wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2025 – 10:12 AM JST

PDB ID	:	9K2N
Title	:	Crystal structure of Glutamine Synthetase-apo
Authors	:	Chandrasekaran, P.; Killivalavan, A.; Vaigundan, D.; Yuvaraj, I.; Manju, B.; Sekar, K.
Deposited on	:	2024-10-17
Resolution	:	3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

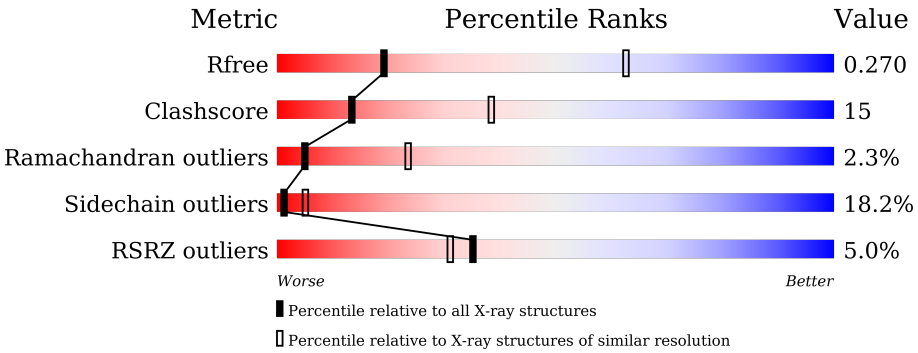
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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	468	3% 60% 32% 7% ·
1	B	468	4% 60% 29% 9% ·
1	C	468	4% 61% 27% 9% ·
1	D	468	6% 65% 27% 6% ·
1	E	468	5% 63% 28% 7% ·
1	F	468	7% 63% 29% 7% ·

2 Entry composition (i)

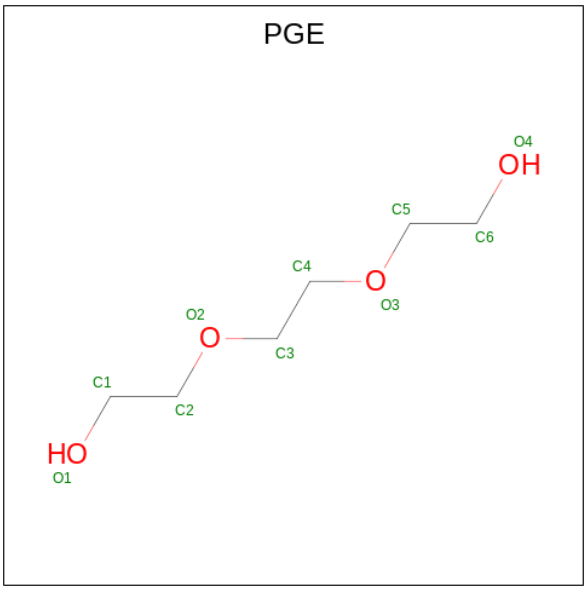
There are 5 unique types of molecules in this entry. The entry contains 43046 atoms, of which 21160 are hydrogens and 0 are deuteriums.

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 Glutamine synthetase.

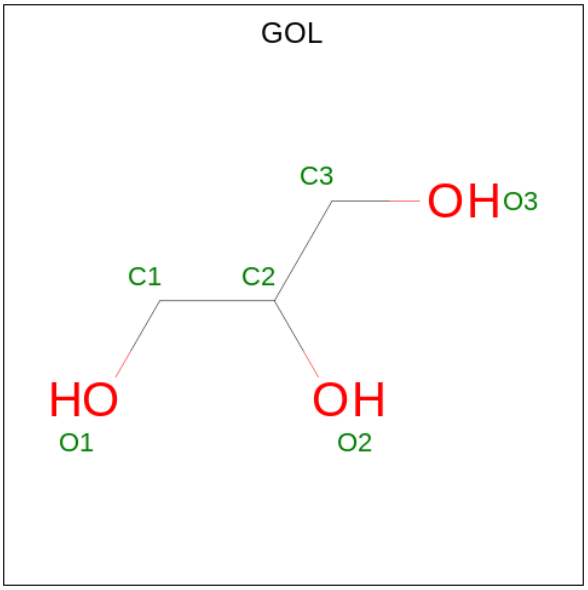
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	468	Total	C	H	N	O	S	111	0	0
			7152	2304	3515	613	699	21			
1	B	468	Total	C	H	N	O	S	111	0	0
			7152	2304	3515	613	699	21			
1	C	468	Total	C	H	N	O	S	111	0	0
			7152	2304	3515	613	699	21			
1	D	468	Total	C	H	N	O	S	111	0	0
			7155	2305	3517	613	699	21			
1	E	468	Total	C	H	N	O	S	113	0	0
			7142	2302	3508	612	699	21			
1	F	468	Total	C	H	N	O	S	110	0	0
			7149	2301	3514	613	700	21			

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	2	0
			24	6	14	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	A	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	B	1	Total	C	H	O	3	0
			14	3	8	3		
3	C	1	Total	C	H	O	3	0
			14	3	8	3		
3	D	1	Total	C	H	O	3	0
			14	3	8	3		
3	E	1	Total	C	H	O	3	0
			14	3	8	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

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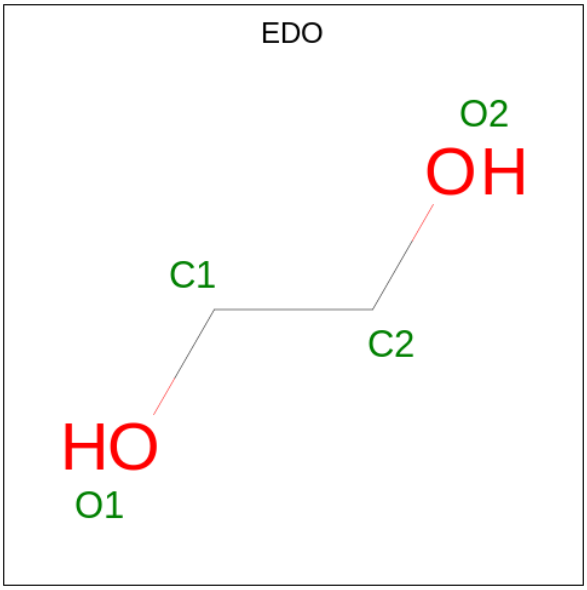
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0
4	E	2	Total Mg 2 2	0	0
4	F	2	Total Mg 2 2	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



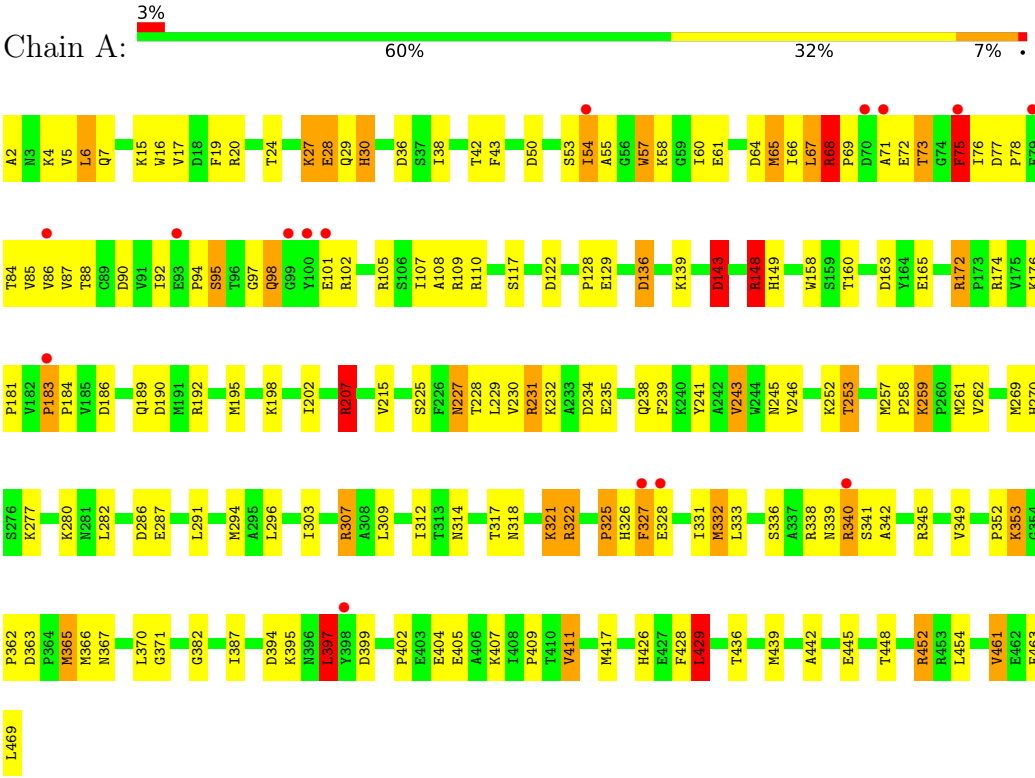
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C H O 10 2 6 2	2	0

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.

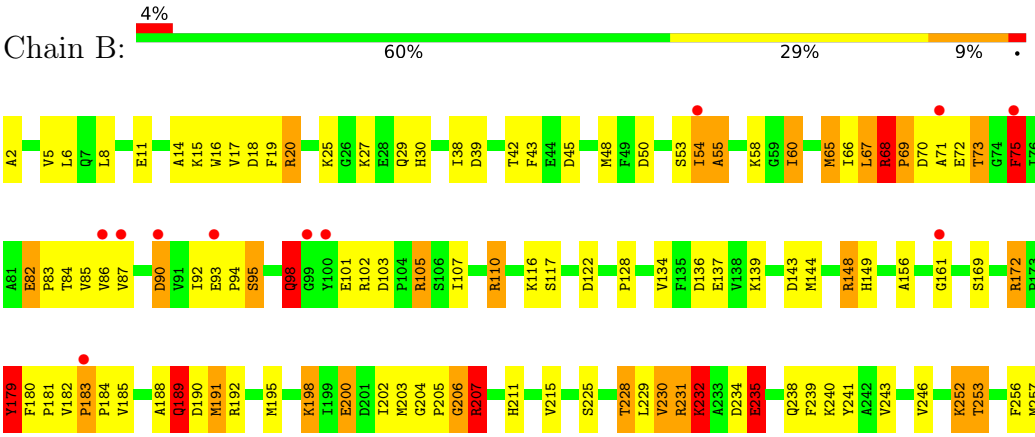
• Molecule 1: Glutamine synthetase

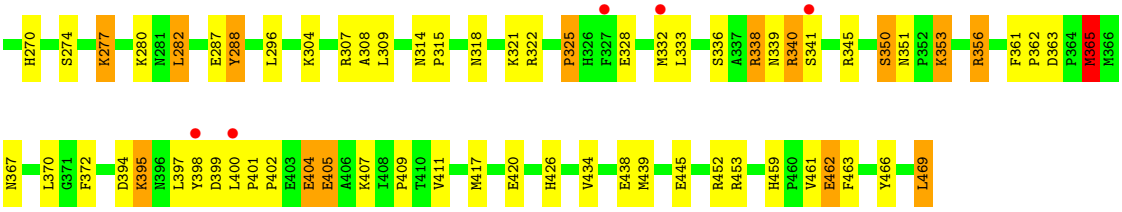
Chain A:



• Molecule 1: Glutamine synthetase

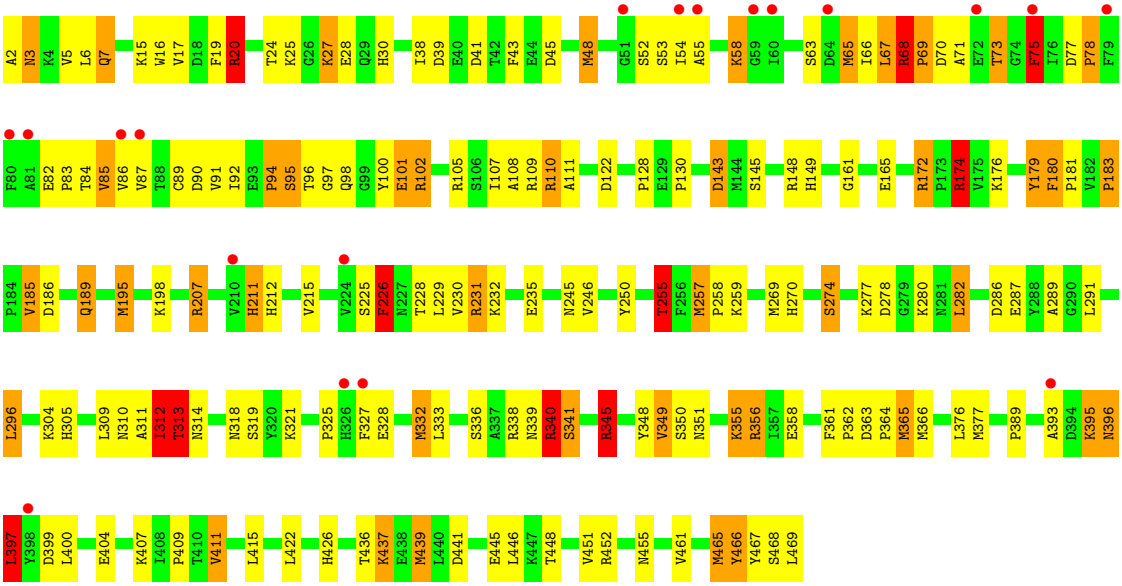
Chain B:





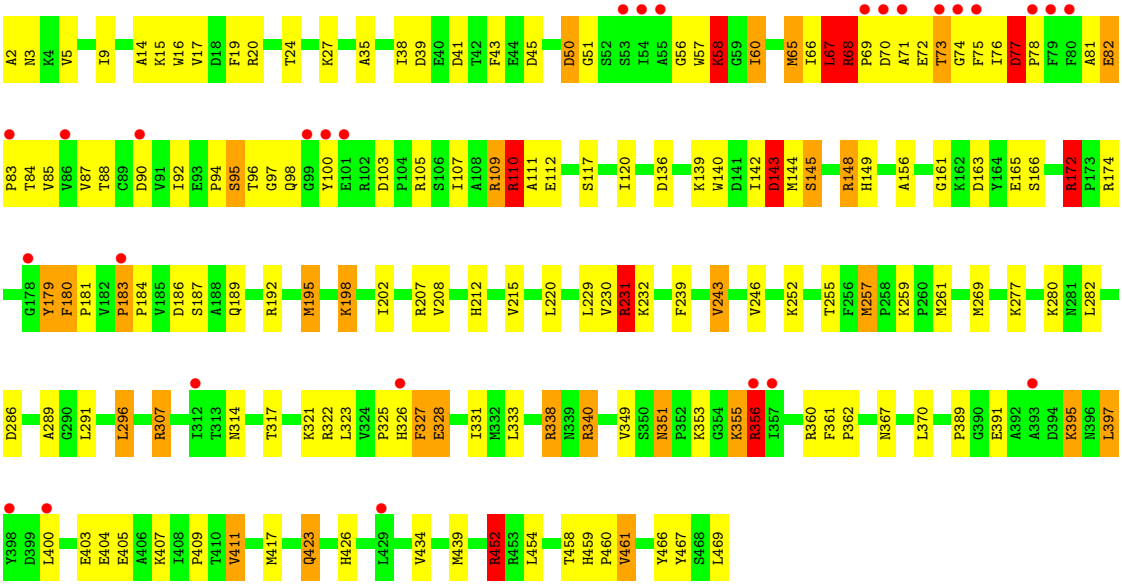
• Molecule 1: Glutamine synthetase

Chain C:



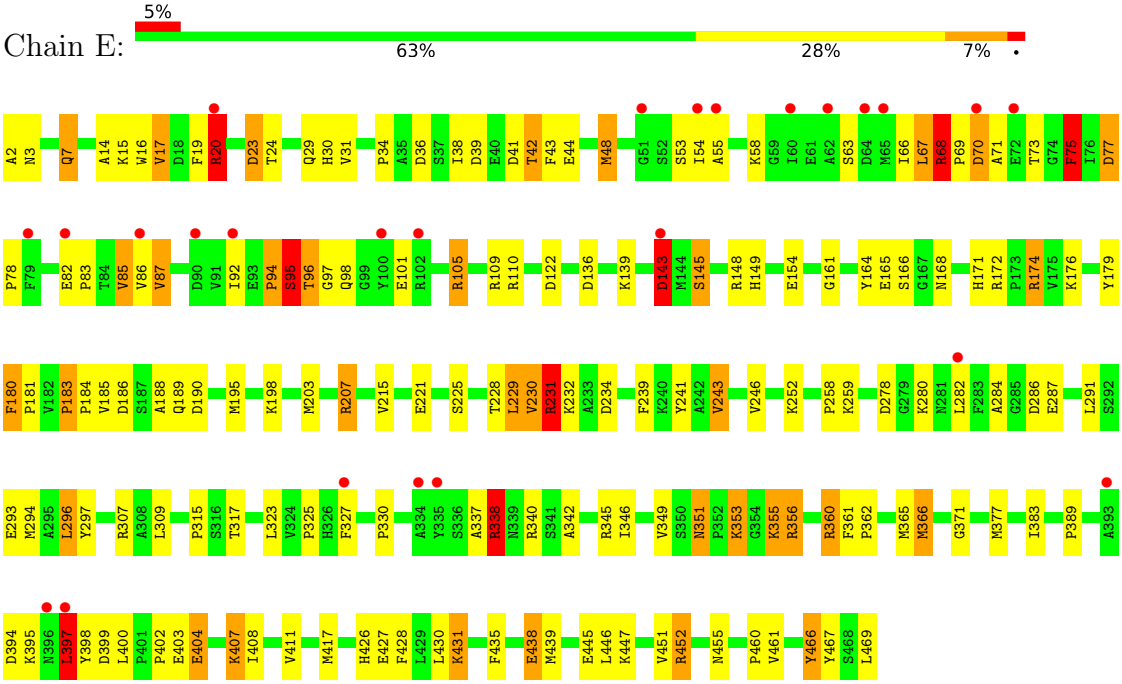
• Molecule 1: Glutamine synthetase

Chain D:



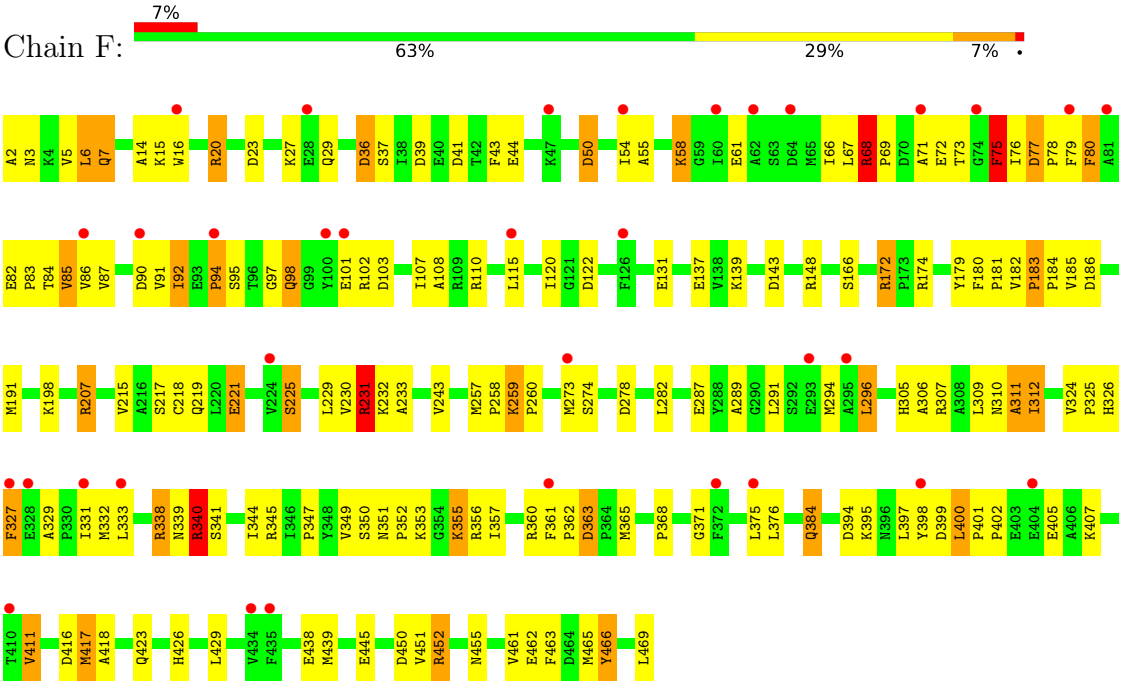
• Molecule 1: Glutamine synthetase

Chain E:



• Molecule 1: Glutamine synthetase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	260.91Å 260.91Å 154.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.22 – 3.40 93.22 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (93.22-3.40) 98.0 (93.22-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 3.41Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.100)	Depositor
R, R_{free}	0.233 , 0.270 0.235 , 0.270	Depositor DCC
R_{free} test set	3606 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.961	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 129.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	43046	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: GOL, PGE, EDO, 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	0.68	1/3729 (0.0%)	1.26	31/5054 (0.6%)
1	B	0.65	1/3729 (0.0%)	1.22	32/5054 (0.6%)
1	C	0.61	1/3729 (0.0%)	1.21	38/5054 (0.8%)
1	D	0.58	2/3730 (0.1%)	1.17	21/5055 (0.4%)
1	E	0.52	1/3726 (0.0%)	1.08	15/5051 (0.3%)
1	F	0.53	0/3726	1.11	19/5049 (0.4%)
All	All	0.60	6/22369 (0.0%)	1.18	156/30317 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	11
1	C	0	8
1	D	0	13
1	E	0	11
1	F	0	6
All	All	0	56

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	GLU	CD-OE2	6.47	1.32	1.25
1	E	145	SER	CA-CB	-5.76	1.44	1.52
1	C	319	SER	CA-CB	-5.54	1.44	1.52
1	D	469	LEU	C-O	5.42	1.33	1.23
1	D	145	SER	CA-CB	-5.26	1.45	1.52

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	20	ARG	NE-CZ-NH1	-15.81	112.39	120.30
1	A	322	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	D	322	ARG	NE-CZ-NH2	-11.87	114.37	120.30
1	B	75	PHE	N-CA-CB	11.34	131.01	110.60
1	E	148	ARG	NE-CZ-NH2	-11.21	114.70	120.30

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain
1	A	148	ARG	Sidechain
1	A	207	ARG	Sidechain
1	A	322	ARG	Sidechain
1	A	68	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3637	3515	3485	137	1
1	B	3637	3515	3485	127	0
1	C	3637	3515	3485	118	0
1	D	3638	3517	3487	113	1
1	E	3634	3508	3476	102	0
1	F	3635	3514	3484	92	0
2	A	10	14	14	0	0
3	A	12	16	16	0	0
3	B	12	16	16	0	0
3	C	6	8	8	0	0
3	D	6	8	8	0	0
3	E	6	8	8	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	F	4	6	6	0	0
All	All	21886	21160	20978	622	1

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 15.

The worst 5 of 622 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:B:75:PHE:CE2	1:B:78:PRO:HG2	1.94	1.03
1:C:2:ALA:HB1	1:C:69:PRO:HB3	1.40	1.01
1:E:67:LEU:HB3	1:E:87:VAL:HB	1.42	0.99
1:C:207:ARG:HH21	1:C:225:SER:HB2	1.30	0.96
1:A:253:THR:OG1	1:D:467:TYR:OH	1.86	0.94

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASP:OD1	1:D:139:LYS:HZ2[8_554]	1.57	0.03

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	466/468 (100%)	421 (90%)	39 (8%)	6 (1%)	10 33
1	B	466/468 (100%)	412 (88%)	36 (8%)	18 (4%)	2 15
1	C	466/468 (100%)	410 (88%)	43 (9%)	13 (3%)	4 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	466/468 (100%)	423 (91%)	37 (8%)	6 (1%)	10 33
1	E	466/468 (100%)	417 (90%)	36 (8%)	13 (3%)	4 20
1	F	466/468 (100%)	422 (91%)	35 (8%)	9 (2%)	6 26
All	All	2796/2808 (100%)	2505 (90%)	226 (8%)	65 (2%)	5 23

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	95	SER
1	B	189	GLN
1	B	288	TYR
1	C	96	THR
1	C	101	GLU

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	381/387 (98%)	316 (83%)	65 (17%)	1 6
1	B	381/387 (98%)	308 (81%)	73 (19%)	1 3
1	C	381/387 (98%)	306 (80%)	75 (20%)	1 3
1	D	381/387 (98%)	327 (86%)	54 (14%)	2 11
1	E	380/387 (98%)	312 (82%)	68 (18%)	1 5
1	F	381/387 (98%)	300 (79%)	81 (21%)	1 2
All	All	2285/2322 (98%)	1869 (82%)	416 (18%)	1 5

5 of 416 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	165	GLU
1	E	98	GLN
1	F	395	LYS
1	D	189	GLN

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Mol	Chain	Res	Type
1	D	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	318	ASN
1	F	396	ASN
1	D	270	HIS
1	E	149	HIS
1	C	396	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 12 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	D	501	-	5,5,5	0.19	0	5,5,5	0.66	0
3	GOL	A	502	-	5,5,5	0.15	0	5,5,5	0.36	0
5	EDO	F	501	-	3,3,3	0.42	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	C	501	-	5,5,5	0.25	0	5,5,5	0.47	0
2	PGE	A	501	-	9,9,9	0.26	0	8,8,8	0.21	0
3	GOL	B	502	-	5,5,5	0.09	0	5,5,5	0.31	0
3	GOL	A	503	-	5,5,5	0.15	0	5,5,5	0.41	0
3	GOL	B	501	-	5,5,5	0.21	0	5,5,5	0.65	0
3	GOL	E	501	-	5,5,5	0.16	0	5,5,5	0.41	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
3	GOL	D	501	-	-	2/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
5	EDO	F	501	-	-	1/1/1/1	-
3	GOL	C	501	-	-	2/4/4/4	-
2	PGE	A	501	-	-	4/7/7/7	-
3	GOL	B	502	-	-	3/4/4/4	-
3	GOL	A	503	-	-	4/4/4/4	-
3	GOL	B	501	-	-	2/4/4/4	-
3	GOL	E	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-C3
3	A	503	GOL	C1-C2-C3-O3
3	B	501	GOL	C1-C2-C3-O3

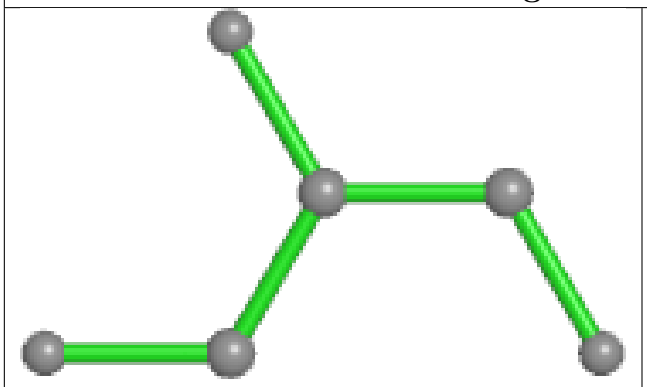
There are no ring outliers.

No monomer is involved in short contacts.

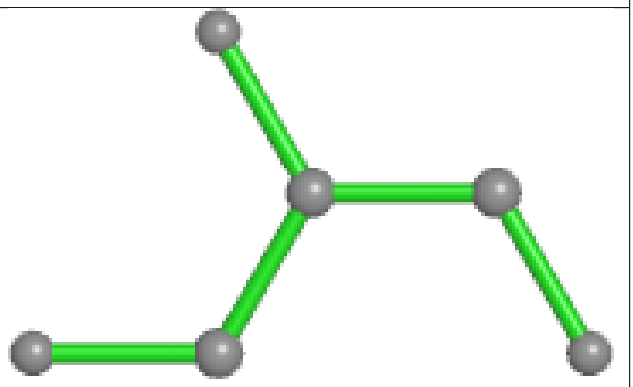
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

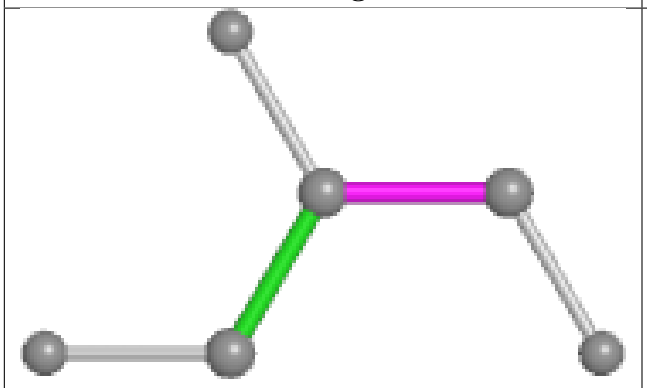
Ligand GOL D 501



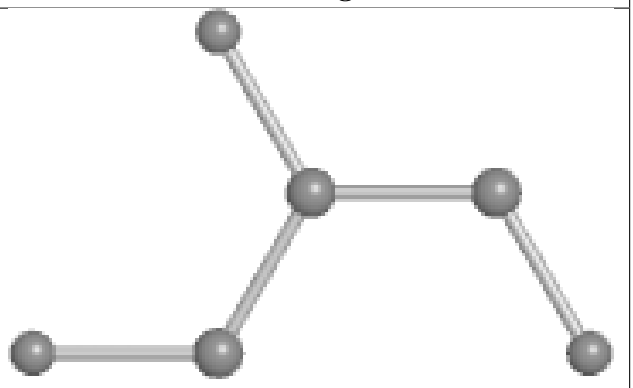
Bond lengths



Bond angles

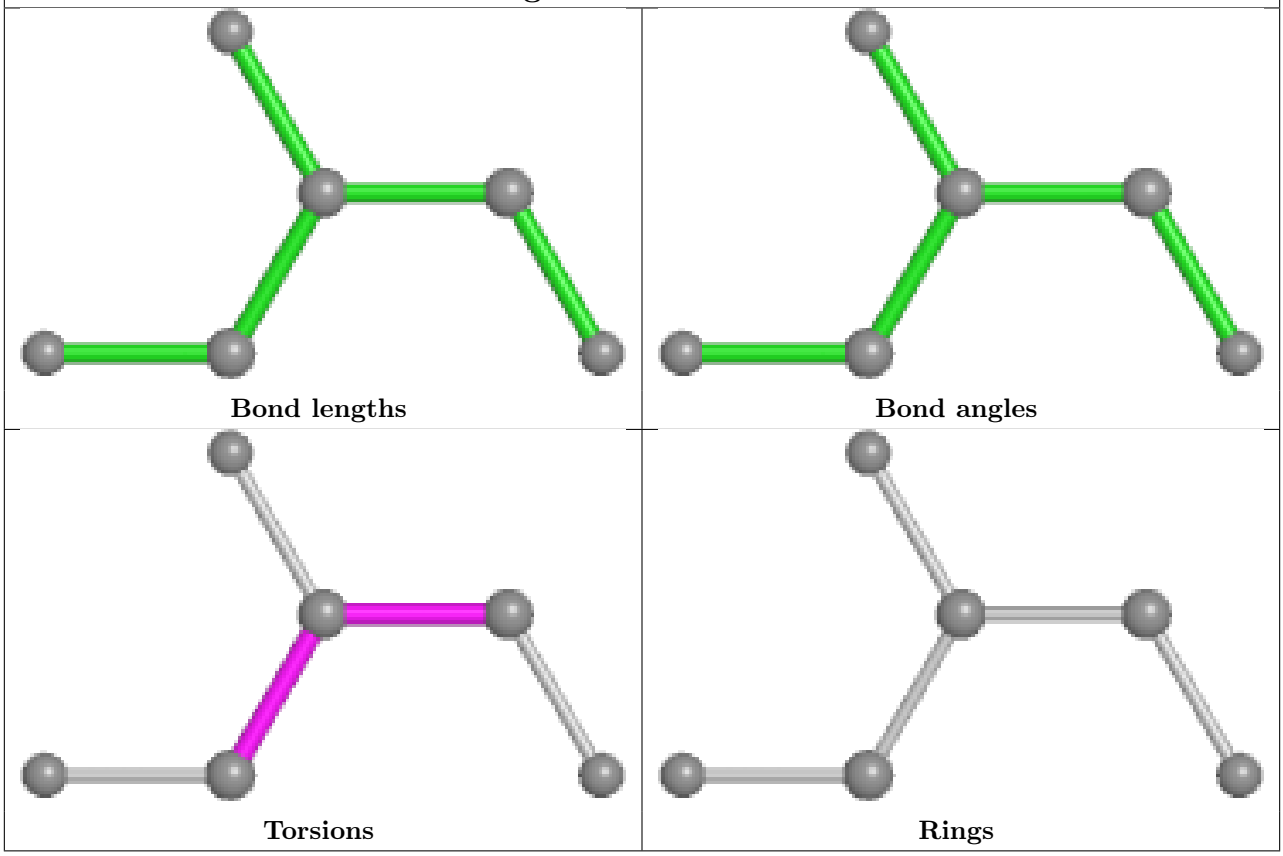


Torsions

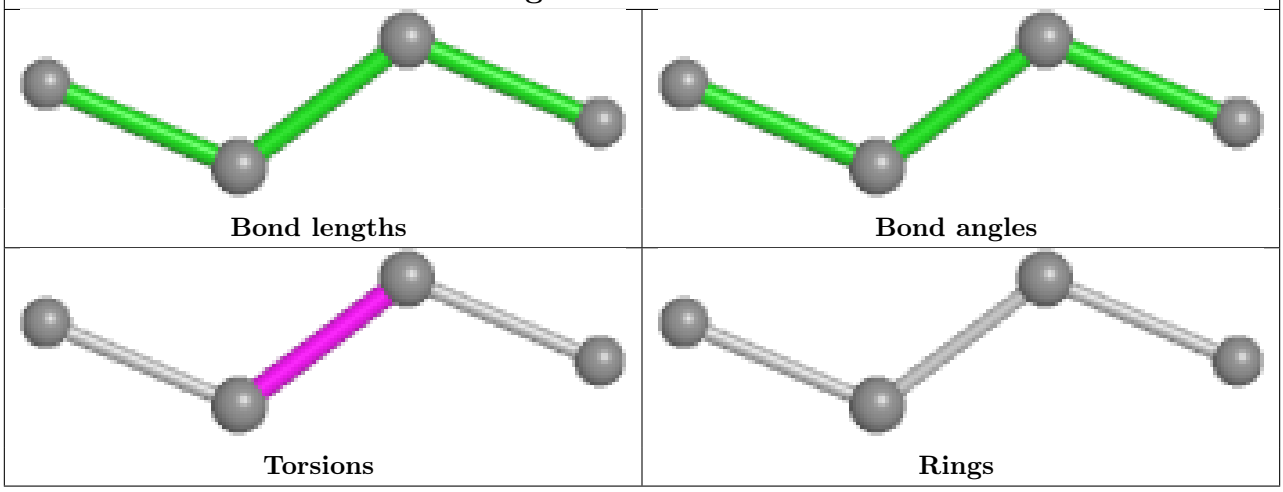


Rings

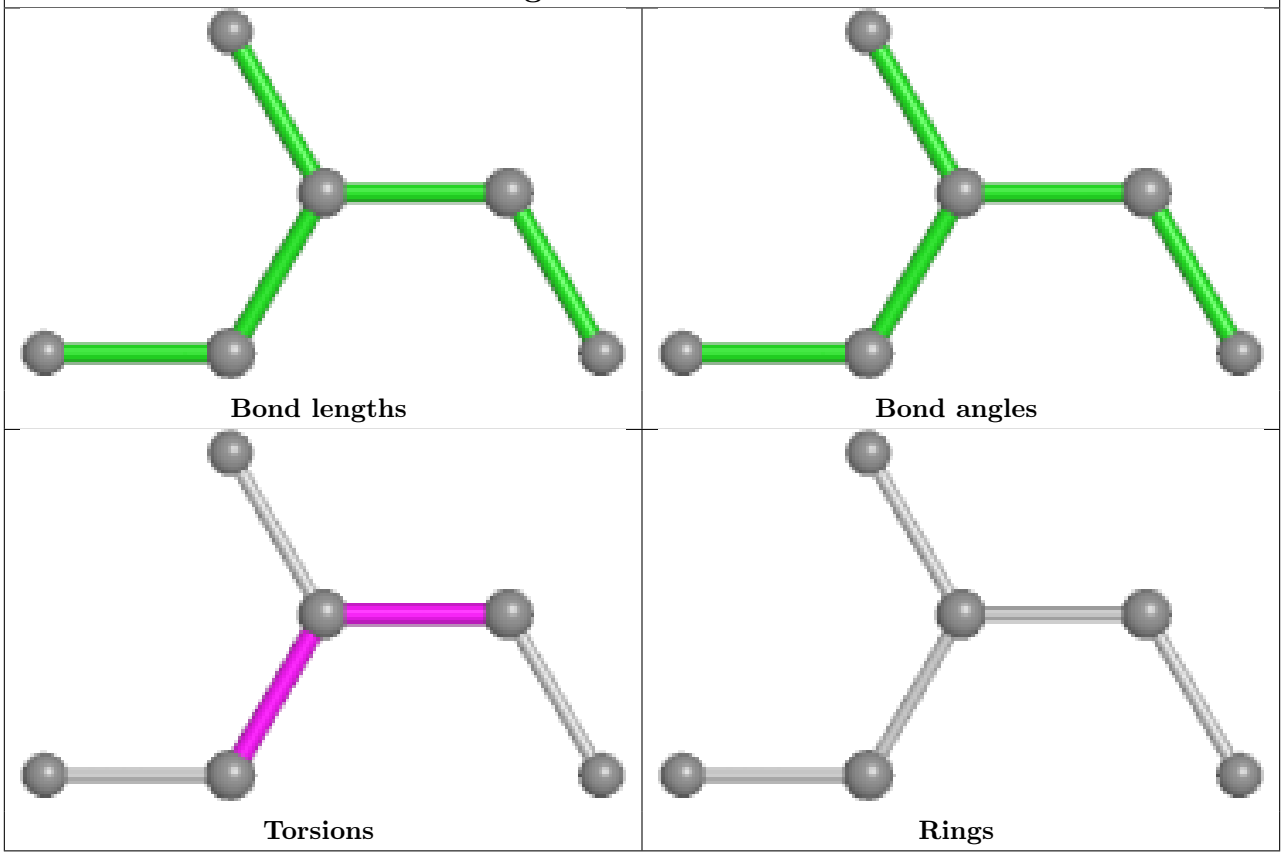
Ligand GOL A 502



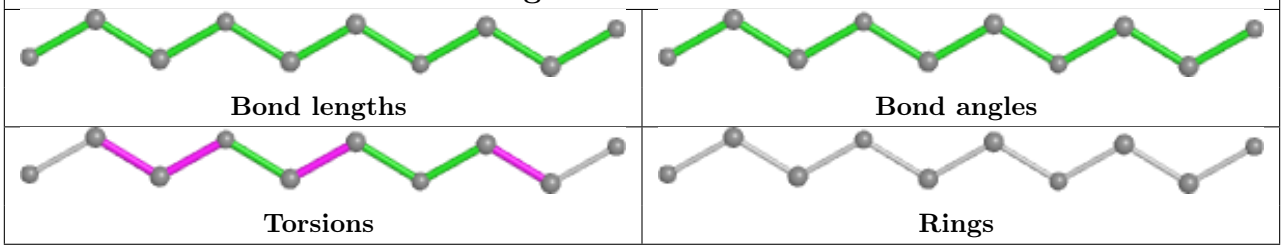
Ligand EDO F 501



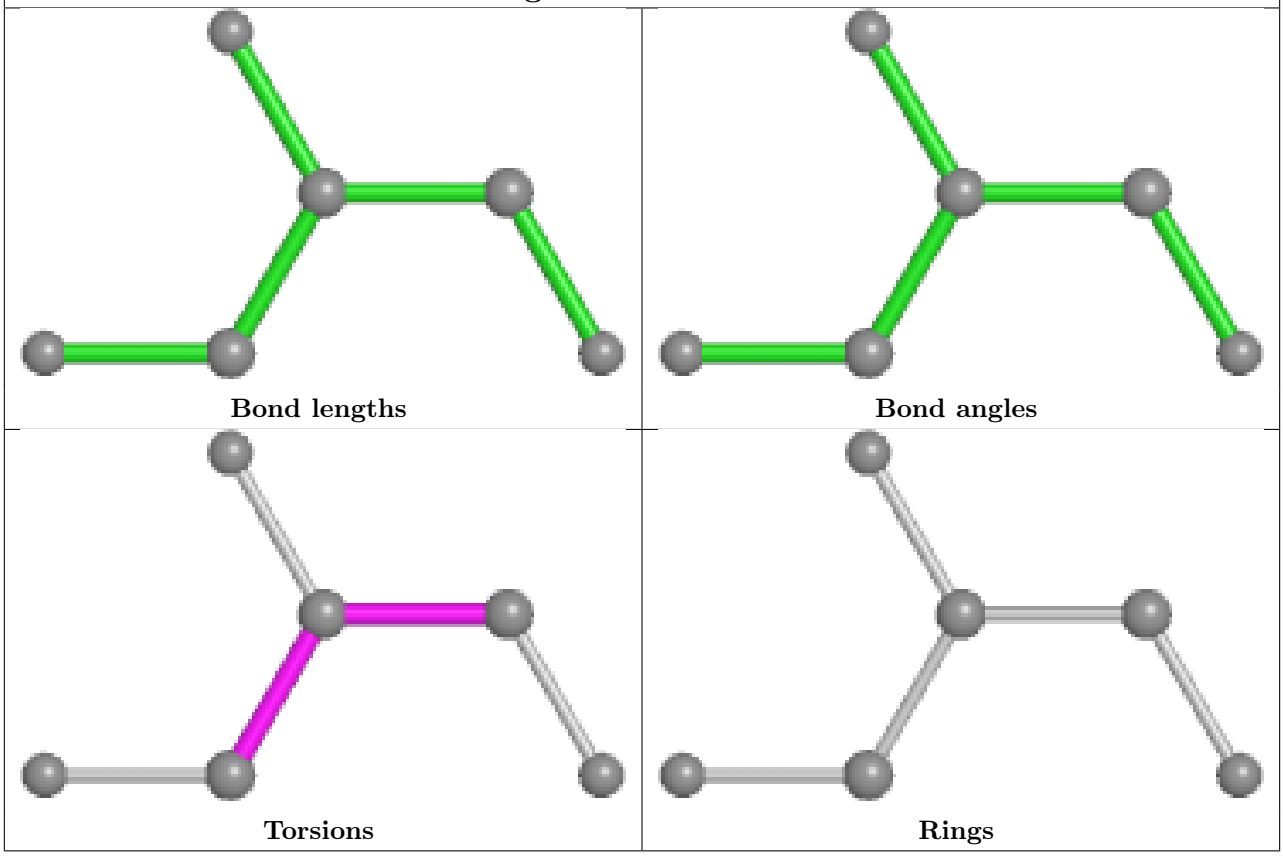
Ligand GOL C 501



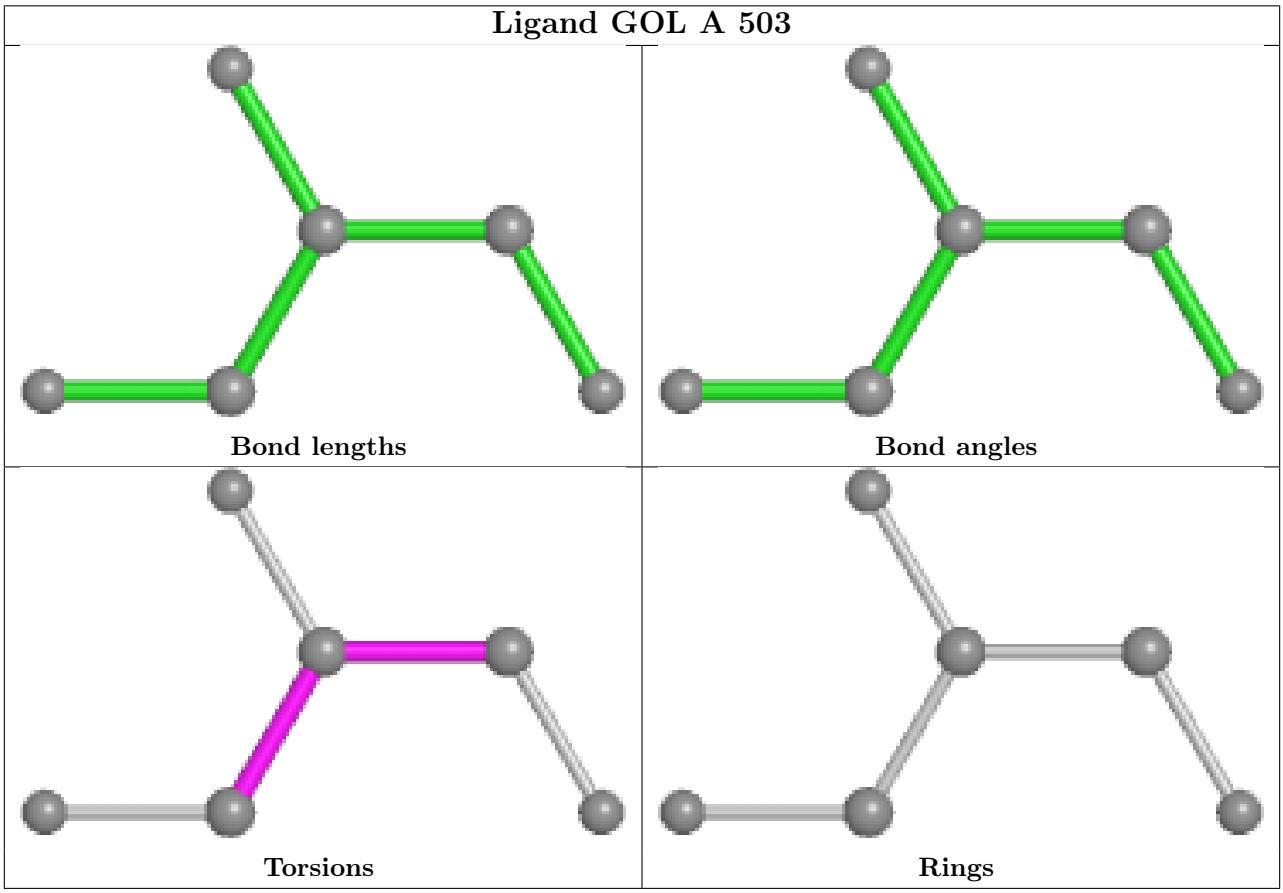
Ligand PGE A 501



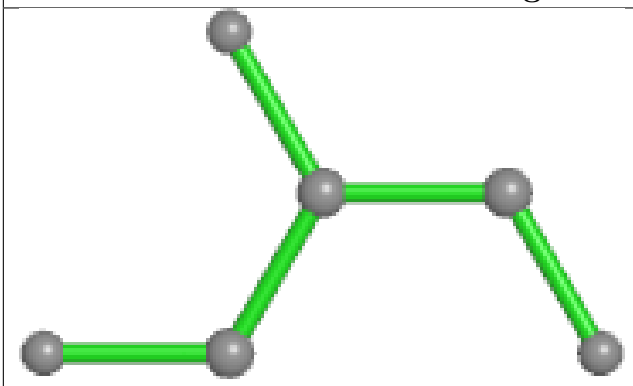
Ligand GOL B 502



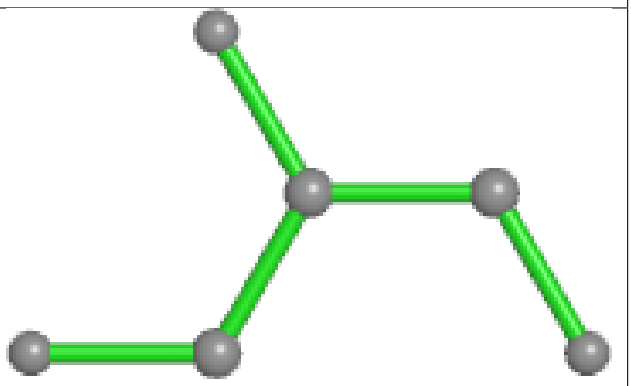
Ligand GOL A 503



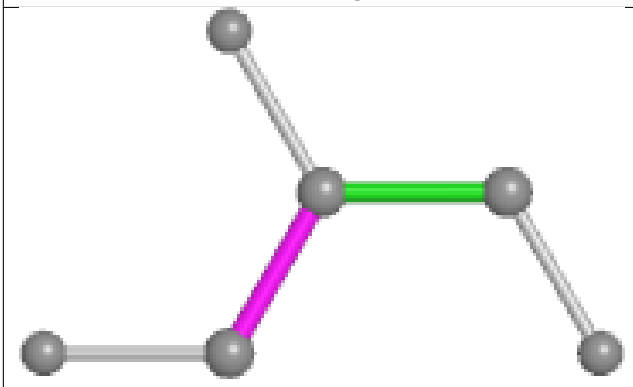
Ligand GOL B 501



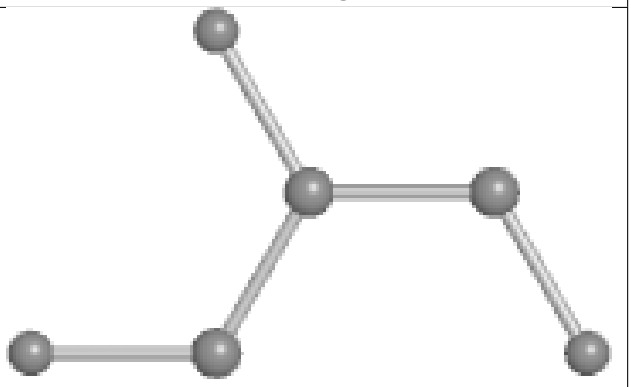
Bond lengths



Bond angles

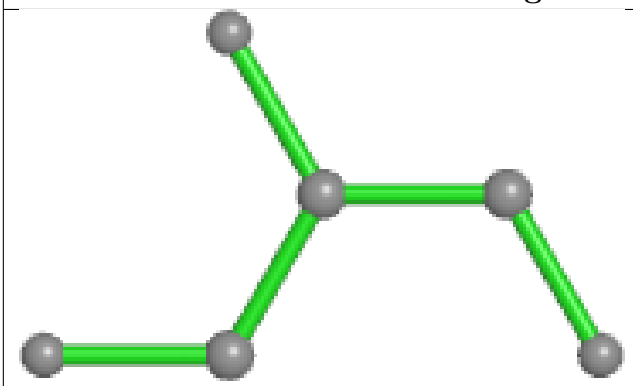


Torsions

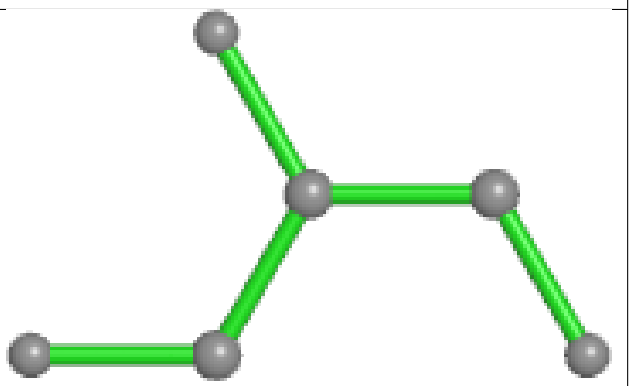


Rings

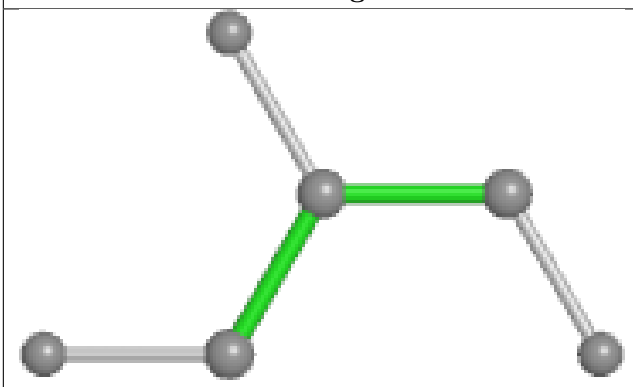
Ligand GOL E 501



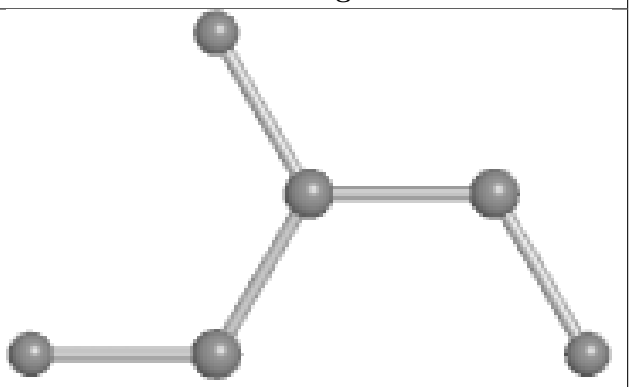
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	468/468 (100%)	0.03	16 (3%)	48	41	31, 70, 148, 235	0
1	B	468/468 (100%)	0.15	17 (3%)	46	39	38, 89, 156, 222	0
1	C	468/468 (100%)	0.30	19 (4%)	42	36	57, 102, 163, 265	0
1	D	468/468 (100%)	0.36	28 (5%)	29	27	41, 103, 183, 239	0
1	E	468/468 (100%)	0.60	25 (5%)	33	29	56, 141, 197, 248	0
1	F	468/468 (100%)	0.62	34 (7%)	22	22	65, 138, 214, 307	0
All	All	2808/2808 (100%)	0.34	139 (4%)	35	31	31, 104, 195, 307	0

The worst 5 of 139 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	86	VAL	6.4
1	F	100	TYR	6.1
1	F	60	ILE	5.2
1	A	54	ILE	5.1
1	B	100	TYR	5.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

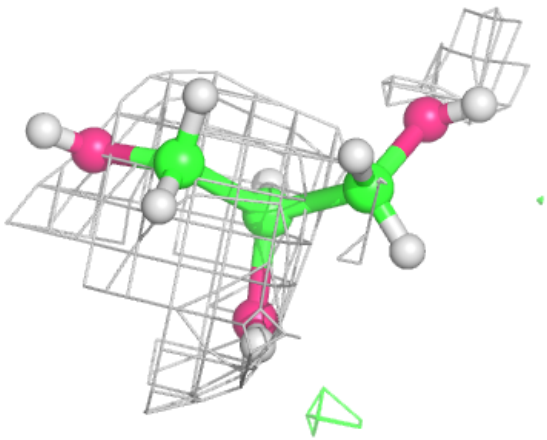
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

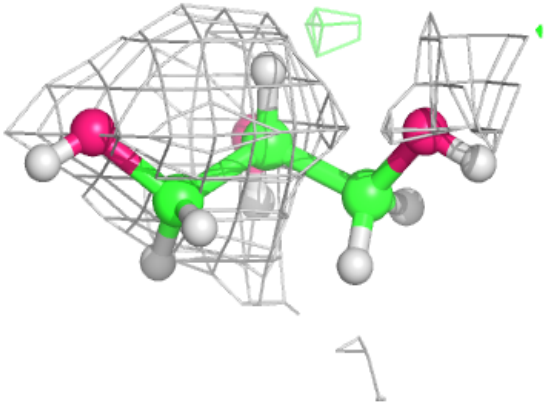
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	502	6/6	0.57	0.17	30,170,175,179	3
3	GOL	C	501	6/6	0.60	0.16	30,130,137,137	3
4	MG	E	503	1/1	0.61	0.22	114,114,114,114	0
3	GOL	B	501	6/6	0.62	0.16	30,118,125,126	3
3	GOL	A	502	6/6	0.73	0.17	30,140,145,146	3
4	MG	E	502	1/1	0.84	0.19	66,66,66,66	0
5	EDO	F	501	4/4	0.85	0.20	30,96,98,99	2
3	GOL	E	501	6/6	0.86	0.13	30,122,131,133	3
3	GOL	D	501	6/6	0.86	0.13	30,103,107,111	3
3	GOL	A	503	6/6	0.89	0.14	30,89,92,92	3
4	MG	B	504	1/1	0.90	0.10	67,67,67,67	0
2	PGE	A	501	10/10	0.90	0.14	30,105,114,114	2
4	MG	D	502	1/1	0.94	0.10	68,68,68,68	0
4	MG	A	505	1/1	0.94	0.12	39,39,39,39	0
4	MG	A	504	1/1	0.95	0.13	49,49,49,49	0
4	MG	F	502	1/1	0.96	0.18	62,62,62,62	0
4	MG	C	502	1/1	0.96	0.16	37,37,37,37	0
4	MG	F	503	1/1	0.97	0.09	68,68,68,68	0
4	MG	D	503	1/1	0.98	0.05	58,58,58,58	0
4	MG	C	503	1/1	0.98	0.05	57,57,57,57	0
4	MG	B	503	1/1	0.98	0.07	41,41,41,41	0

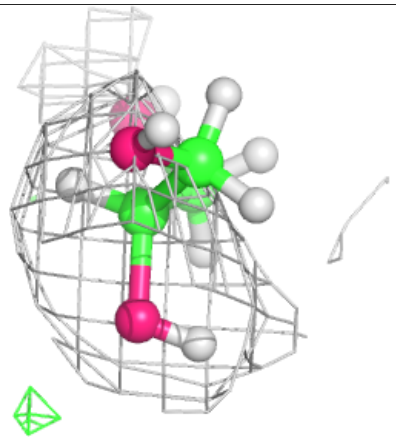
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GOL B 502:

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

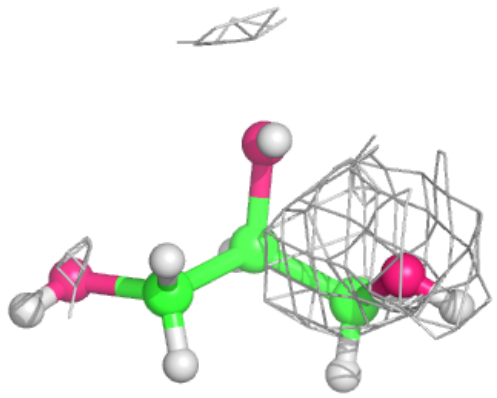


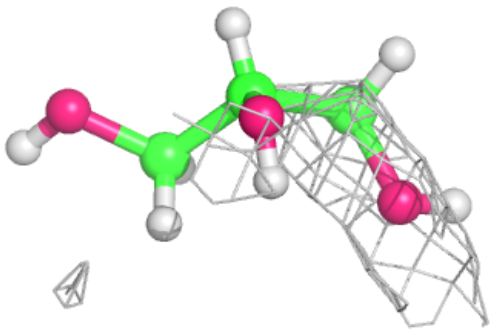


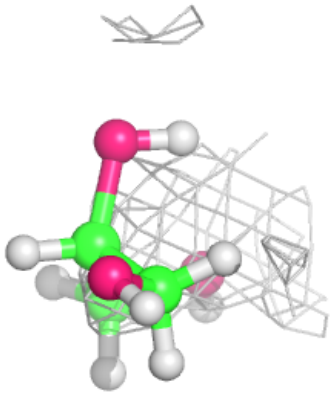


Electron density around GOL C 501:

$2mF_o$-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 E 503:

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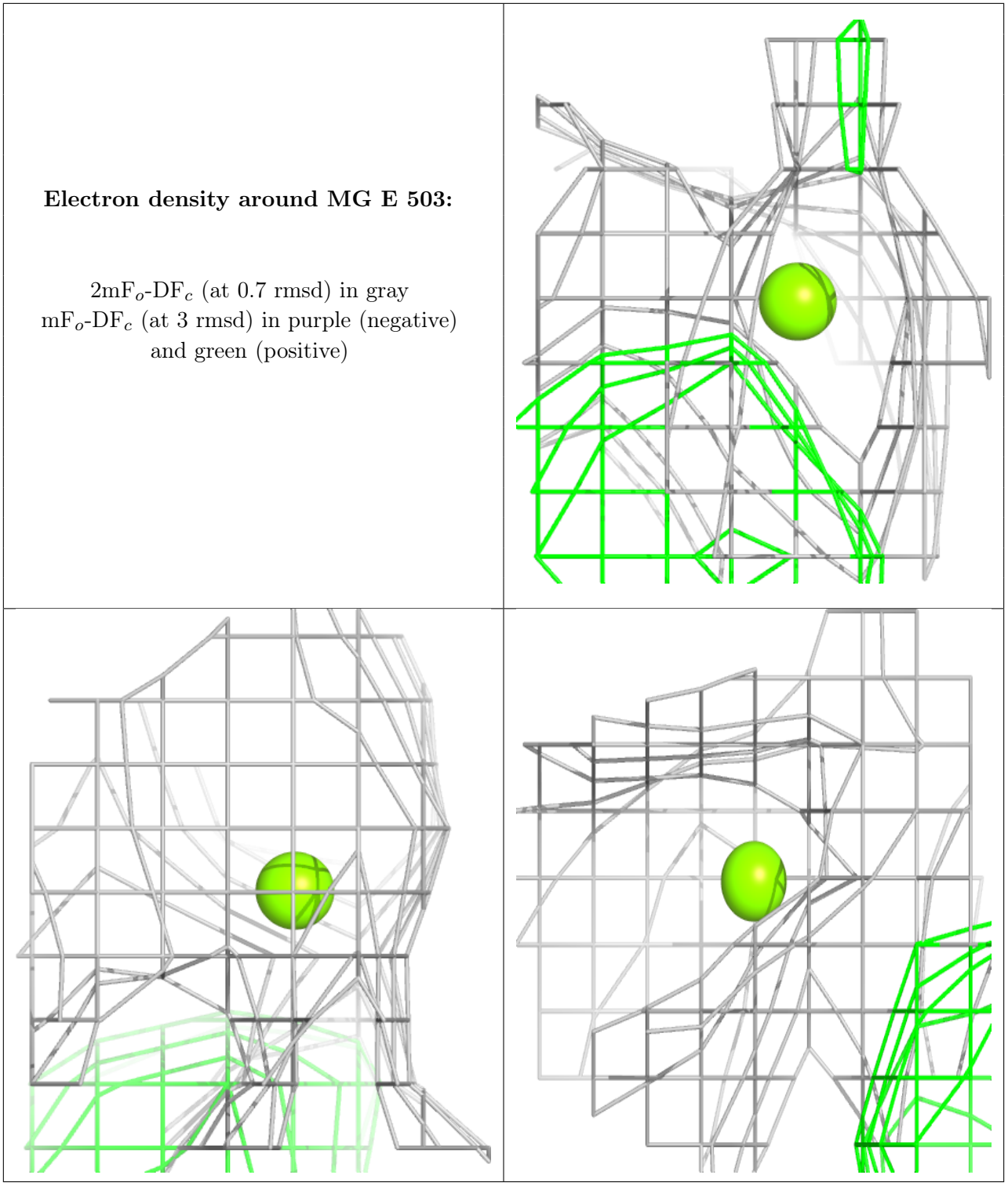
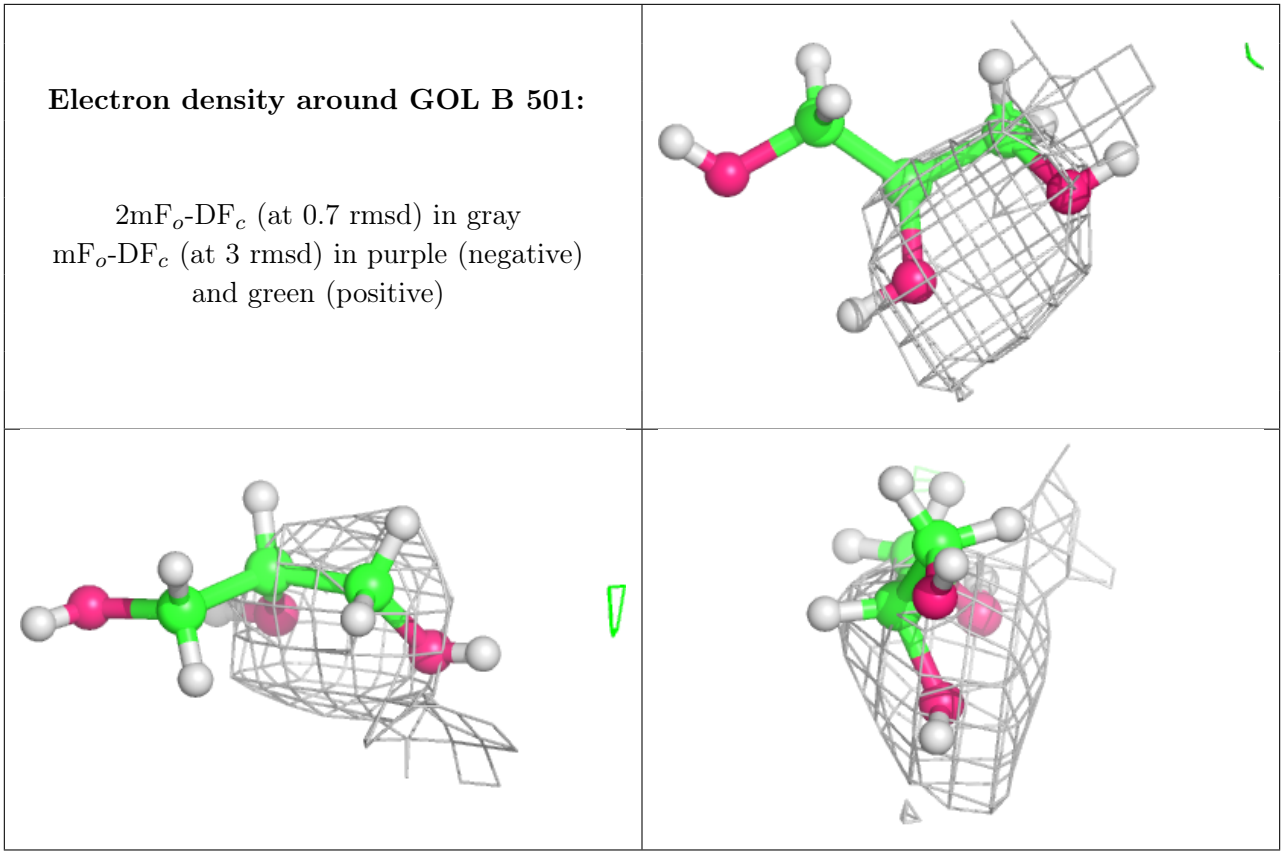
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



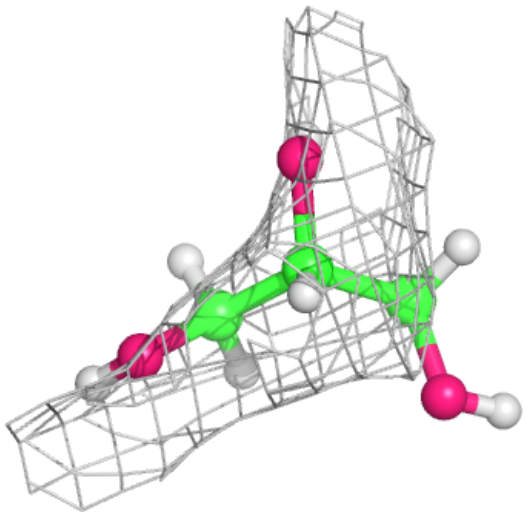
Electron density around GOL B 501:

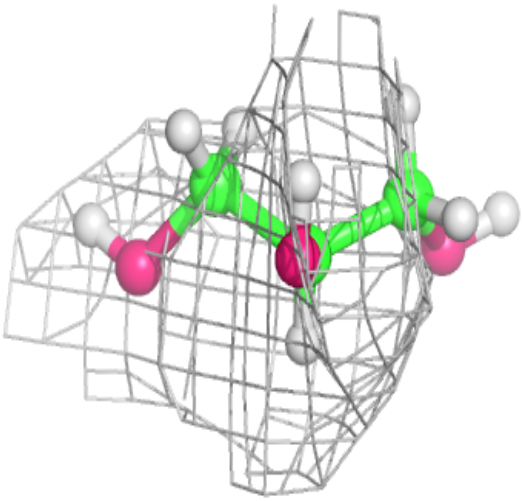
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

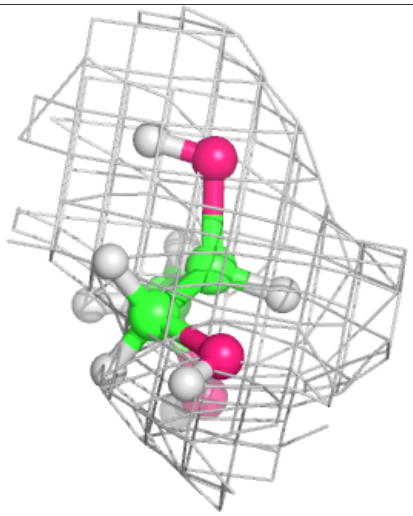


Electron density around GOL A 502:

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

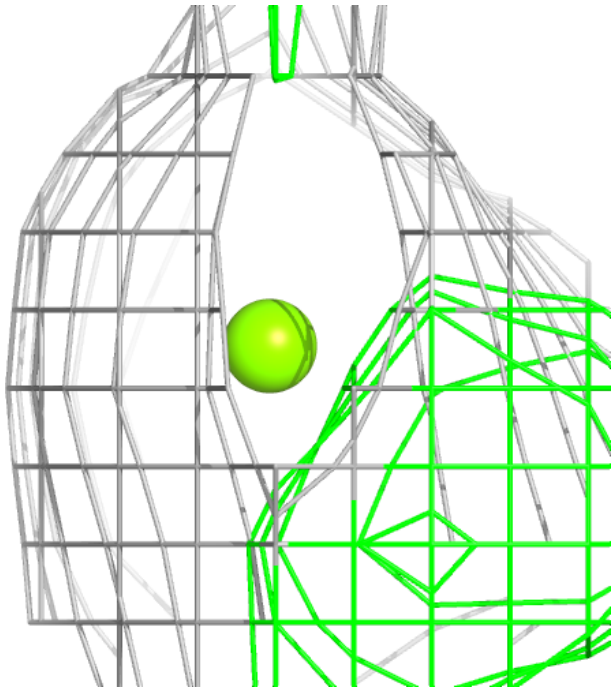


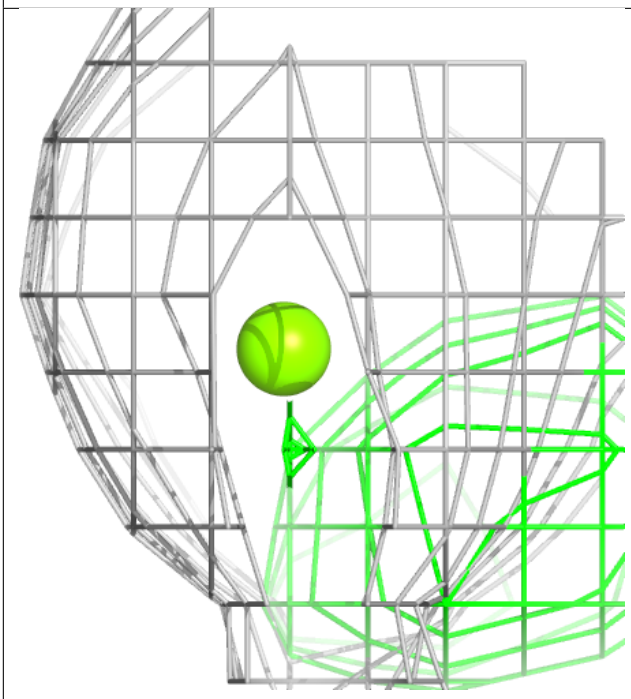


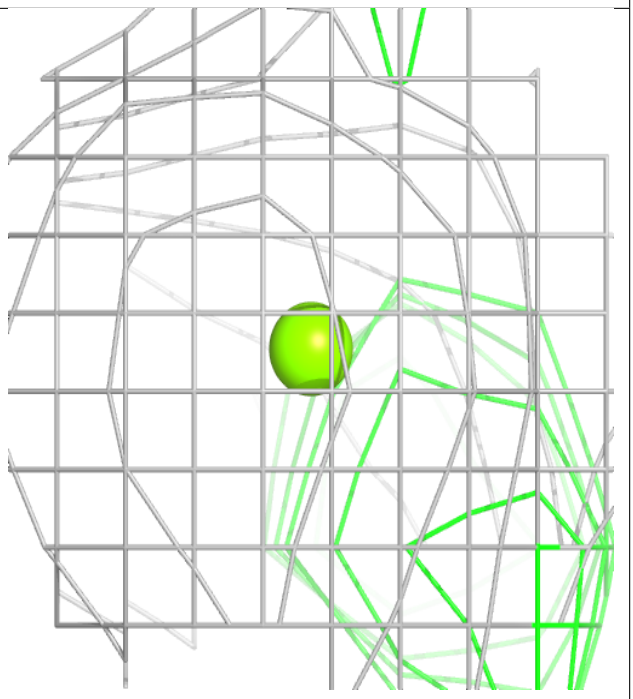


Electron density around MG E 502:

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

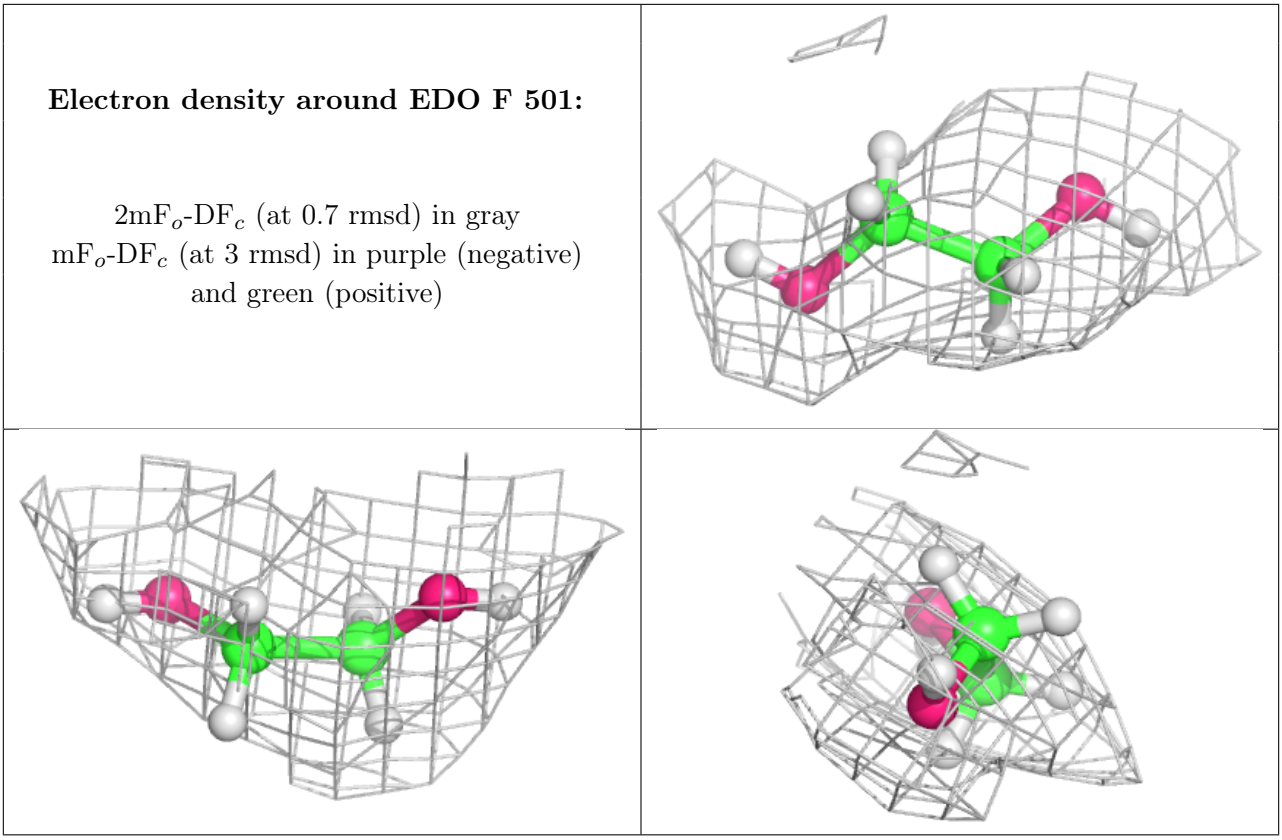






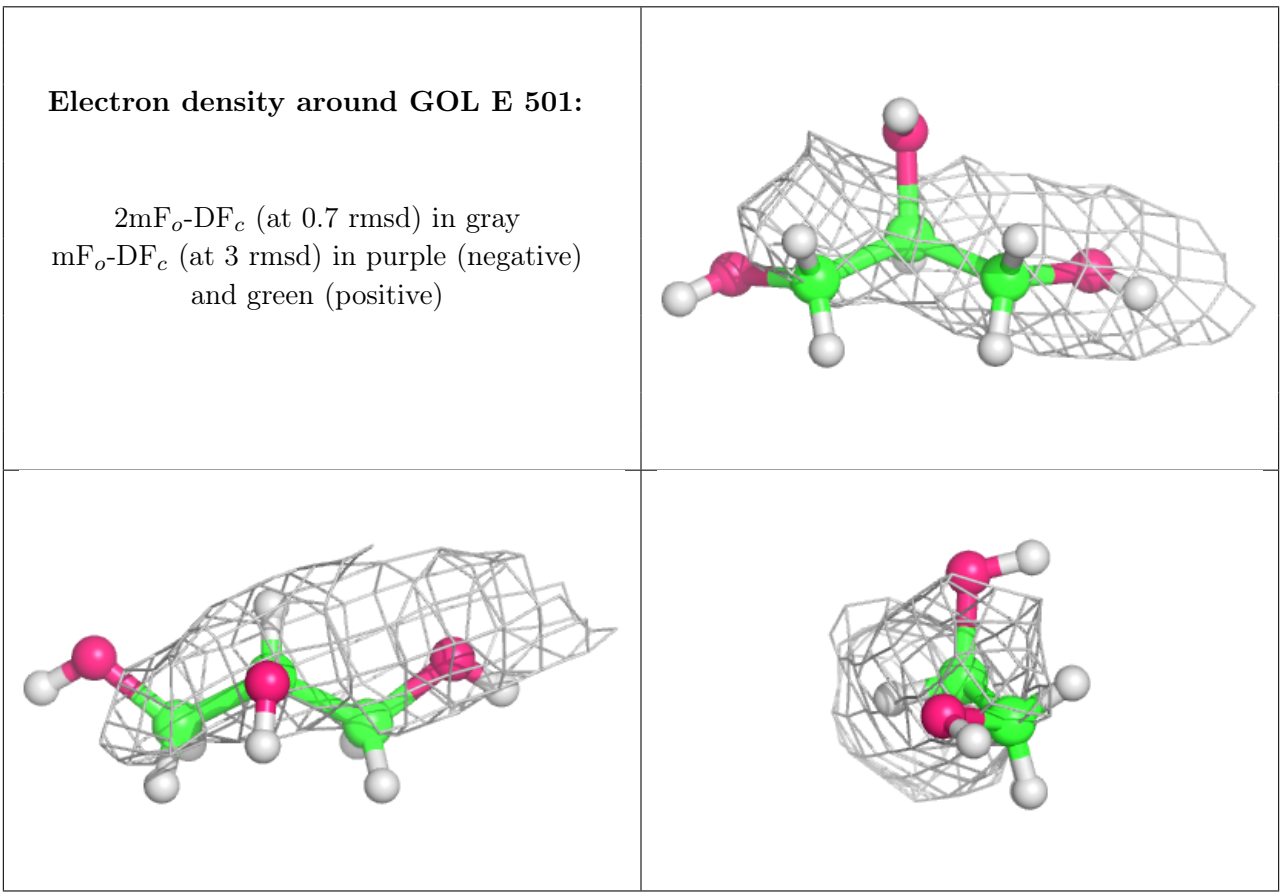
Electron density around EDO F 501:

$2mF_o$-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 501:

$2mF_o$-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 501:

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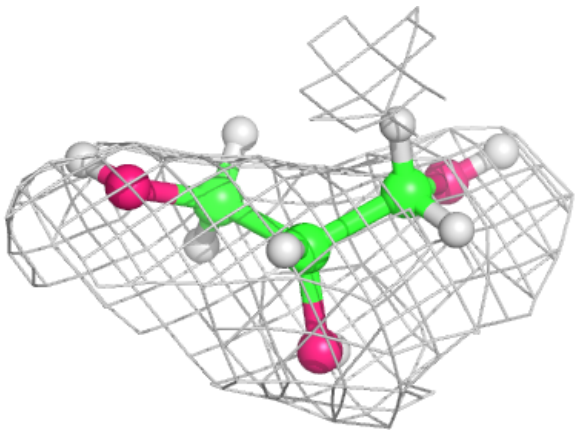
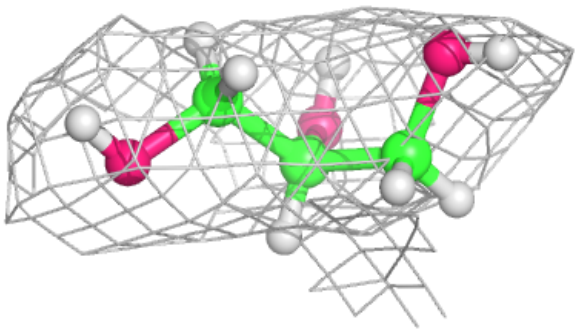
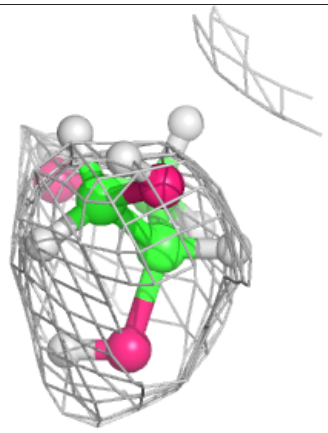
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

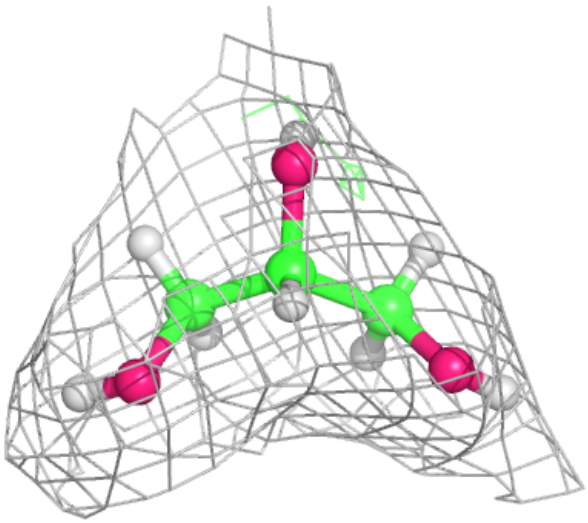


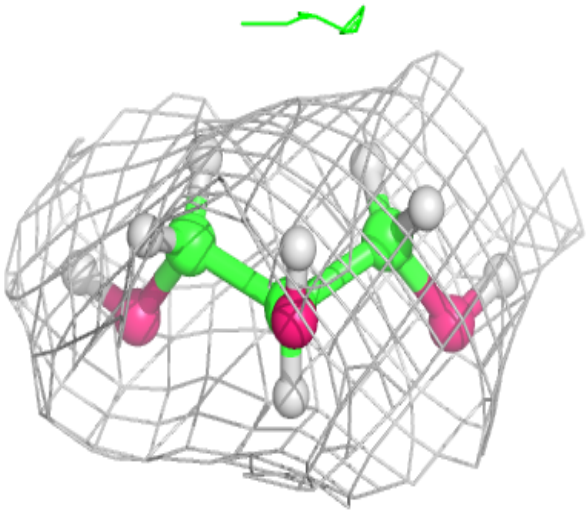


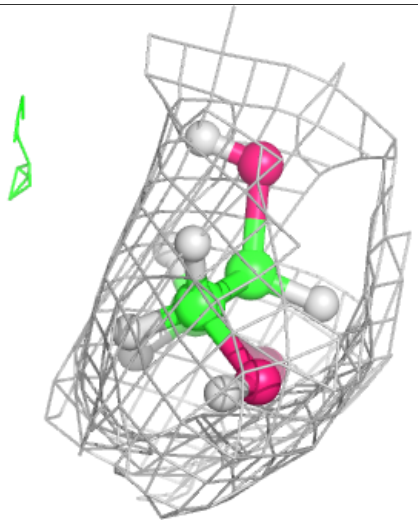


Electron density around GOL A 503:

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

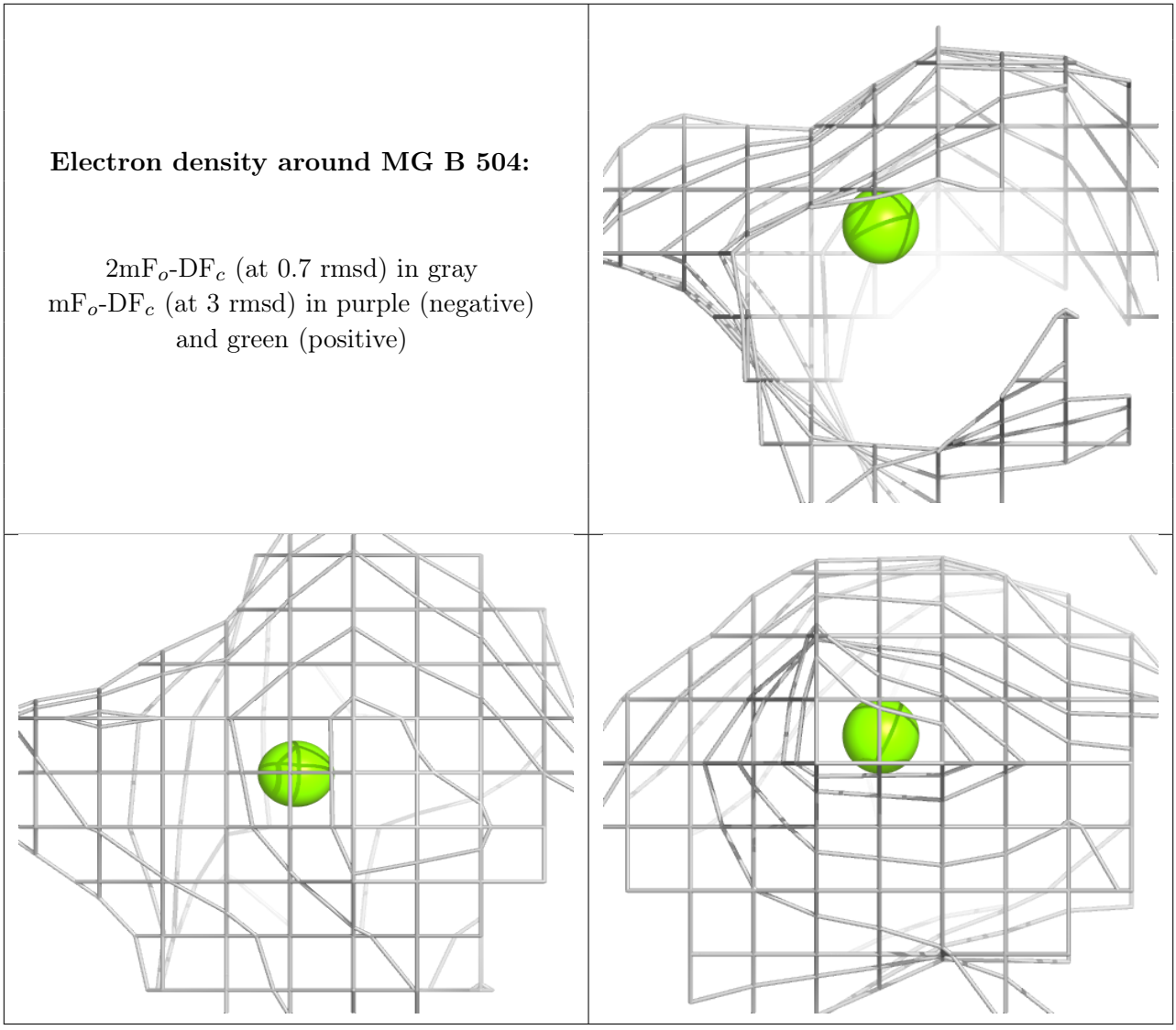






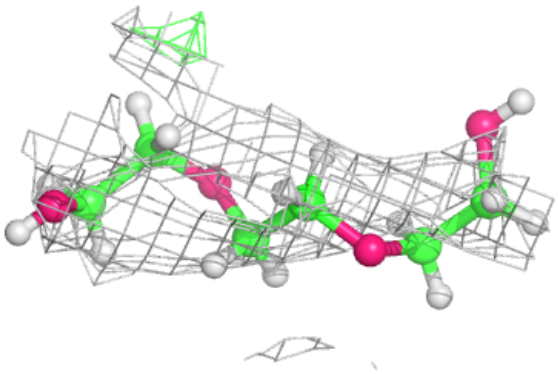
Electron density around MG B 504:

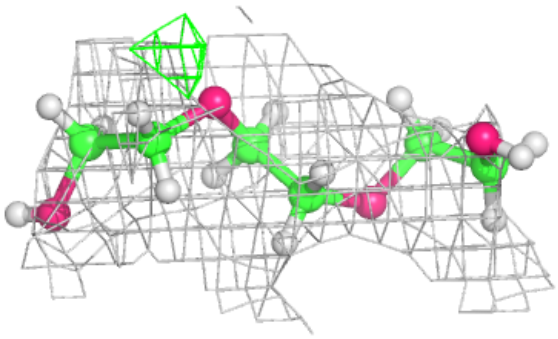
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

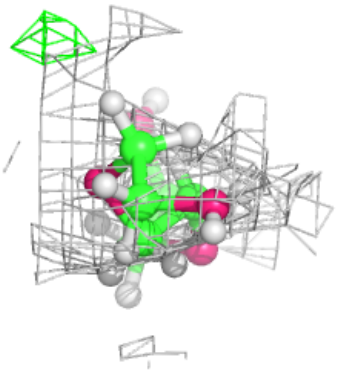


Electron density around PGE A 501:

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

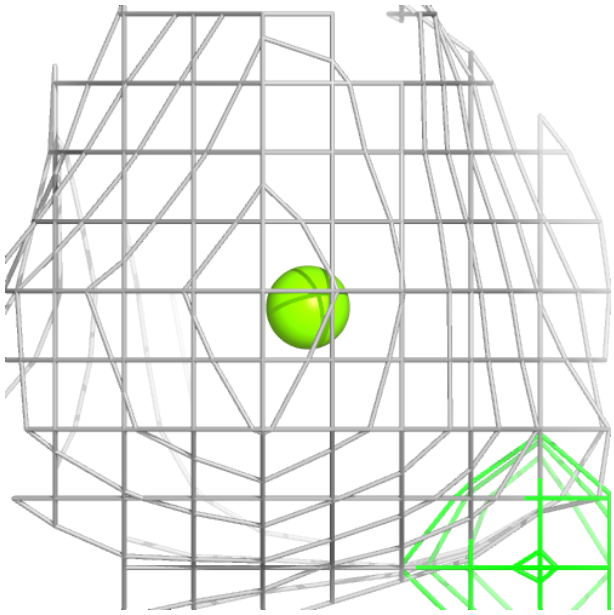


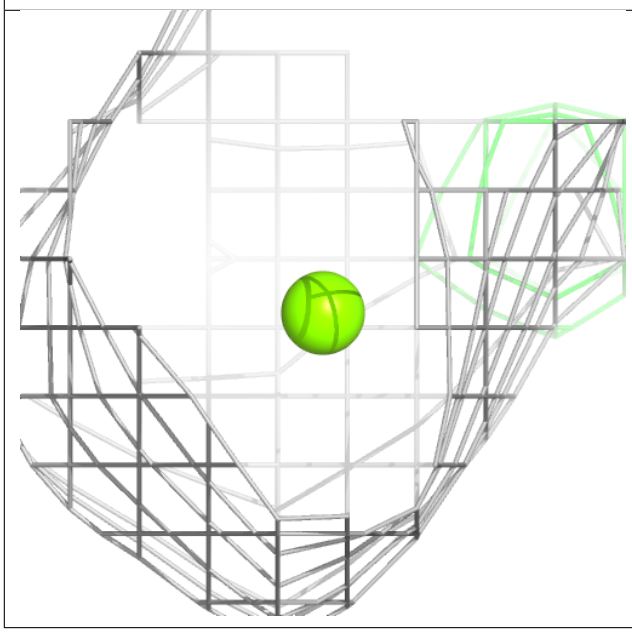


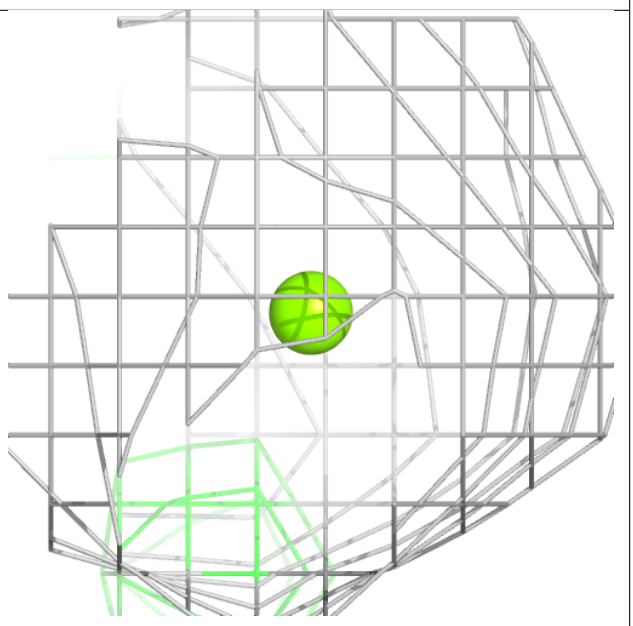


Electron density around MG D 502:

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

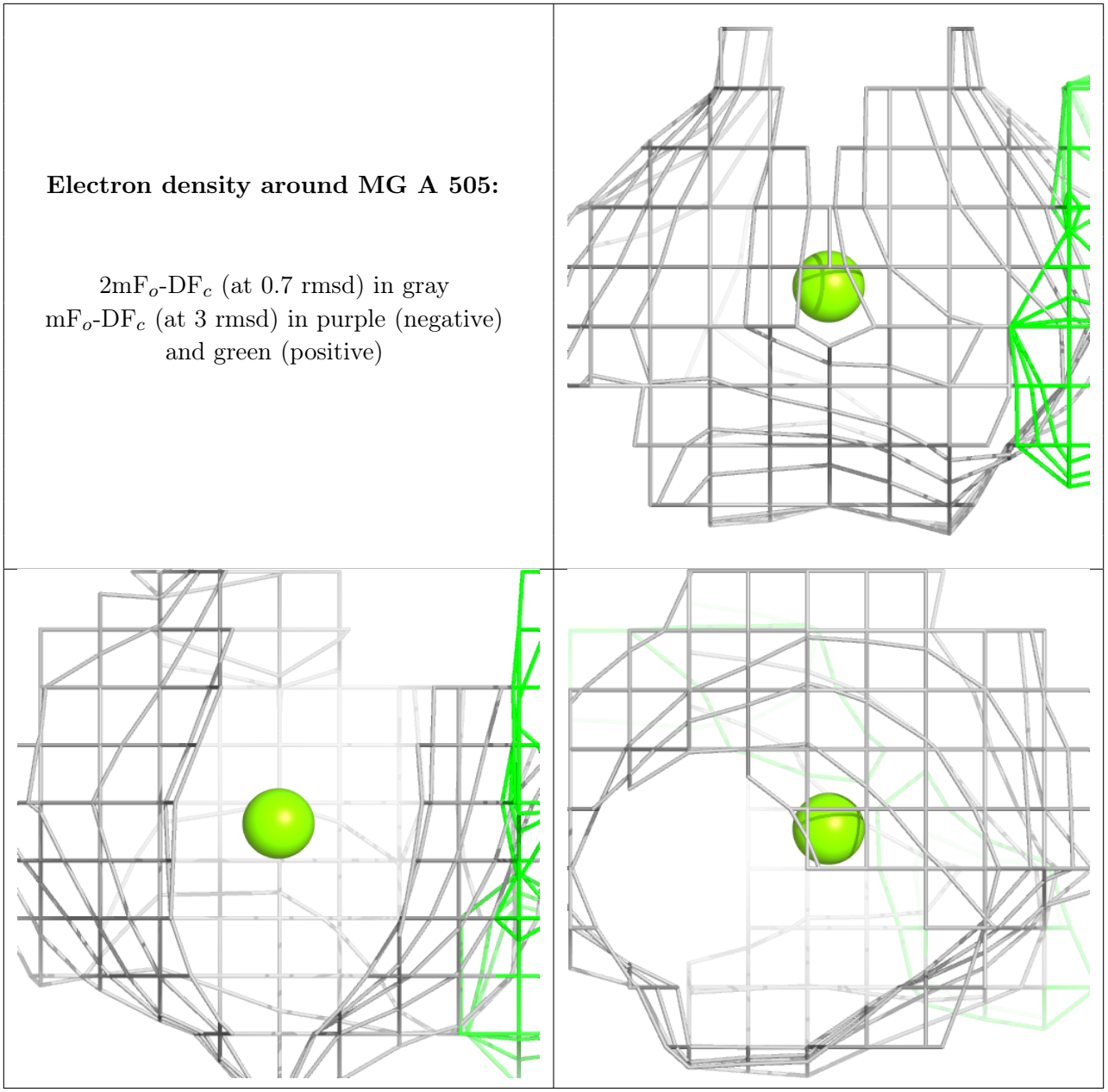






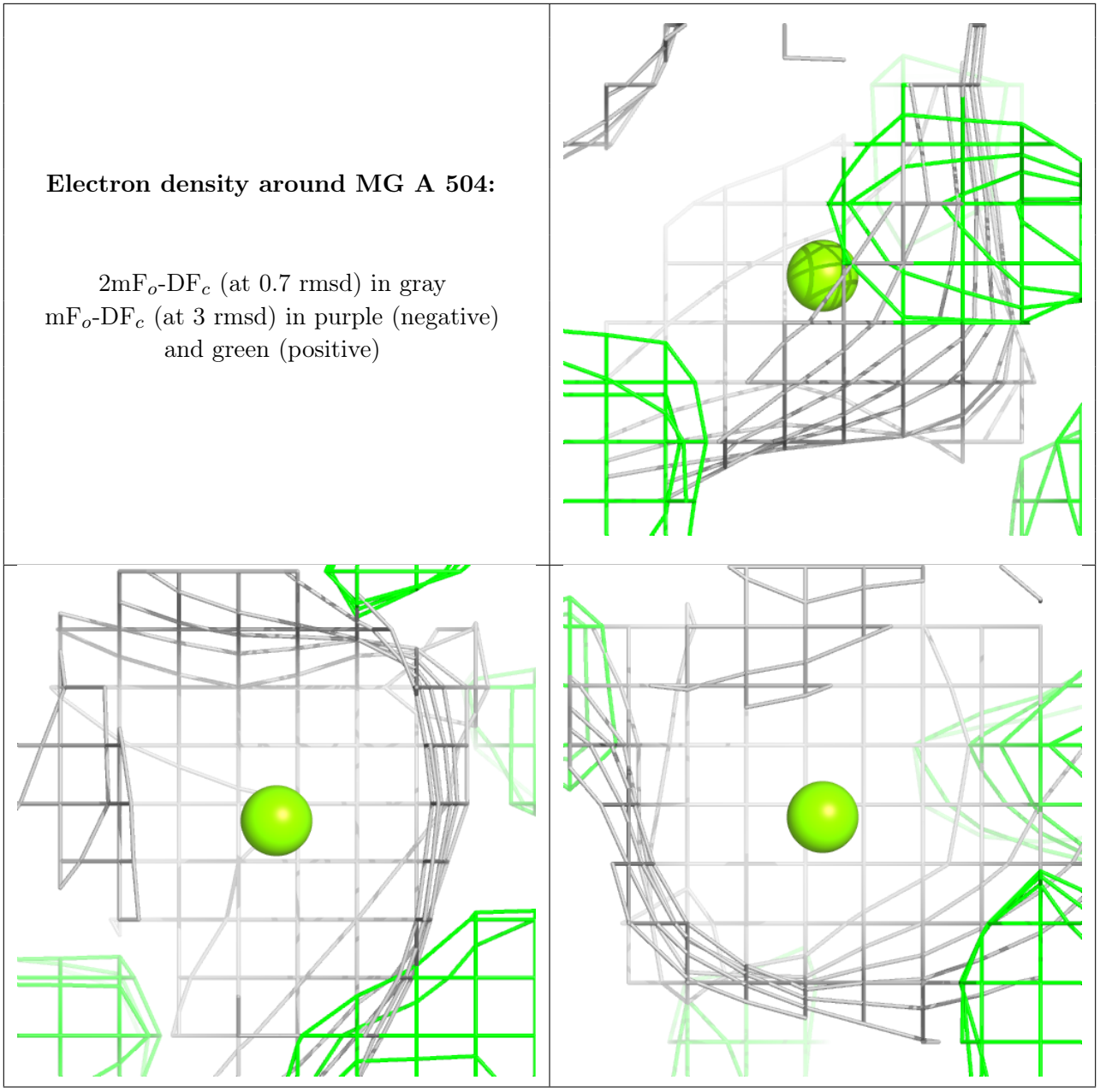
Electron density around MG A 505:

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



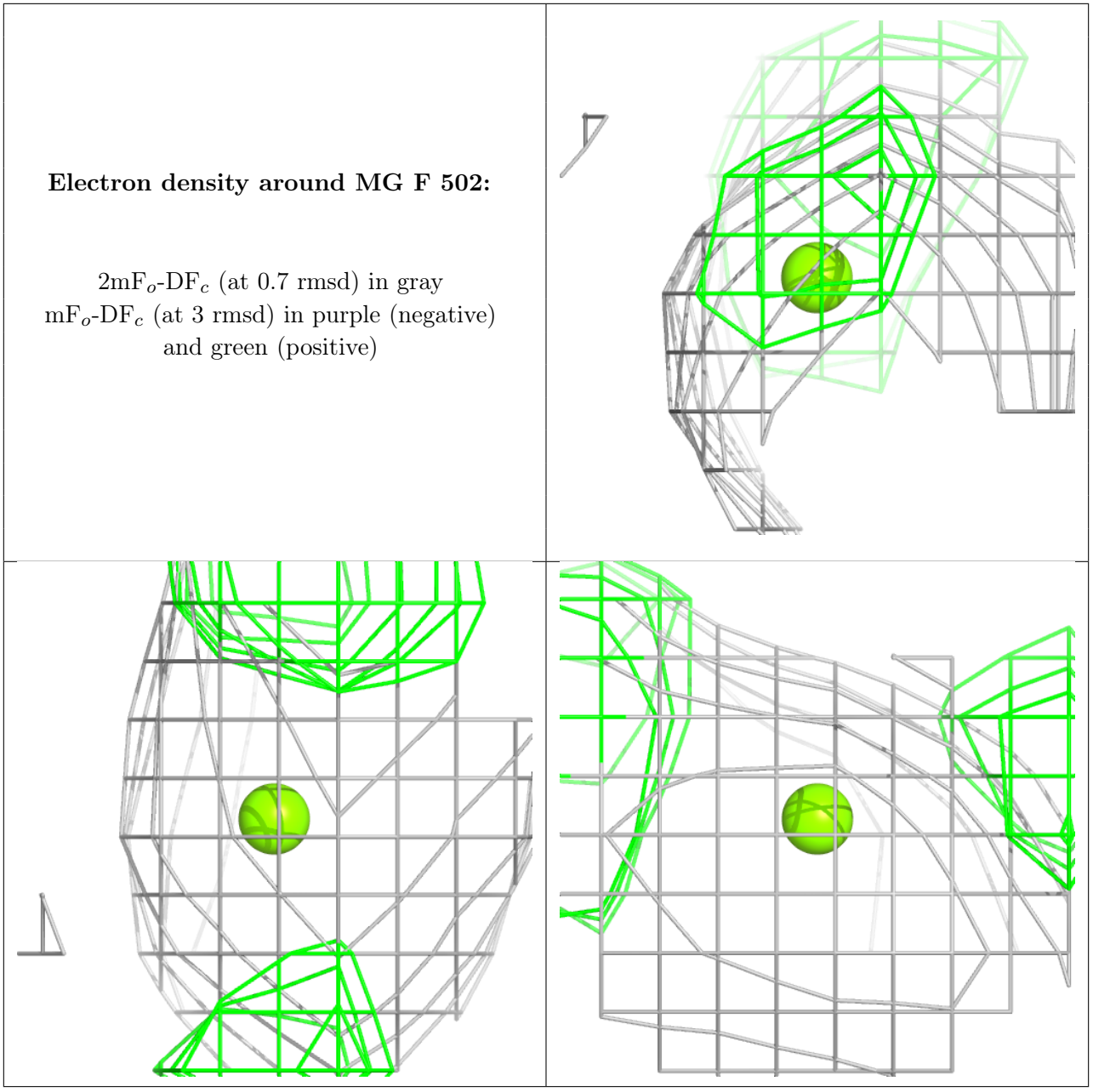
Electron density around MG A 504:

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



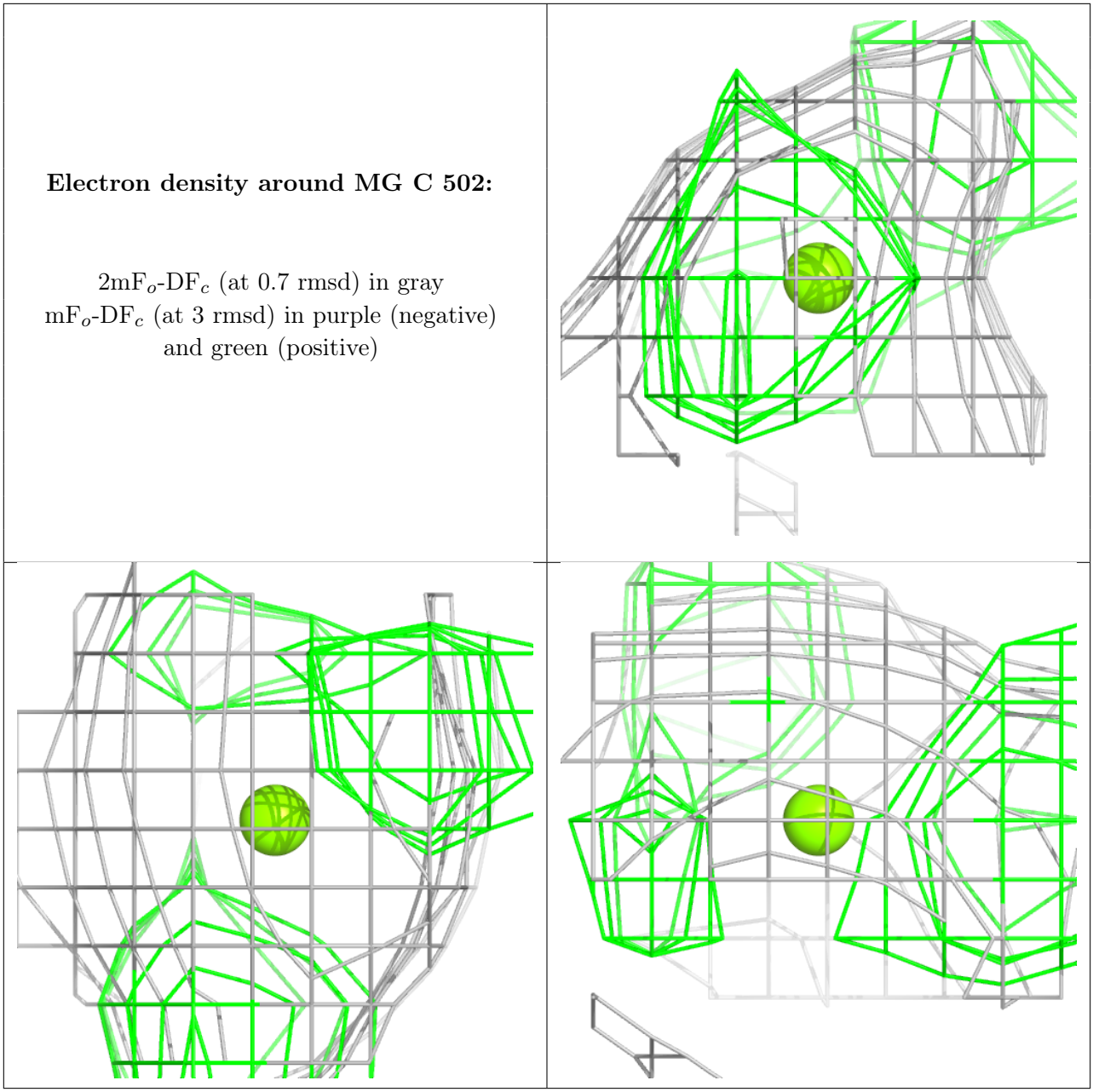
Electron density around MG F 502:

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



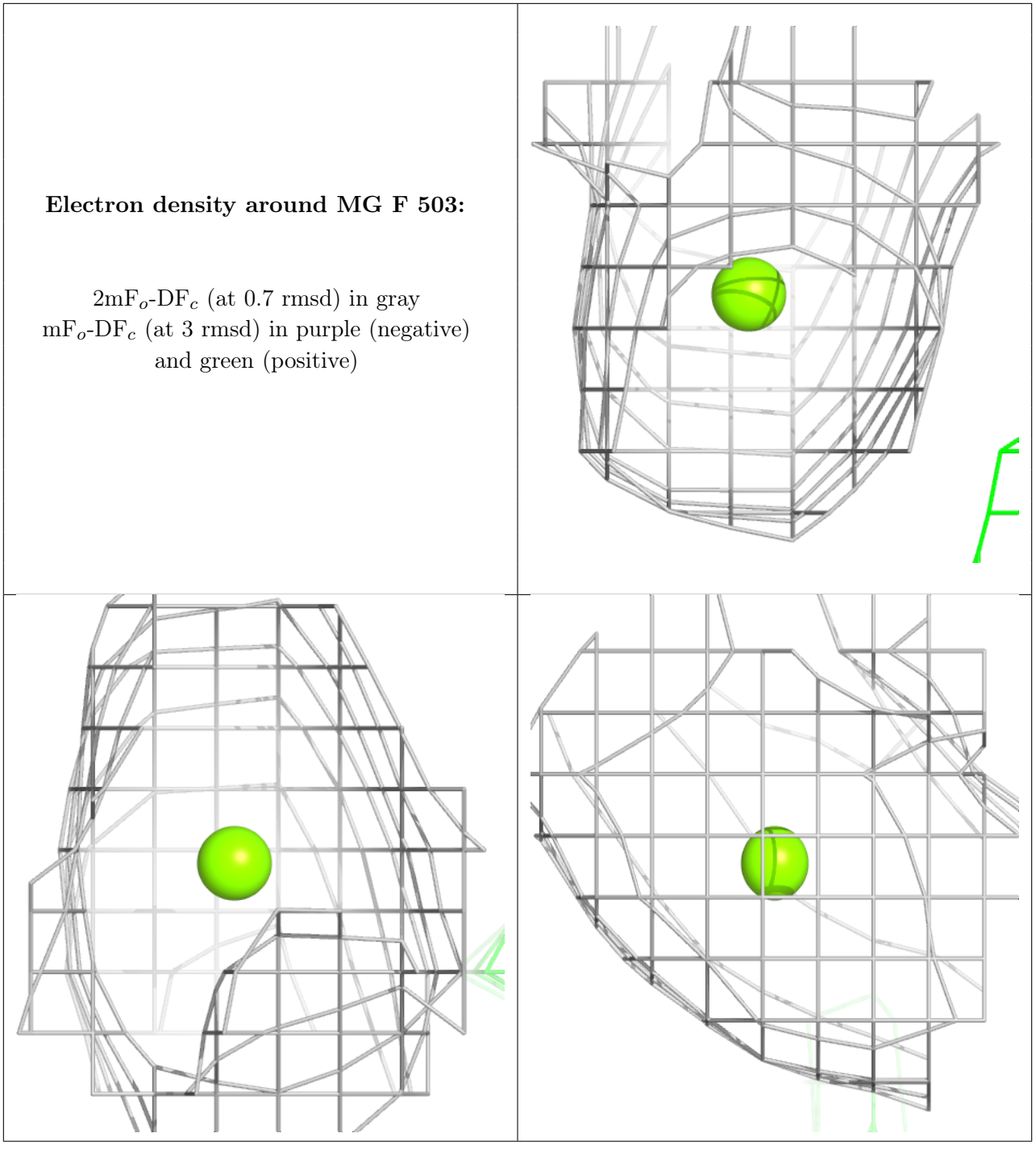
Electron density around MG C 502:

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



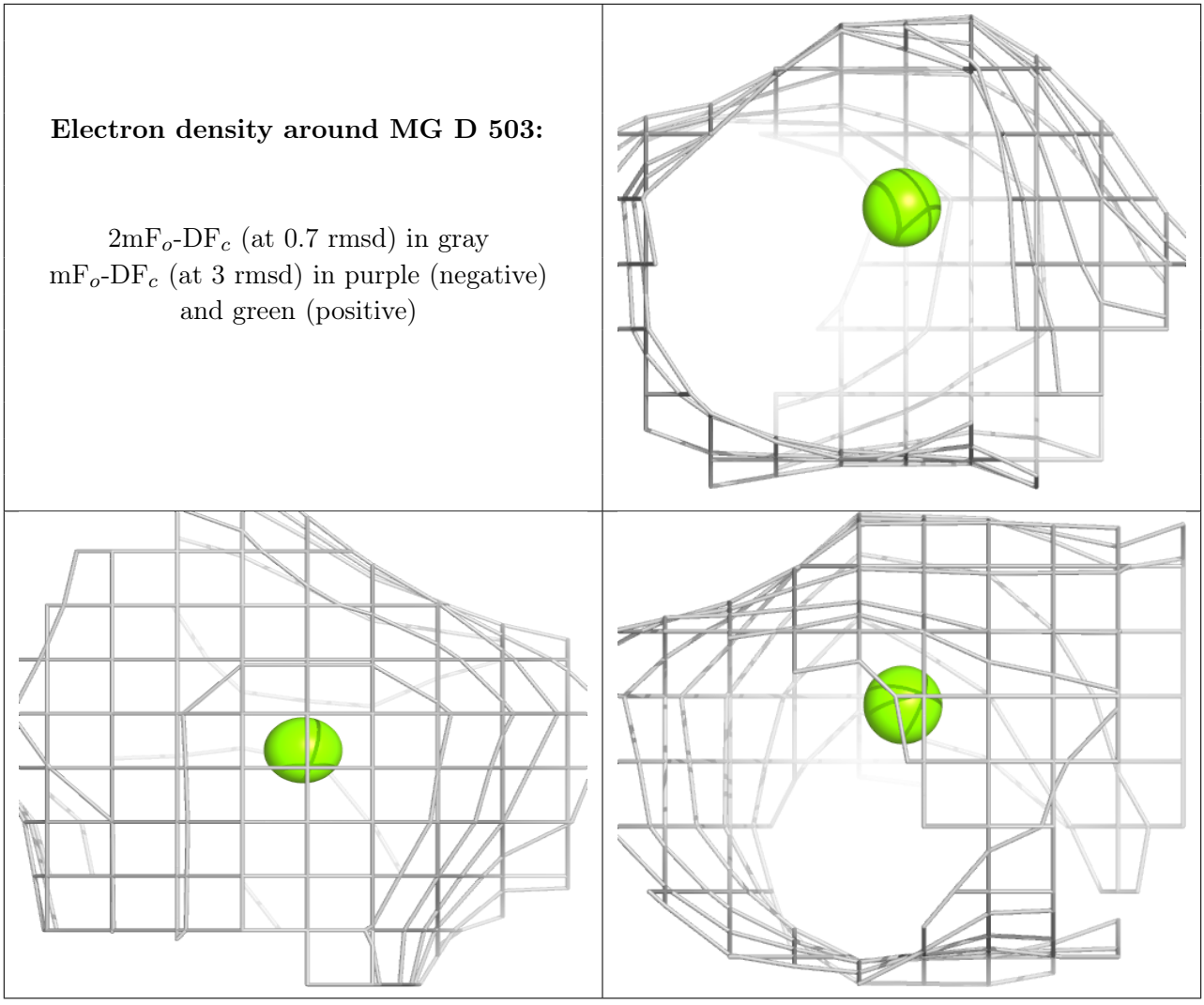
Electron density around MG F 503:

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



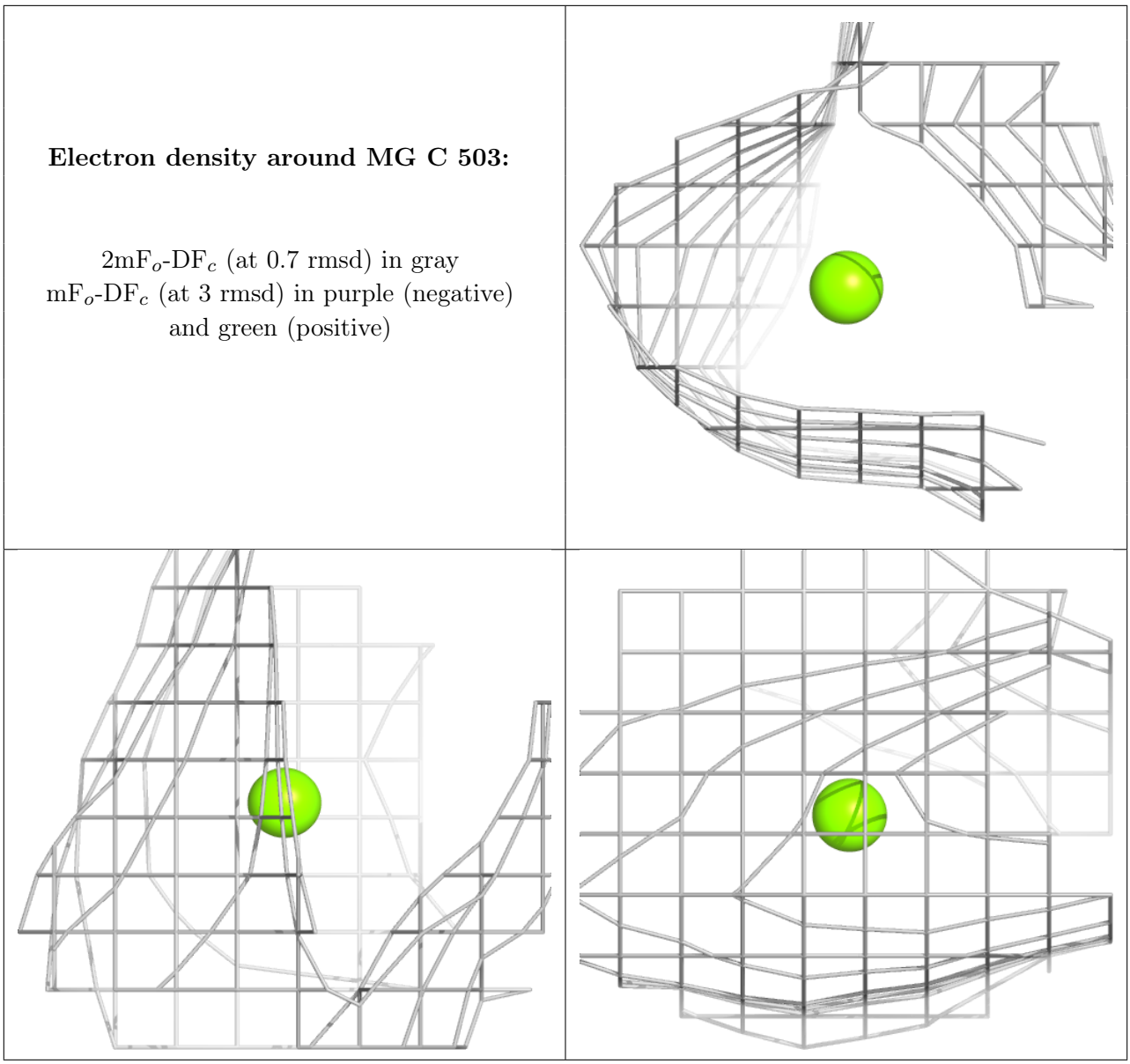
Electron density around MG D 503:

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



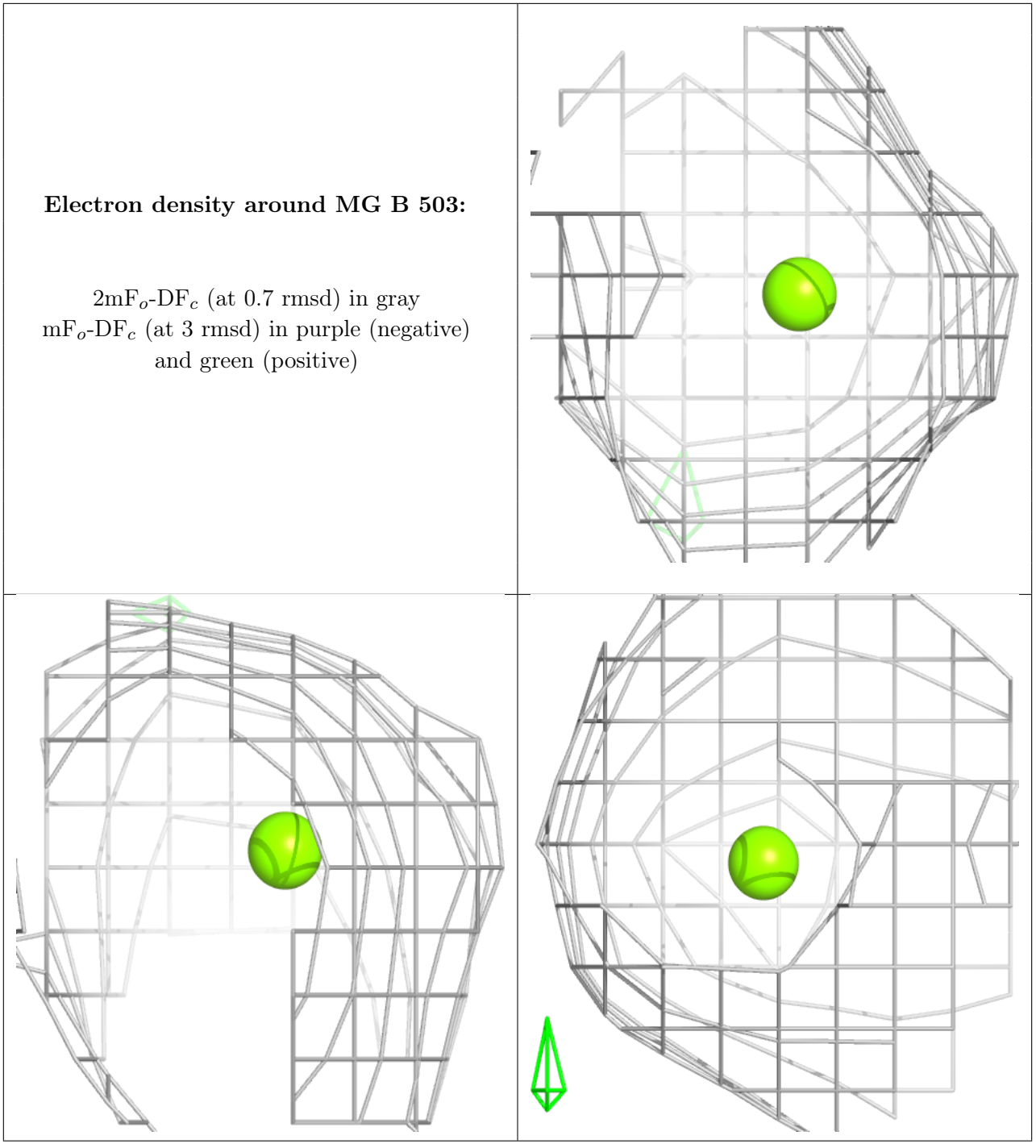
Electron density around MG C 503:

$2mF_o$-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 B 503:

$2mF_o$-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.