



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:41 PM UTC

PDB ID : 9K2N / pdb_00009k2n
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

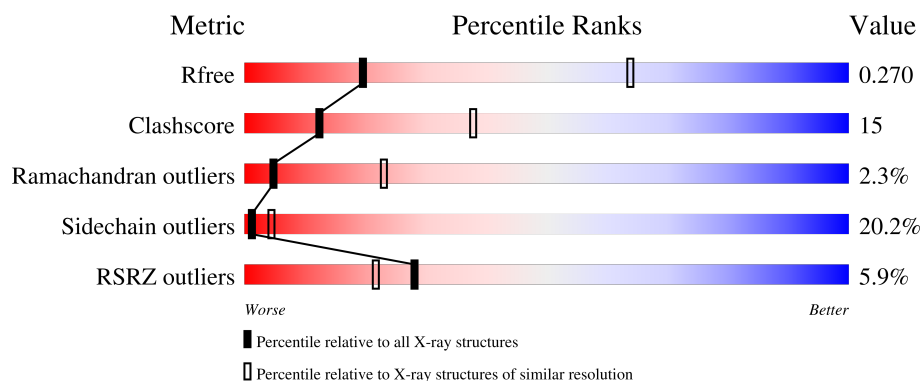
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	468	
1	B	468	
1	C	468	
1	D	468	
1	E	468	

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Mol	Chain	Length	Quality of chain
1	F	468	

2 Entry composition [i](#)

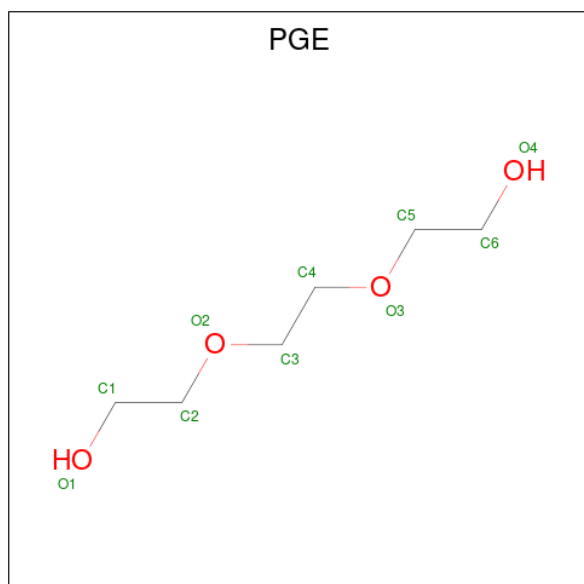
There are 5 unique types of molecules in this entry. The entry contains 43046 atoms, of which 21160 are hydrogens and 0 are deuteriums.

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.

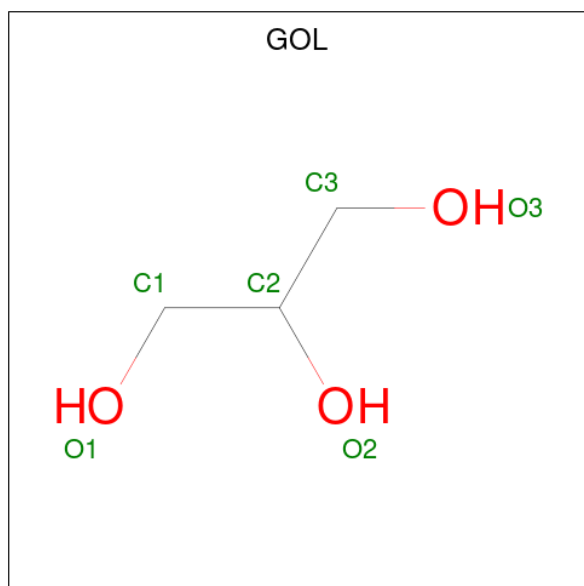
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	468	Total	C	H	N	O	S	111	0	0
			7152	2304	3515	613	699	21			
1	B	468	Total	C	H	N	O	S	111	0	0
			7152	2304	3515	613	699	21			
1	C	468	Total	C	H	N	O	S	111	0	0
			7152	2304	3515	613	699	21			
1	D	468	Total	C	H	N	O	S	111	0	0
			7155	2305	3517	613	699	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 (CCD ID: 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 (CCD ID: 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 (CCD ID: 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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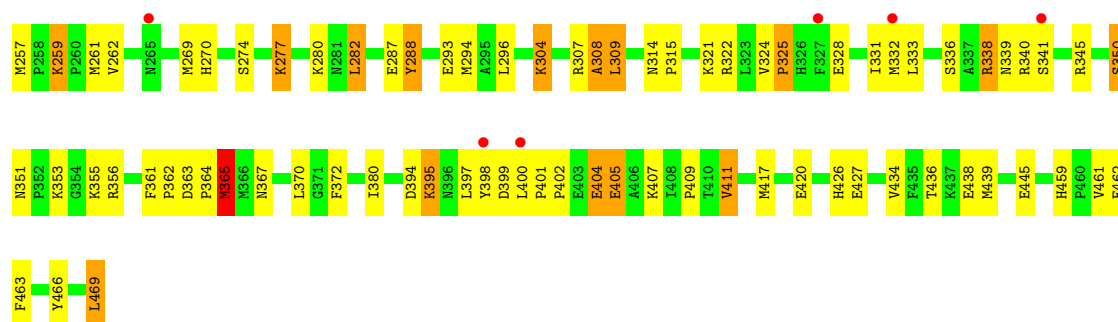
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		

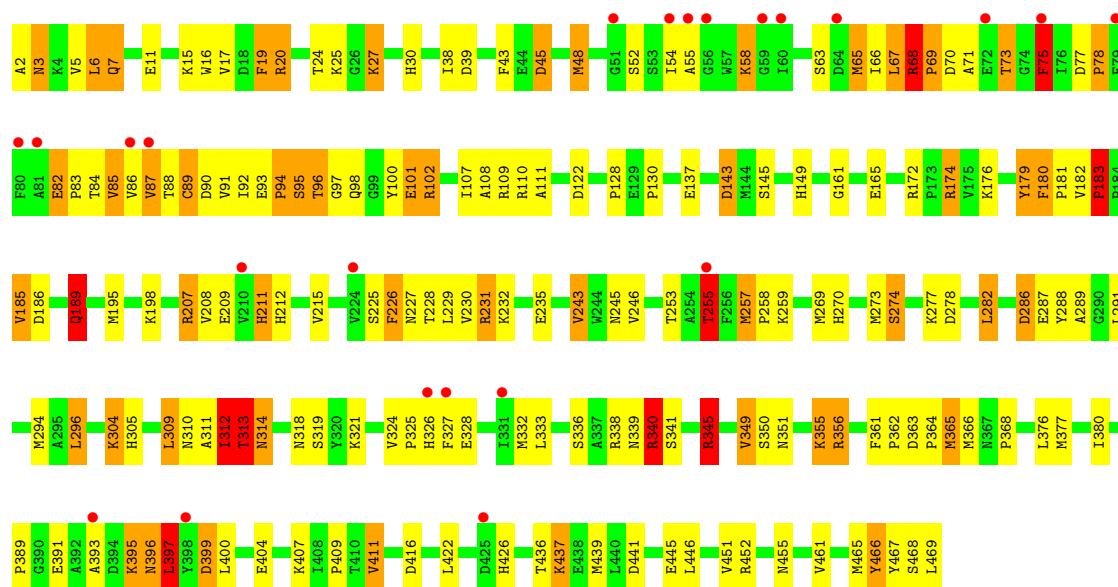
- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



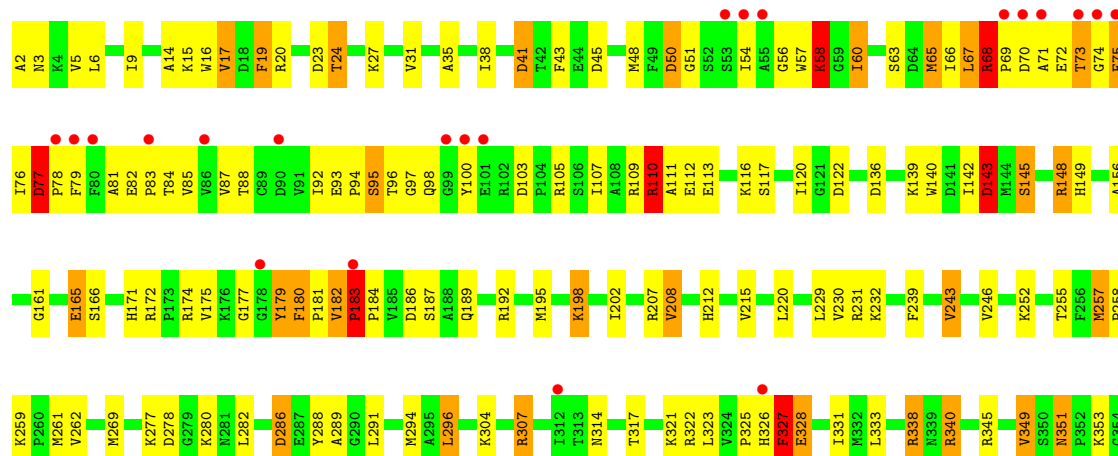
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	1	Total	C	H	O	2	0
			10	2	6	2		

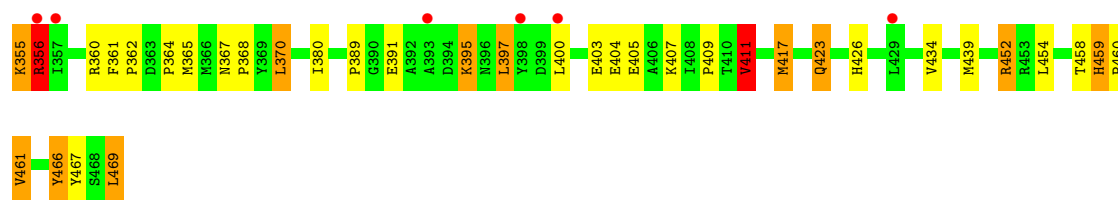


• Molecule 1: Glutamine synthetase

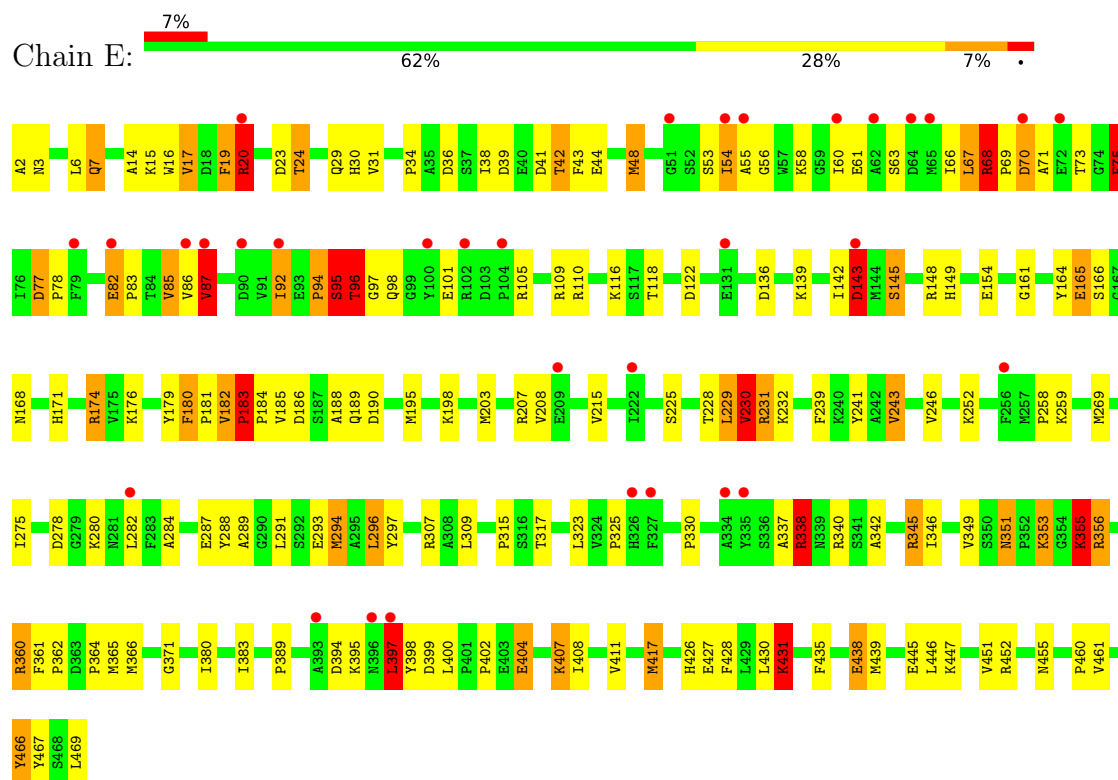


• Molecule 1: Glutamine synthetase

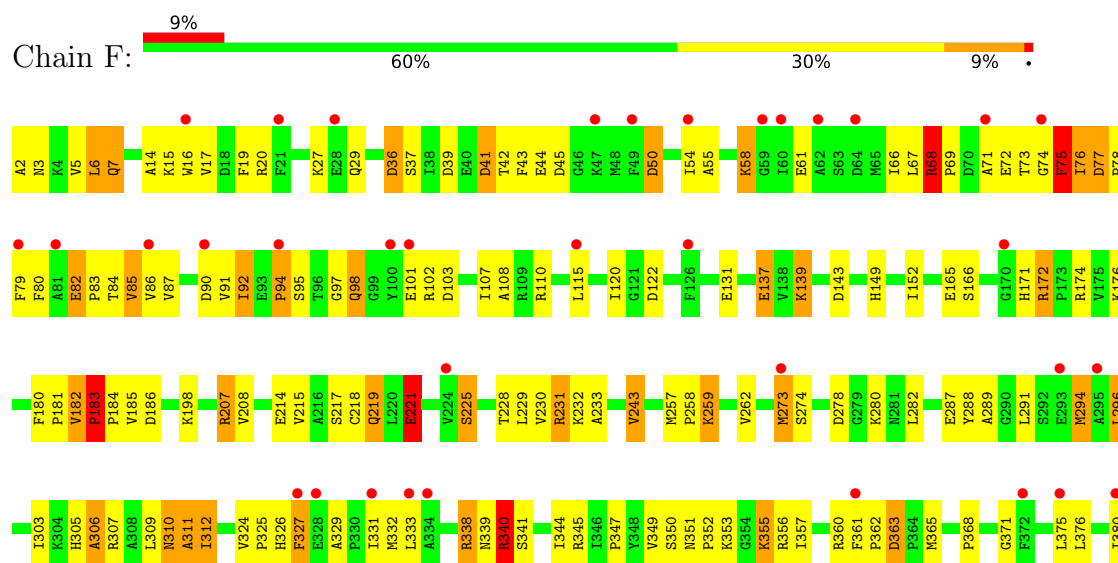


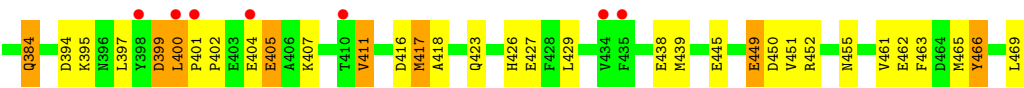


• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	3545 reflections (4.83%)	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	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, MG, GOL, EDO

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	0.87	0/3729	1.52	44/5054 (0.9%)
1	B	0.83	0/3729	1.49	48/5054 (0.9%)
1	C	0.81	1/3729 (0.0%)	1.45	39/5054 (0.8%)
1	D	0.78	2/3730 (0.1%)	1.43	35/5055 (0.7%)
1	E	0.72	1/3726 (0.0%)	1.33	21/5051 (0.4%)
1	F	0.73	1/3726 (0.0%)	1.36	33/5049 (0.7%)
All	All	0.79	5/22369 (0.0%)	1.43	220/30317 (0.7%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	171	HIS	CG-CD2	-6.08	1.29	1.35
1	E	145	SER	CA-CB	-5.77	1.44	1.53
1	C	319	SER	CA-CB	-5.29	1.44	1.53
1	D	145	SER	CA-CB	-5.28	1.45	1.53
1	D	469	LEU	C-O	5.05	1.33	1.23

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	PHE	N-CA-CB	12.14	131.01	110.49
1	D	77	ASP	CA-CB-CG	11.87	124.47	112.60
1	B	75	PHE	CB-CA-C	-11.19	88.15	110.42
1	B	77	ASP	CB-CA-C	10.89	130.66	113.57
1	D	75	PHE	CA-CB-CG	10.63	124.43	113.80

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	147	1
1	B	3637	3515	3485	129	0
1	C	3637	3515	3485	125	0
1	D	3638	3517	3487	125	1
1	E	3634	3508	3476	107	0
1	F	3635	3514	3484	99	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	662	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 662 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%)	9	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	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	466/468 (100%)	423 (91%)	37 (8%)	6 (1%)	9	33
1	E	466/468 (100%)	417 (90%)	36 (8%)	13 (3%)	4	19
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 ⓘ

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%)	305 (80%)	76 (20%)	1	5
1	B	381/387 (98%)	299 (78%)	82 (22%)	1	3
1	C	381/387 (98%)	300 (79%)	81 (21%)	1	3
1	D	381/387 (98%)	320 (84%)	61 (16%)	2	10
1	E	380/387 (98%)	308 (81%)	72 (19%)	1	6
1	F	381/387 (98%)	291 (76%)	90 (24%)	1	2
All	All	2285/2322 (98%)	1823 (80%)	462 (20%)	1	4

5 of 462 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	436	THR
1	F	397	LEU
1	D	355	LYS
1	F	375	LEU

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Mol	Chain	Res	Type
1	F	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	396	ASN
1	F	396	ASN
1	D	351	ASN
1	F	339	ASN
1	F	189	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	A	503	-	5,5,5	0.15	0	5,5,5	0.42	0
5	EDO	F	501	-	3,3,3	0.41	0	2,2,2	0.44	0
3	GOL	A	502	-	5,5,5	0.15	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	501	-	5,5,5	0.22	0	5,5,5	0.68	0
3	GOL	C	501	-	5,5,5	0.26	0	5,5,5	0.48	0
3	GOL	B	502	-	5,5,5	0.09	0	5,5,5	0.30	0
2	PGE	A	501	-	9,9,9	0.26	0	8,8,8	0.20	0
3	GOL	D	501	-	5,5,5	0.19	0	5,5,5	0.68	0
3	GOL	E	501	-	5,5,5	0.17	0	5,5,5	0.42	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	A	503	-	-	4/4/4/4	-
5	EDO	F	501	-	-	1/1/1/1	-
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	B	501	-	-	2/4/4/4	-
3	GOL	C	501	-	-	2/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
2	PGE	A	501	-	-	4/7/7/7	-
3	GOL	D	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 21 torsion outliers are listed below:

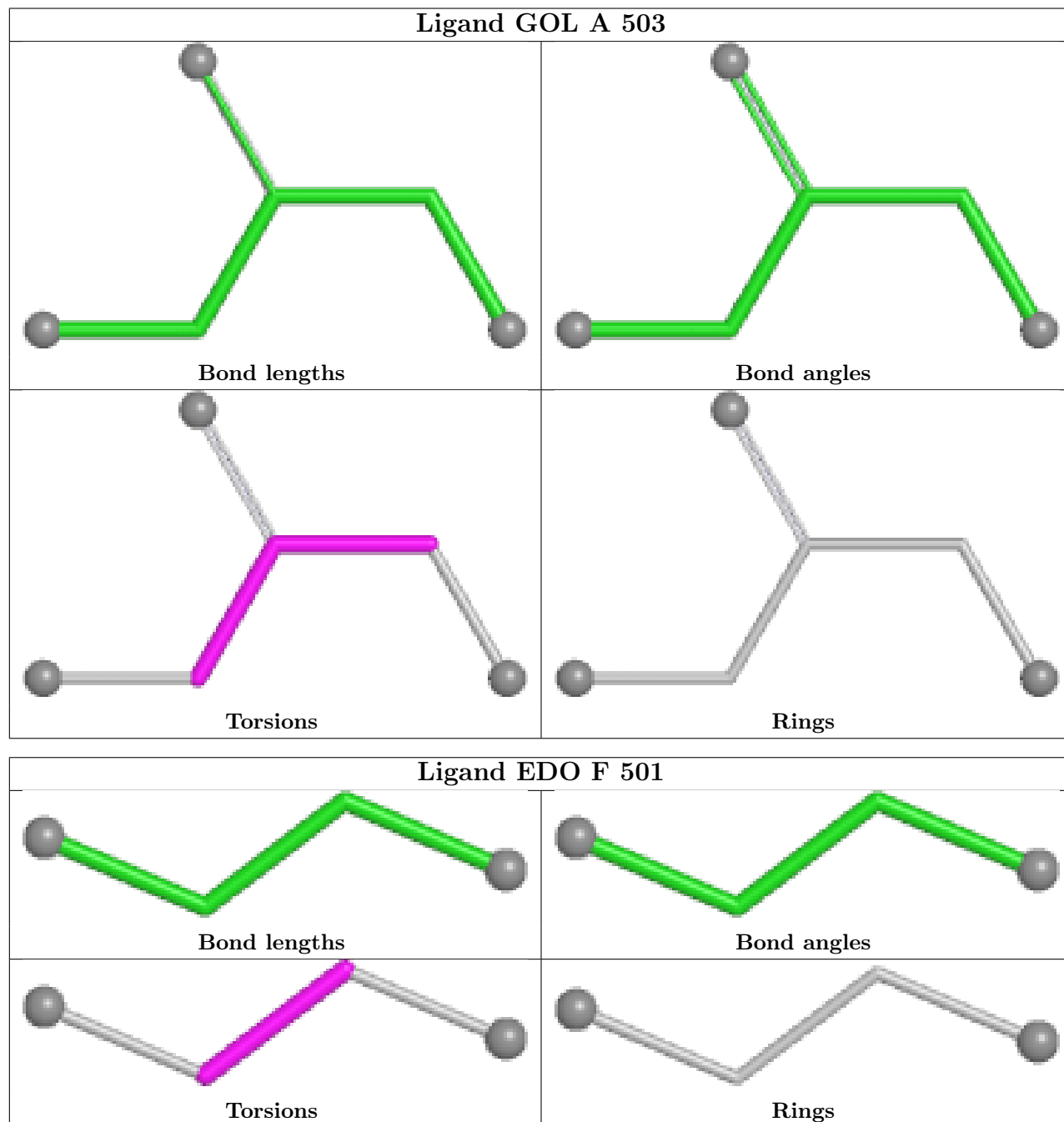
Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	A	503	GOL	O1-C1-C2-O2
3	A	503	GOL	O1-C1-C2-C3
3	A	503	GOL	C1-C2-C3-O3
3	B	501	GOL	C1-C2-C3-O3

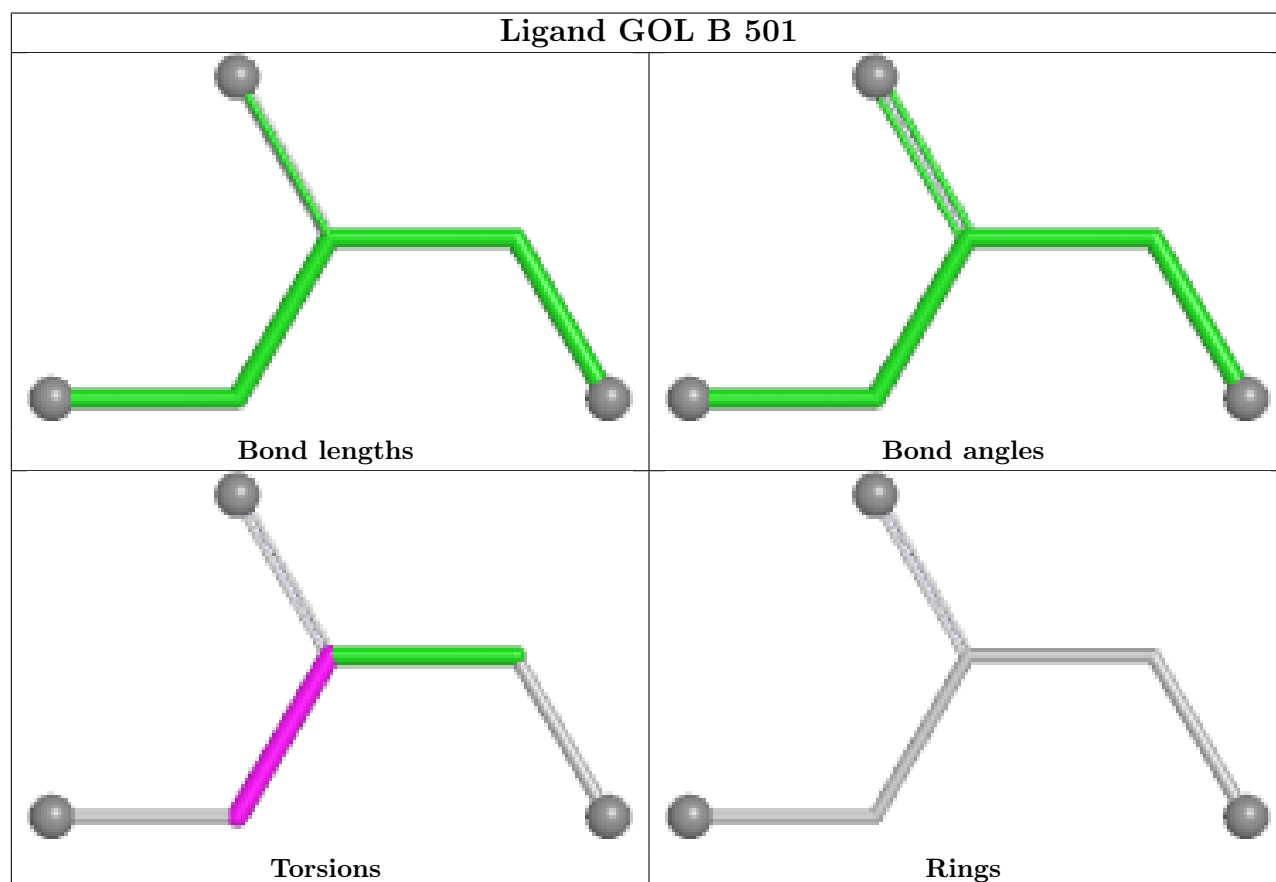
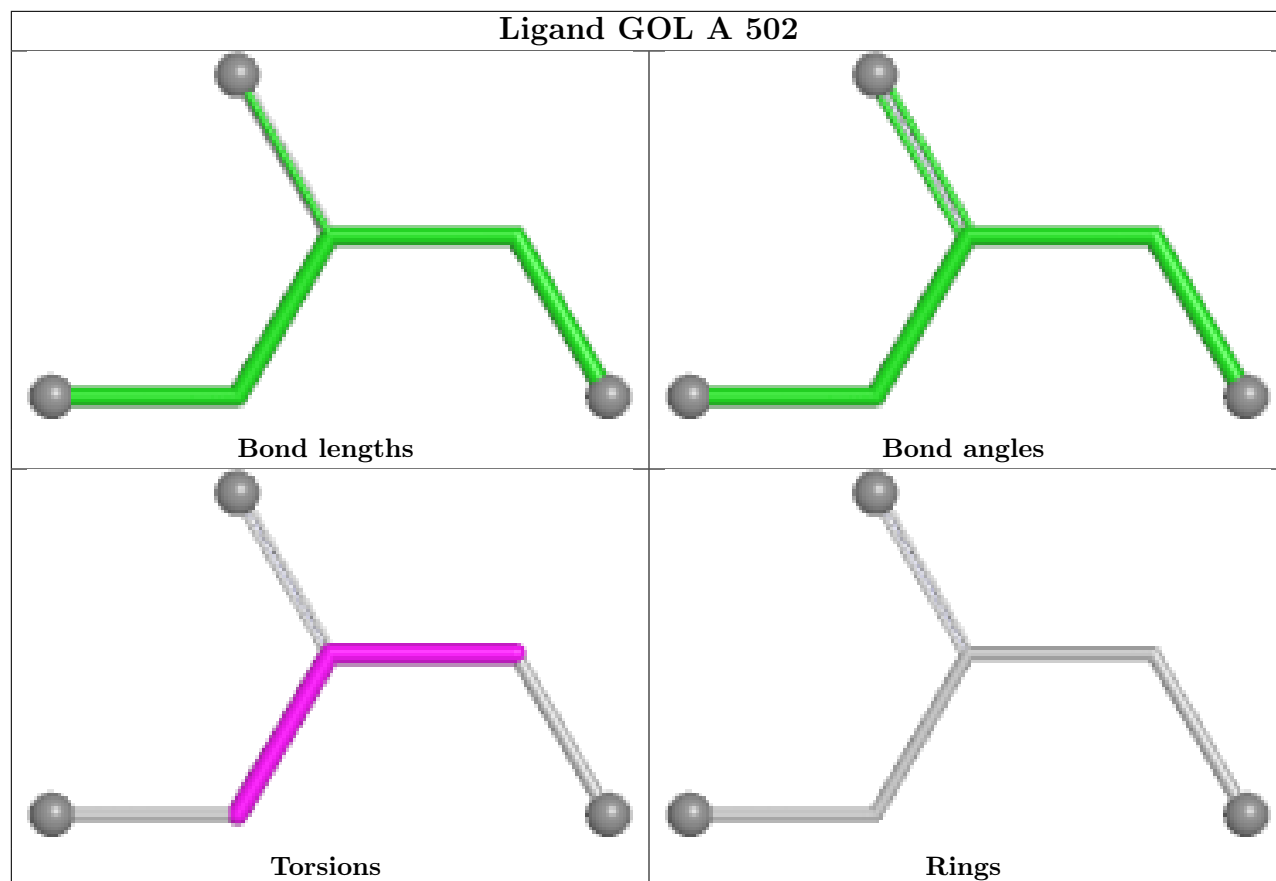
There are no ring outliers.

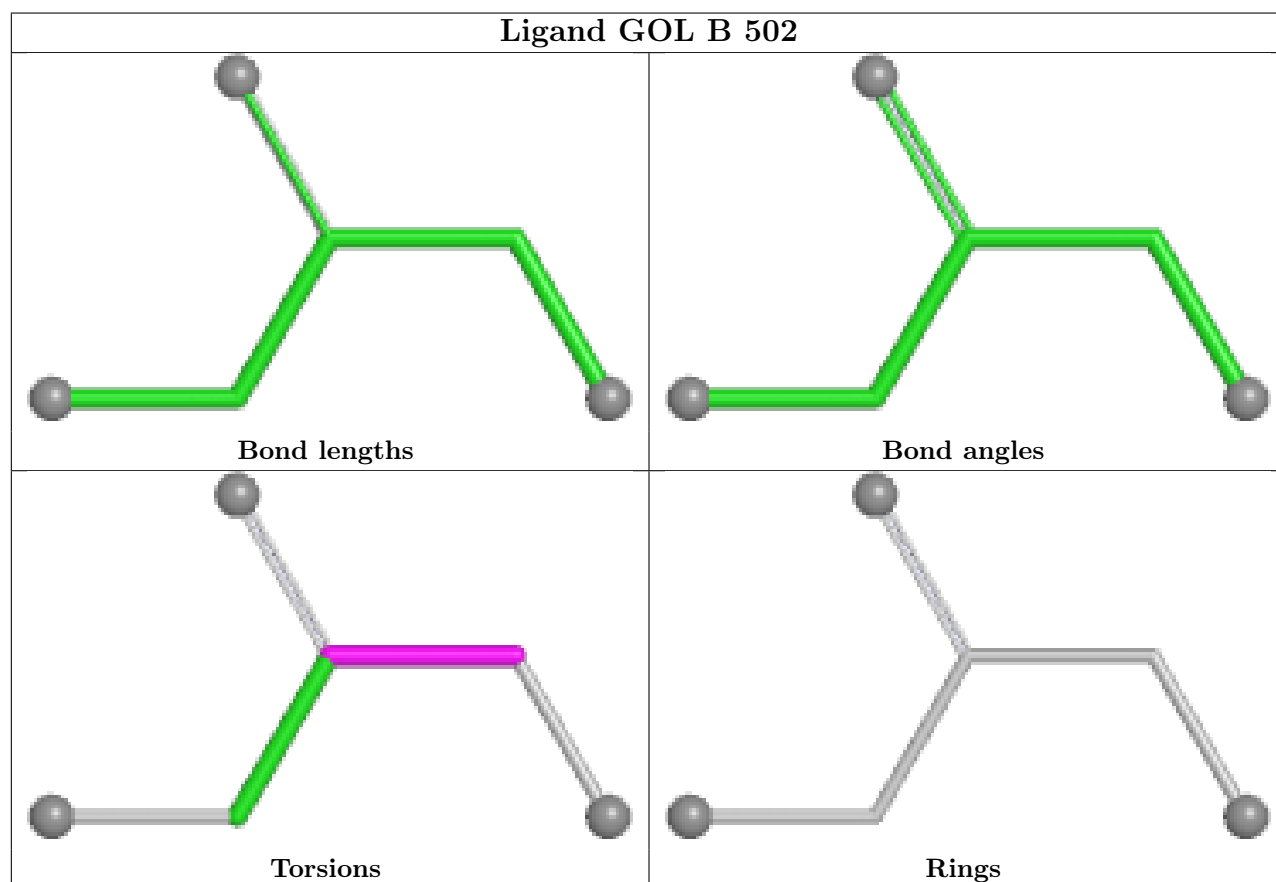
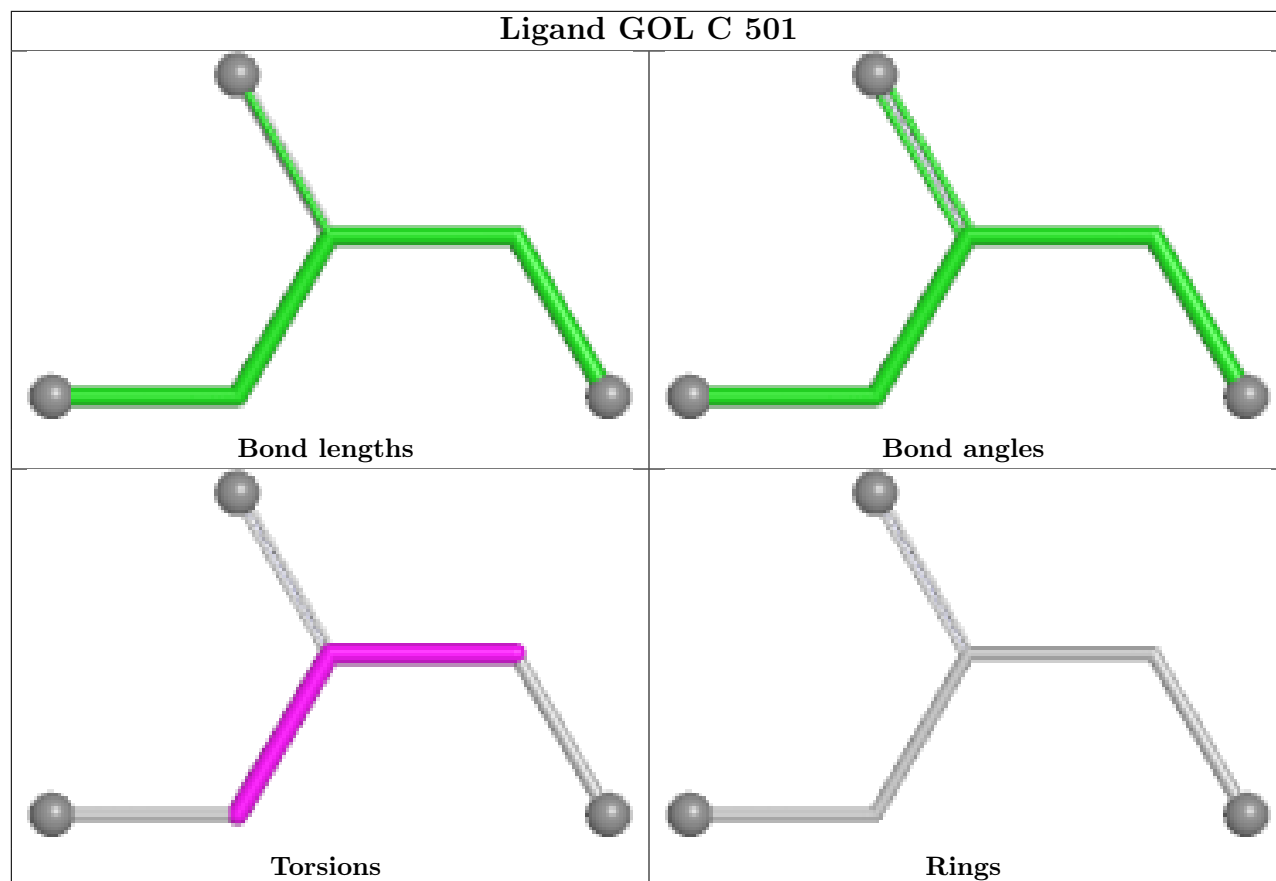
No monomer is involved in short contacts.

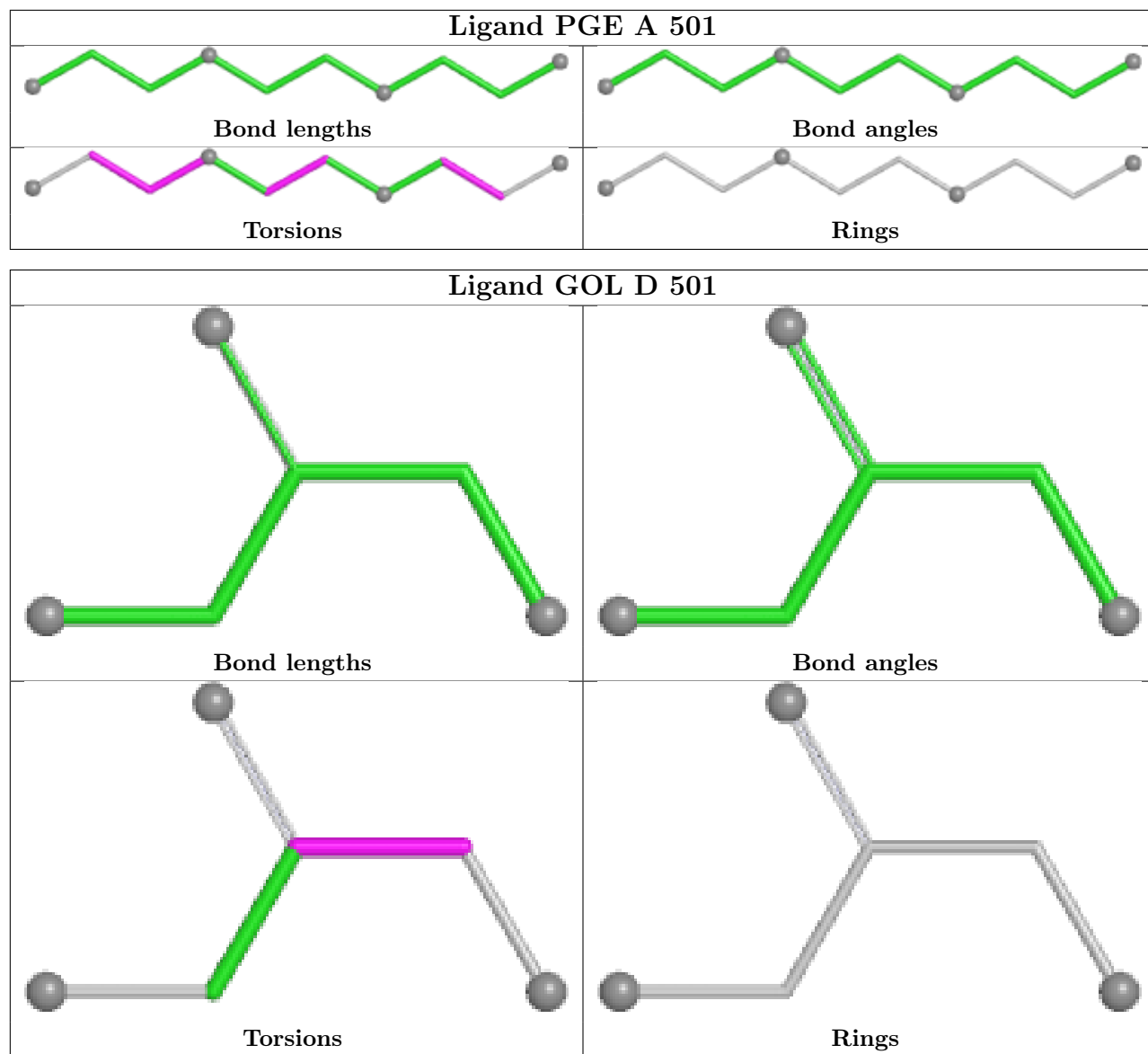
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

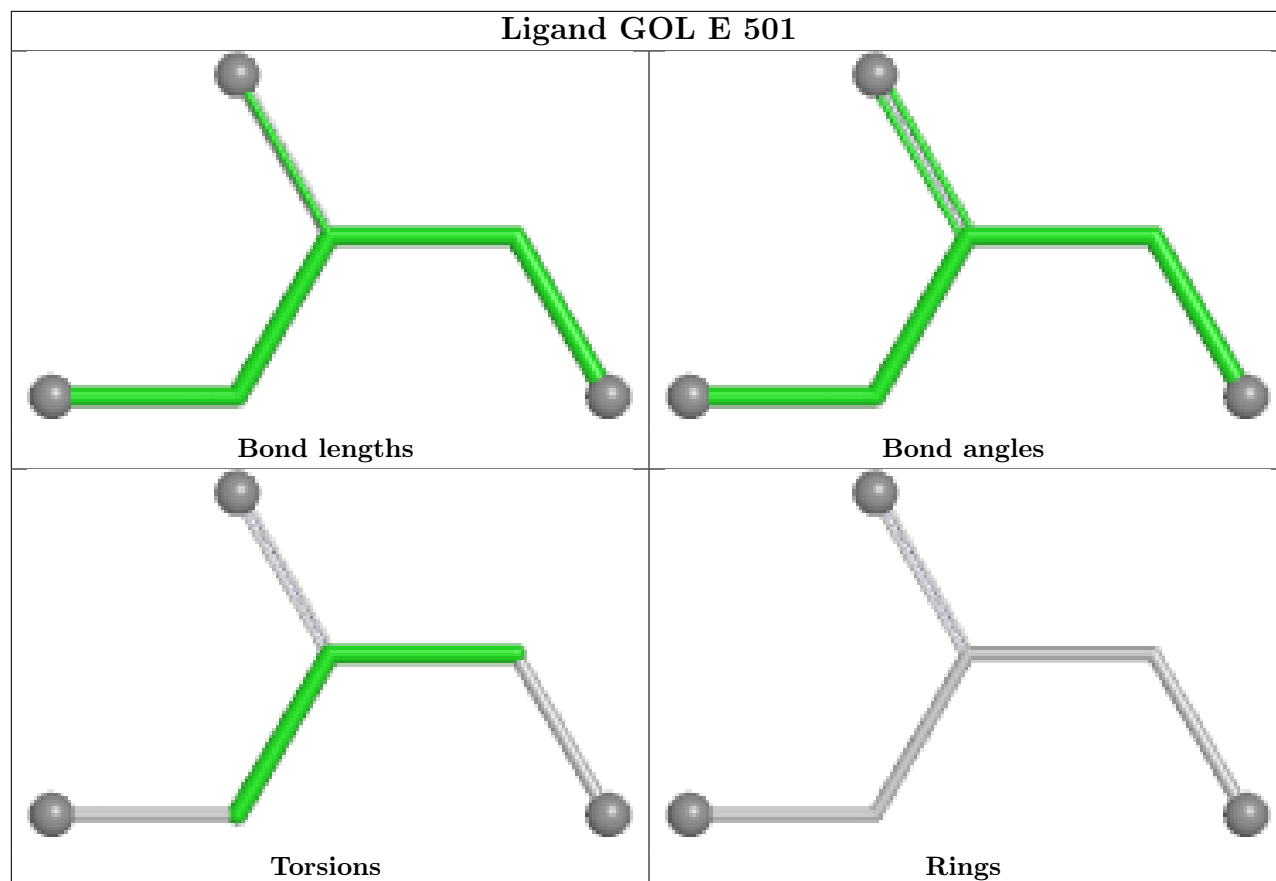
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	468/468 (100%)	0.18	19 (4%)	41	29	31, 70, 148, 235	0
1	B	468/468 (100%)	0.29	23 (4%)	35	26	38, 89, 156, 222	0
1	C	468/468 (100%)	0.45	23 (4%)	35	26	57, 102, 163, 265	0
1	D	468/468 (100%)	0.51	28 (5%)	27	21	41, 103, 183, 239	0
1	E	468/468 (100%)	0.75	32 (6%)	23	19	56, 141, 197, 248	0
1	F	468/468 (100%)	0.77	42 (8%)	15	14	65, 138, 214, 307	0
All	All	2808/2808 (100%)	0.49	167 (5%)	28	22	31, 104, 195, 307	0

The worst 5 of 167 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	86	VAL	6.6
1	F	100	TYR	6.3
1	F	60	ILE	5.4
1	A	54	ILE	5.3
1	B	100	TYR	5.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

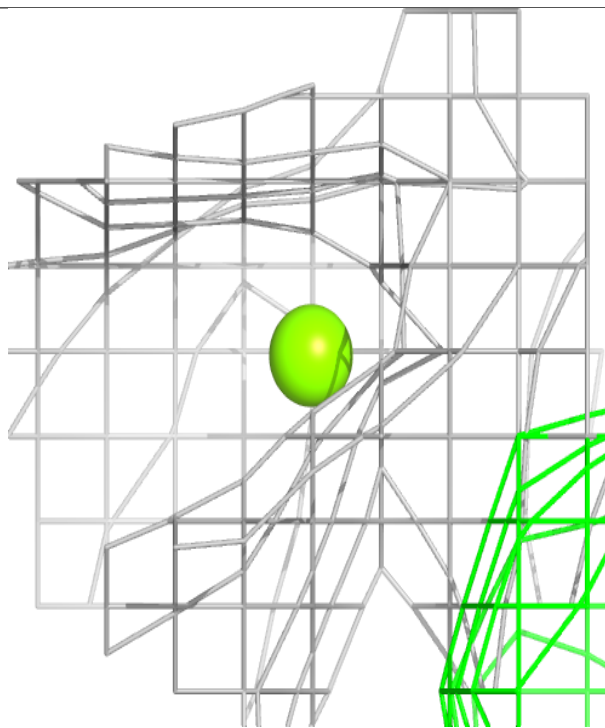
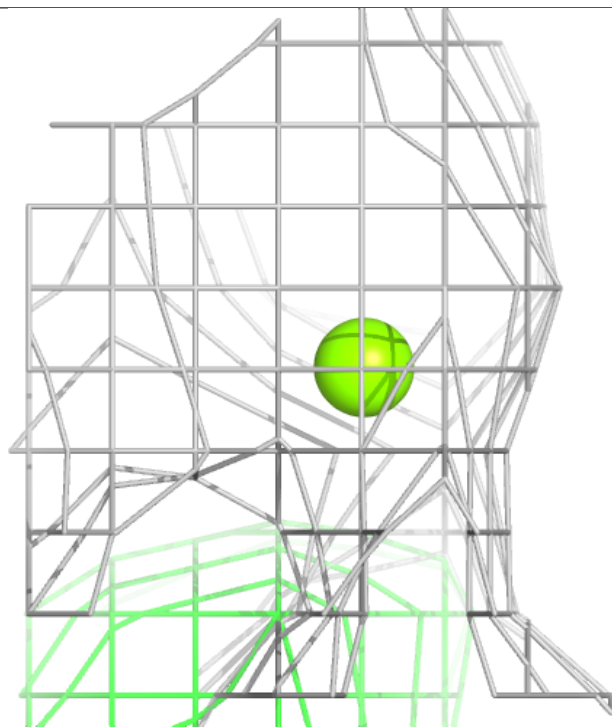
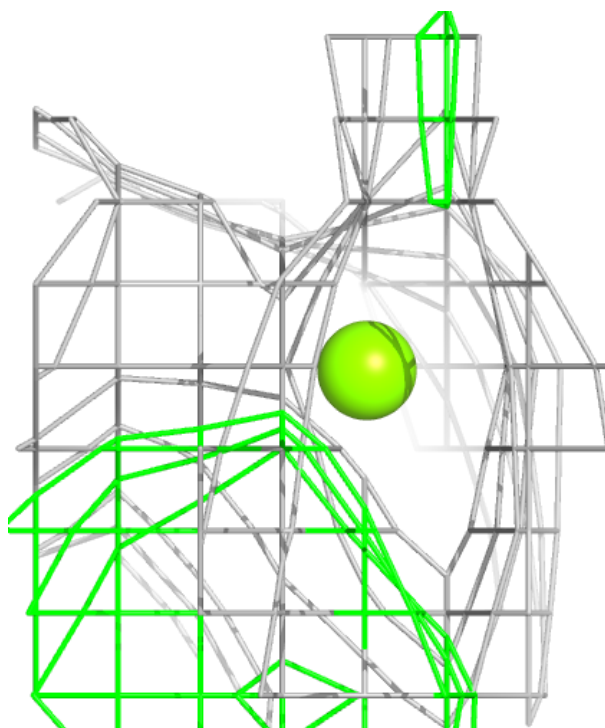
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	E	503	1/1	0.52	0.21	114,114,114,114	0
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
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
5	EDO	F	501	4/4	0.85	0.20	30,96,98,99	2
3	GOL	D	501	6/6	0.86	0.13	30,103,107,111	3
3	GOL	E	501	6/6	0.86	0.13	30,122,131,133	3
4	MG	E	502	1/1	0.88	0.16	66,66,66,66	0
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	0.93	0.10	68,68,68,68	0
4	MG	A	504	1/1	0.95	0.13	49,49,49,49	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	F	502	1/1	0.97	0.17	62,62,62,62	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	0.99	0.06	41,41,41,41	0
4	MG	A	505	1/1	1.00	0.07	39,39,39,39	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.

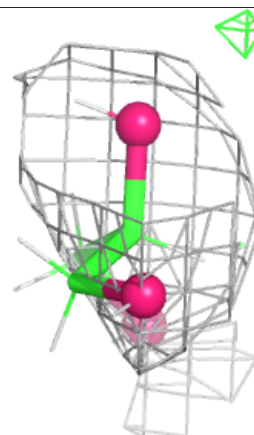
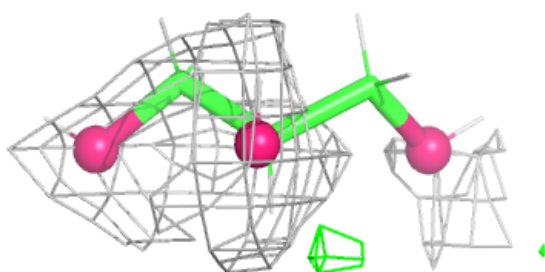
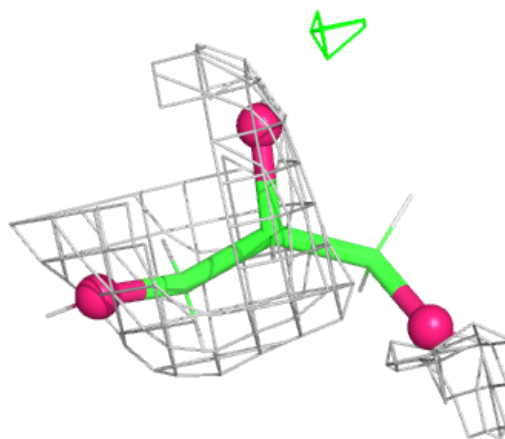
Electron density around MG E 503:

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



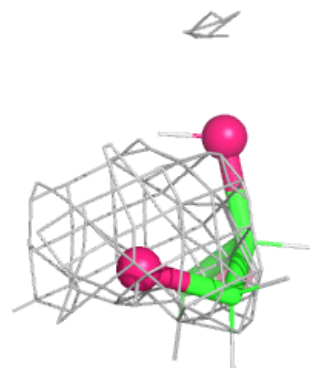
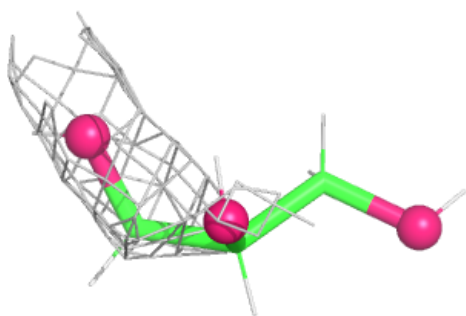
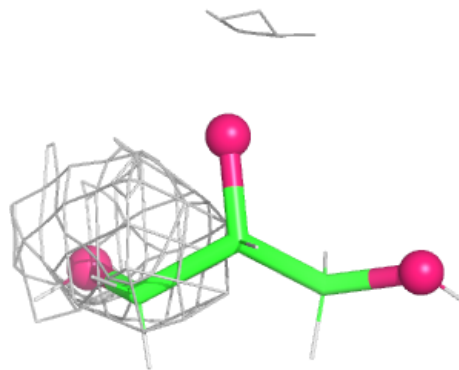
Electron density around GOL B 502:

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and green (positive)

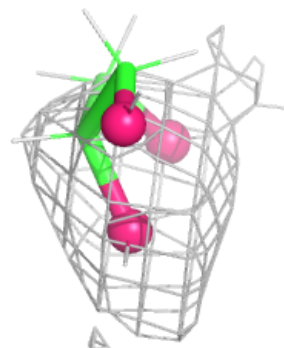
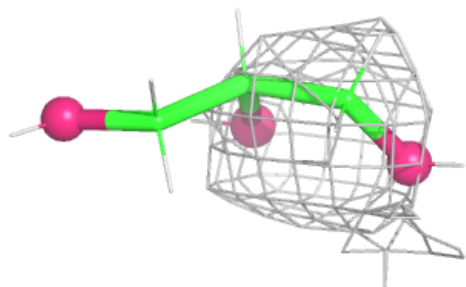
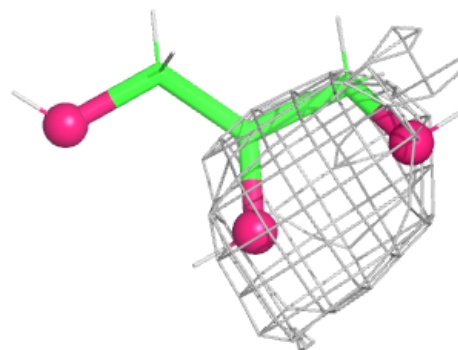


Electron density around GOL C 501:

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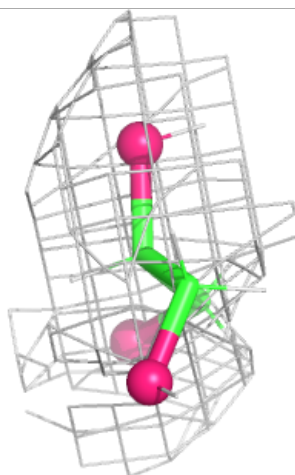
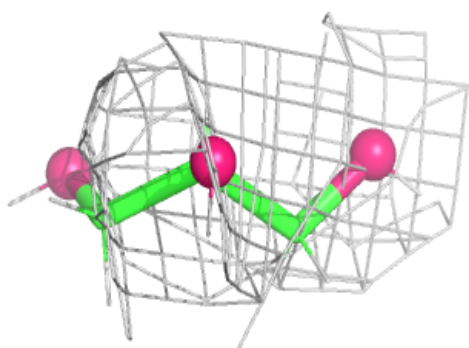
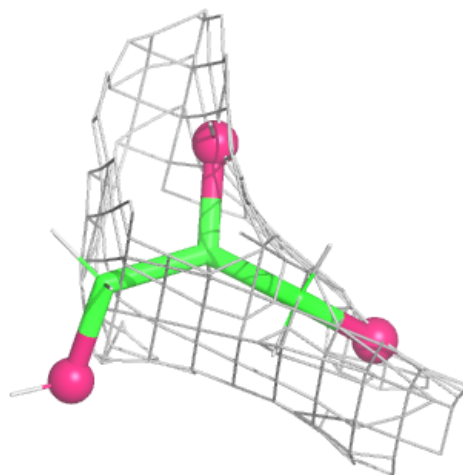
**Electron density around GOL B 501:**

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and green (positive)



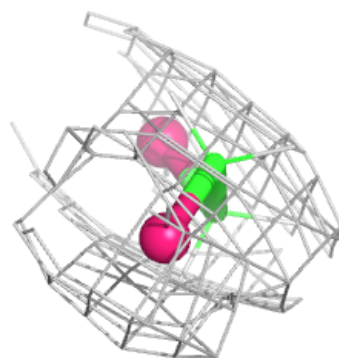
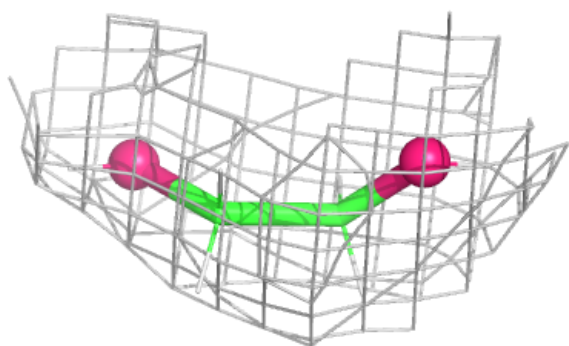
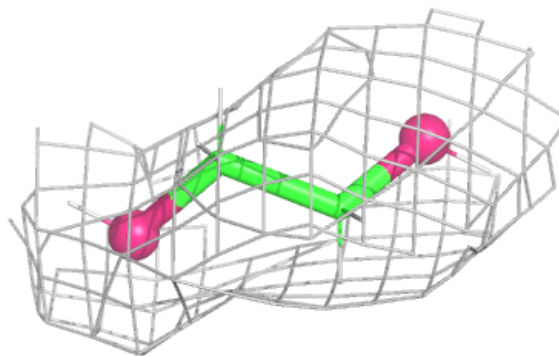
Electron density around GOL A 502:

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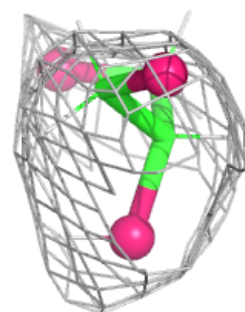
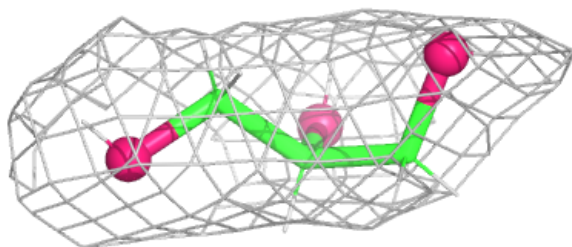
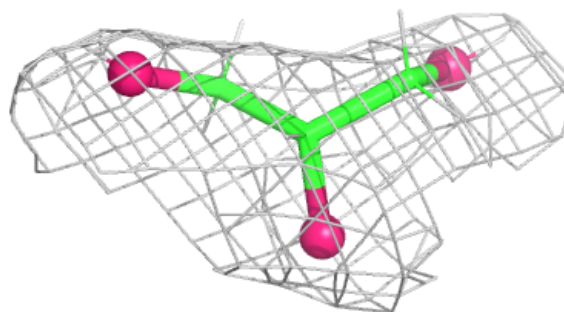


Electron density around EDO F 501:

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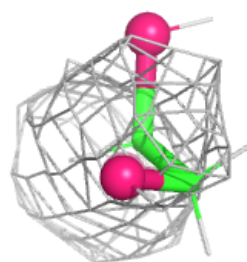
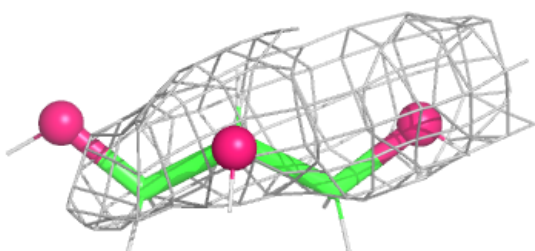
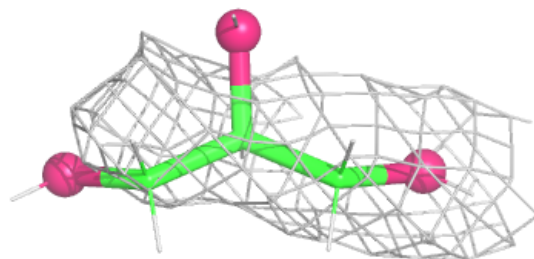
**Electron density around GOL D 501:**

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and green (positive)



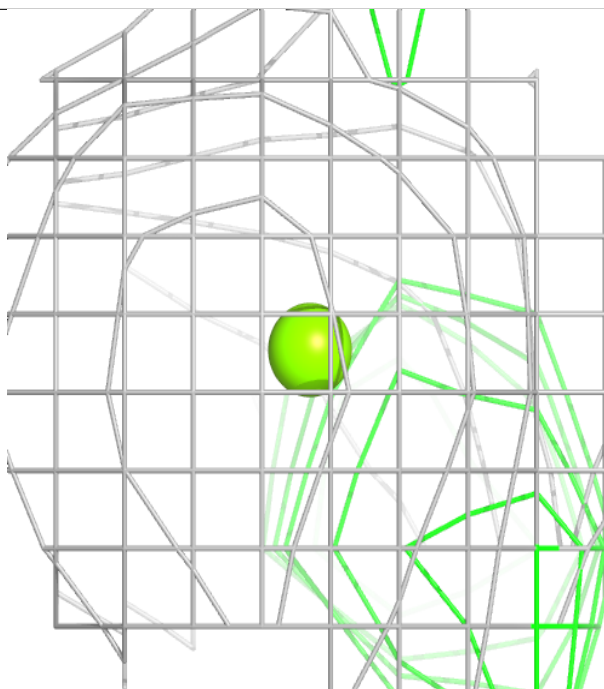
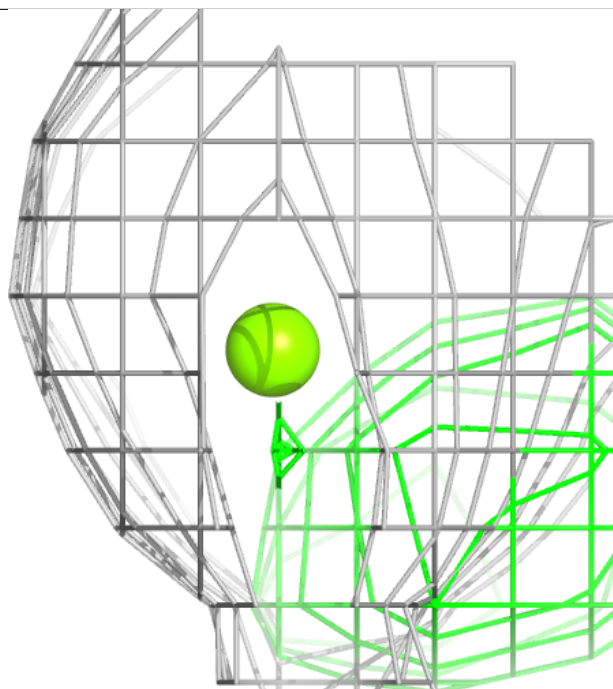
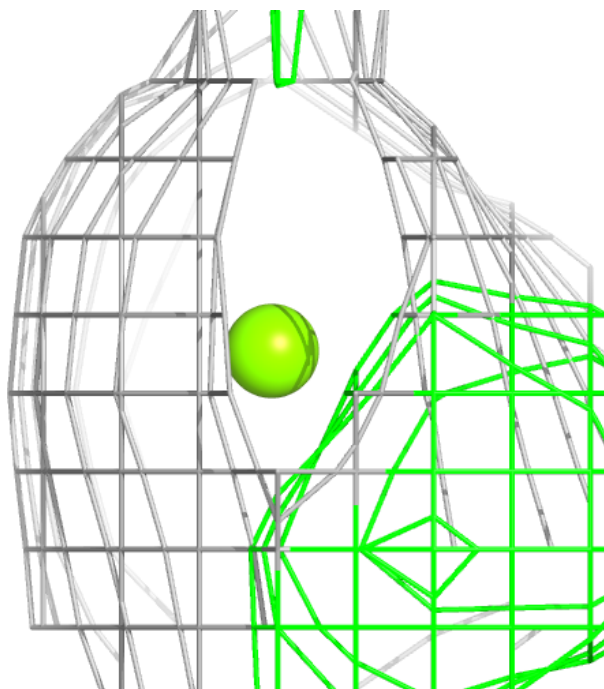
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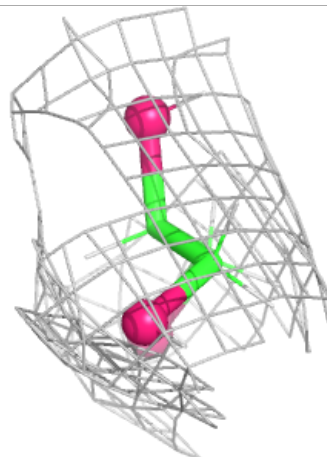
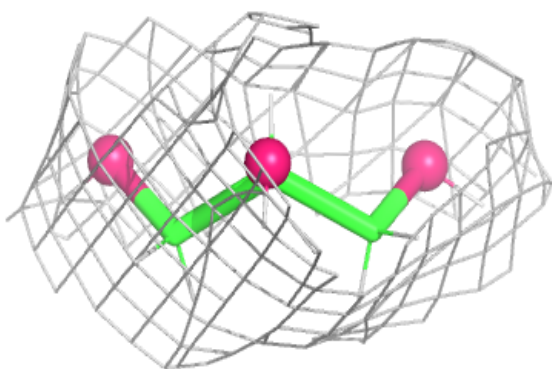
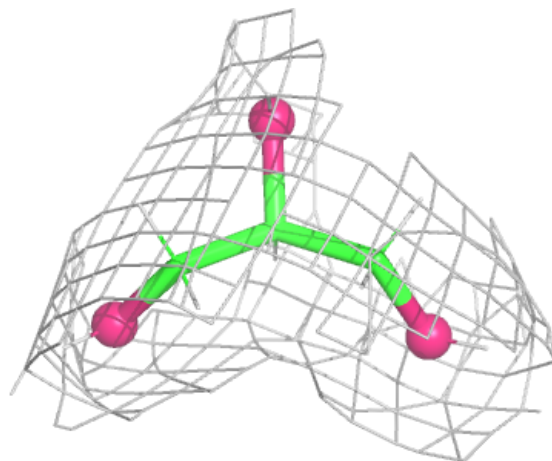
Electron density around MG E 502:

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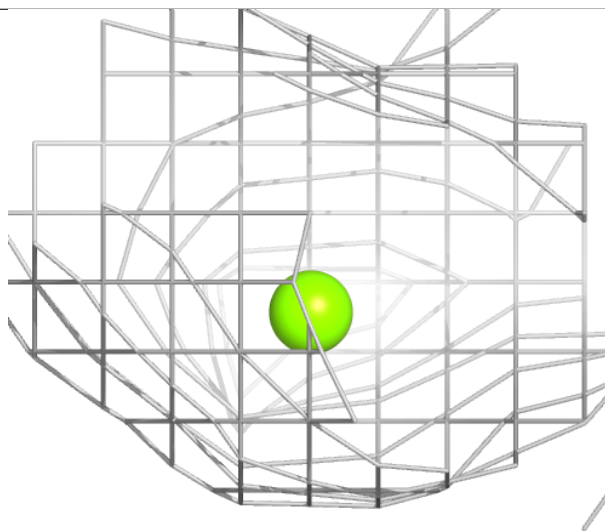
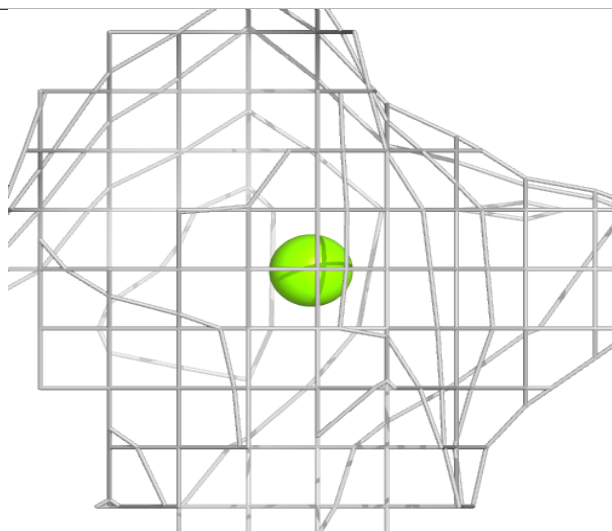
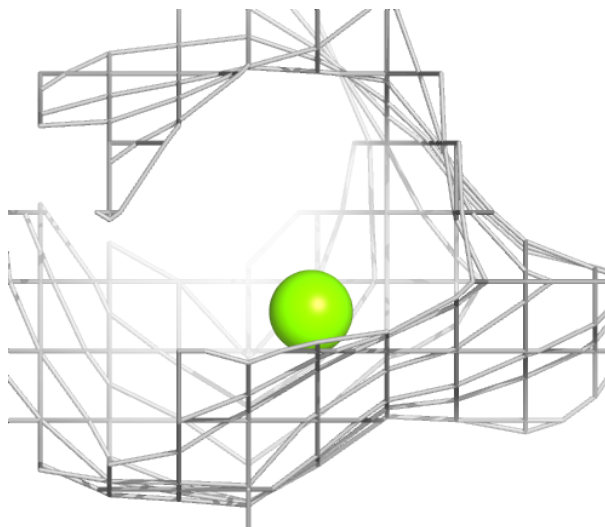
Electron density around GOL A 503:

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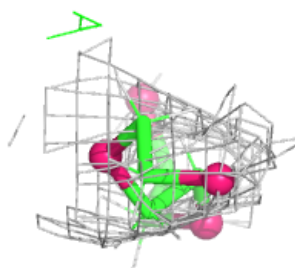
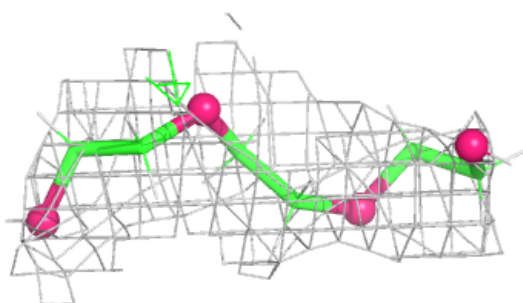
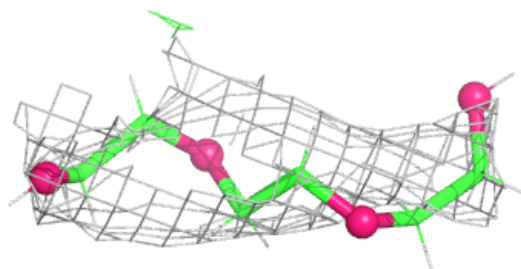
Electron density around MG B 504:

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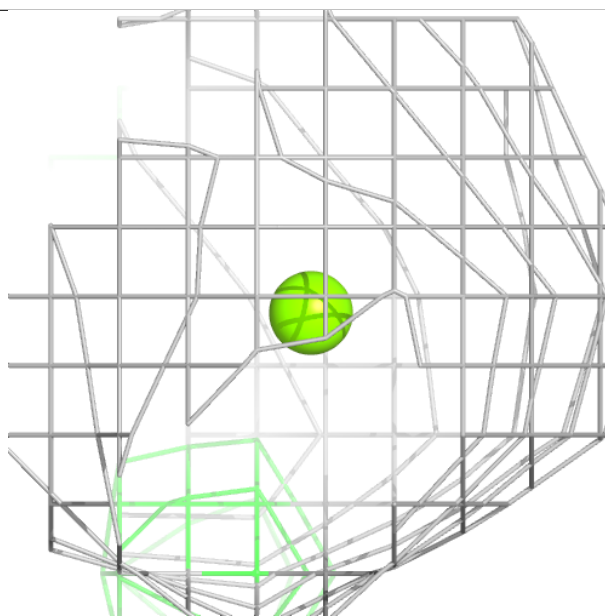
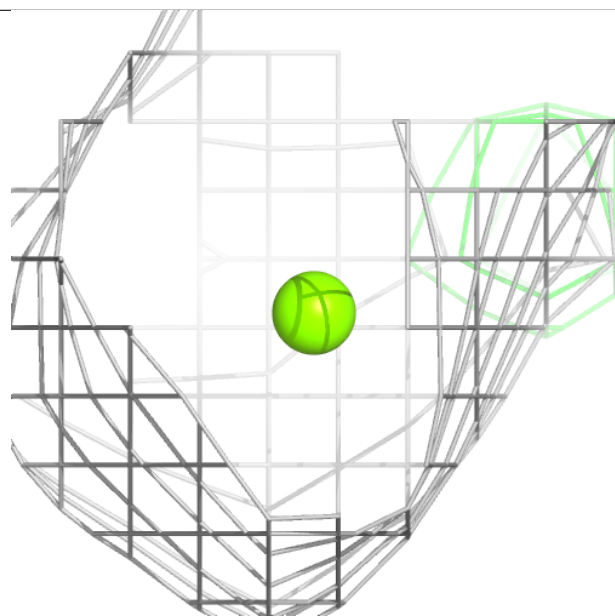
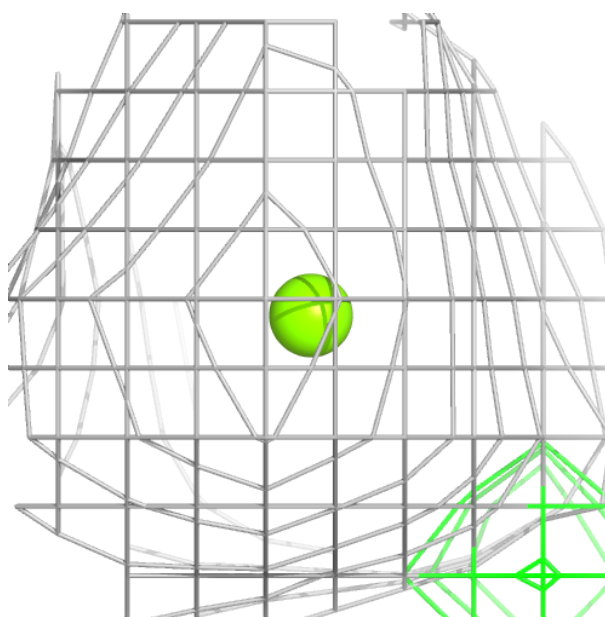
Electron density around PGE A 501:

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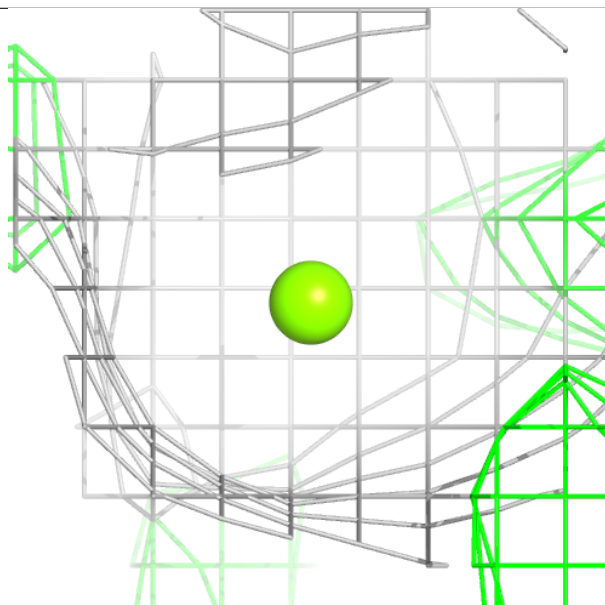
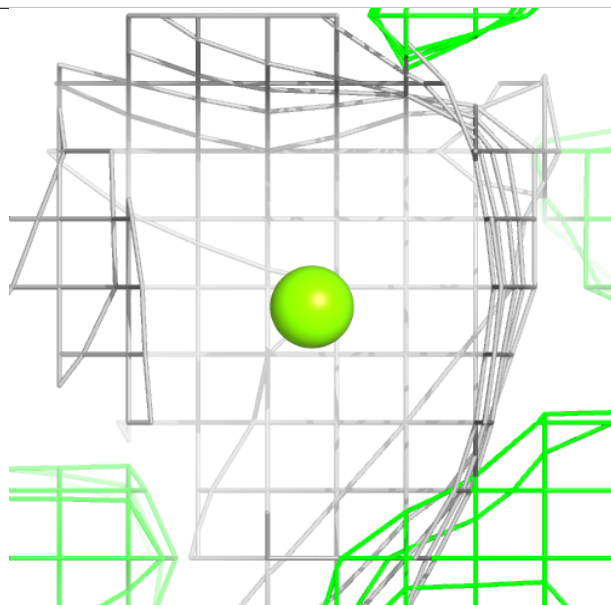
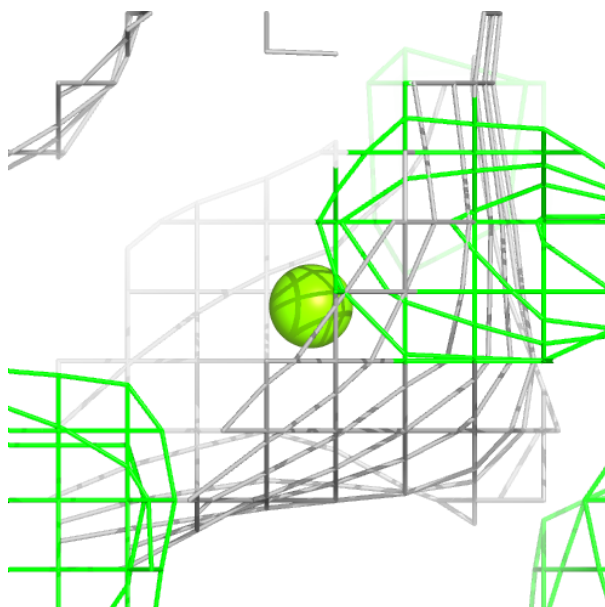
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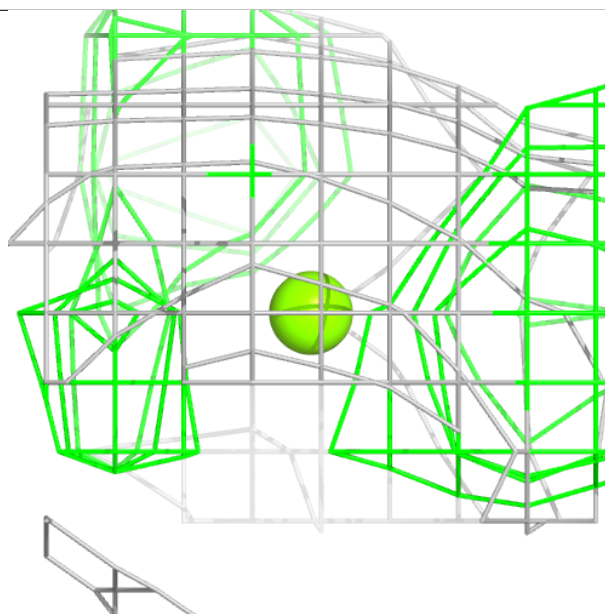
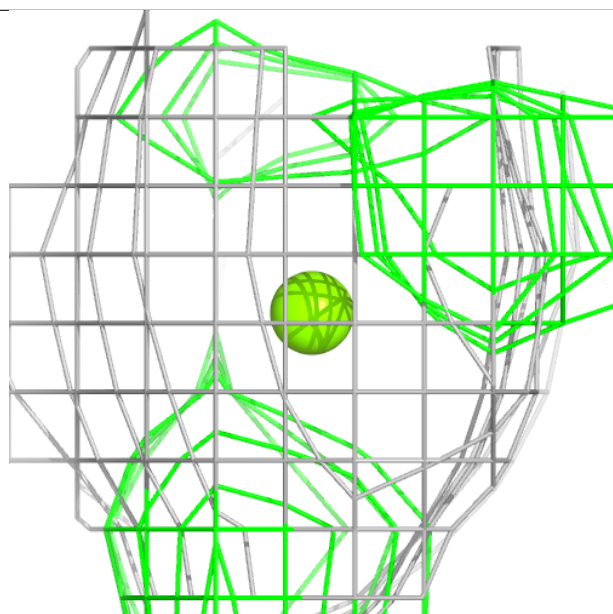
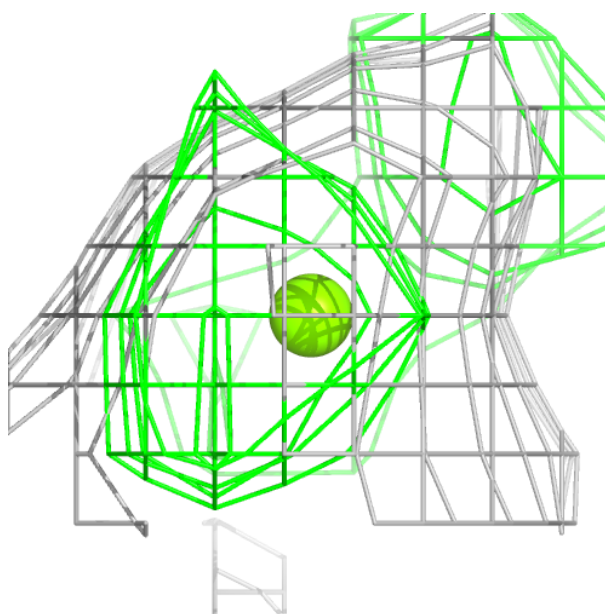
Electron density around MG A 504:

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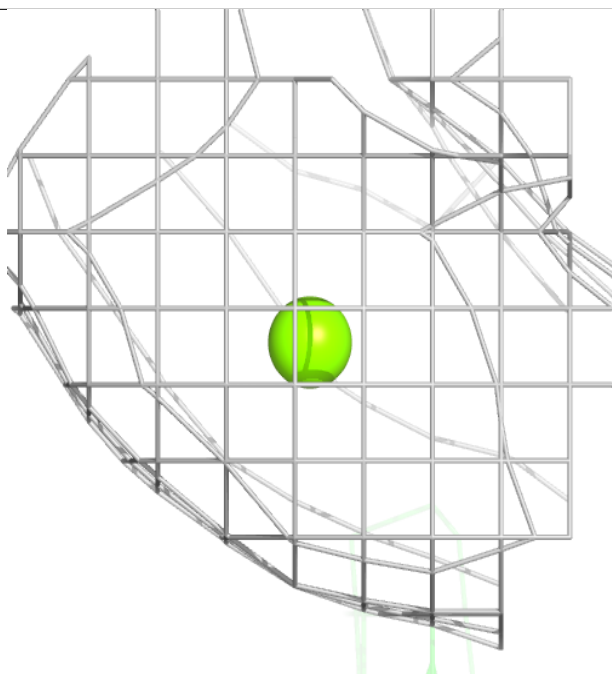
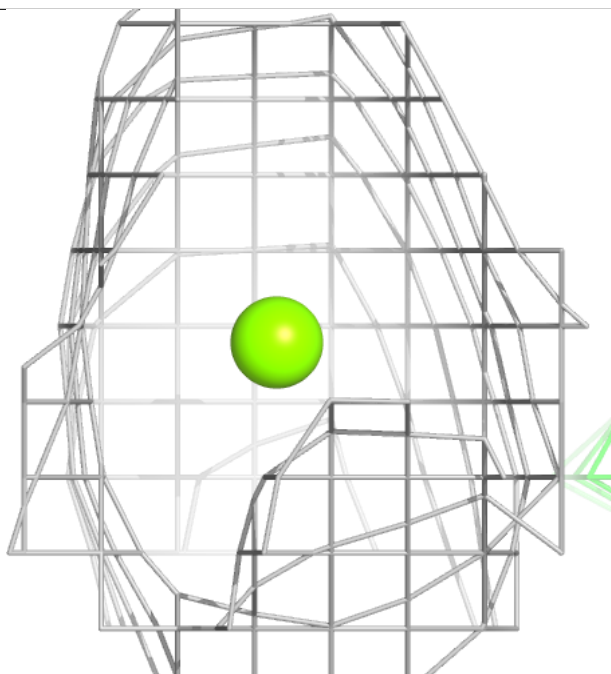
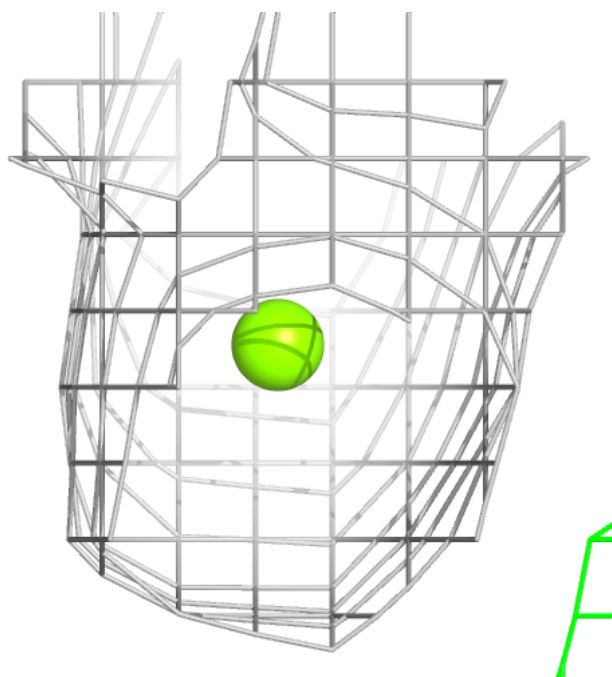
Electron density around MG C 502:

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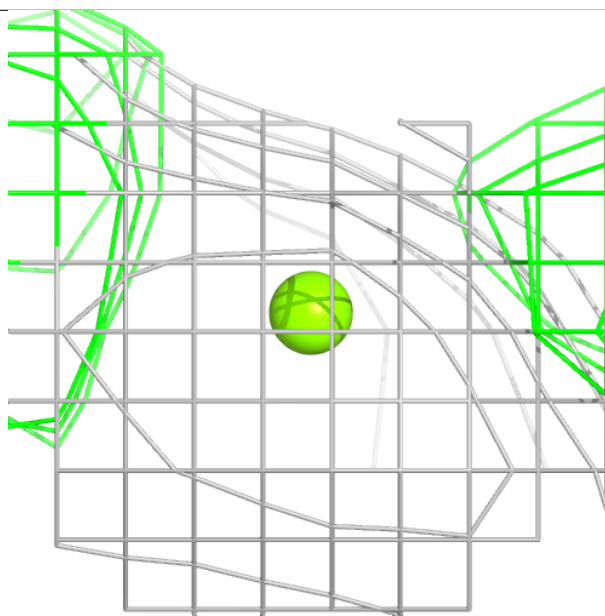
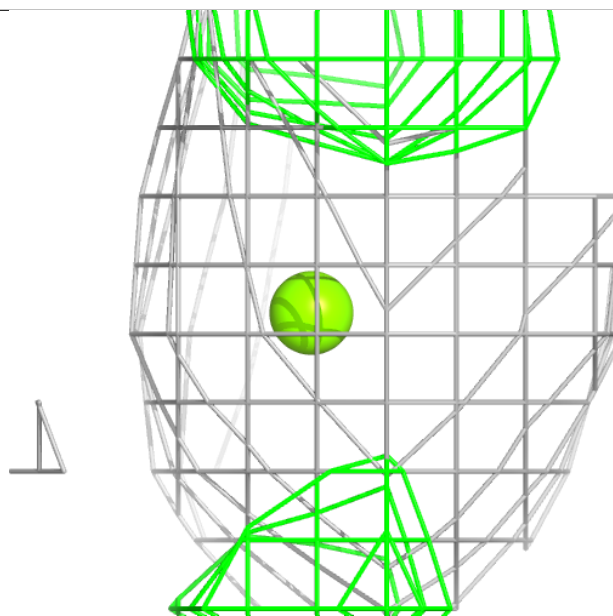
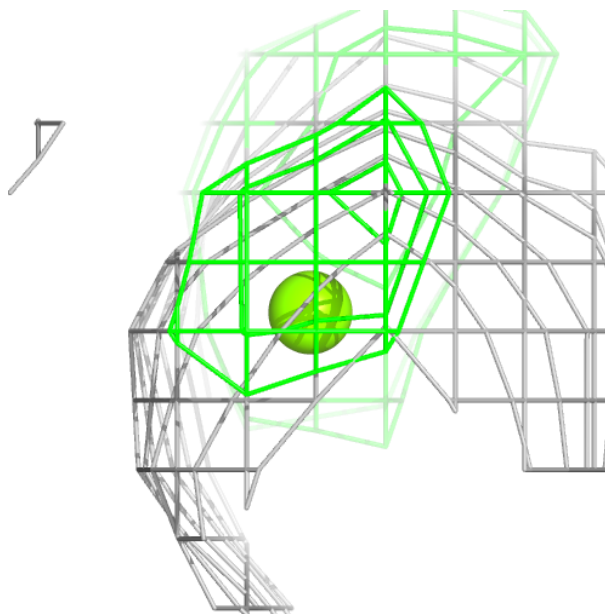
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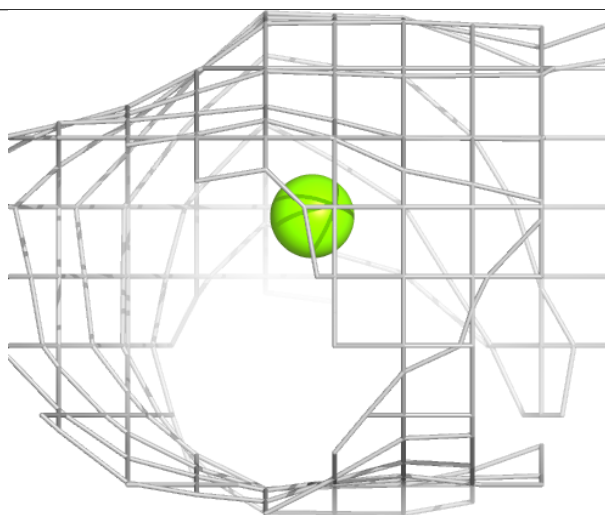
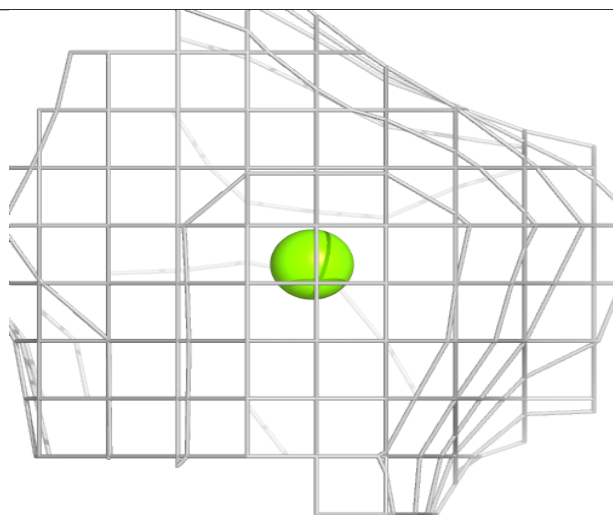
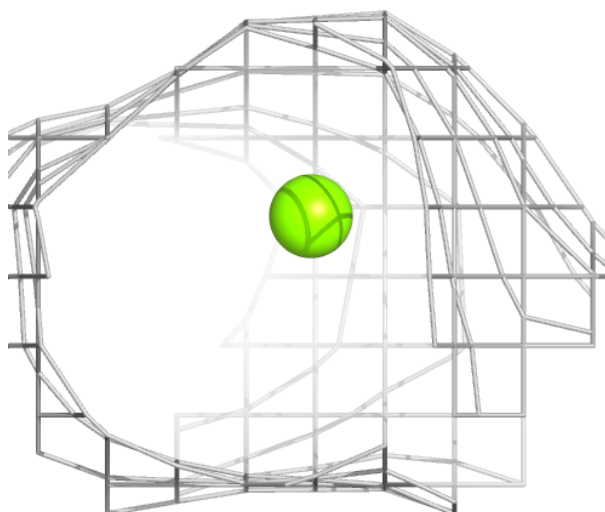
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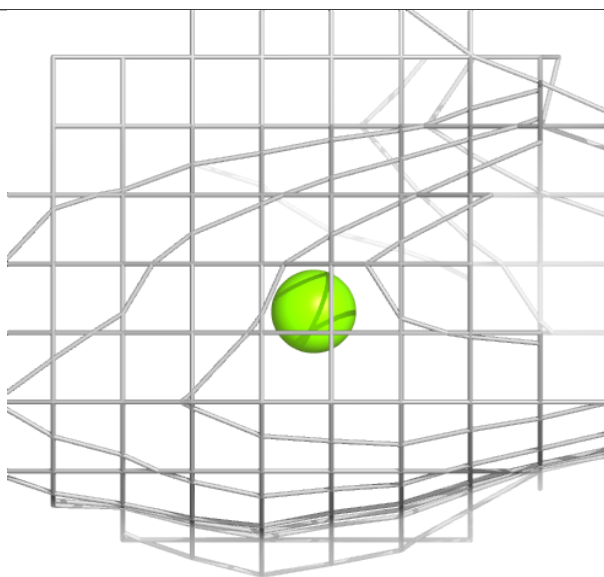
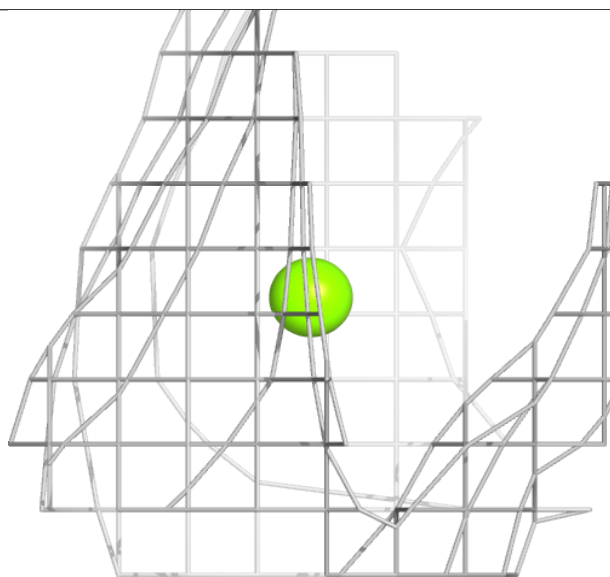
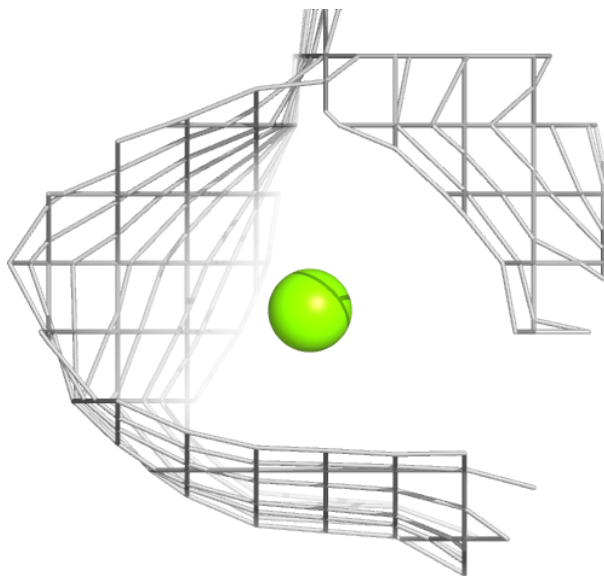
Electron density around MG D 503:

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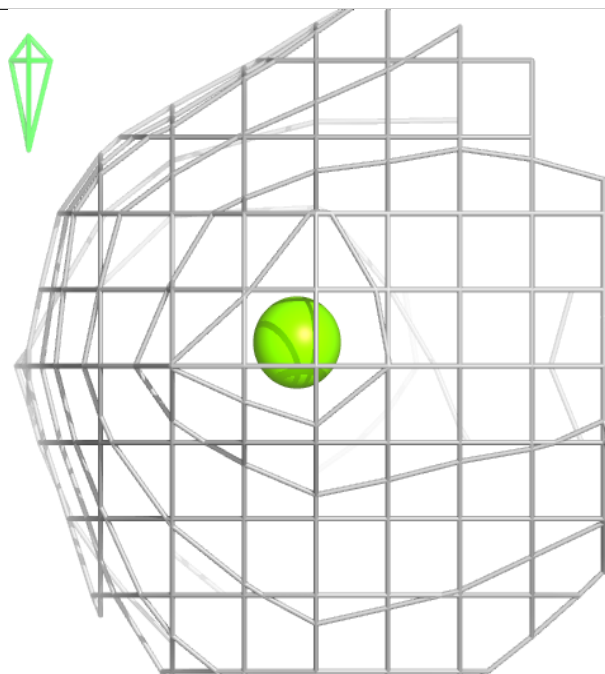
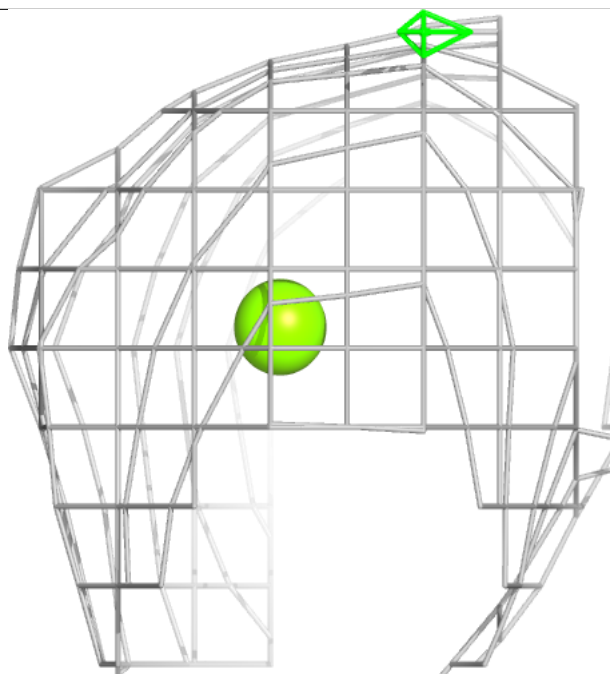
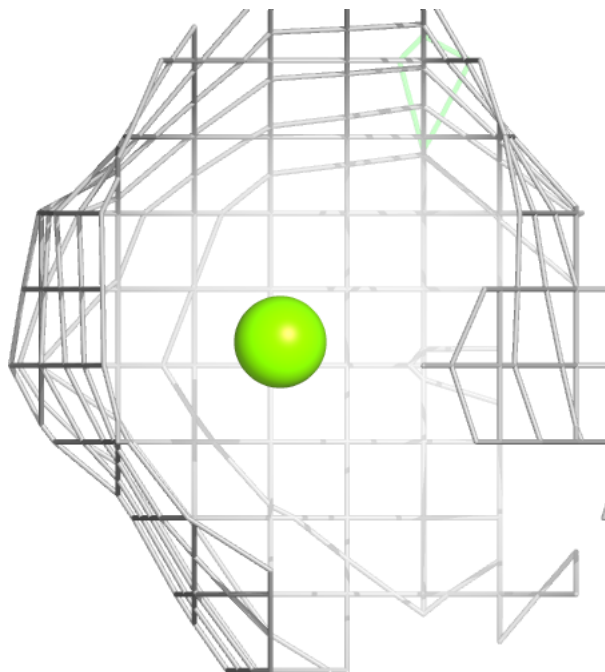
Electron density around MG C 503:

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



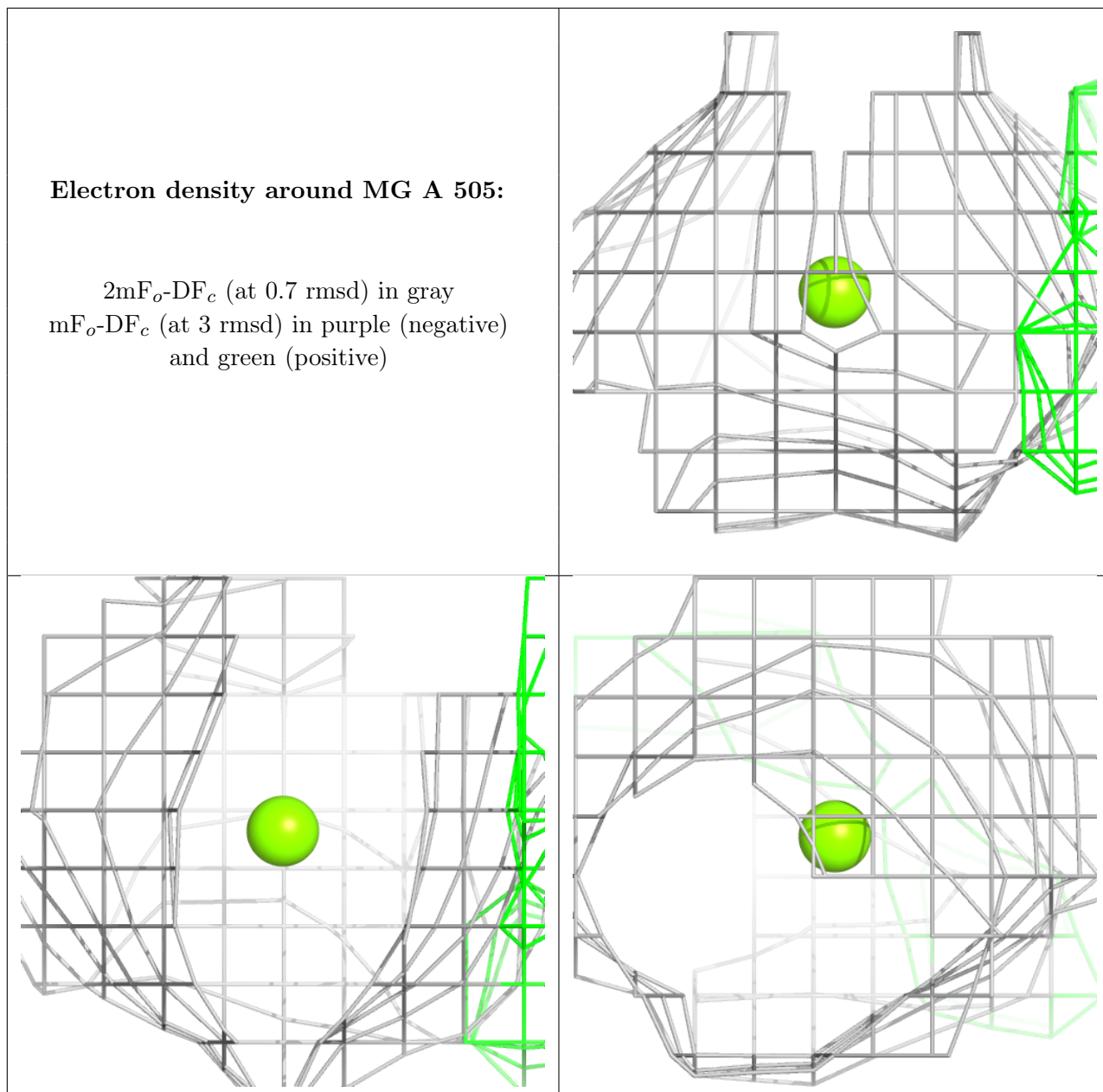
Electron density around MG B 503:

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



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)



6.5 Other polymers ⓘ

There are no such residues in this entry.