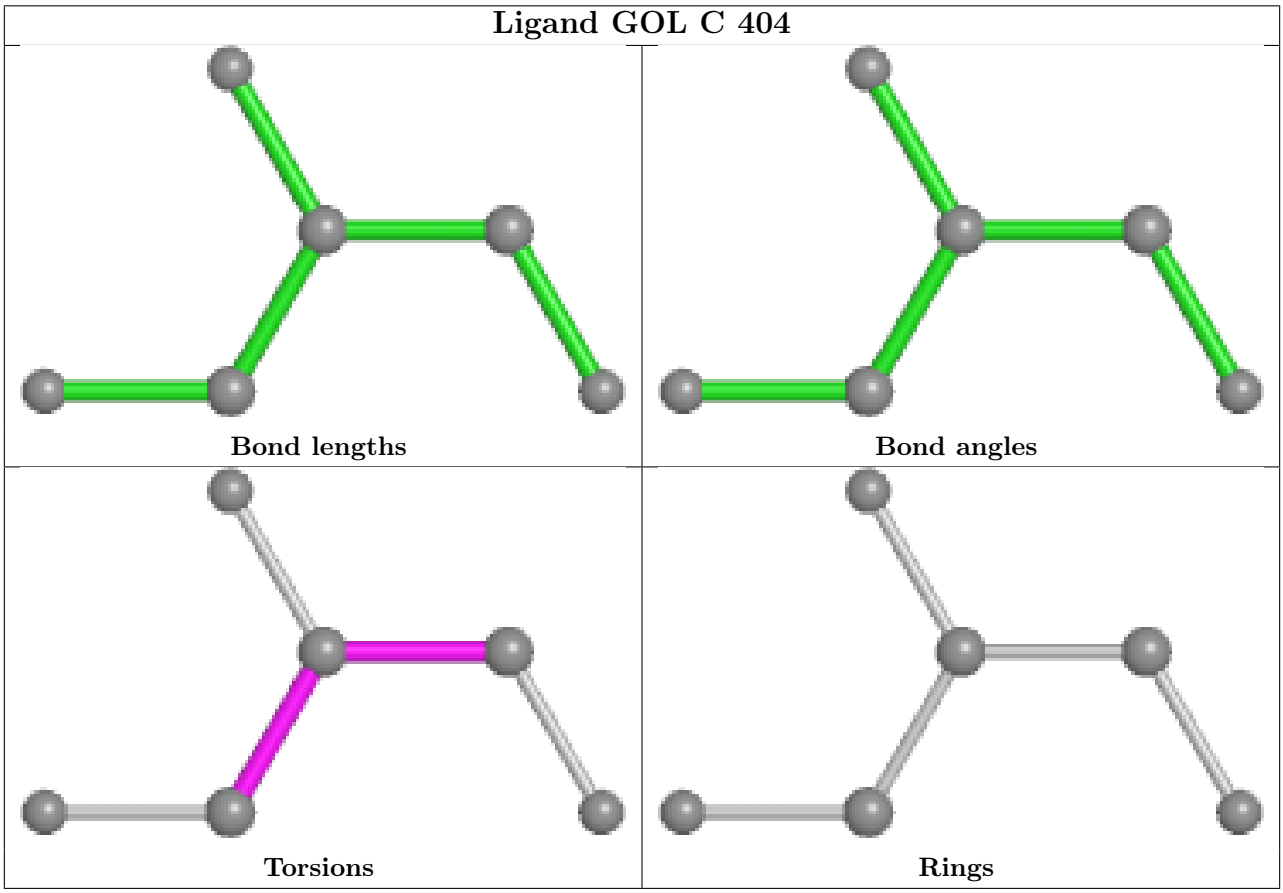
No monomer is involved in short contacts.

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

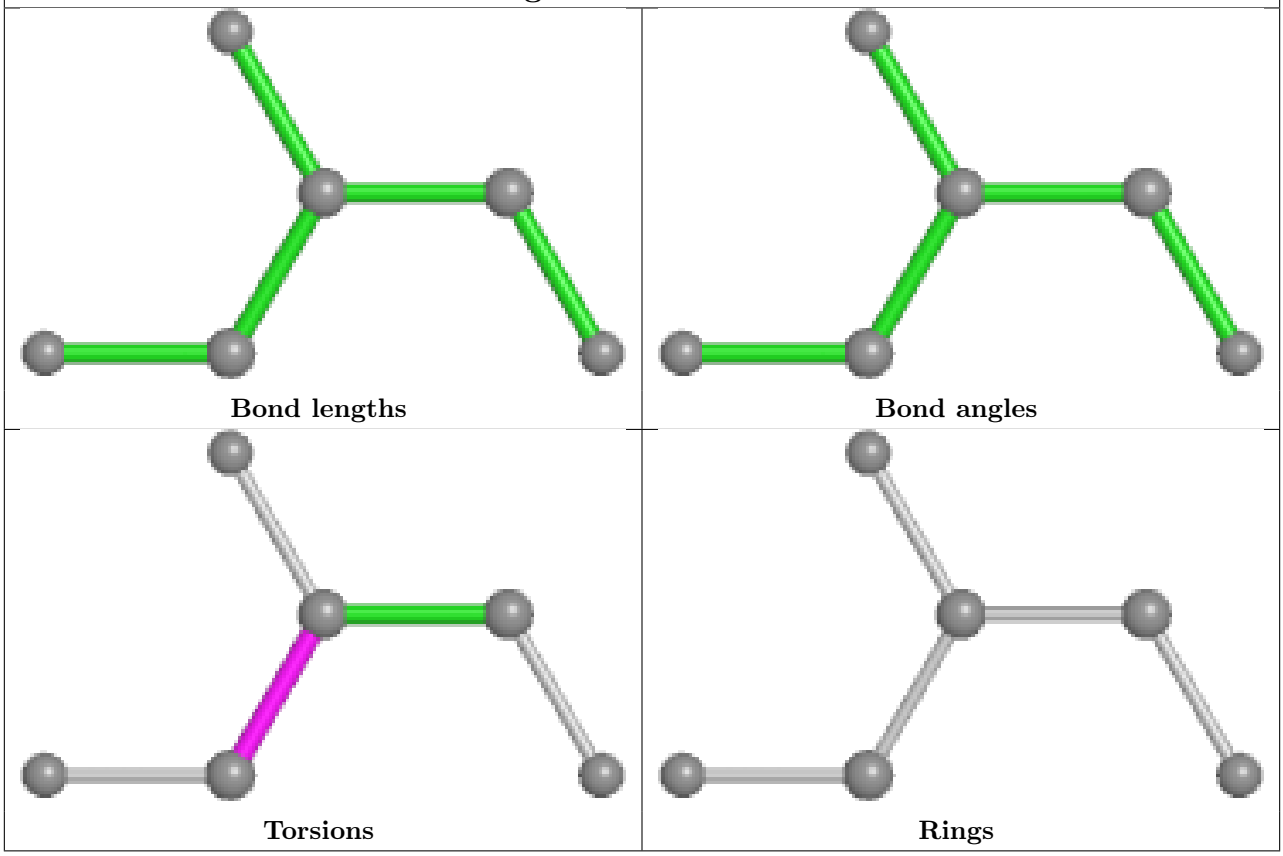
Ligand GOL F 403



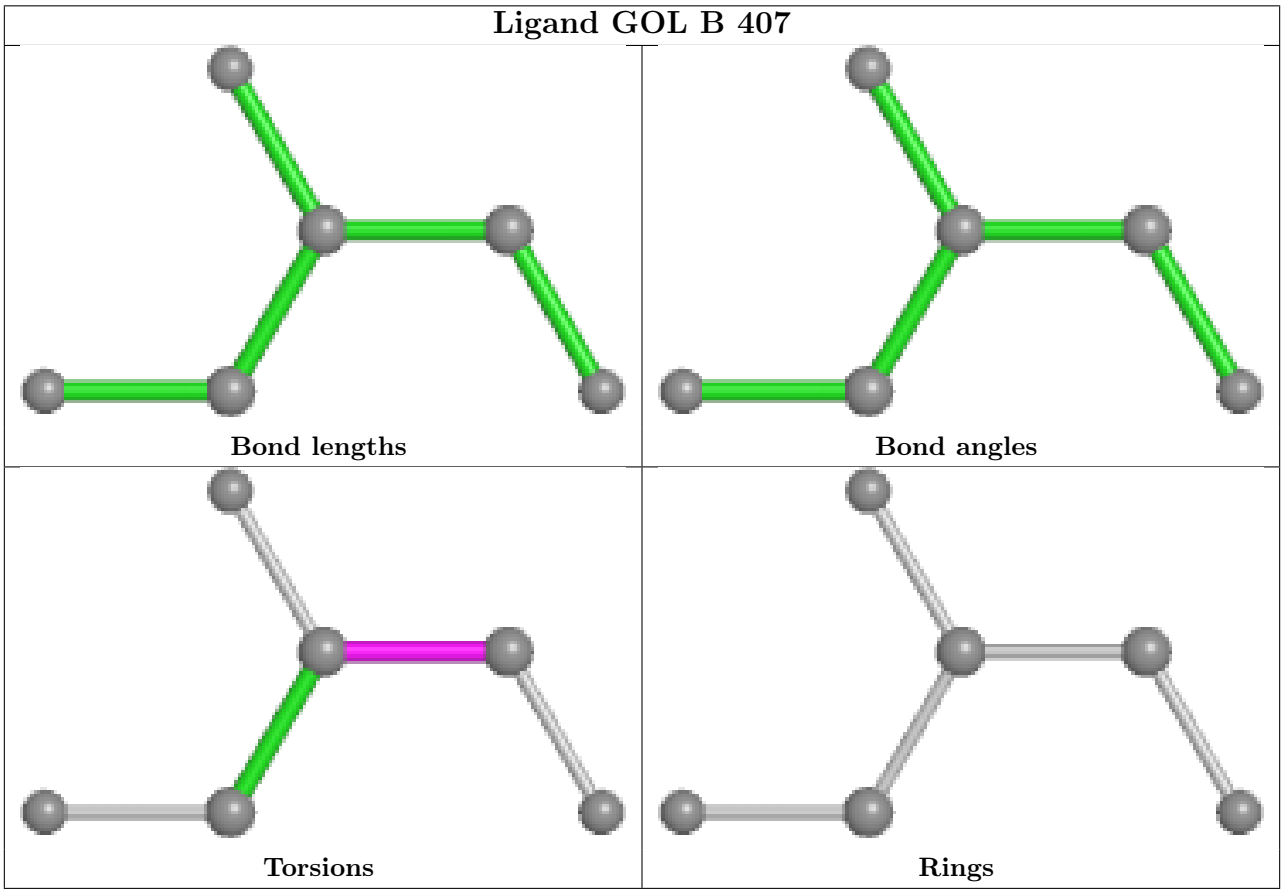
Ligand GOL C 404



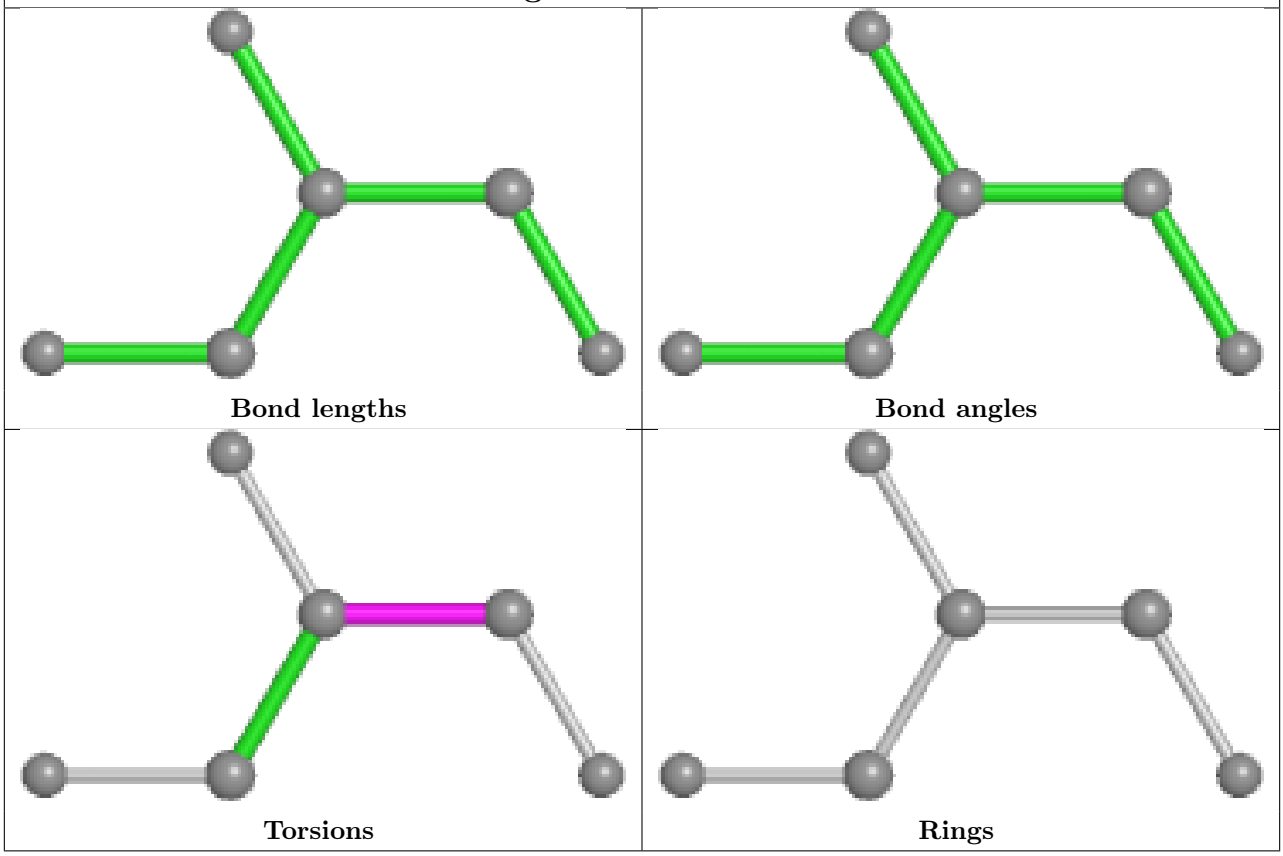
Ligand GOL B 405



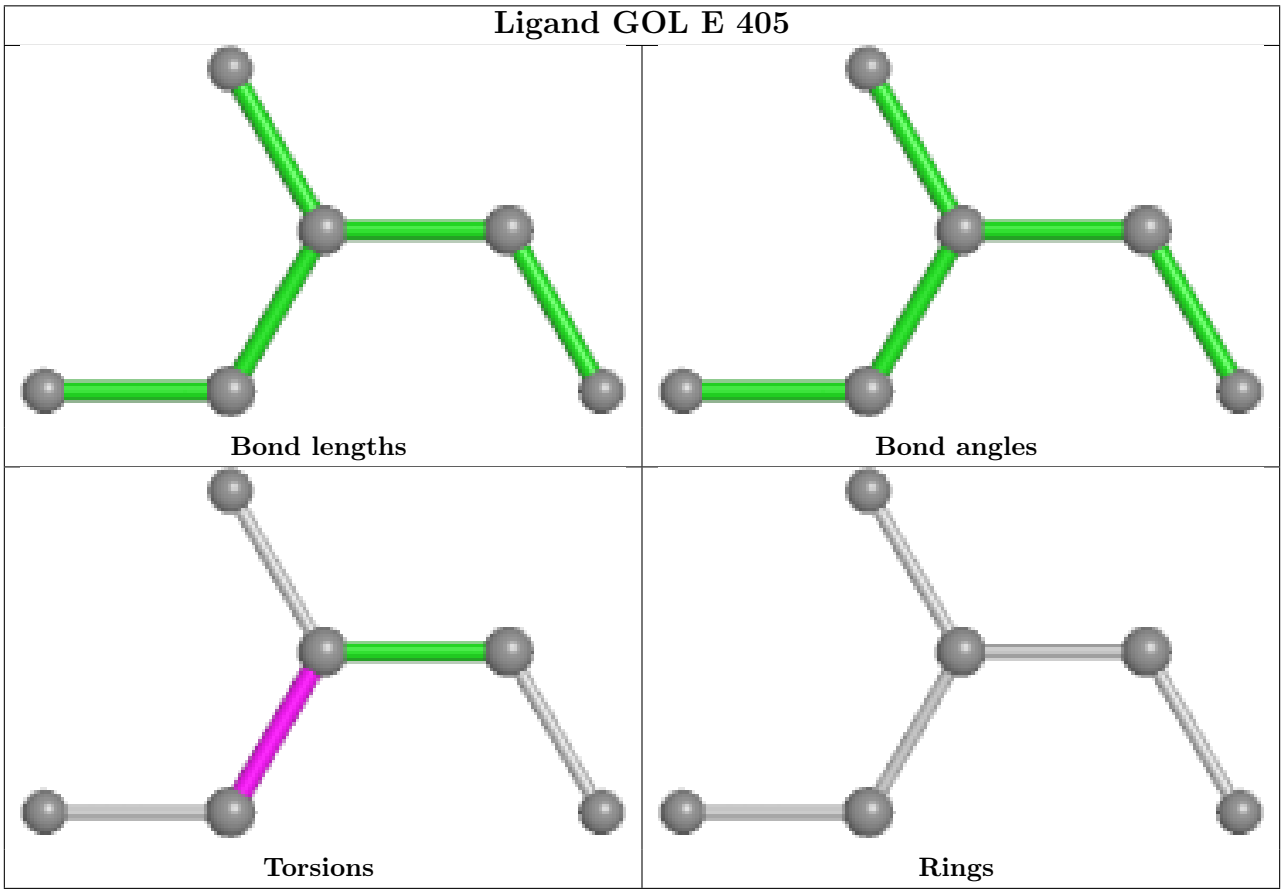
Ligand GOL B 407



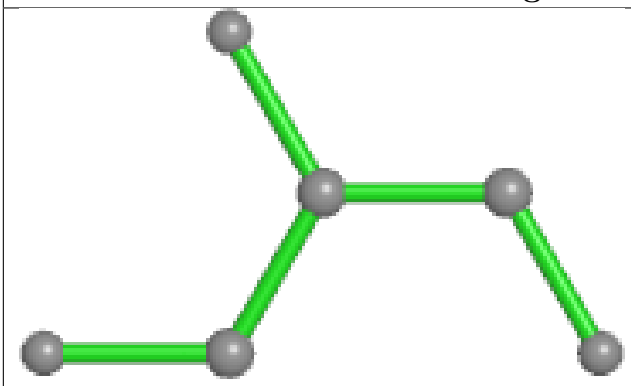
Ligand GOL C 405



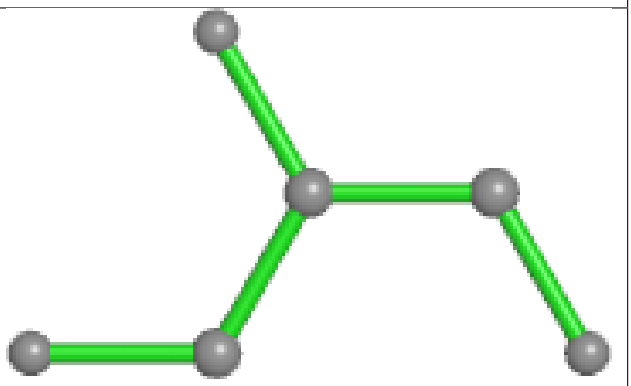
Ligand GOL E 405



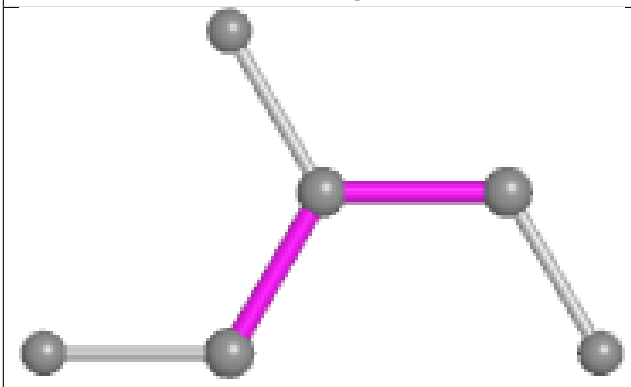
Ligand GOL B 406



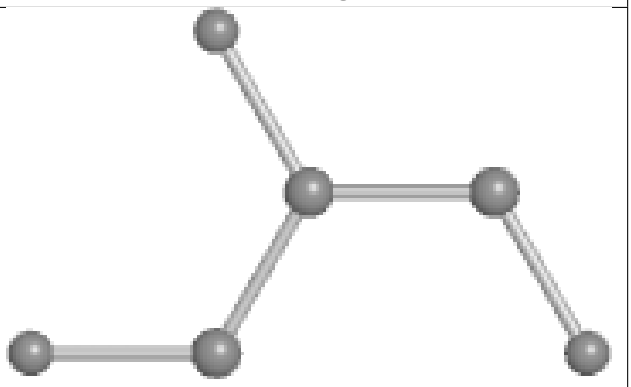
Bond lengths



Bond angles

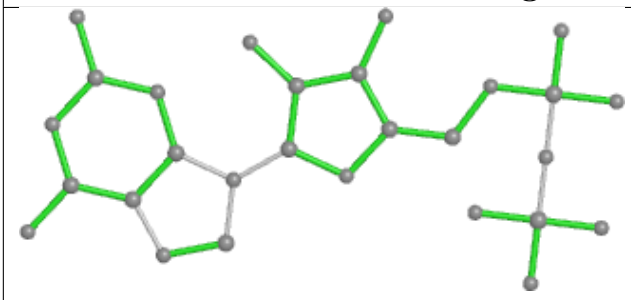


Torsions

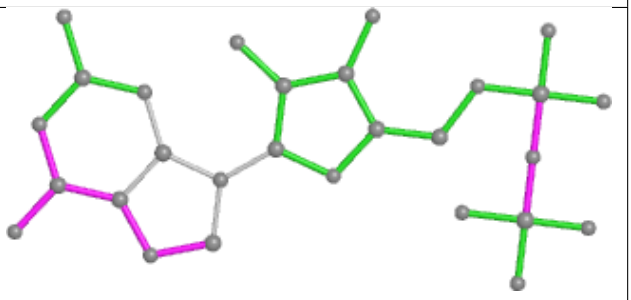


Rings

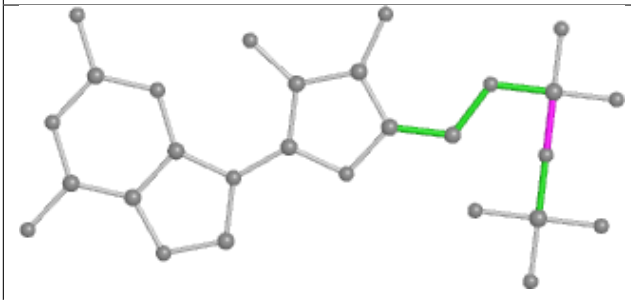
Ligand GDP A 402



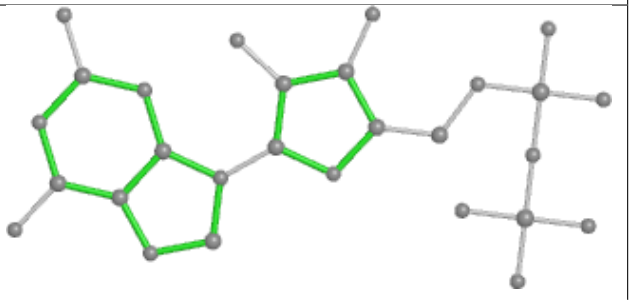
Bond lengths



Bond angles

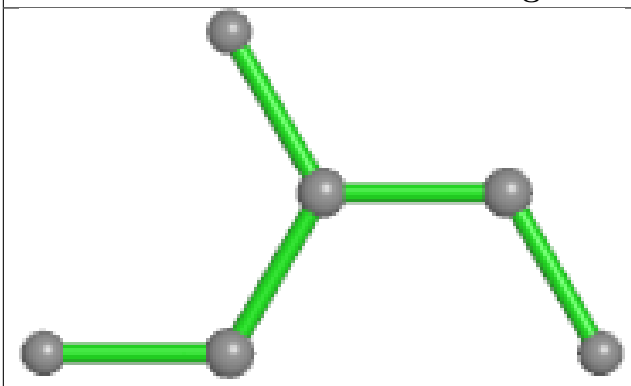


Torsions

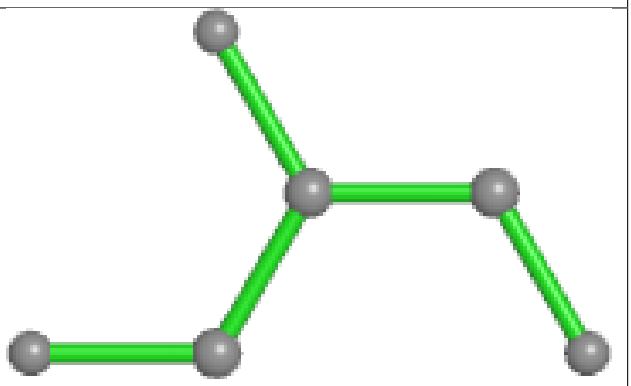


Rings

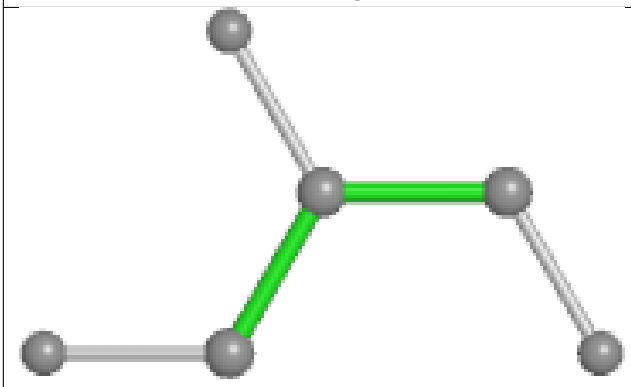
Ligand GOL A 405



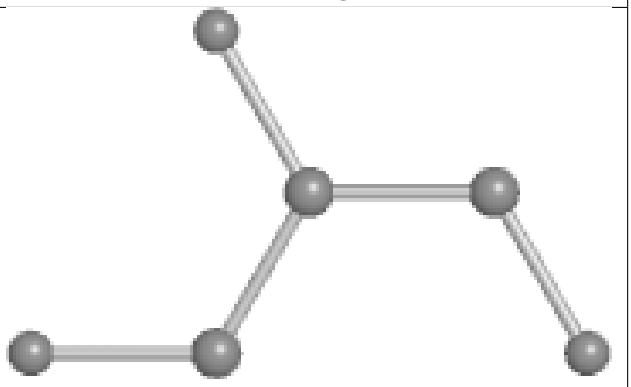
Bond lengths



Bond angles

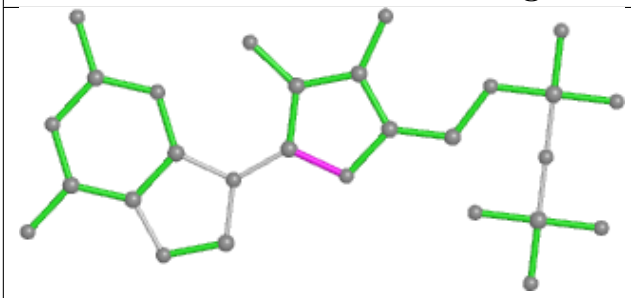


Torsions

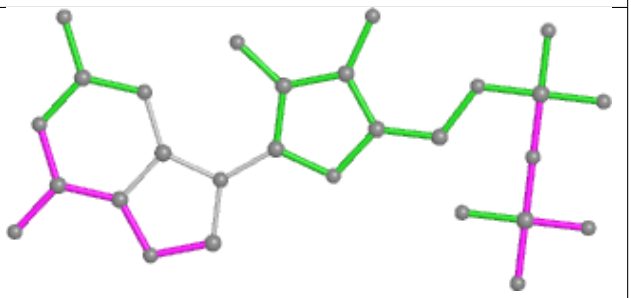


Rings

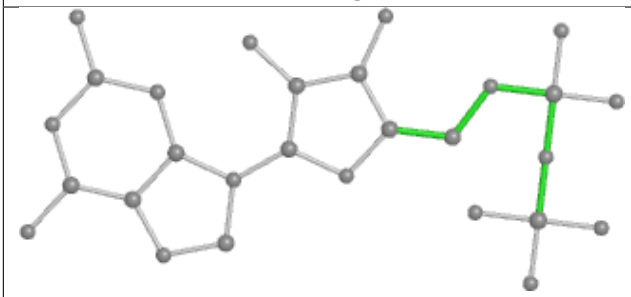
Ligand GDP E 402



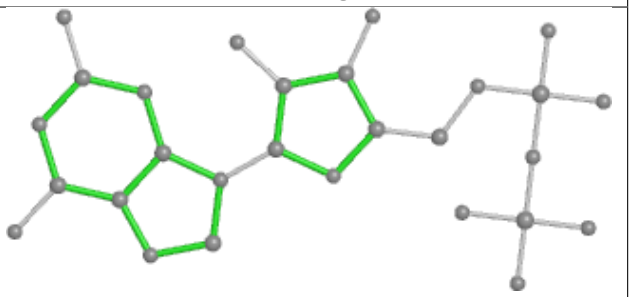
Bond lengths



Bond angles

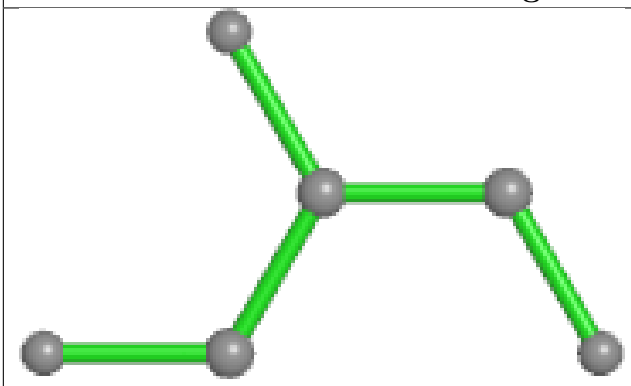


Torsions

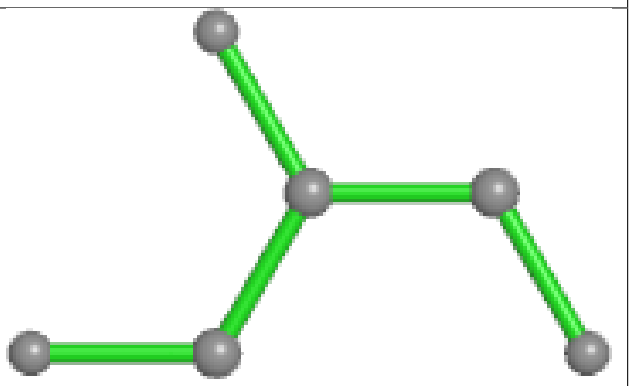


Rings

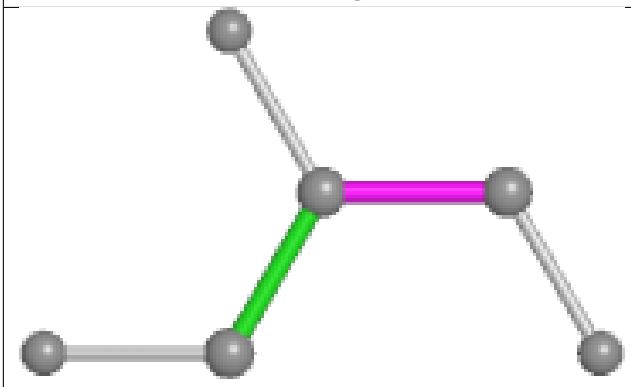
Ligand GOL A 406



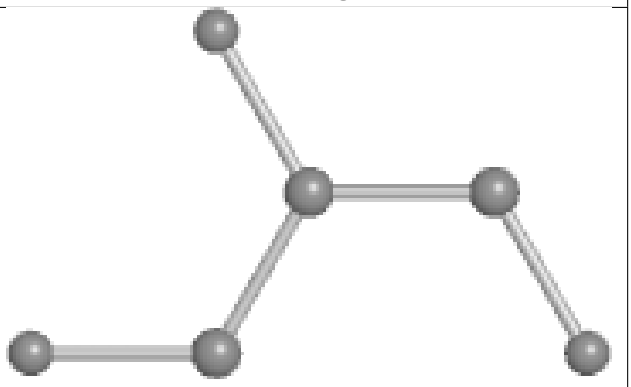
Bond lengths



Bond angles

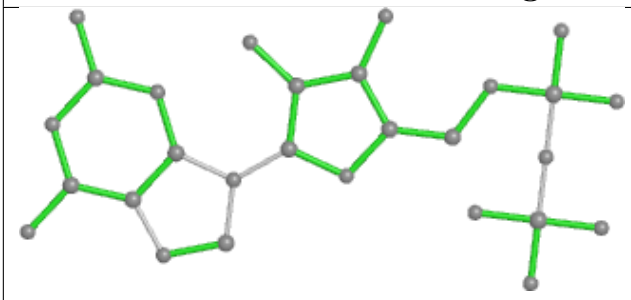


Torsions

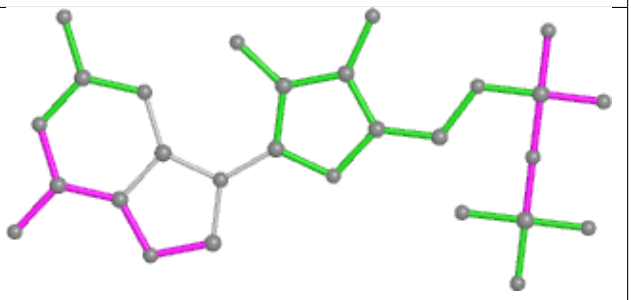


Rings

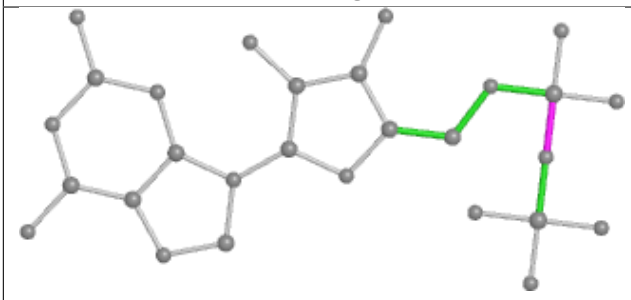
Ligand GDP B 402



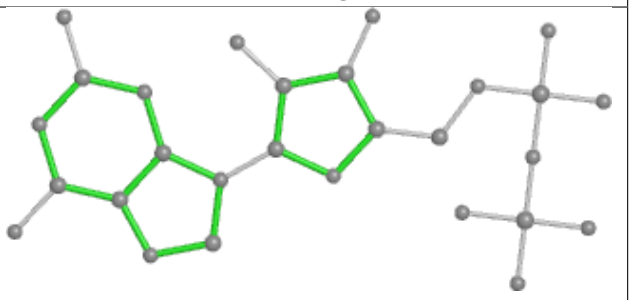
Bond lengths



Bond angles

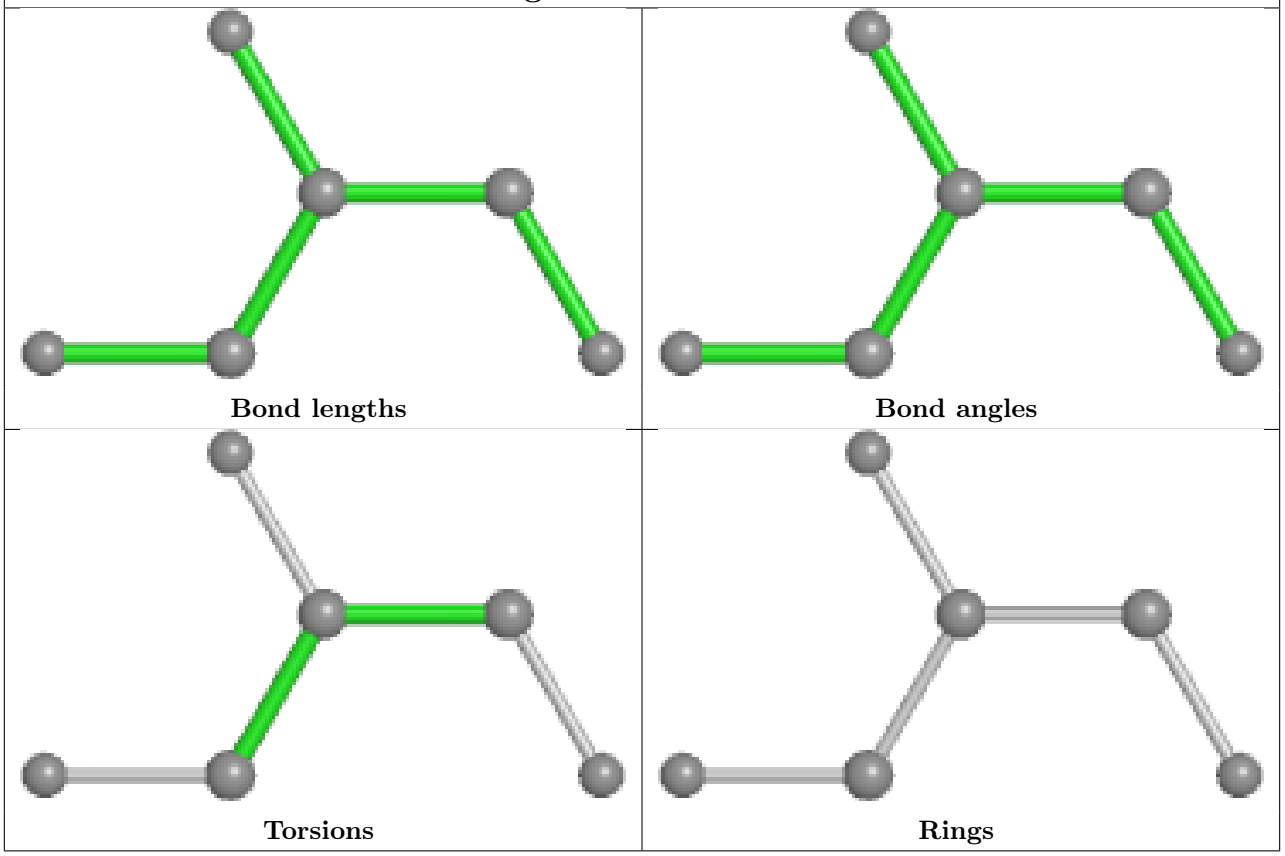


Torsions

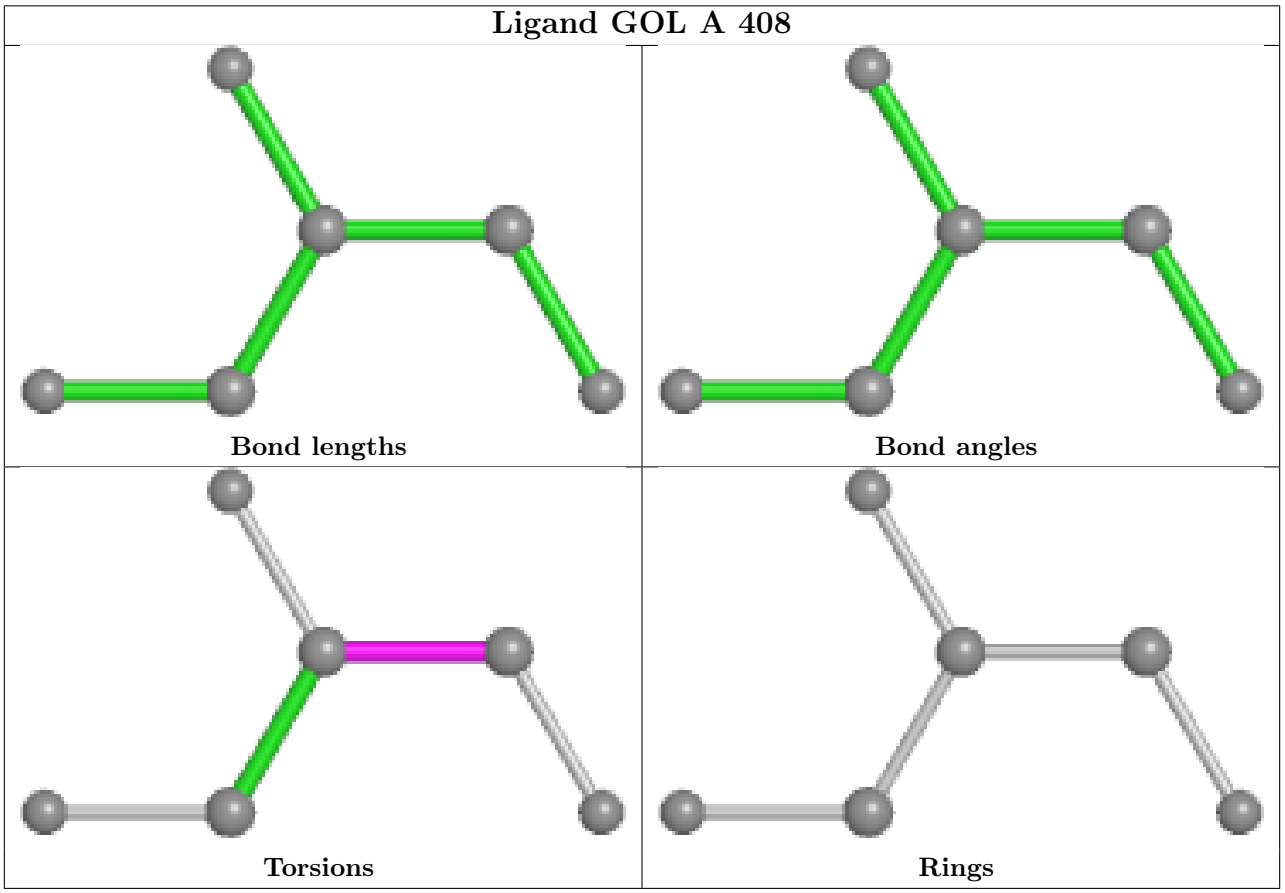


Rings

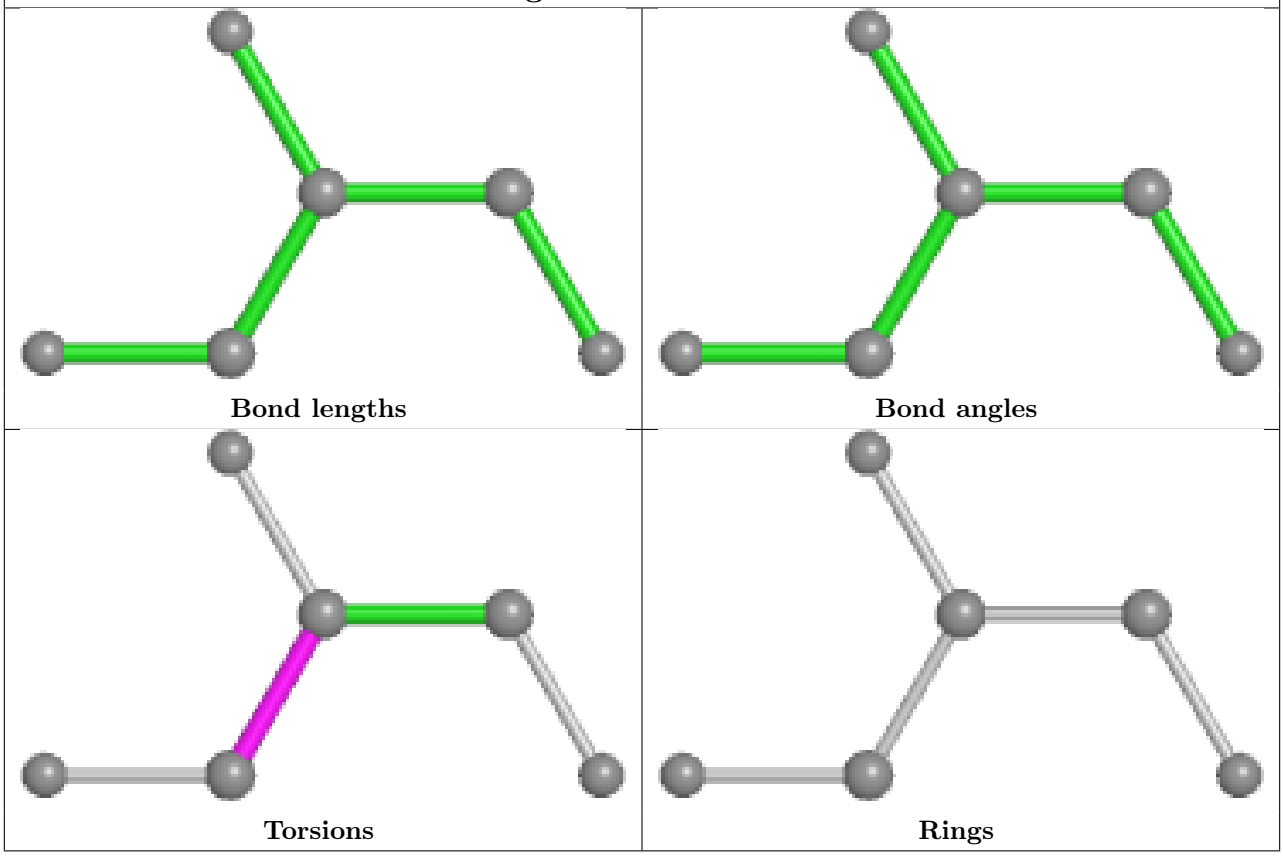
Ligand GOL B 408



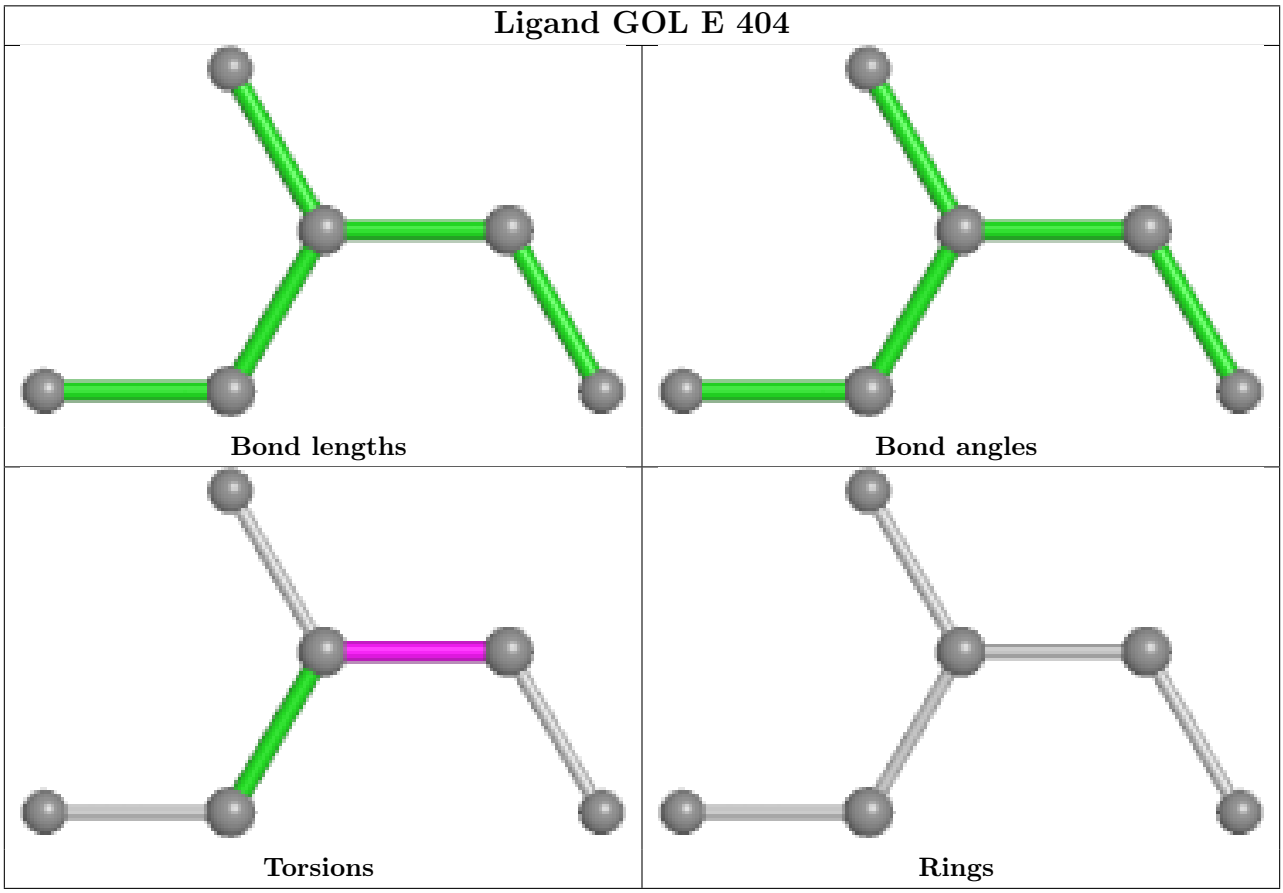
Ligand GOL A 408



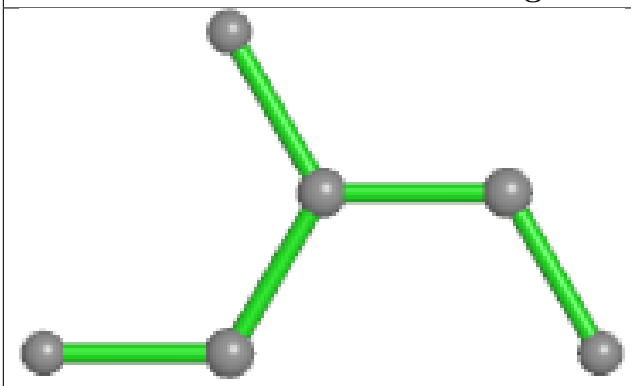
Ligand GOL E 406



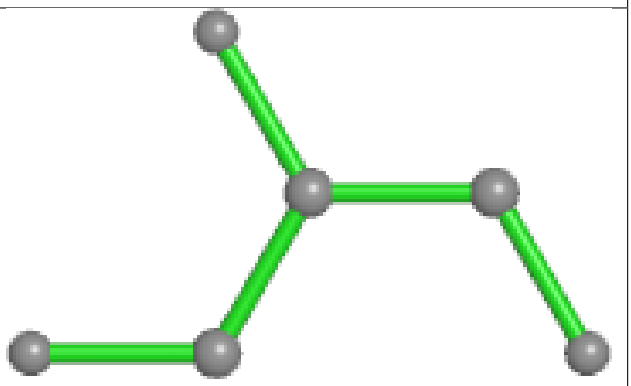
Ligand GOL E 404



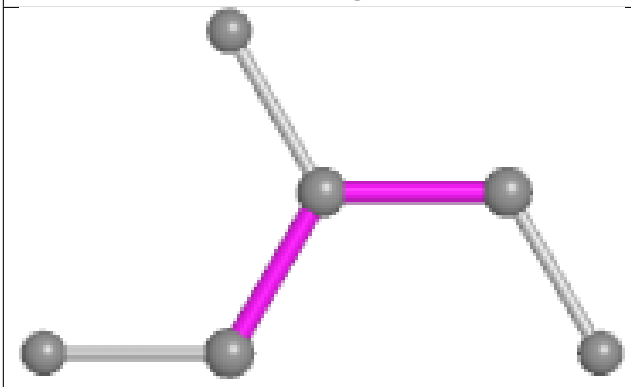
Ligand GOL E 403



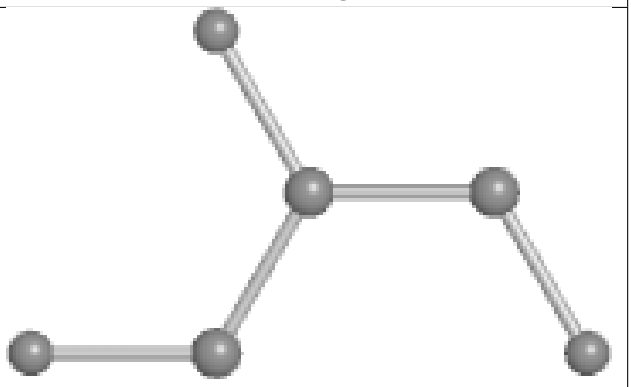
Bond lengths



Bond angles

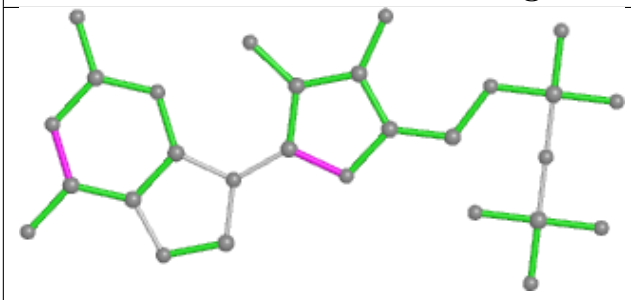


Torsions

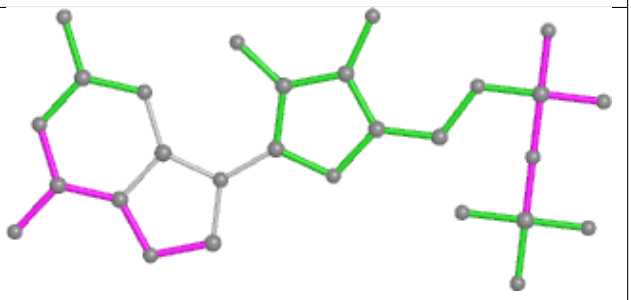


Rings

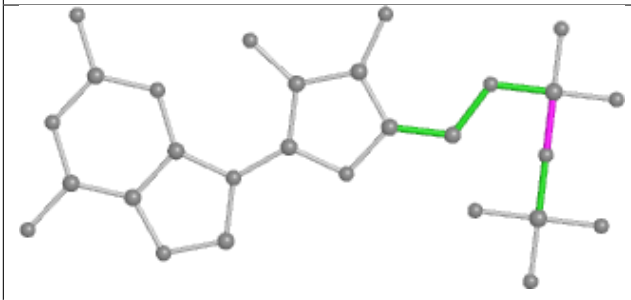
Ligand GDP F 402



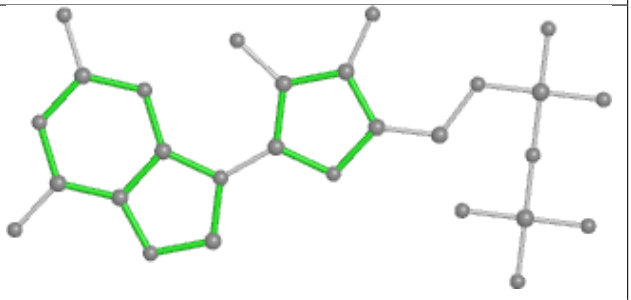
Bond lengths



Bond angles

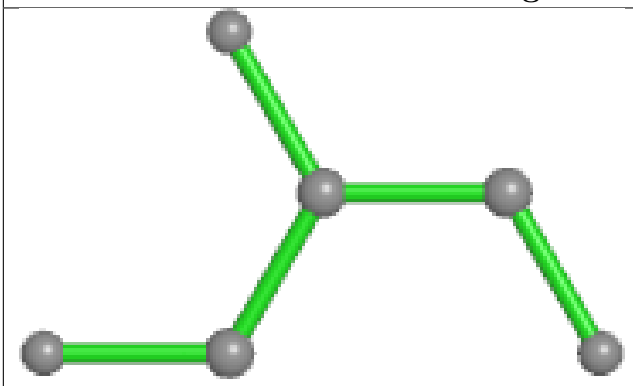


Torsions

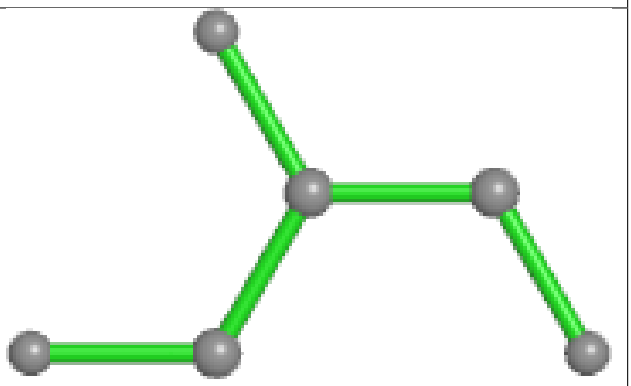


Rings

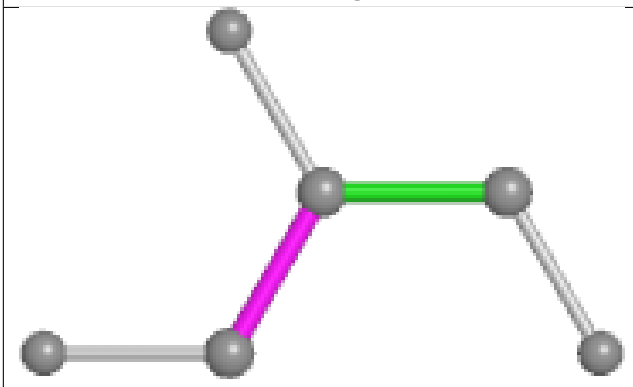
Ligand GOL D 407



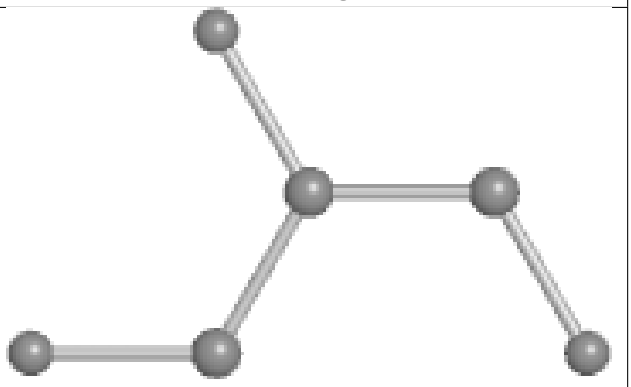
Bond lengths



Bond angles

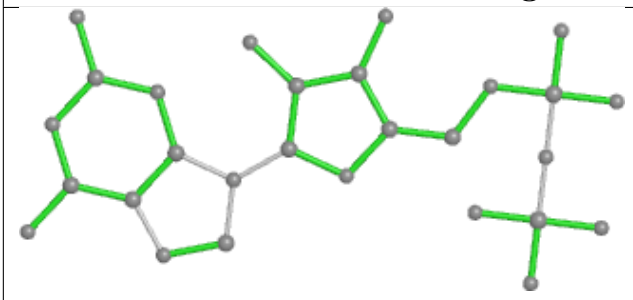


Torsions

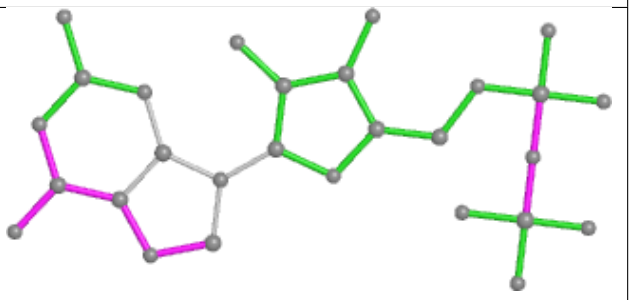


Rings

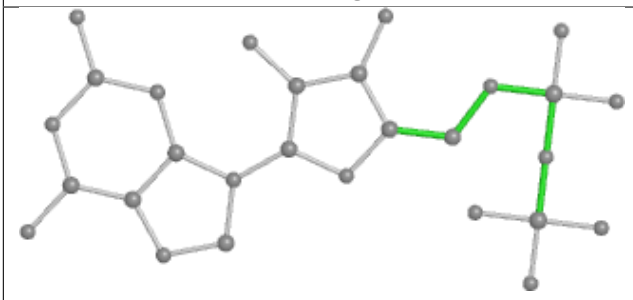
Ligand GDP D 402



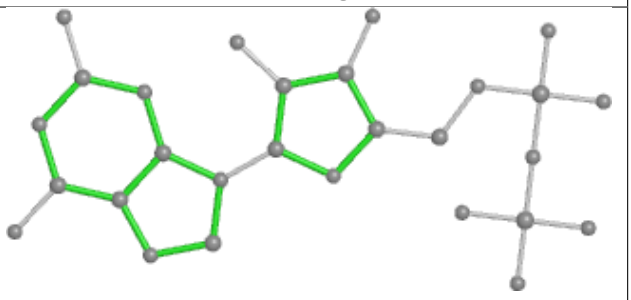
Bond lengths



Bond angles

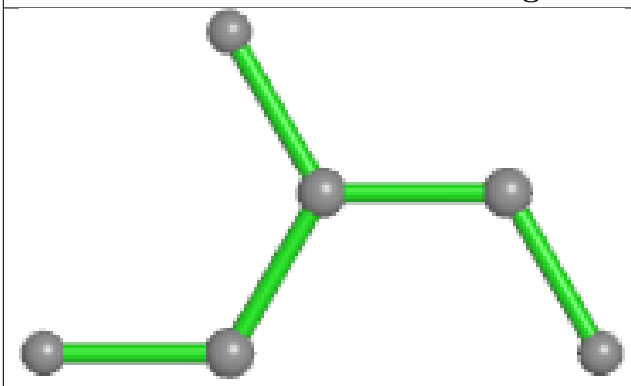


Torsions

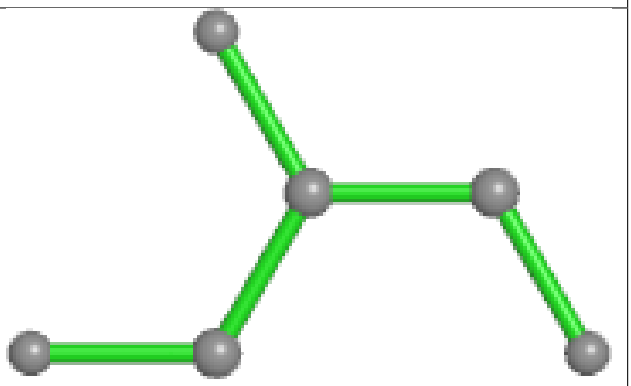


Rings

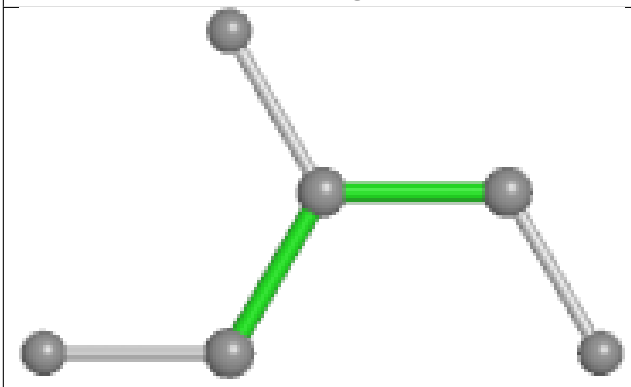
Ligand GOL D 405



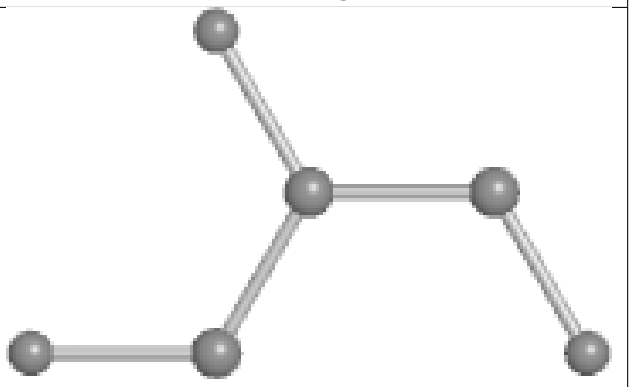
Bond lengths



Bond angles

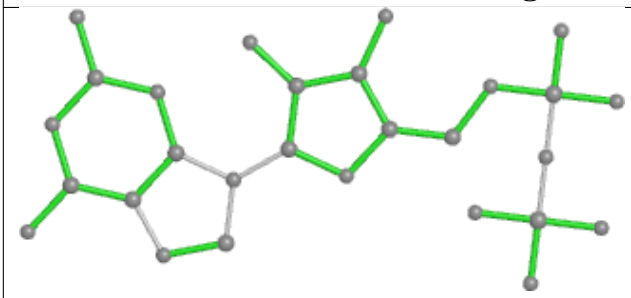


Torsions

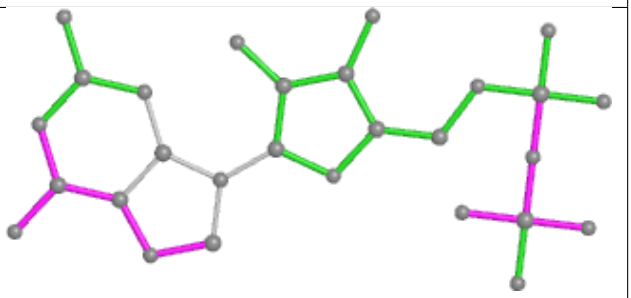


Rings

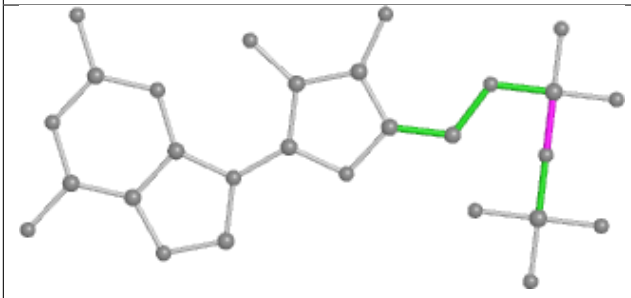
Ligand GDP C 402



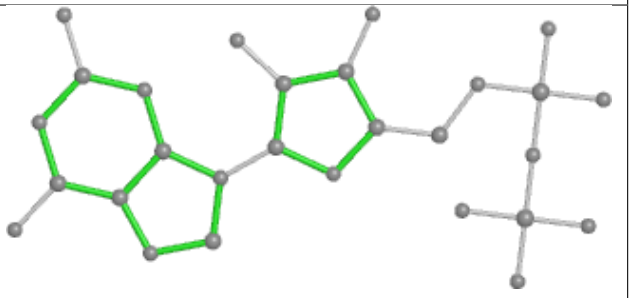
Bond lengths



Bond angles

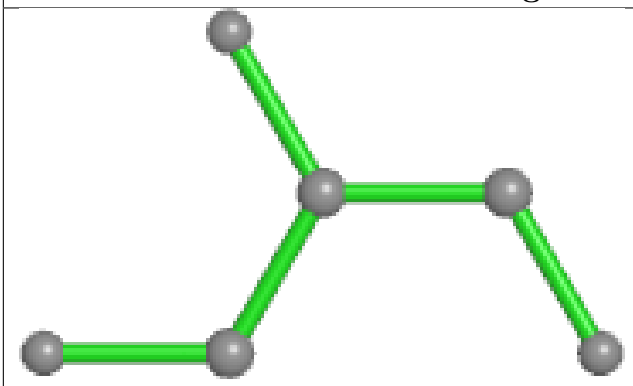


Torsions

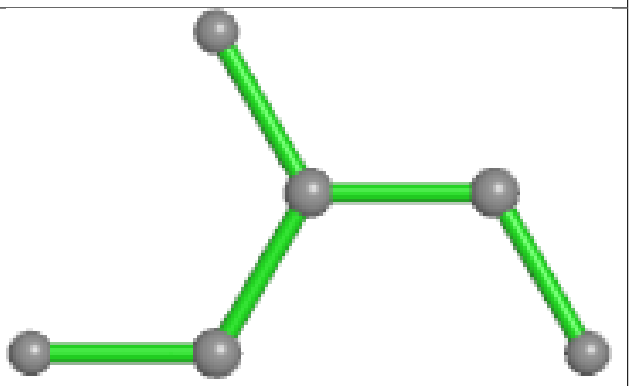


Rings

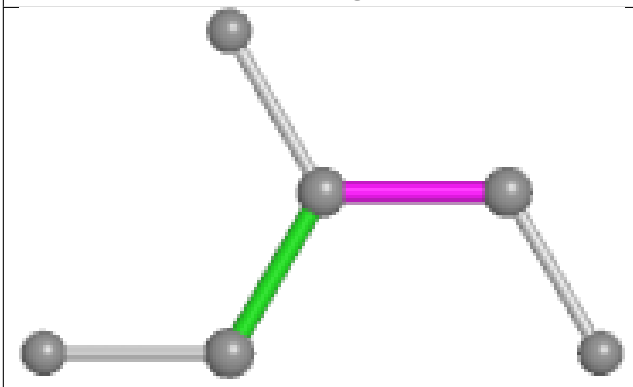
Ligand GOL A 407



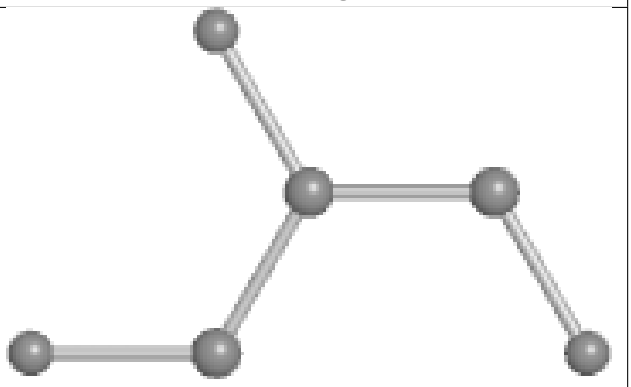
Bond lengths



Bond angles

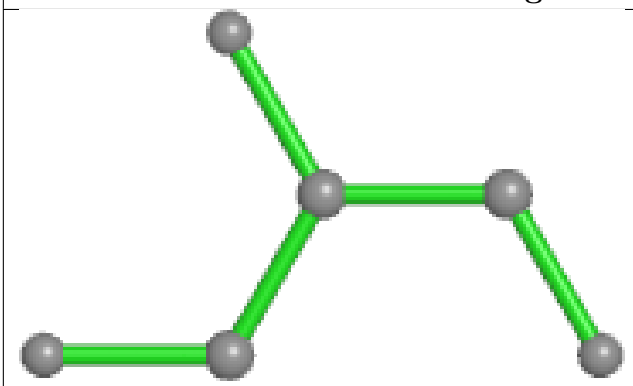


Torsions

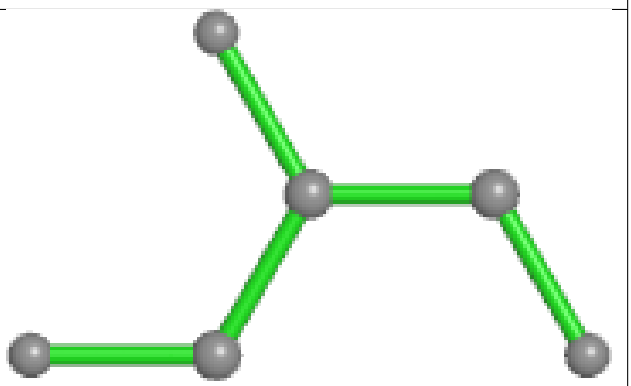


Rings

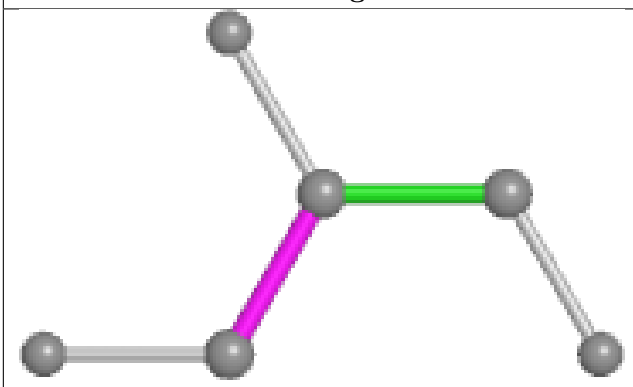
Ligand GOL F 404



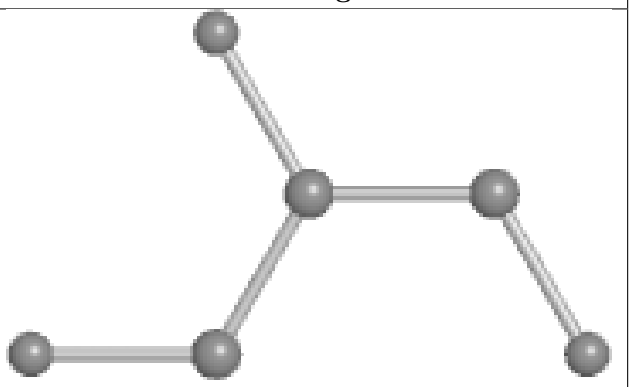
Bond lengths



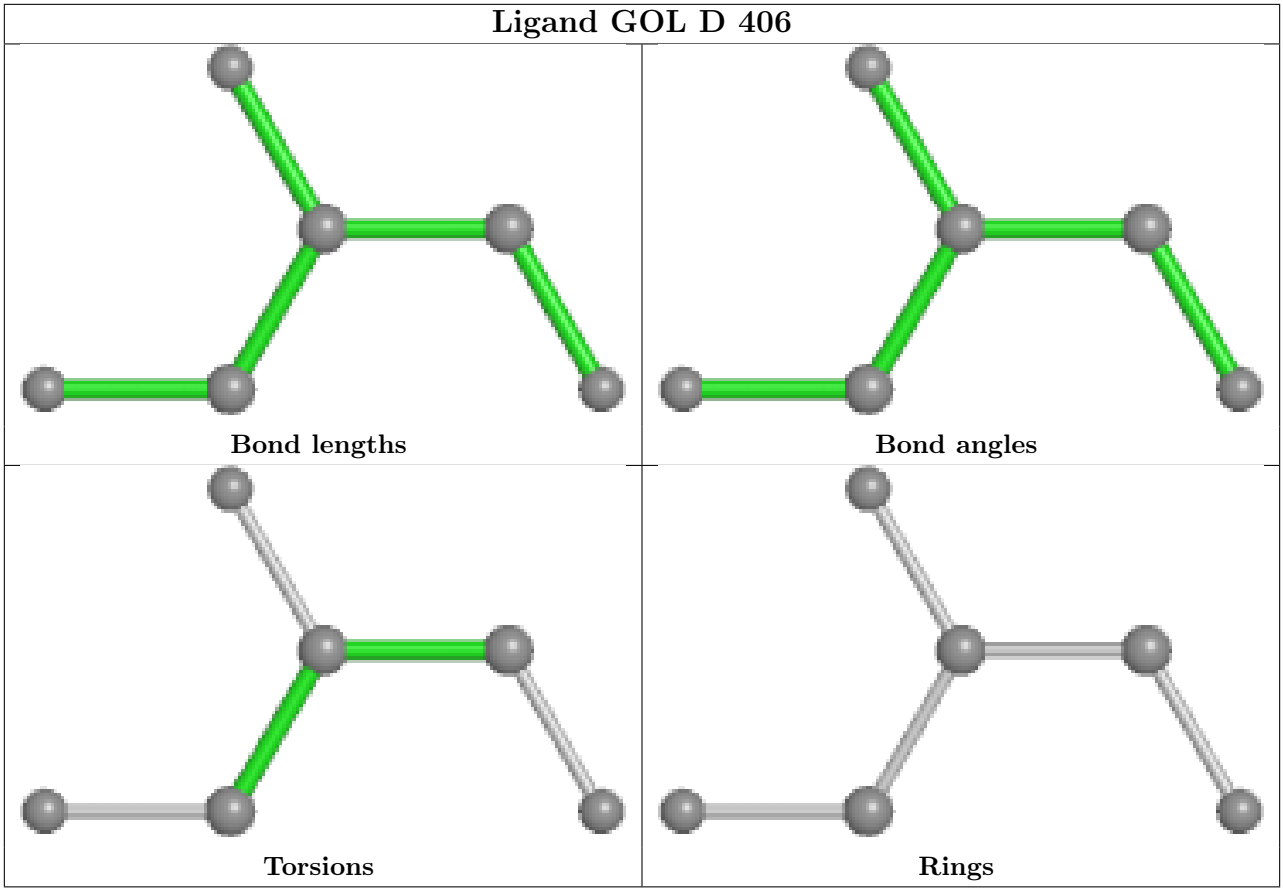
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	365/386 (94%)	0.36	15 (4%)	37	40	27, 34, 52, 93	0
1	B	365/386 (94%)	0.35	19 (5%)	27	30	27, 34, 51, 104	0
1	C	372/386 (96%)	-0.06	10 (2%)	54	57	28, 36, 56, 85	0
1	D	365/386 (94%)	0.57	35 (9%)	8	9	26, 36, 58, 96	0
1	E	372/386 (96%)	0.02	13 (3%)	44	47	28, 40, 60, 94	0
1	F	372/386 (96%)	0.05	13 (3%)	44	47	30, 40, 61, 89	0
All	All	2211/2316 (95%)	0.21	105 (4%)	31	34	26, 37, 58, 104	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	34	ILE	9.2
1	B	33	PHE	8.4
1	F	73	ALA	8.2
1	A	34	ILE	7.6
1	D	34	ILE	7.4
1	A	33	PHE	7.2
1	B	39	LYS	6.7
1	C	74	HIS	6.7
1	D	33	PHE	6.6
1	F	74	HIS	6.6
1	E	74	HIS	6.3
1	E	73	ALA	6.2
1	B	32	SER	5.9
1	B	29	HIS	5.6
1	C	73	ALA	5.3
1	B	40	GLU	5.2
1	A	28	SER	5.2
1	D	32	SER	4.8
1	D	28	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	31	PRO	4.4
1	B	30	GLY	4.4
1	D	71	ASN	4.4
1	A	32	SER	4.4
1	D	29	HIS	4.2
1	D	40	GLU	4.1
1	C	174	ASP	4.0
1	E	171	GLN	4.0
1	A	40	GLU	3.8
1	A	30	GLY	3.8
1	D	64[A]	ASP	3.7
1	E	71	ASN	3.7
1	A	29	HIS	3.7
1	D	63	ALA	3.6
1	F	174	ASP	3.6
1	F	172	TYR	3.2
1	C	368	LYS	3.1
1	E	172	TYR	3.1
1	D	73	ALA	3.0
1	A	64	ASP	2.9
1	D	330	VAL	2.9
1	D	242	VAL	2.9
1	D	31	PRO	2.9
1	B	330	VAL	2.8
1	D	131	ALA	2.8
1	F	64	ASP	2.8
1	A	31	PRO	2.7
1	B	64	ASP	2.7
1	D	290	PHE	2.7
1	F	71	ASN	2.7
1	D	123	GLU	2.7
1	D	65	ASP	2.6
1	D	333	ILE	2.6
1	B	71	ASN	2.6
1	A	144	LYS	2.6
1	B	65	ASP	2.6
1	B	235	LEU	2.6
1	D	245	LEU	2.6
1	E	145	GLU	2.6
1	D	124	GLU	2.5
1	D	136	LYS	2.5
1	C	173	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	127	LYS	2.5
1	B	245	LEU	2.5
1	C	171	GLN	2.5
1	E	174	ASP	2.5
1	F	196	LYS	2.4
1	D	151	GLU	2.4
1	D	125	PHE	2.4
1	D	30	GLY	2.4
1	E	119	LYS	2.4
1	E	151	GLU	2.4
1	F	39	LYS	2.4
1	F	169	LYS	2.4
1	D	45	LYS	2.3
1	D	249	THR	2.3
1	A	333	ILE	2.3
1	D	76	ALA	2.3
1	B	333	ILE	2.3
1	B	329	PRO	2.2
1	C	167	GLU	2.2
1	F	167	GLU	2.2
1	C	169	LYS	2.2
1	D	70	PRO	2.2
1	B	45	LYS	2.2
1	E	368	LYS	2.2
1	F	72	SER	2.2
1	C	172	TYR	2.1
1	C	170	ILE	2.1
1	A	235	LEU	2.1
1	F	156	GLU	2.1
1	D	335	LEU	2.1
1	A	326	GLY	2.1
1	A	151	GLU	2.1
1	B	151	GLU	2.1
1	D	128	ARG	2.1
1	D	325	TRP	2.1
1	B	41	TYR	2.0
1	E	64	ASP	2.0
1	D	61	TRP	2.0
1	D	134	LYS	2.0
1	D	329	PRO	2.0
1	F	151	GLU	2.0
1	A	65	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	169	LYS	2.0
1	E	166	THR	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 monosaccharides 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, 95^{th} 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
5	GOL	B	407	6/6	0.37	0.37	73,77,82,82	0
5	GOL	E	405	6/6	0.60	0.29	65,71,73,75	0
5	GOL	A	408	6/6	0.80	0.27	44,58,60,67	0
5	GOL	F	403	6/6	0.81	0.20	51,65,71,73	0
4	NA	D	404	1/1	0.82	0.37	51,51,51,51	0
5	GOL	E	403	6/6	0.82	0.21	53,72,75,76	0
5	GOL	C	405	6/6	0.84	0.24	48,59,63,65	0
5	GOL	B	406	6/6	0.85	0.20	42,57,61,62	0
5	GOL	D	405	6/6	0.87	0.23	46,56,58,65	0
5	GOL	E	406	6/6	0.87	0.31	55,63,66,69	0
5	GOL	A	406	6/6	0.87	0.19	47,58,62,71	0
5	GOL	E	404	6/6	0.88	0.34	58,61,62,63	0
5	GOL	B	405	6/6	0.88	0.19	37,43,51,54	0
5	GOL	A	405	6/6	0.89	0.15	41,45,52,55	0
5	GOL	D	407	6/6	0.90	0.24	47,66,70,71	0
5	GOL	B	408	6/6	0.90	0.19	50,53,55,56	0
5	GOL	C	404	6/6	0.92	0.26	46,52,53,55	0
5	GOL	D	406	6/6	0.92	0.13	36,46,50,56	0
5	GOL	F	404	6/6	0.92	0.28	57,59,63,64	0
4	NA	C	403	1/1	0.93	0.31	49,49,49,49	0
3	GDP	F	402	28/28	0.93	0.11	42,46,54,55	0

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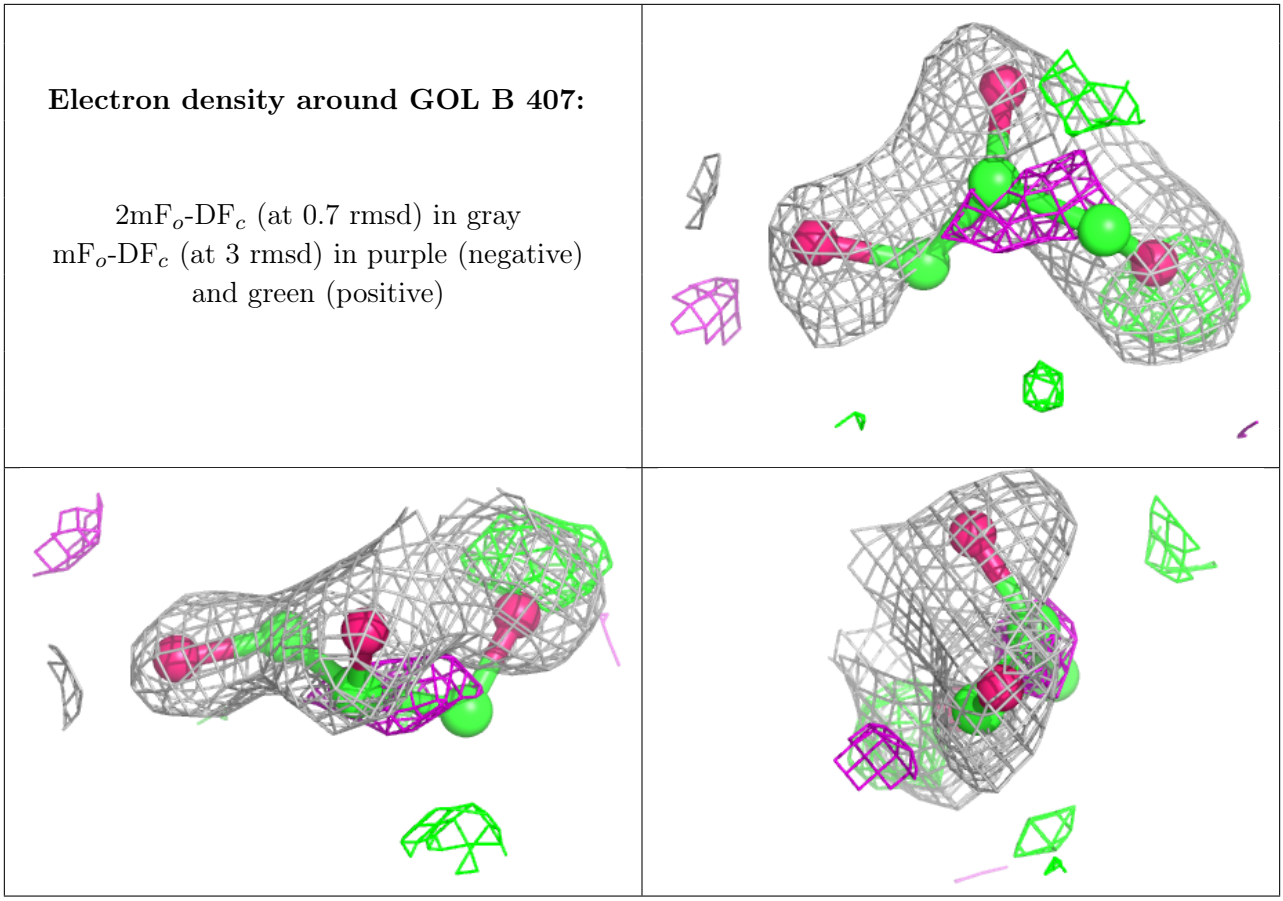
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GDP	C	402	28/28	0.94	0.10	37,41,50,51	0
3	GDP	E	402	28/28	0.94	0.12	45,48,54,56	0
3	GDP	A	402	28/28	0.94	0.10	41,45,49,50	0
5	GOL	A	407	6/6	0.94	0.30	52,55,55,57	0
3	GDP	B	402	28/28	0.94	0.09	39,43,51,55	0
3	GDP	D	402	28/28	0.95	0.09	42,46,50,53	0
2	MN	E	401	1/1	0.95	0.04	49,49,49,49	0
4	NA	B	404	1/1	0.96	0.42	41,41,41,41	0
4	NA	D	403	1/1	0.96	0.09	30,30,30,30	0
4	NA	A	404	1/1	0.97	0.08	31,31,31,31	0
2	MN	C	401	1/1	0.97	0.04	45,45,45,45	0
2	MN	A	401	1/1	0.98	0.05	43,43,43,43	0
2	MN	F	401	1/1	0.98	0.05	49,49,49,49	0
4	NA	A	403	1/1	0.98	0.24	36,36,36,36	0
4	NA	B	403	1/1	0.99	0.07	32,32,32,32	0
2	MN	B	401	1/1	0.99	0.05	42,42,42,42	0
2	MN	D	401	1/1	0.99	0.04	44,44,44,44	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.

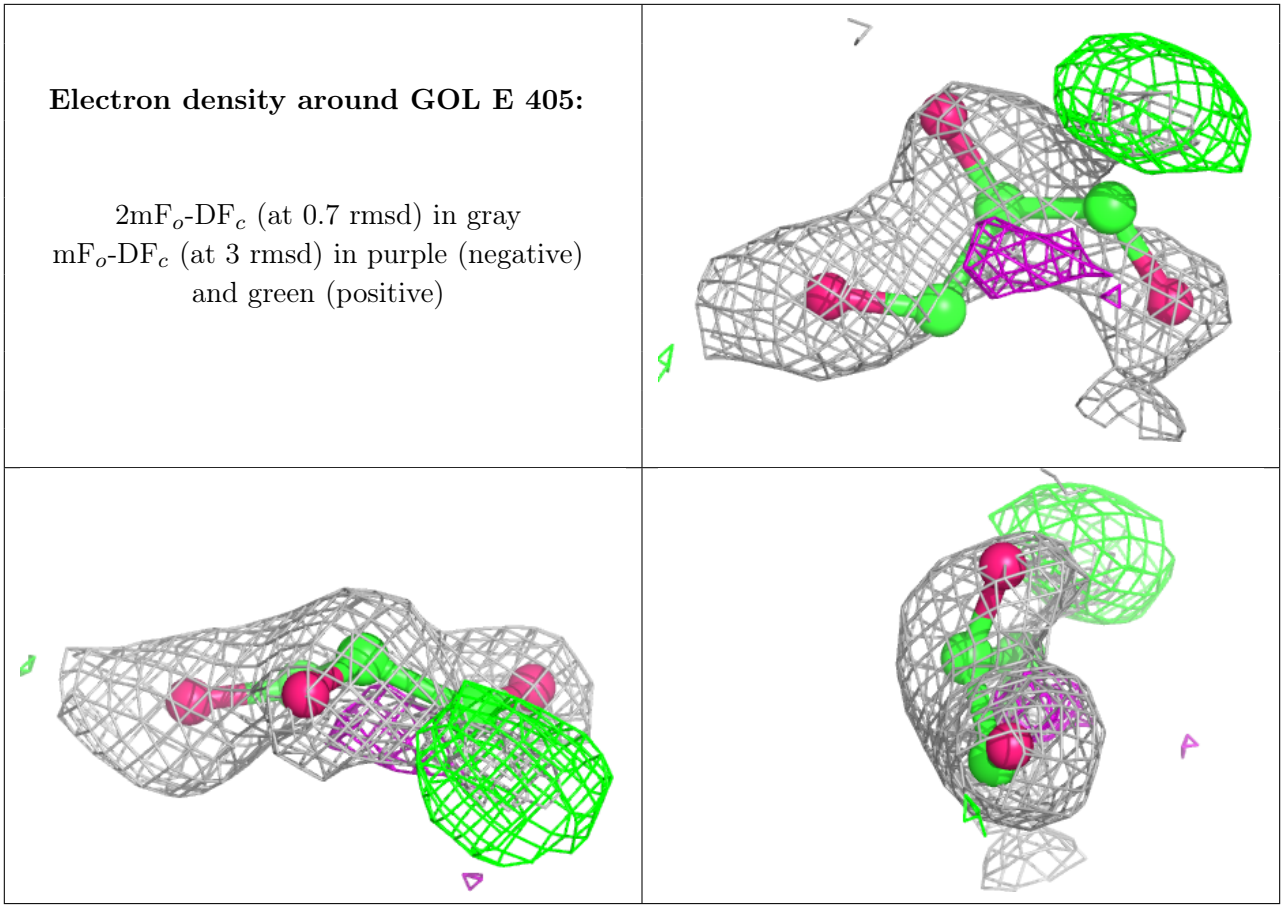
Electron density around GOL B 407:

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



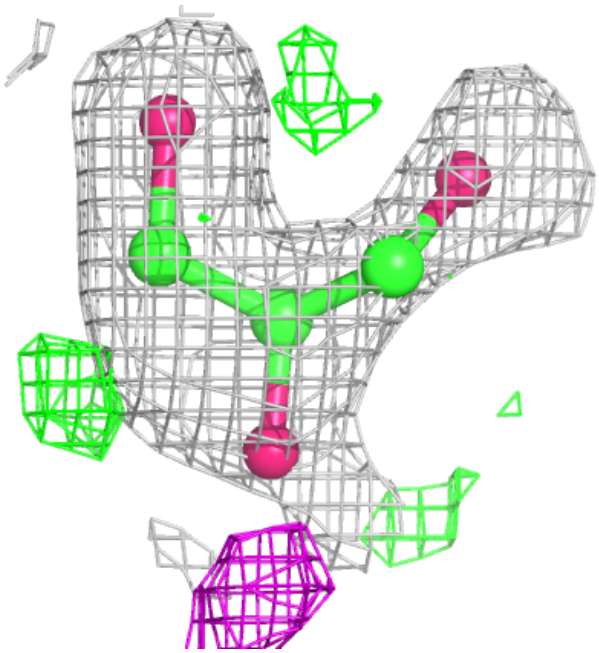
Electron density around GOL E 405:

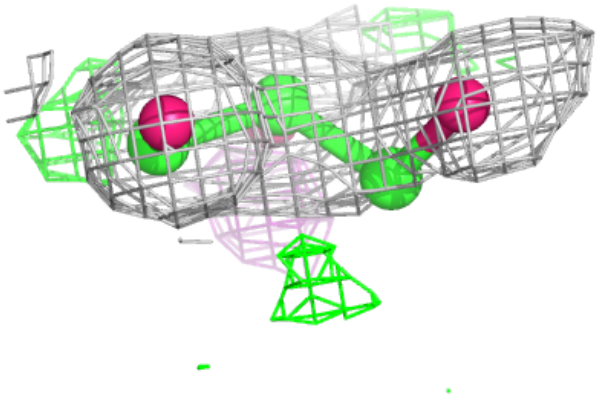
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

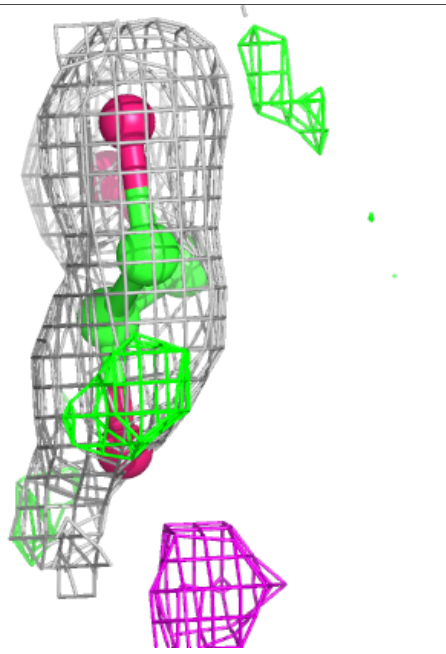


Electron density around GOL A 408:

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

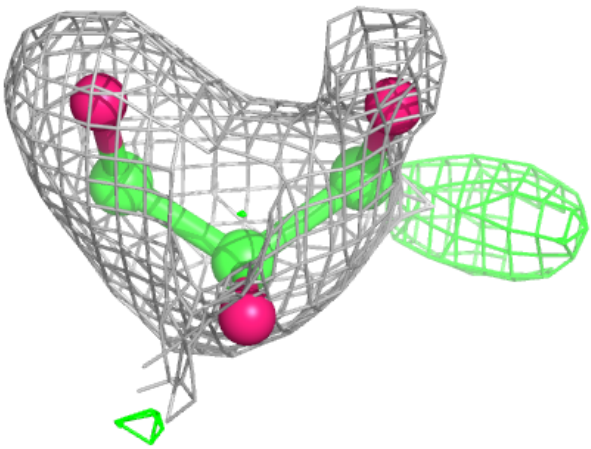


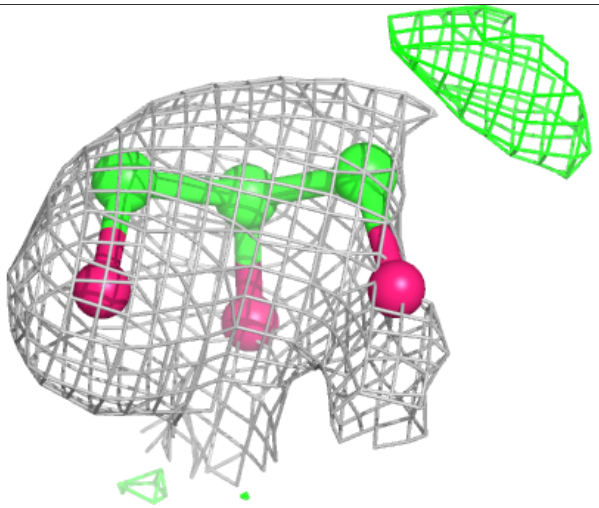


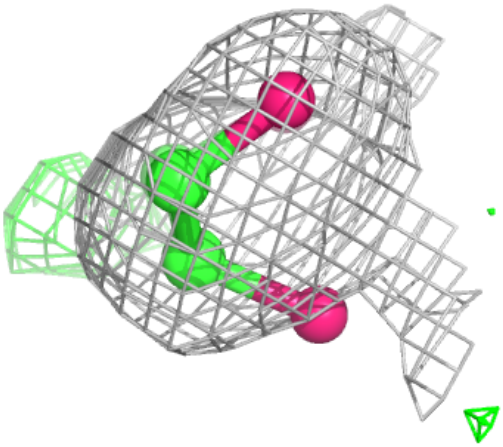


Electron density around GOL F 403:

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

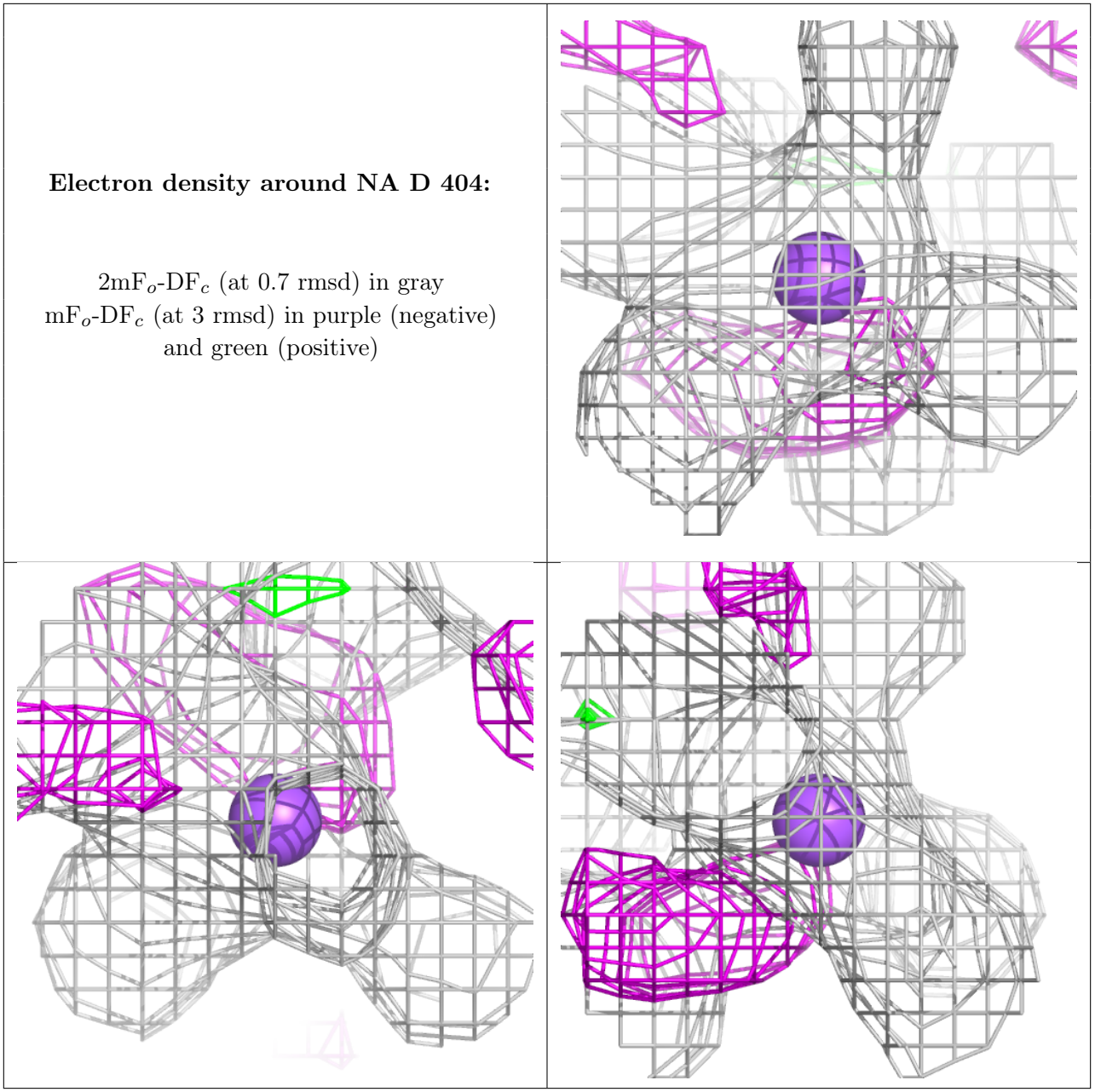






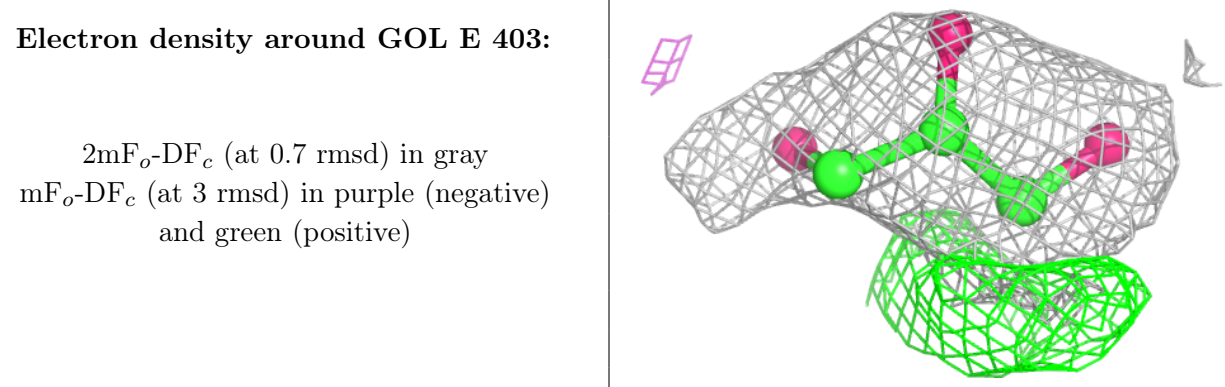
Electron density around NA D 404:

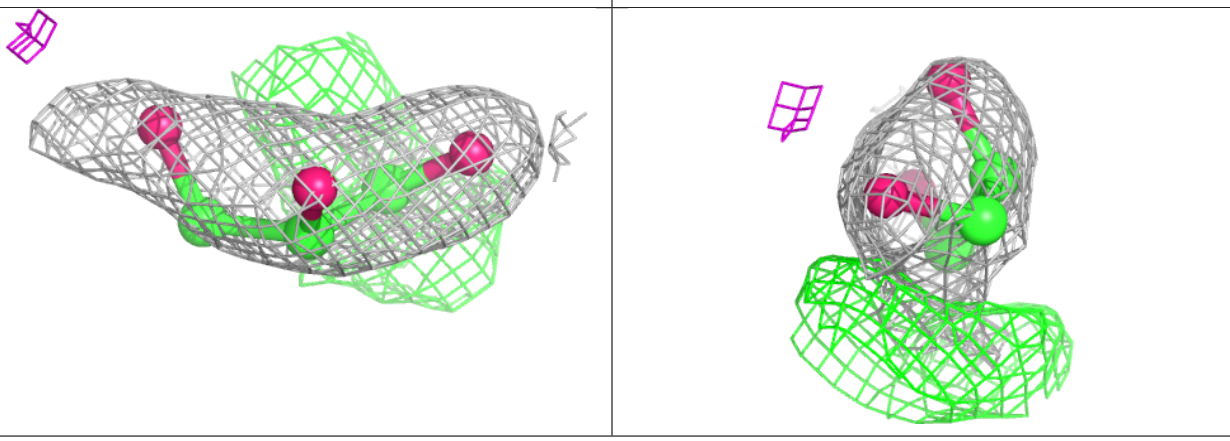
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GOL E 403:

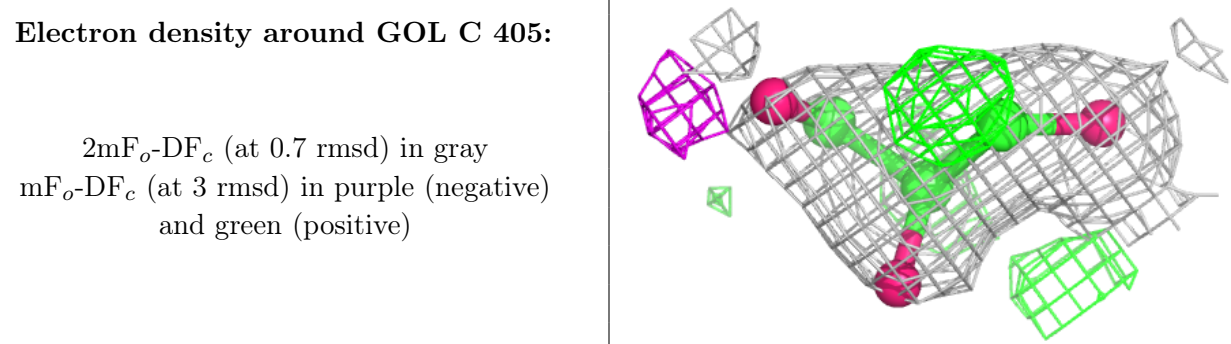
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

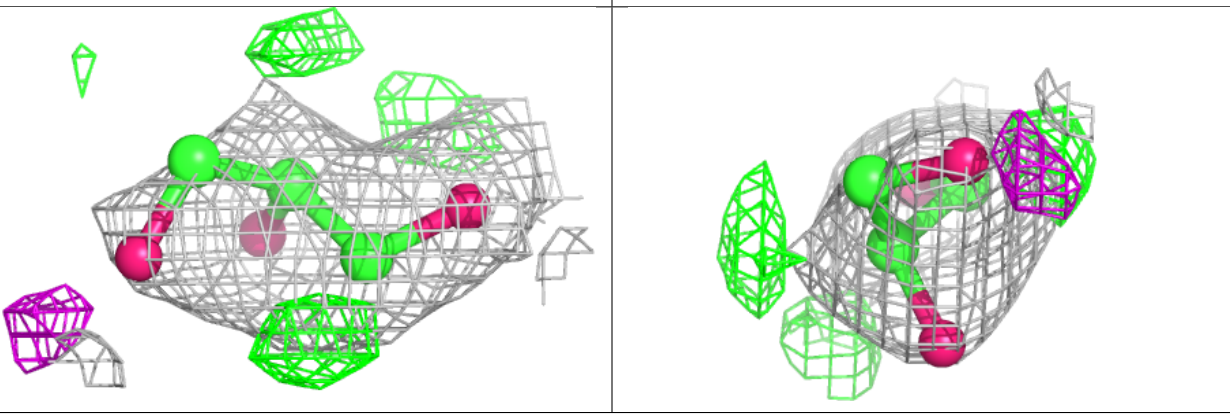




Electron density around GOL C 405:

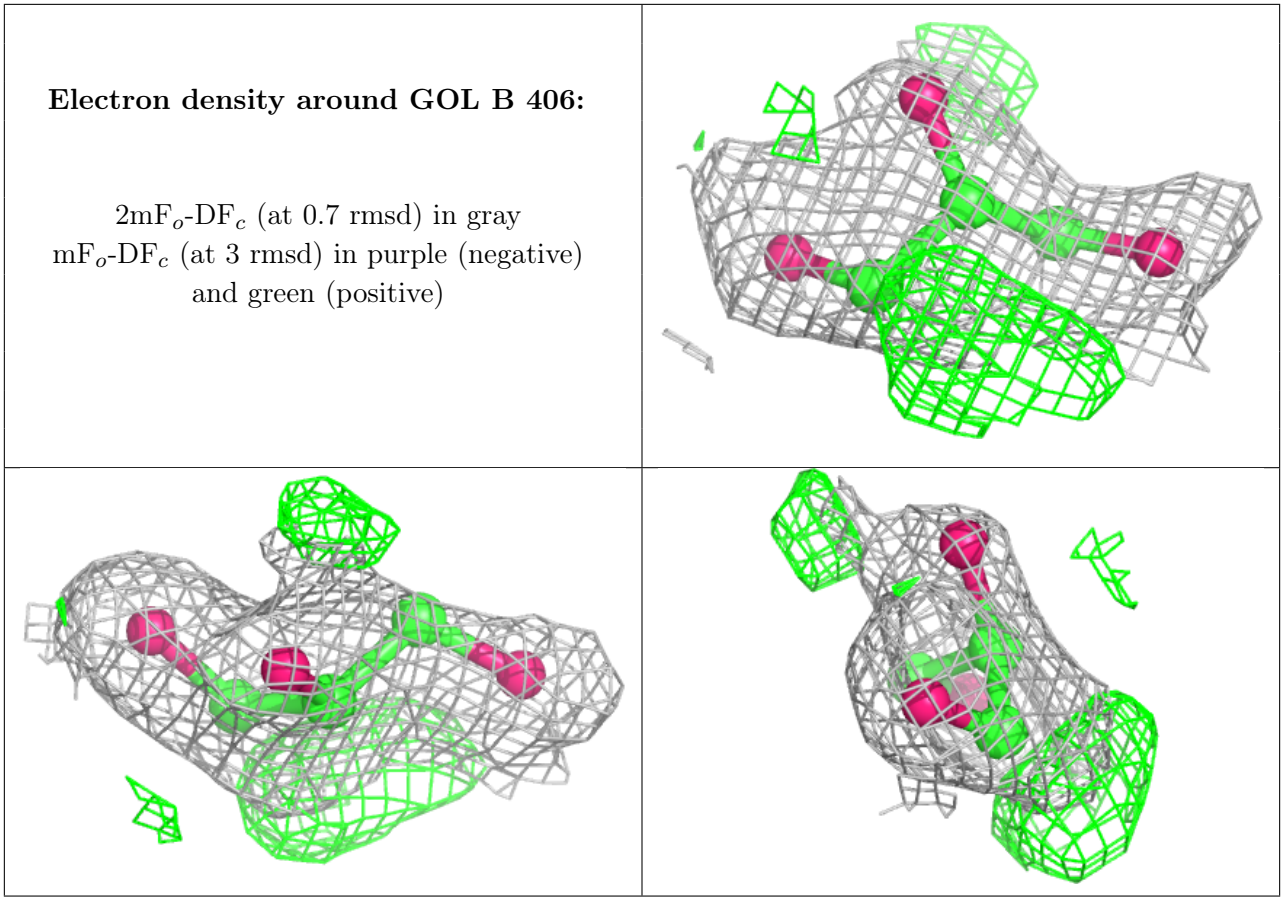
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





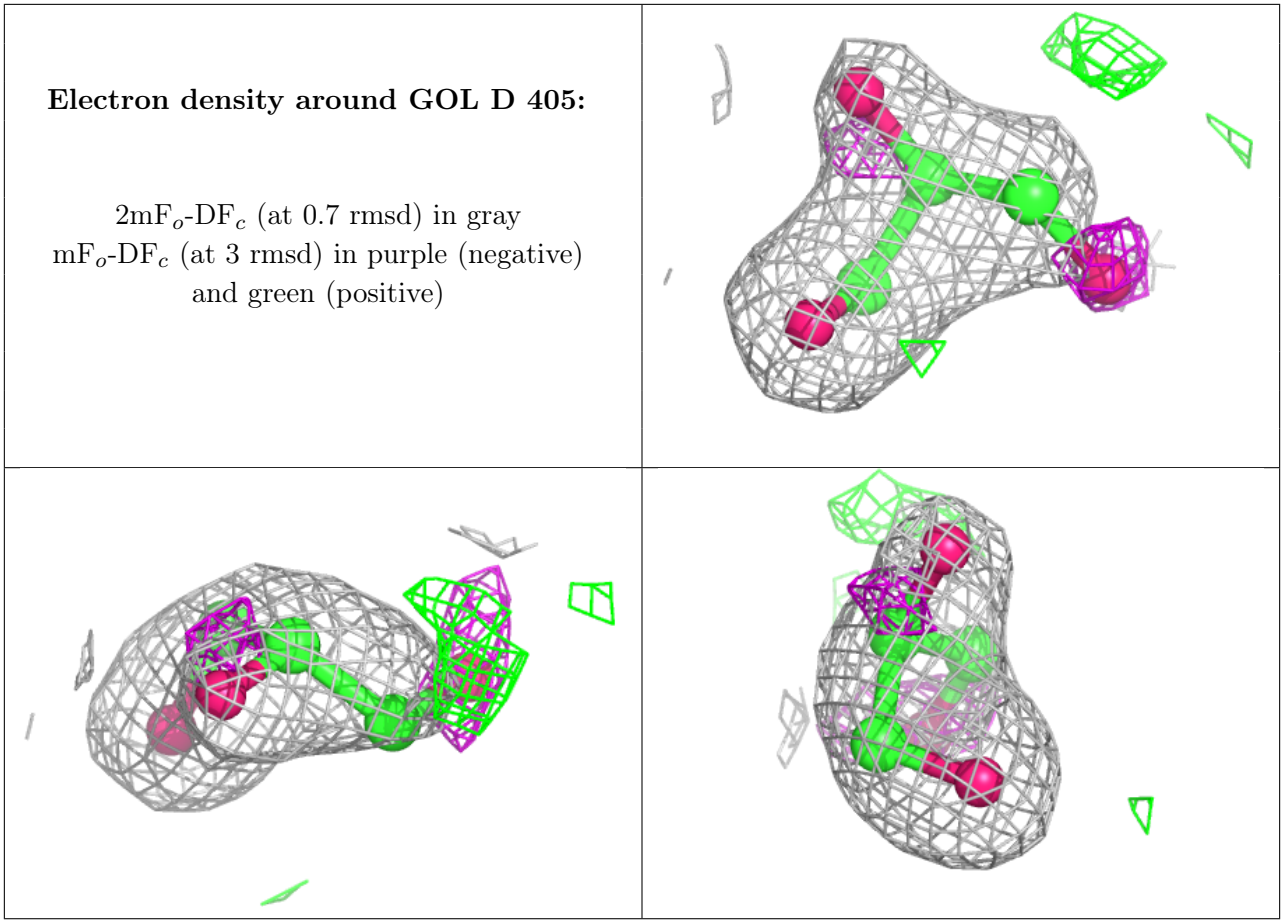
Electron density around GOL B 406:

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



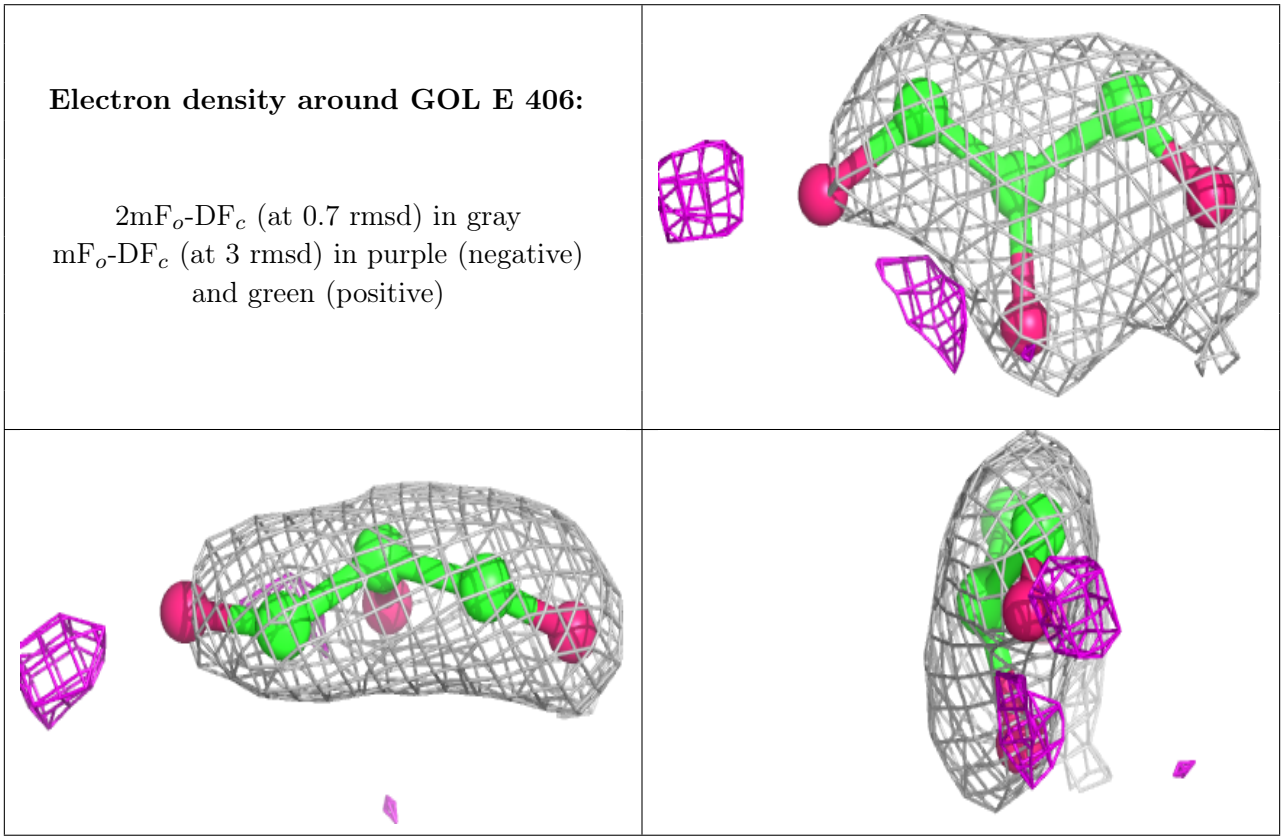
Electron density around GOL D 405:

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



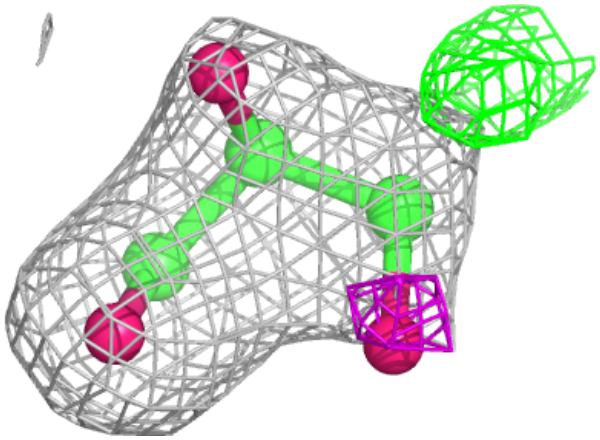
Electron density around GOL E 406:

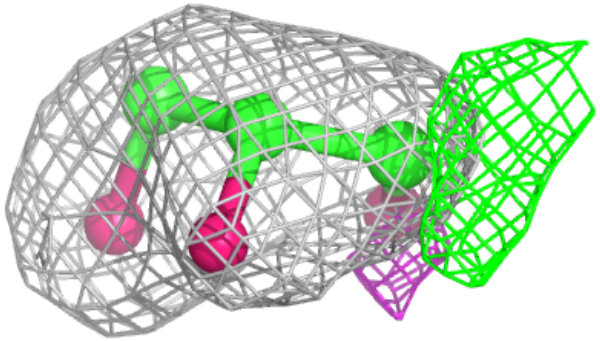
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

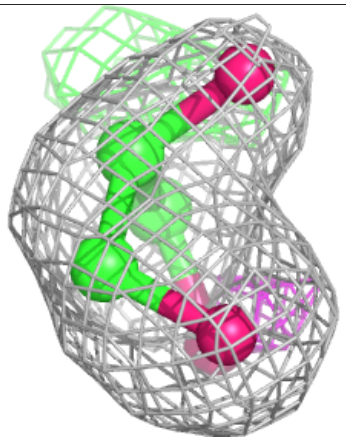


Electron density around GOL A 406:

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

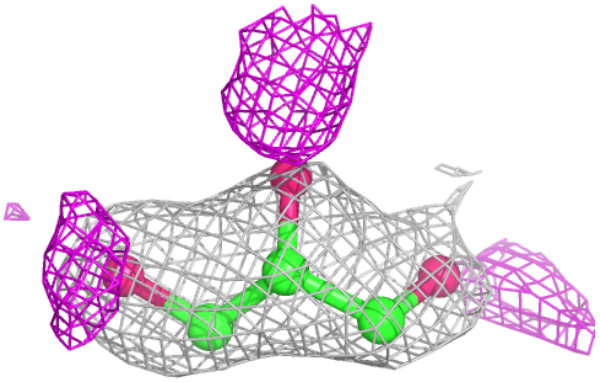


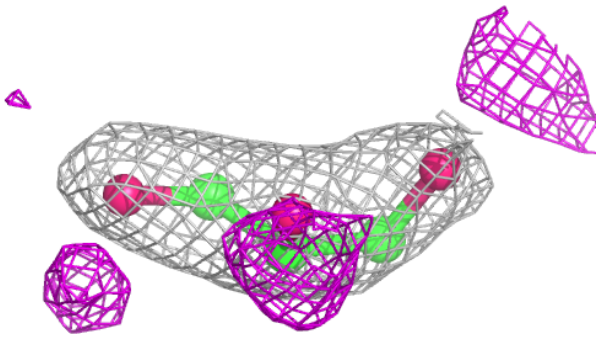


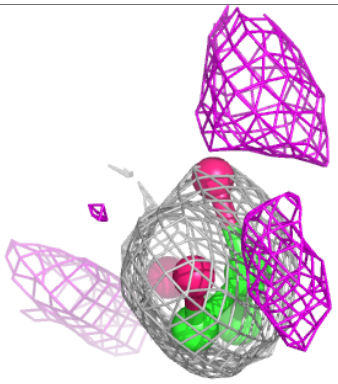


Electron density around GOL E 404:

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

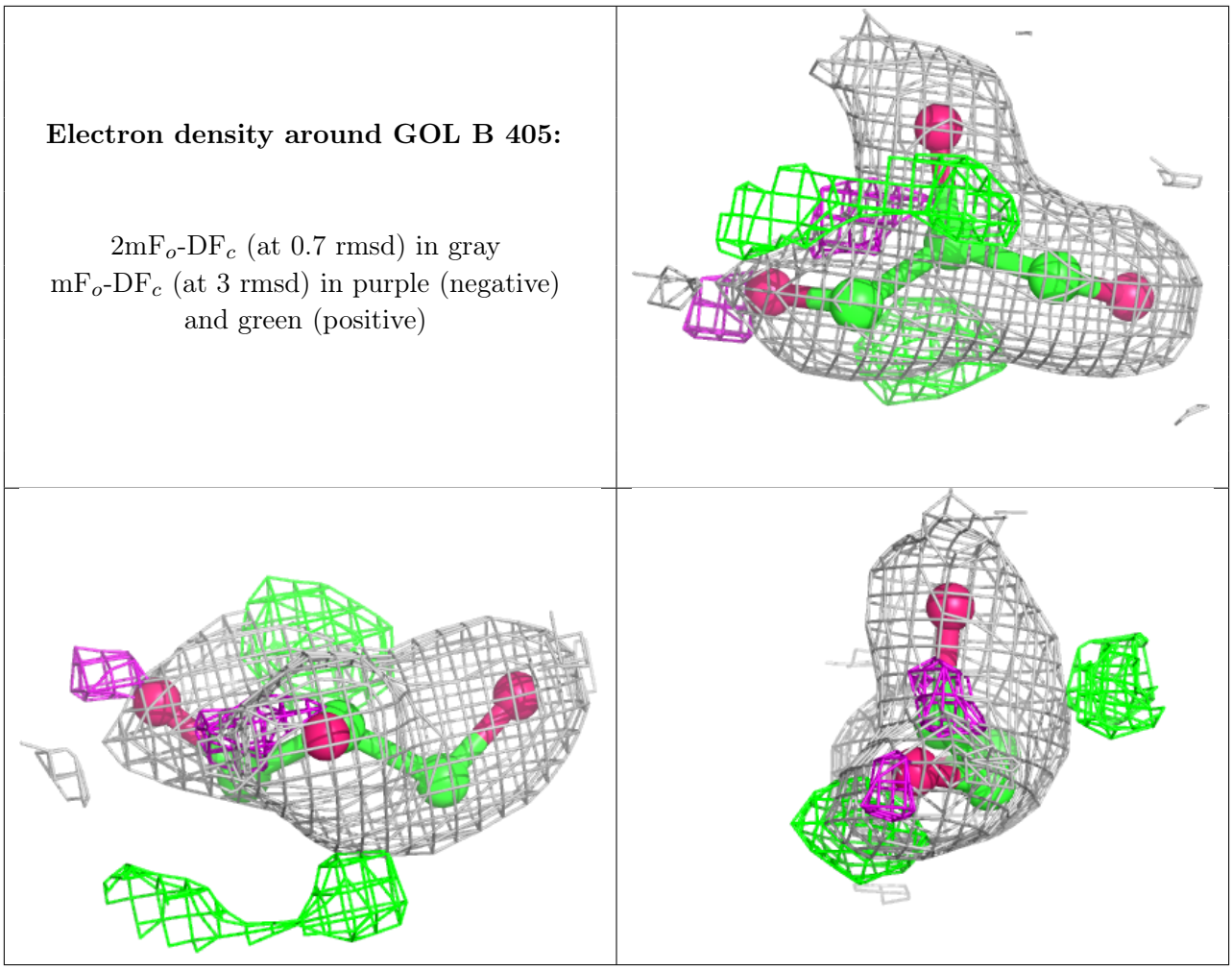






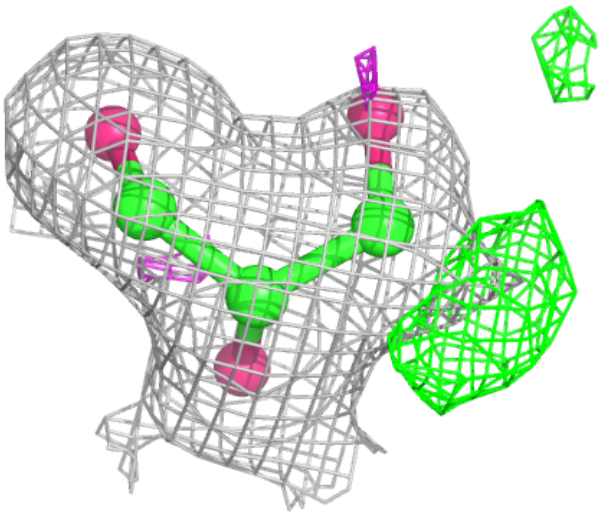
Electron density around GOL B 405:

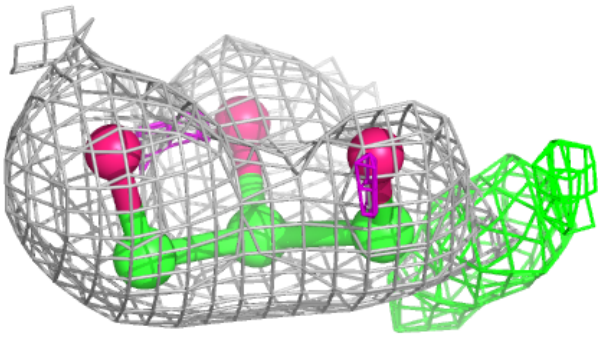
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

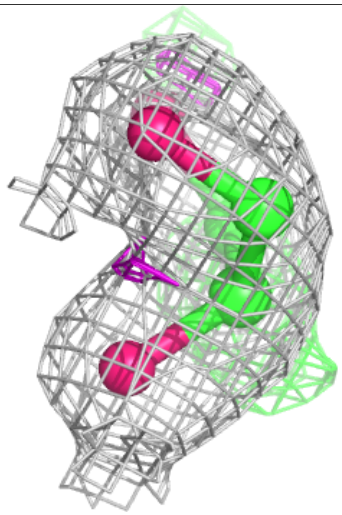


Electron density around GOL A 405:

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

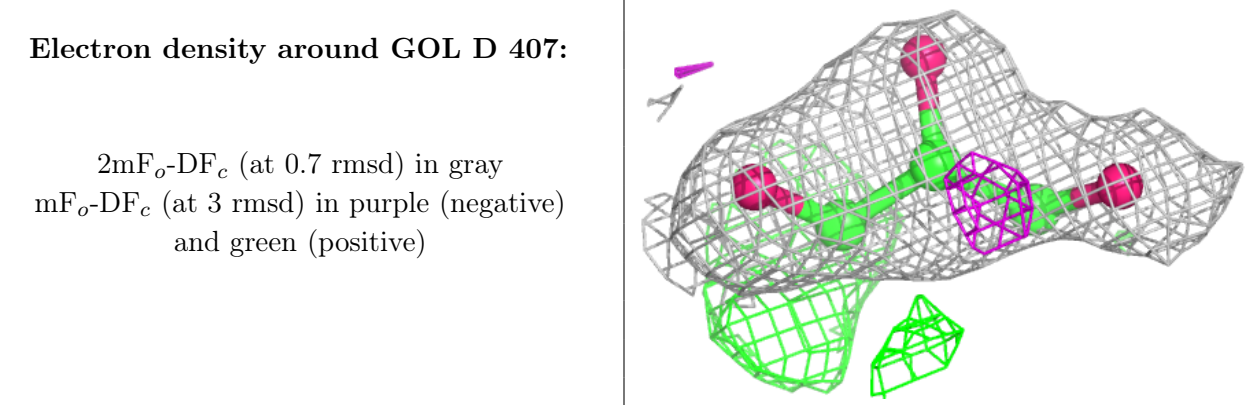


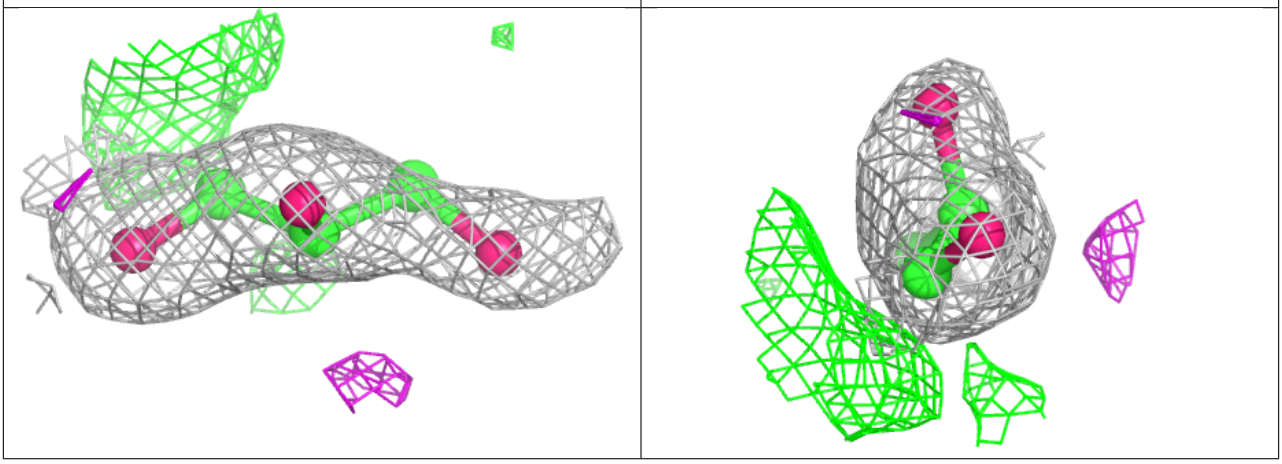




Electron density around GOL D 407:

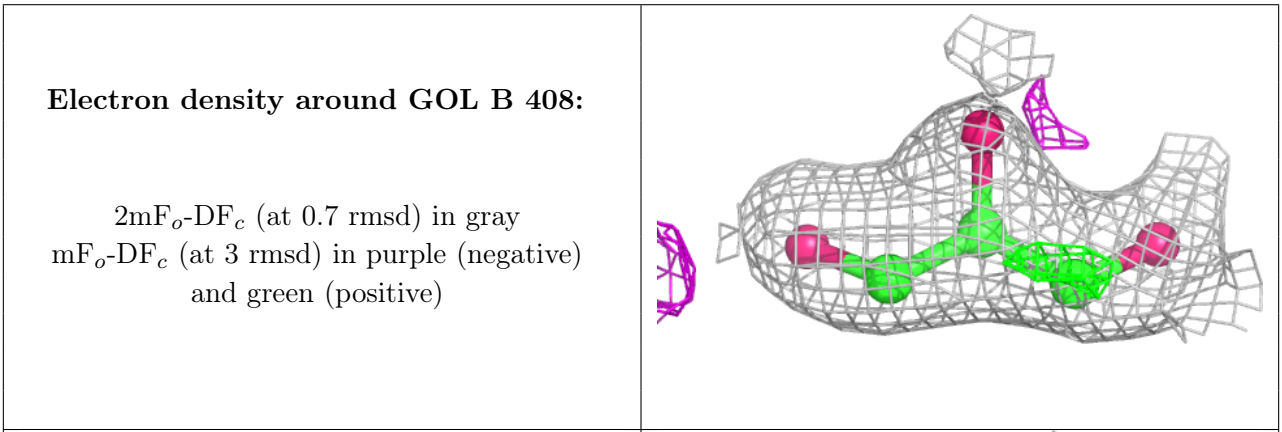
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

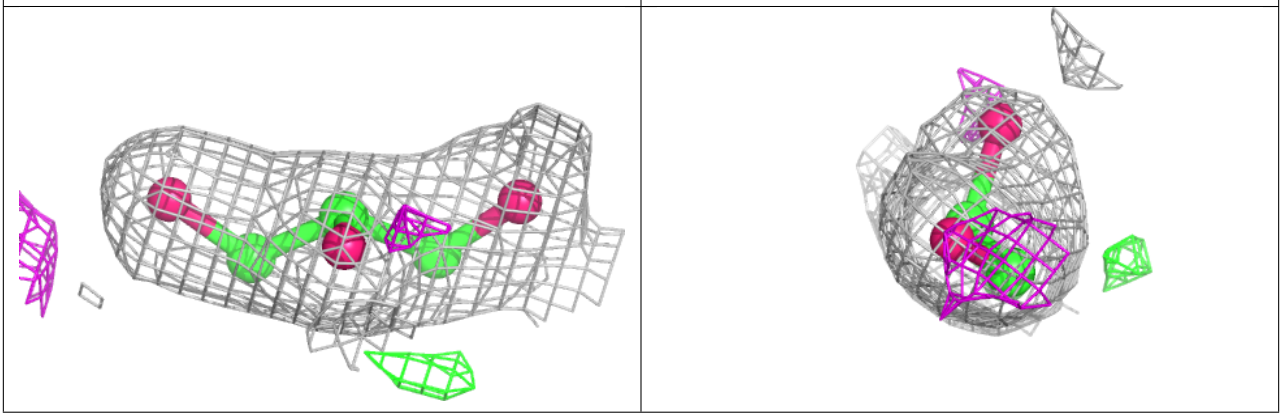




Electron density around GOL B 408:

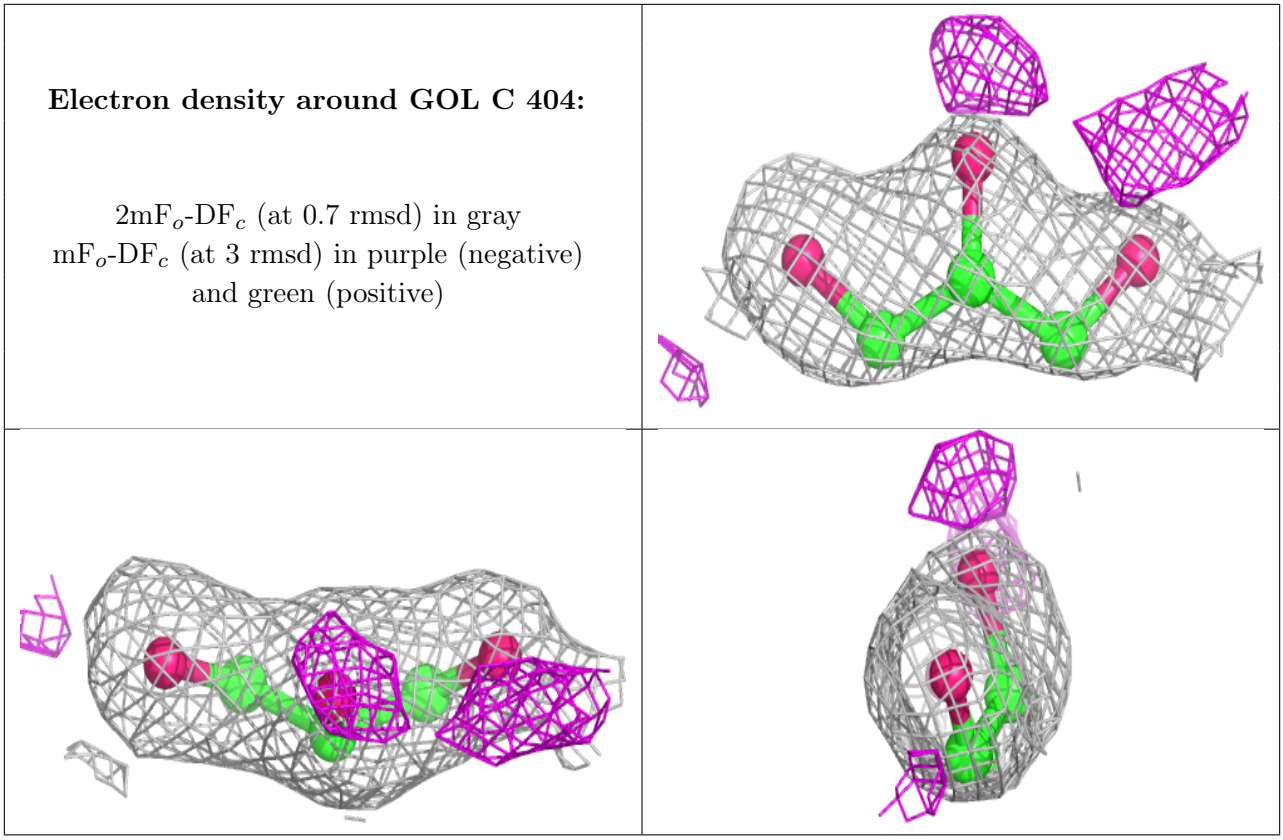
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





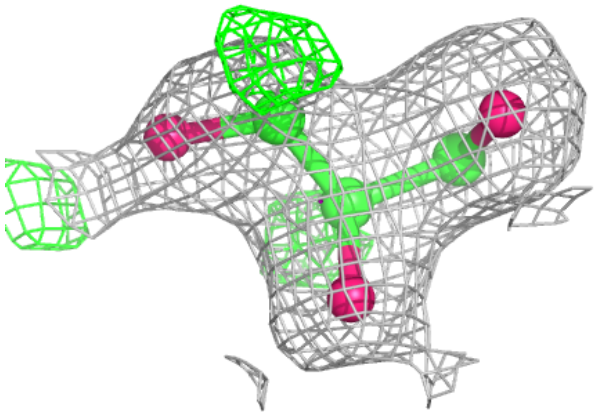
Electron density around GOL C 404:

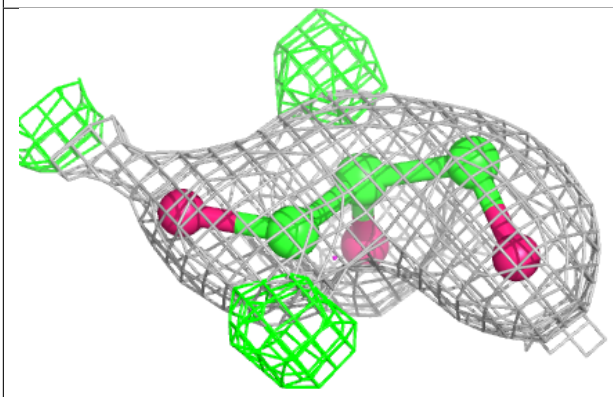
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

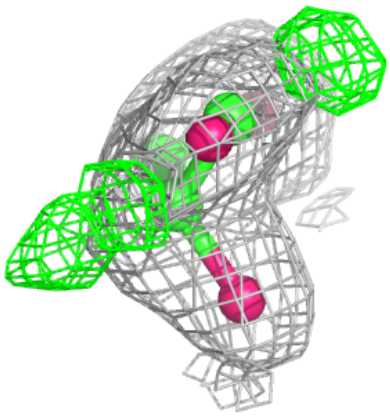


Electron density around GOL D 406:

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

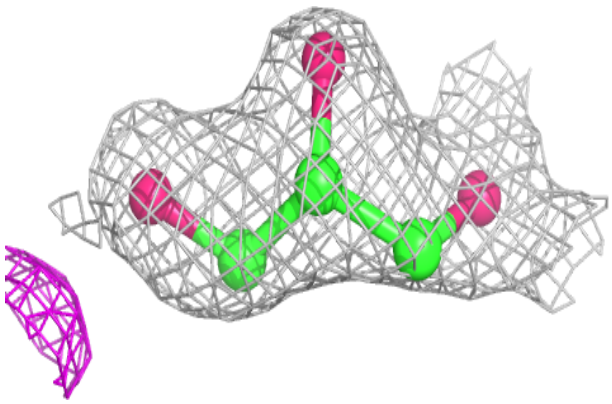


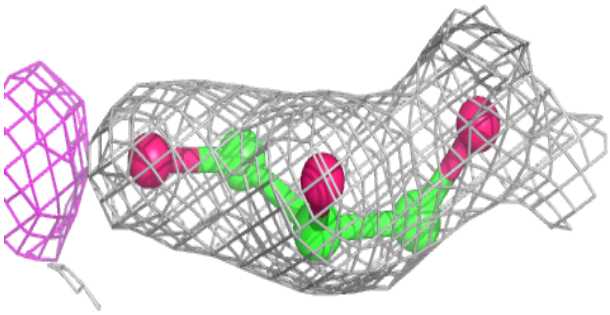


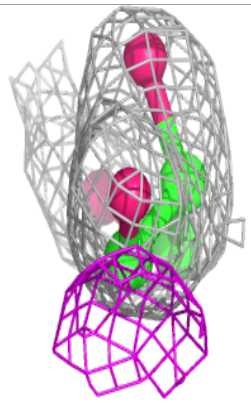


Electron density around GOL F 404:

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

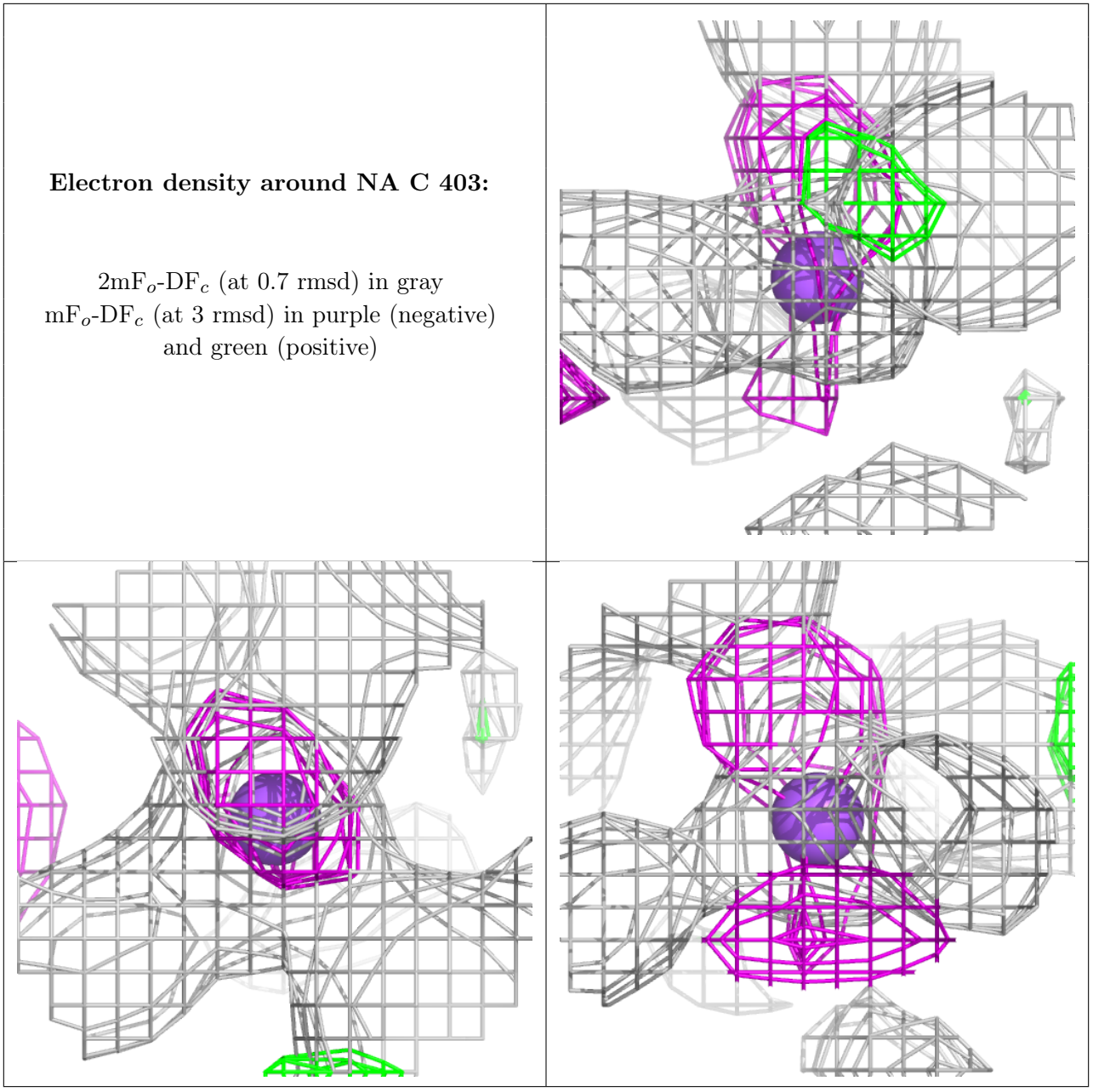






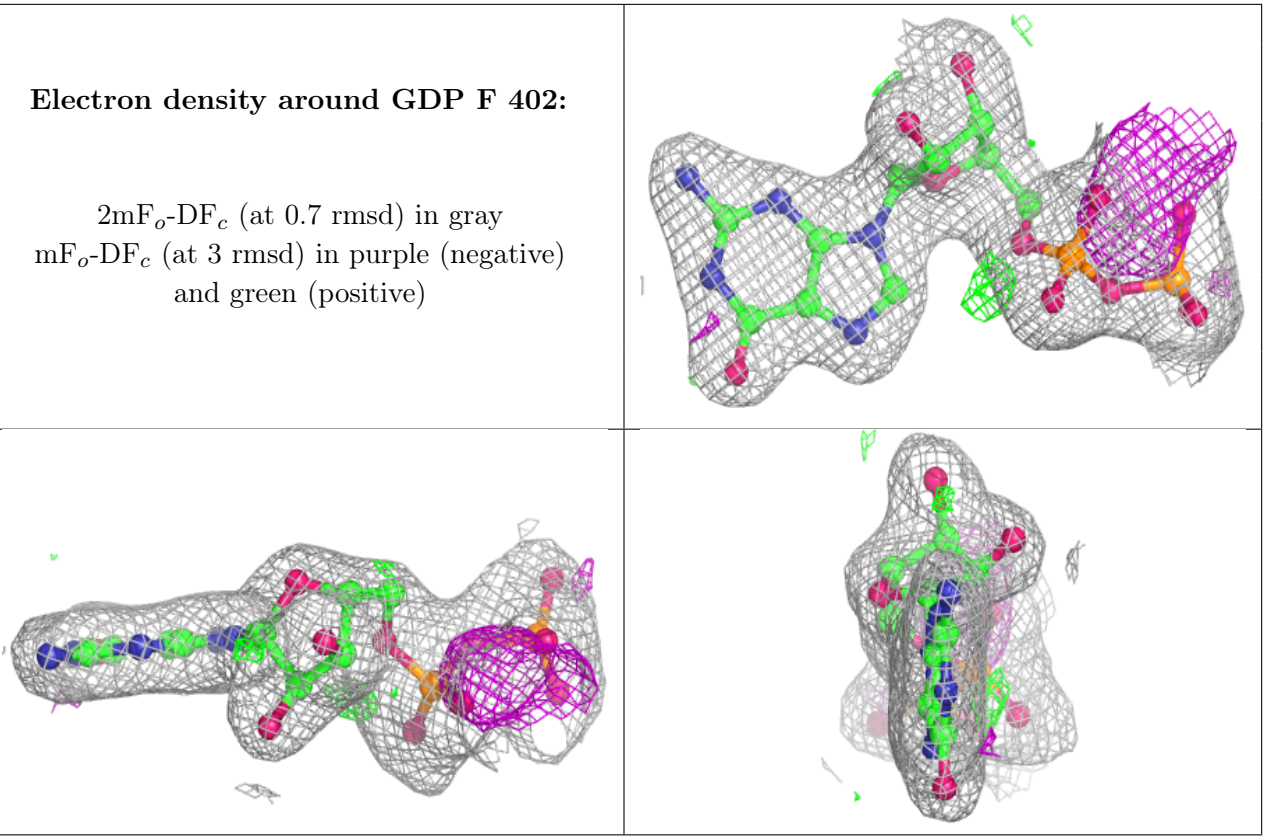
Electron density around NA C 403:

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



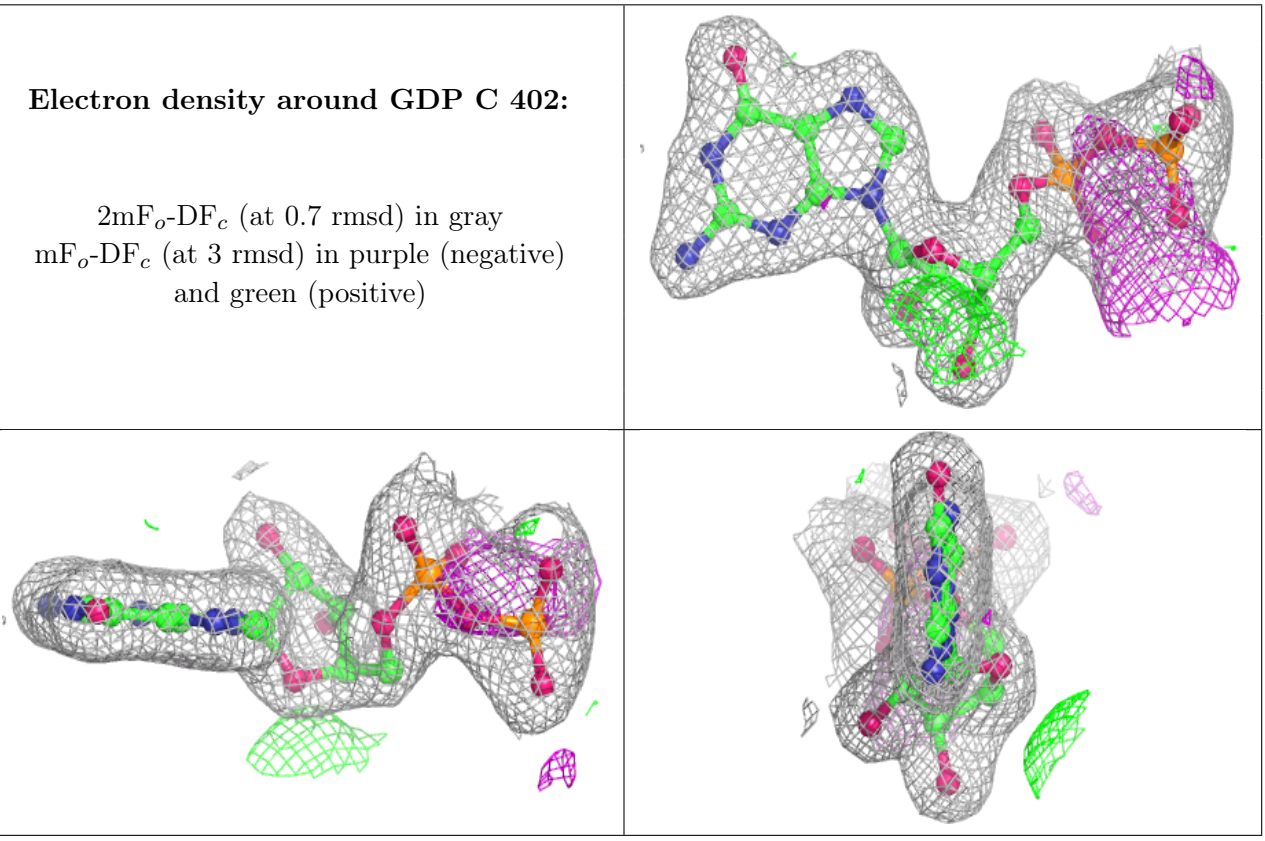
Electron density around GDP F 402:

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



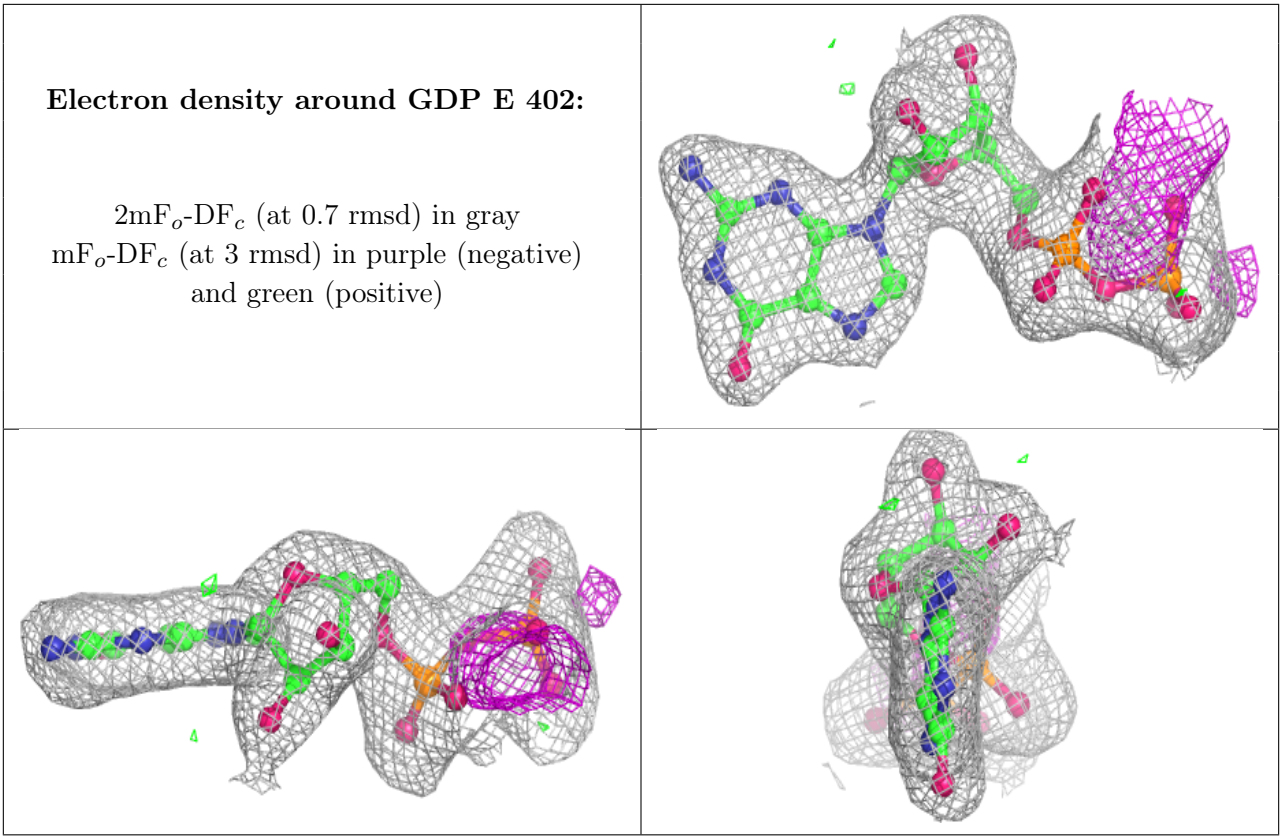
Electron density around GDP C 402:

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



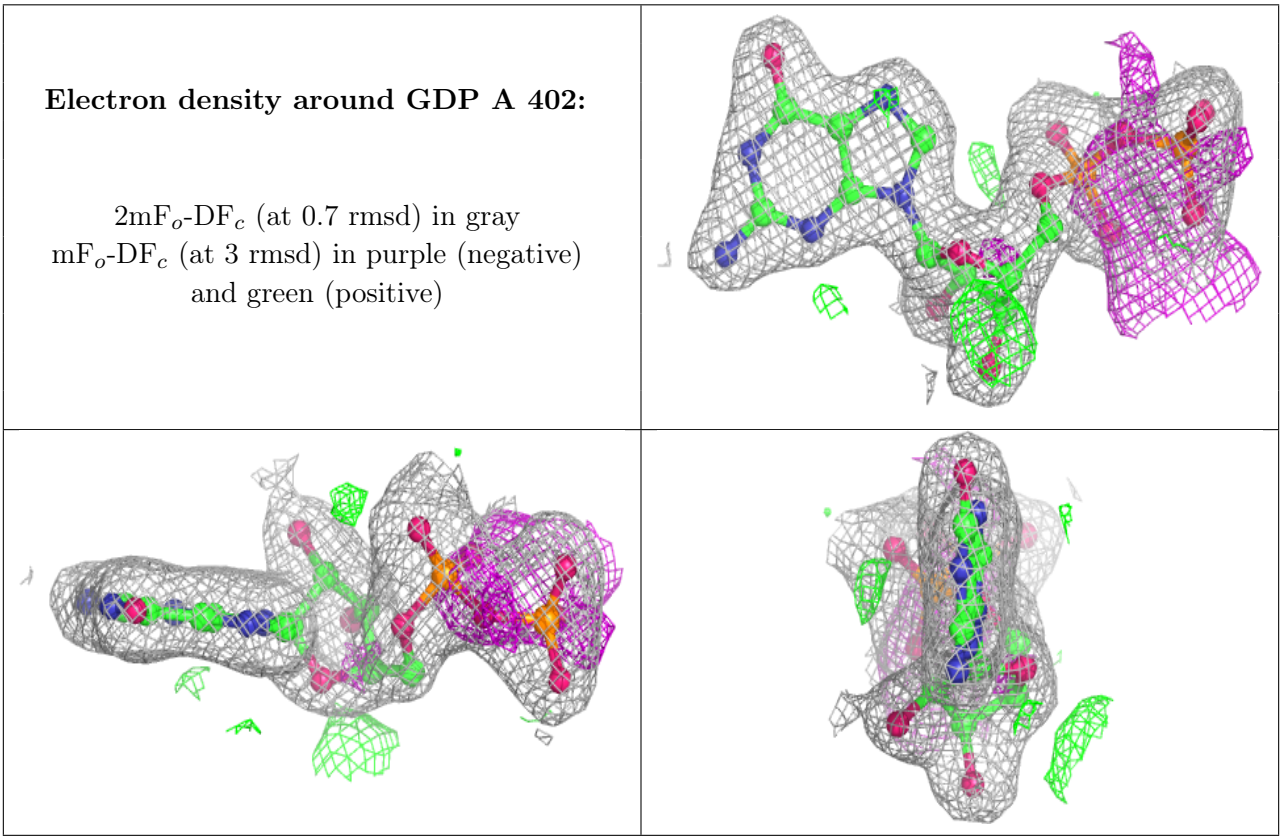
Electron density around GDP E 402:

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



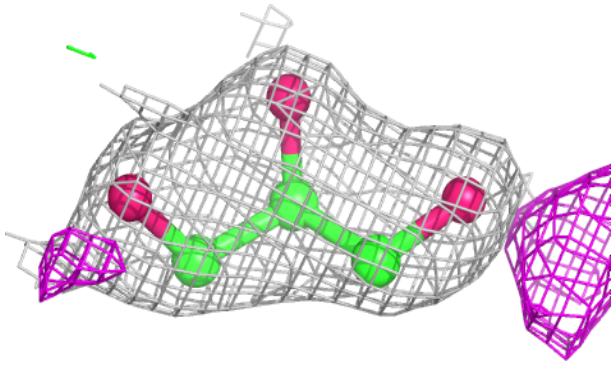
Electron density around GDP A 402:

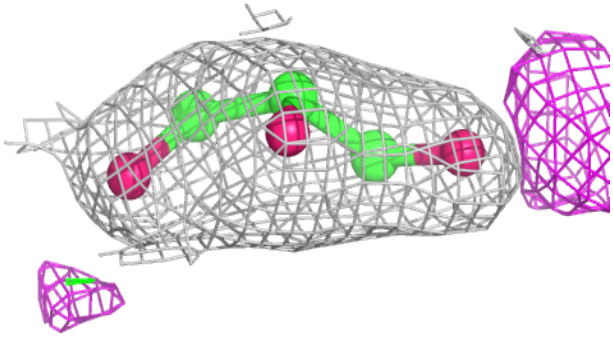
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

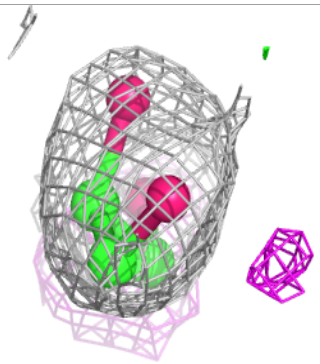


Electron density around GOL A 407:

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

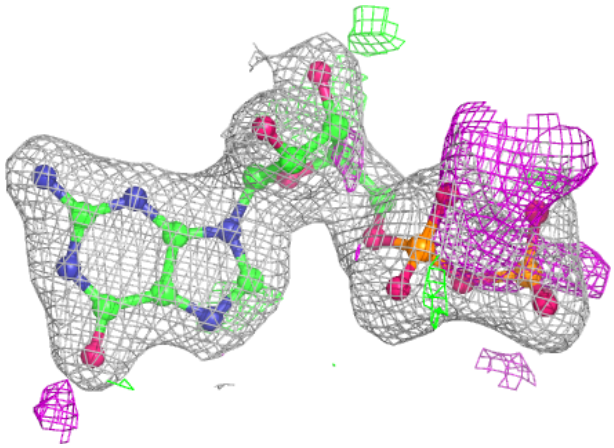


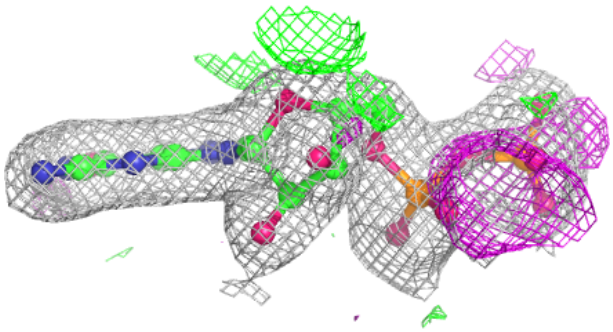


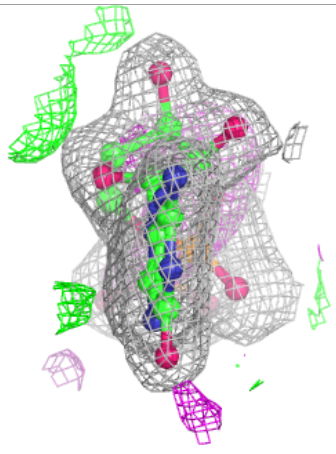


Electron density around GDP B 402:

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

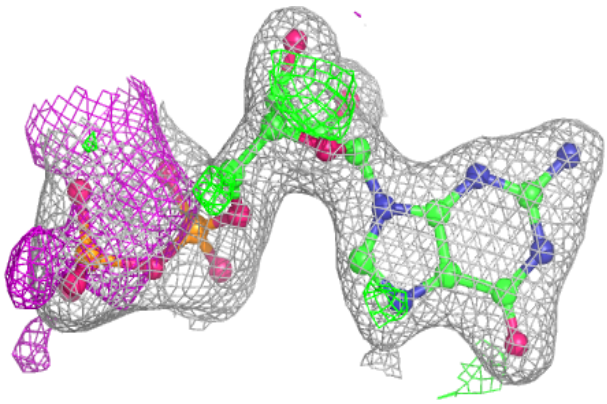


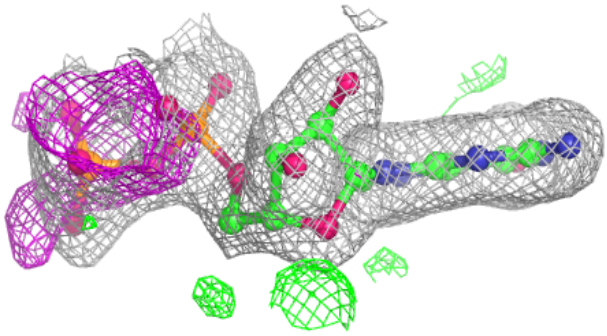


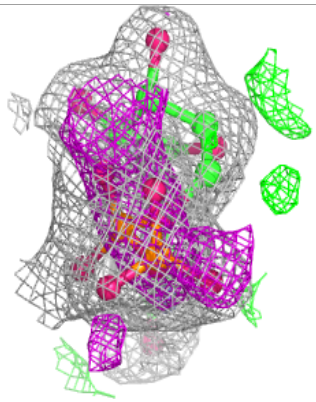


Electron density around GDP D 402:

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

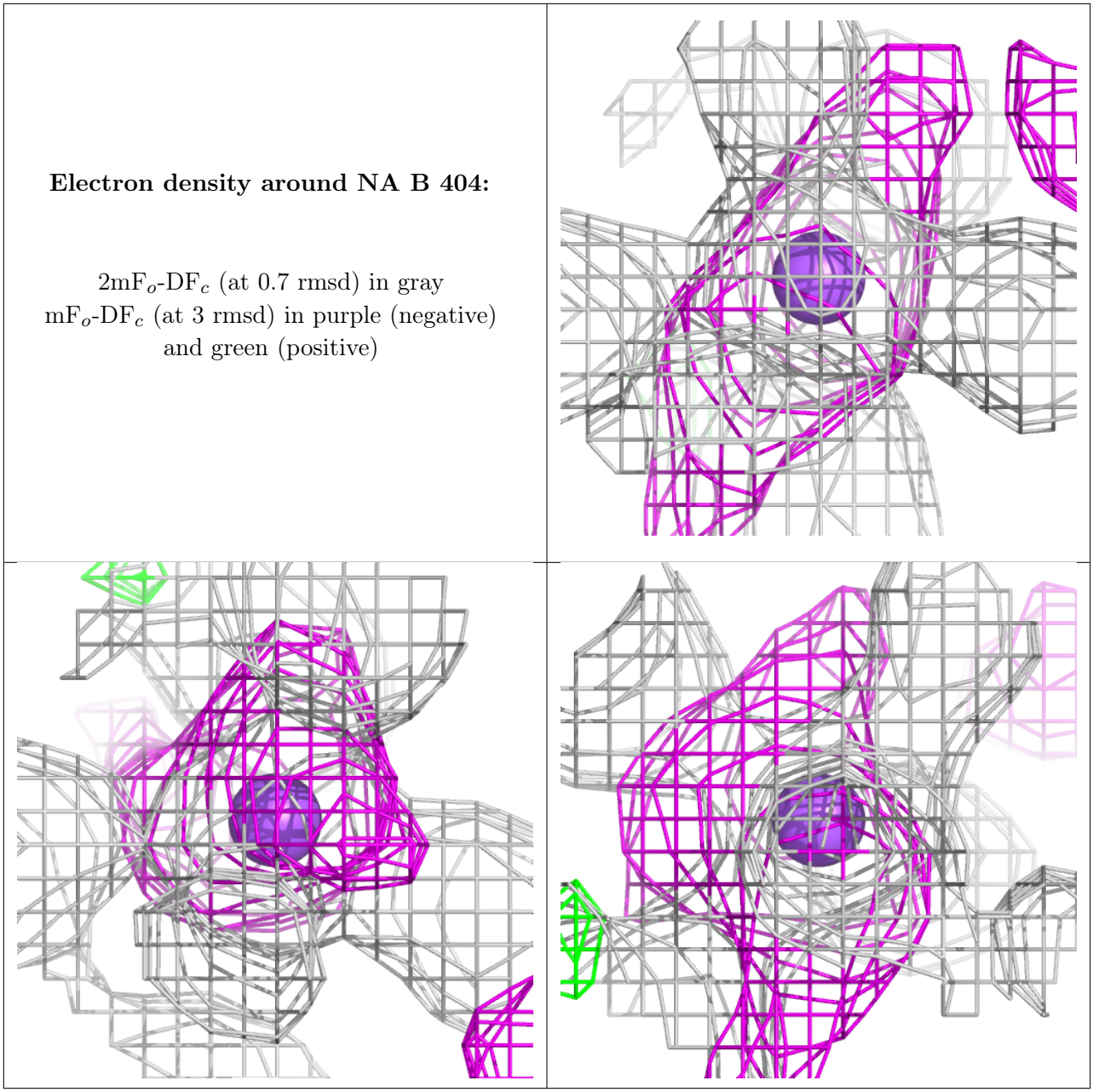






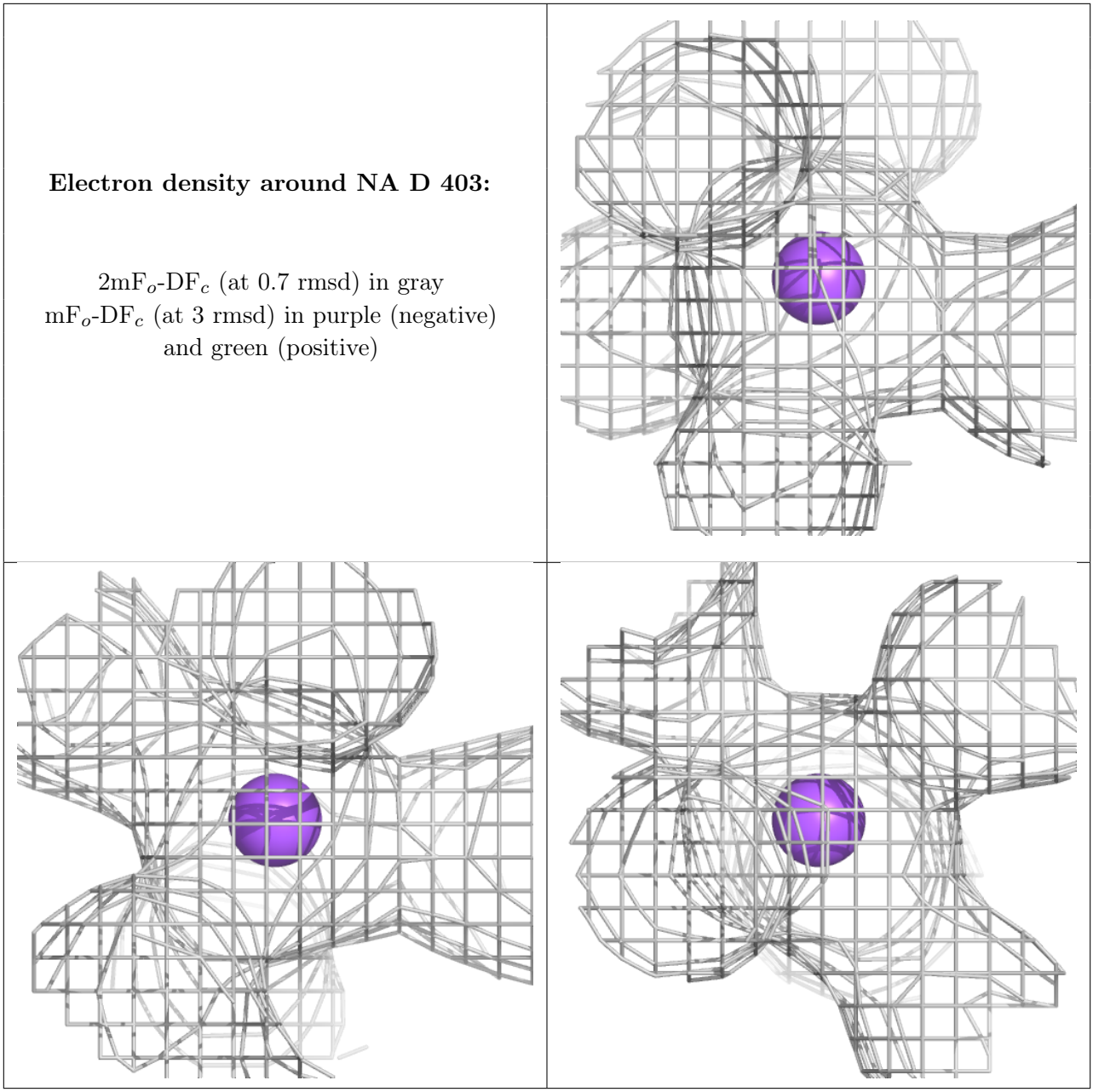
Electron density around NA B 404:

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



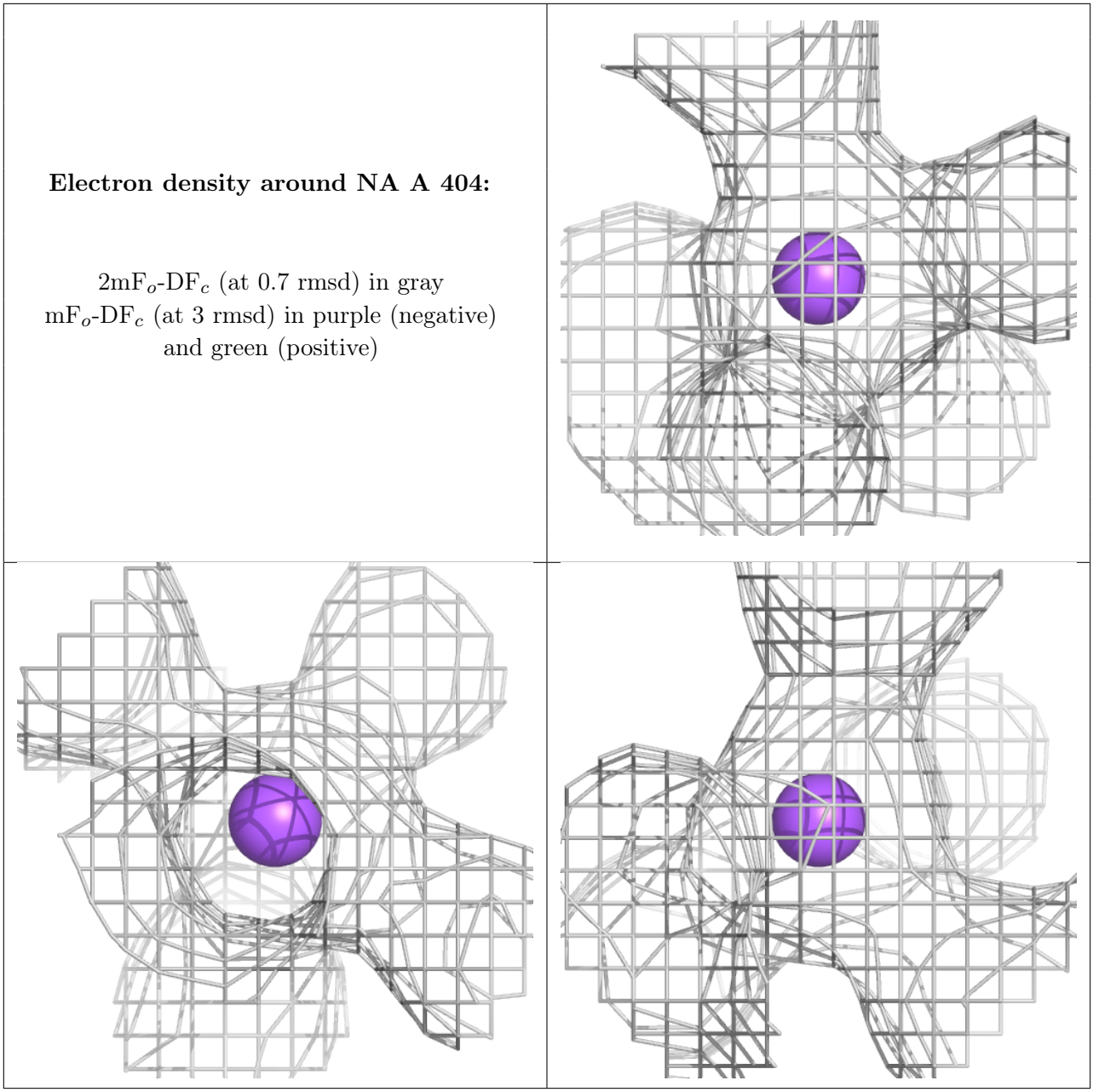
Electron density around NA D 403:

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



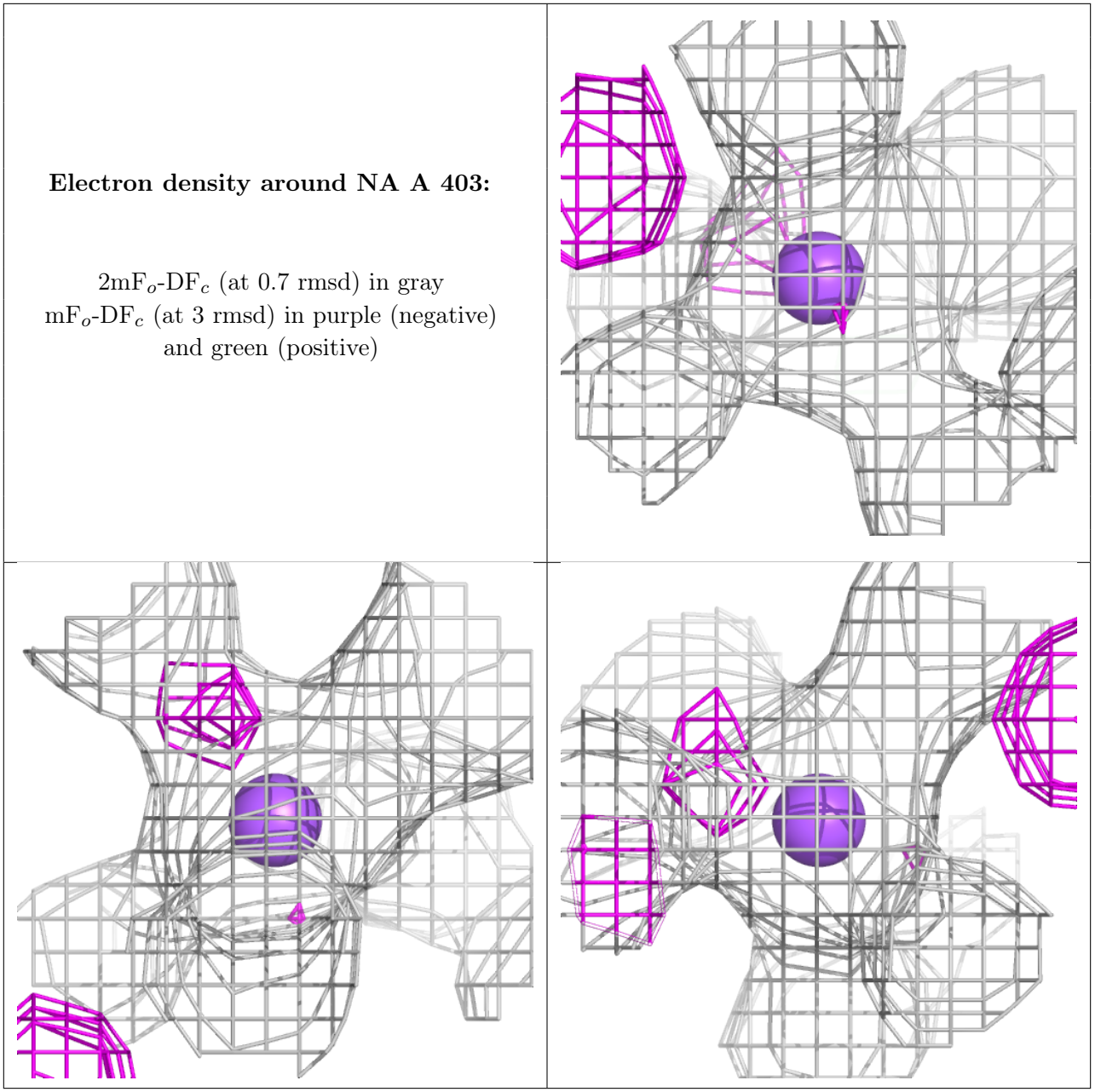
Electron density around NA A 404:

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



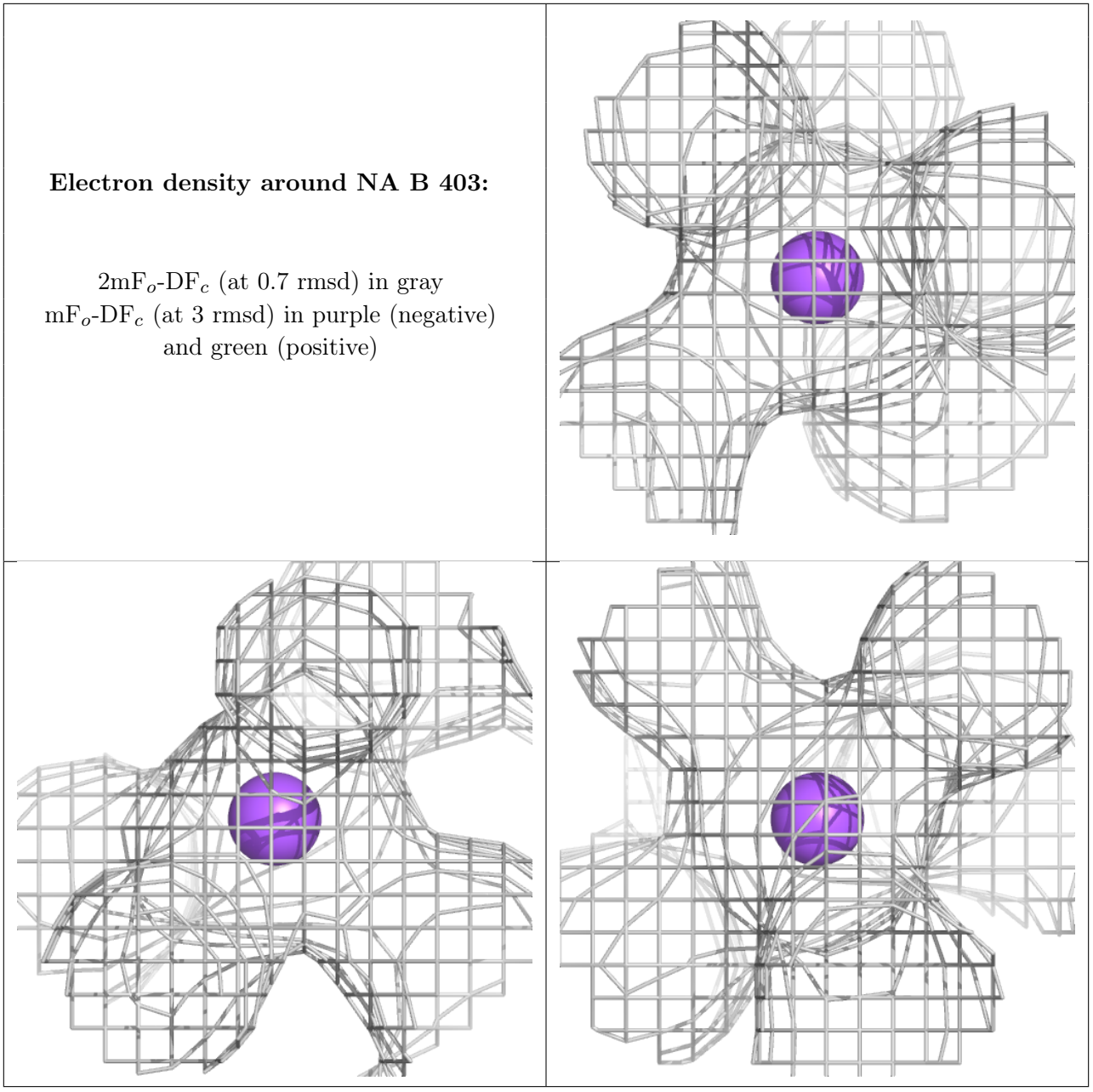
Electron density around NA A 403:

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



Electron density around NA B 403:

$2mF_o$-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.