Full wwPDB X-ray Structure Validation Report (i)

Jan 9, 2024 – 03:41 pm GMT

PDB ID	:	8OE2
Title	:	Structure of hyperstable haloalkane dehalogenase variant DhaA223
Authors	:	Marek, M.
Deposited on	:	2023-03-10
Resolution	:	1.51 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 (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:

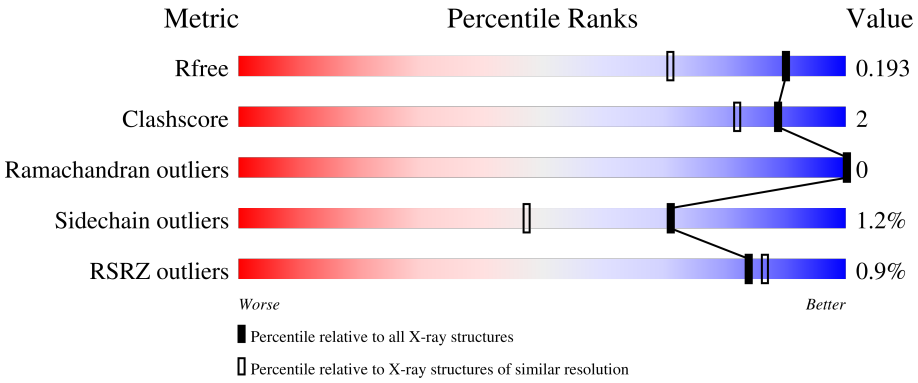
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.51 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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	299	92% 6%
1	B	299	93%
1	C	299	93%
1	D	299	91% 6%
1	E	299	93%

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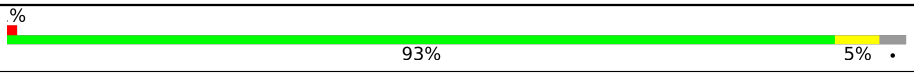
Mol	Chain	Length	Quality of chain
1	F	299	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	303	-	X	-	-
6	TRS	A	306	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16472 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 Haloalkane dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	7	0
			2460	1615	411	428	6			
1	B	290	Total	C	N	O	S	0	1	0
			2382	1561	398	417	6			
1	C	292	Total	C	N	O	S	0	3	0
			2416	1585	405	420	6			
1	D	293	Total	C	N	O	S	0	2	0
			2414	1584	404	420	6			
1	E	289	Total	C	N	O	S	0	2	0
			2386	1567	398	415	6			
1	F	291	Total	C	N	O	S	0	2	0
			2399	1576	400	417	6			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	GLU	conflict	UNP P0A3G4
A	80	ARG	PHE	conflict	UNP P0A3G4
A	128	PHE	CYS	conflict	UNP P0A3G4
A	148	LEU	THR	conflict	UNP P0A3G4
A	155	PRO	ALA	conflict	UNP P0A3G4
A	165	TYR	GLN	conflict	UNP P0A3G4
A	171	ILE	GLY	conflict	UNP P0A3G4
A	172	ILE	ALA	conflict	UNP P0A3G4
A	176	PHE	CYS	conflict	UNP P0A3G4
A	184	GLU	VAL	conflict	UNP P0A3G4
A	197	GLU	VAL	conflict	UNP P0A3G4
A	198	TRP	ASP	conflict	UNP P0A3G4
A	212	ASN	ALA	conflict	UNP P0A3G4
A	217	ASP	ASN	conflict	UNP P0A3G4
A	219	TRP	VAL	conflict	UNP P0A3G4
A	262	LEU	CYS	conflict	UNP P0A3G4
A	266	PHE	ASP	conflict	UNP P0A3G4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	294	HIS	-	expression tag	UNP P0A3G4
A	295	HIS	-	expression tag	UNP P0A3G4
A	296	HIS	-	expression tag	UNP P0A3G4
A	297	HIS	-	expression tag	UNP P0A3G4
A	298	HIS	-	expression tag	UNP P0A3G4
A	299	HIS	-	expression tag	UNP P0A3G4
B	20	SER	GLU	conflict	UNP P0A3G4
B	80	ARG	PHE	conflict	UNP P0A3G4
B	128	PHE	CYS	conflict	UNP P0A3G4
B	148	LEU	THR	conflict	UNP P0A3G4
B	155	PRO	ALA	conflict	UNP P0A3G4
B	165	TYR	GLN	conflict	UNP P0A3G4
B	171	ILE	GLY	conflict	UNP P0A3G4
B	172	ILE	ALA	conflict	UNP P0A3G4
B	176	PHE	CYS	conflict	UNP P0A3G4
B	184	GLU	VAL	conflict	UNP P0A3G4
B	197	GLU	VAL	conflict	UNP P0A3G4
B	198	TRP	ASP	conflict	UNP P0A3G4
B	212	ASN	ALA	conflict	UNP P0A3G4
B	217	ASP	ASN	conflict	UNP P0A3G4
B	219	TRP	VAL	conflict	UNP P0A3G4
B	262	LEU	CYS	conflict	UNP P0A3G4
B	266	PHE	ASP	conflict	UNP P0A3G4
B	294	HIS	-	expression tag	UNP P0A3G4
B	295	HIS	-	expression tag	UNP P0A3G4
B	296	HIS	-	expression tag	UNP P0A3G4
B	297	HIS	-	expression tag	UNP P0A3G4
B	298	HIS	-	expression tag	UNP P0A3G4
B	299	HIS	-	expression tag	UNP P0A3G4
C	20	SER	GLU	conflict	UNP P0A3G4
C	80	ARG	PHE	conflict	UNP P0A3G4
C	128	PHE	CYS	conflict	UNP P0A3G4
C	148	LEU	THR	conflict	UNP P0A3G4
C	155	PRO	ALA	conflict	UNP P0A3G4
C	165	TYR	GLN	conflict	UNP P0A3G4
C	171	ILE	GLY	conflict	UNP P0A3G4
C	172	ILE	ALA	conflict	UNP P0A3G4
C	176	PHE	CYS	conflict	UNP P0A3G4
C	184	GLU	VAL	conflict	UNP P0A3G4
C	197	GLU	VAL	conflict	UNP P0A3G4
C	198	TRP	ASP	conflict	UNP P0A3G4
C	212	ASN	ALA	conflict	UNP P0A3G4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	217	ASP	ASN	conflict	UNP P0A3G4
C	219	TRP	VAL	conflict	UNP P0A3G4
C	262	LEU	CYS	conflict	UNP P0A3G4
C	266	PHE	ASP	conflict	UNP P0A3G4
C	294	HIS	-	expression tag	UNP P0A3G4
C	295	HIS	-	expression tag	UNP P0A3G4
C	296	HIS	-	expression tag	UNP P0A3G4
C	297	HIS	-	expression tag	UNP P0A3G4
C	298	HIS	-	expression tag	UNP P0A3G4
C	299	HIS	-	expression tag	UNP P0A3G4
D	20	SER	GLU	conflict	UNP P0A3G4
D	80	ARG	PHE	conflict	UNP P0A3G4
D	128	PHE	CYS	conflict	UNP P0A3G4
D	148	LEU	THR	conflict	UNP P0A3G4
D	155	PRO	ALA	conflict	UNP P0A3G4
D	165	TYR	GLN	conflict	UNP P0A3G4
D	171	ILE	GLY	conflict	UNP P0A3G4
D	172	ILE	ALA	conflict	UNP P0A3G4
D	176	PHE	CYS	conflict	UNP P0A3G4
D	184	GLU	VAL	conflict	UNP P0A3G4
D	197	GLU	VAL	conflict	UNP P0A3G4
D	198	TRP	ASP	conflict	UNP P0A3G4
D	212	ASN	ALA	conflict	UNP P0A3G4
D	217	ASP	ASN	conflict	UNP P0A3G4
D	219	TRP	VAL	conflict	UNP P0A3G4
D	262	LEU	CYS	conflict	UNP P0A3G4
D	266	PHE	ASP	conflict	UNP P0A3G4
D	294	HIS	-	expression tag	UNP P0A3G4
D	295	HIS	-	expression tag	UNP P0A3G4
D	296	HIS	-	expression tag	UNP P0A3G4
D	297	HIS	-	expression tag	UNP P0A3G4
D	298	HIS	-	expression tag	UNP P0A3G4
D	299	HIS	-	expression tag	UNP P0A3G4
E	20	SER	GLU	conflict	UNP P0A3G4
E	80	ARG	PHE	conflict	UNP P0A3G4
E	128	PHE	CYS	conflict	UNP P0A3G4
E	148	LEU	THR	conflict	UNP P0A3G4
E	155	PRO	ALA	conflict	UNP P0A3G4
E	165	TYR	GLN	conflict	UNP P0A3G4
E	171	ILE	GLY	conflict	UNP P0A3G4
E	172	ILE	ALA	conflict	UNP P0A3G4
E	176	PHE	CYS	conflict	UNP P0A3G4

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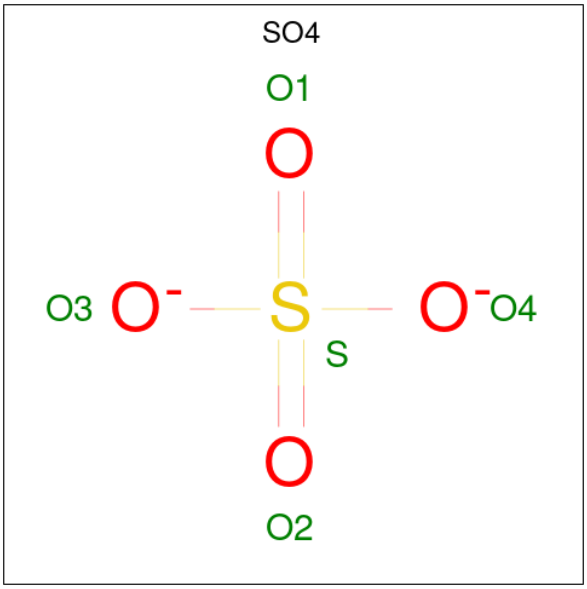
Chain	Residue	Modelled	Actual	Comment	Reference
E	184	GLU	VAL	conflict	UNP P0A3G4
E	197	GLU	VAL	conflict	UNP P0A3G4
E	198	TRP	ASP	conflict	UNP P0A3G4
E	212	ASN	ALA	conflict	UNP P0A3G4
E	217	ASP	ASN	conflict	UNP P0A3G4
E	219	TRP	VAL	conflict	UNP P0A3G4
E	262	LEU	CYS	conflict	UNP P0A3G4
E	266	PHE	ASP	conflict	UNP P0A3G4
E	294	HIS	-	expression tag	UNP P0A3G4
E	295	HIS	-	expression tag	UNP P0A3G4
E	296	HIS	-	expression tag	UNP P0A3G4
E	297	HIS	-	expression tag	UNP P0A3G4
E	298	HIS	-	expression tag	UNP P0A3G4
E	299	HIS	-	expression tag	UNP P0A3G4
F	20	SER	GLU	conflict	UNP P0A3G4
F	80	ARG	PHE	conflict	UNP P0A3G4
F	128	PHE	CYS	conflict	UNP P0A3G4
F	148	LEU	THR	conflict	UNP P0A3G4
F	155	PRO	ALA	conflict	UNP P0A3G4
F	165	TYR	GLN	conflict	UNP P0A3G4
F	171	ILE	GLY	conflict	UNP P0A3G4
F	172	ILE	ALA	conflict	UNP P0A3G4
F	176	PHE	CYS	conflict	UNP P0A3G4
F	184	GLU	VAL	conflict	UNP P0A3G4
F	197	GLU	VAL	conflict	UNP P0A3G4
F	198	TRP	ASP	conflict	UNP P0A3G4
F	212	ASN	ALA	conflict	UNP P0A3G4
F	217	ASP	ASN	conflict	UNP P0A3G4
F	219	TRP	VAL	conflict	UNP P0A3G4
F	262	LEU	CYS	conflict	UNP P0A3G4
F	266	PHE	ASP	conflict	UNP P0A3G4
F	294	HIS	-	expression tag	UNP P0A3G4
F	295	HIS	-	expression tag	UNP P0A3G4
F	296	HIS	-	expression tag	UNP P0A3G4
F	297	HIS	-	expression tag	UNP P0A3G4
F	298	HIS	-	expression tag	UNP P0A3G4
F	299	HIS	-	expression tag	UNP P0A3G4

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

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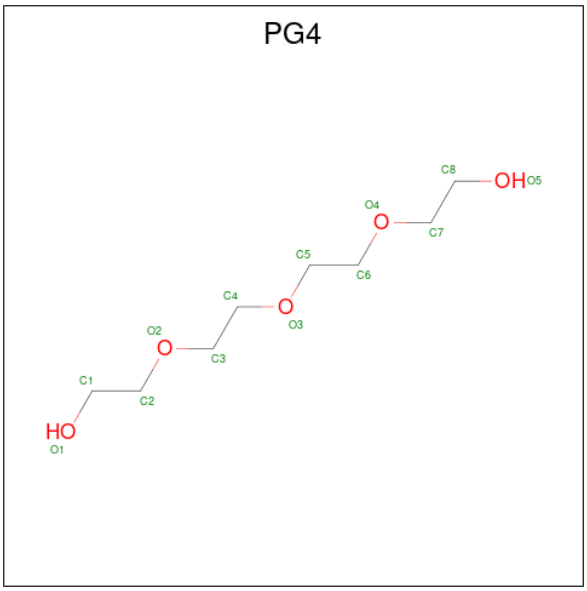
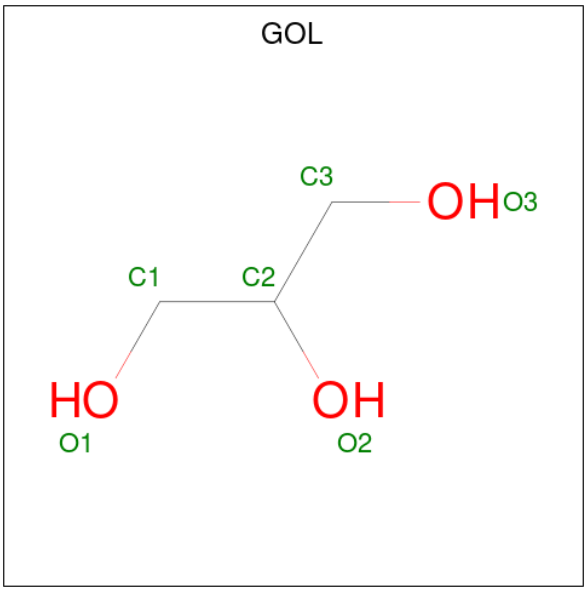
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



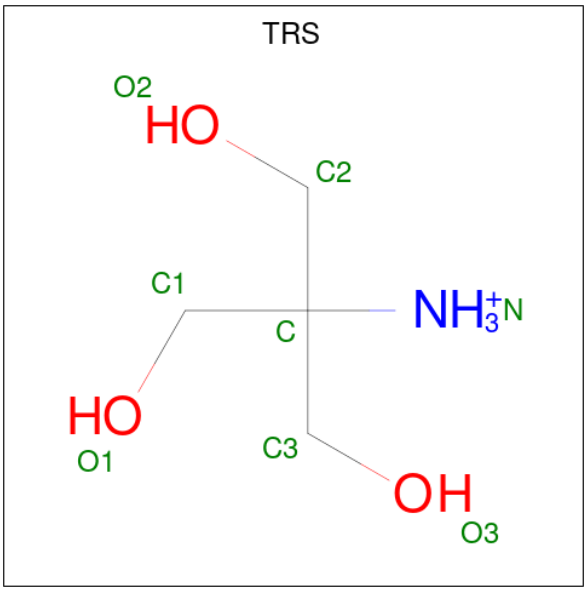
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	D	1	Total C O 13 8 5	0	0
4	E	1	Total C O 13 8 5	0	0

- 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	C	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	F	1	Total C O 6 3 3	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 8 4 1 3	0	0

- Molecule 7 is water.

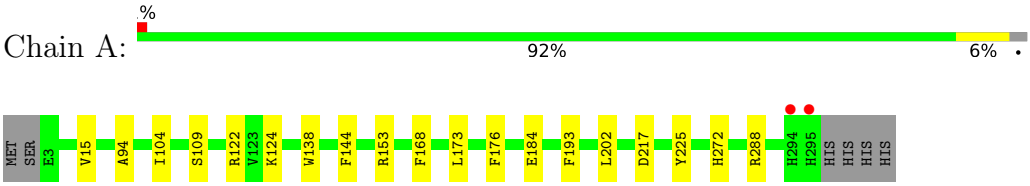
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	366	Total O 367 367	0	1
7	B	315	Total O 315 315	0	0
7	C	315	Total O 316 316	0	1
7	D	283	Total O 283 283	0	0
7	E	308	Total O 308 308	0	0
7	F	266	Total O 266 266	0	0

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.

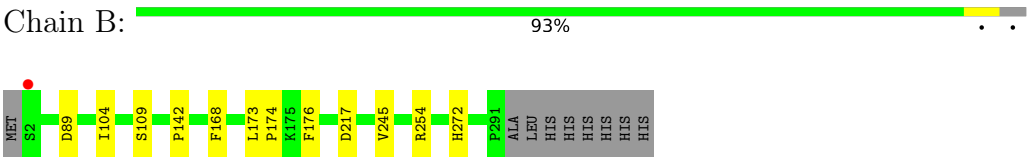
• Molecule 1: Haloalkane dehalogenase

Chain A:



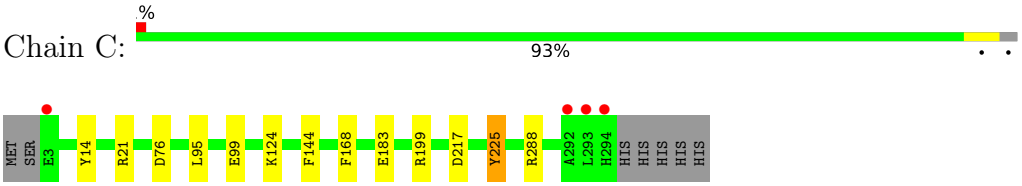
• Molecule 1: Haloalkane dehalogenase

Chain B:



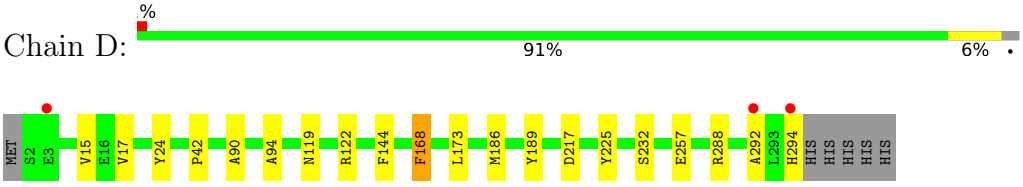
• Molecule 1: Haloalkane dehalogenase

Chain C:



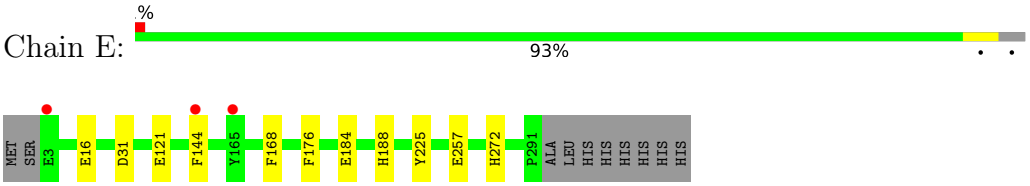
• Molecule 1: Haloalkane dehalogenase

Chain D:



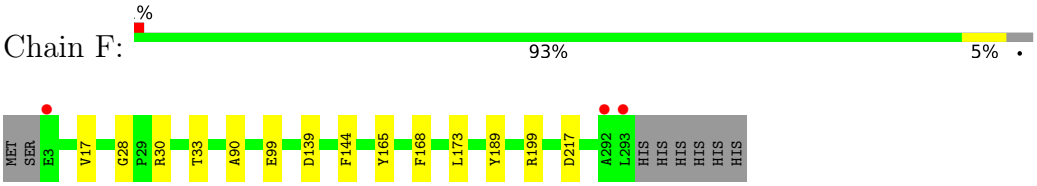
• Molecule 1: Haloalkane dehalogenase

Chain E:



• Molecule 1: Haloalkane dehalogenase

Chain F:


%
93%
5%
MET
SER
E3
V17
G28
P29
R30
T33
A90
E99
D139
F144
Y165
F168
L173
Y189
R199
D217
A292
L293
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	67.35Å 143.14Å 106.68Å 90.00° 108.38° 90.00°	Depositor
Resolution (Å)	47.72 – 1.51 47.72 – 1.51	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.72-1.51) 98.1 (47.72-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.168 , 0.195 0.168 , 0.193	Depositor DCC
R_{free} test set	14654 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	13.9	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16472	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1671e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: SO4, PG4, TRS, CL, GOL

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	0.80	0/2551	0.81	3/3494 (0.1%)
1	B	0.81	0/2471	0.84	2/3382 (0.1%)
1	C	0.81	0/2506	0.83	3/3429 (0.1%)
1	D	0.84	1/2504 (0.0%)	0.84	1/3429 (0.0%)
1	E	0.82	1/2475 (0.0%)	0.80	1/3388 (0.0%)
1	F	0.87	1/2488 (0.0%)	0.86	3/3406 (0.1%)
All	All	0.83	3/14995 (0.0%)	0.83	13/20528 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	165	TYR	CD2-CE2	8.29	1.51	1.39
1	D	232	SER	C-N	6.49	1.46	1.34
1	E	16	GLU	CB-CG	-5.08	1.42	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	30	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	B	217	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	217	ASP	CB-CG-OD1	6.52	124.17	118.30
1	F	217	ASP	CB-CG-OD1	6.48	124.14	118.30
1	F	199	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	89	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	D	217	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C	217	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	199	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	173[A]	LEU	CB-CG-CD2	-5.30	102.00	111.00
1	A	173[B]	LEU	CB-CG-CD2	-5.30	102.00	111.00
1	E	31	ASP	CB-CG-OD2	-5.11	113.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	225	TYR	CB-CG-CD2	-5.04	117.98	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2460	0	2386	17	0
1	B	2382	0	2305	5	0
1	C	2416	0	2345	6	0
1	D	2414	0	2343	12	0
1	E	2386	0	2316	4	0
1	F	2399	0	2332	5	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	5	0	0	0	0
3	B	5	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
4	A	13	0	18	0	0
4	D	13	0	18	3	0
4	E	13	0	18	3	0
5	A	24	0	32	1	0
5	B	12	0	15	1	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
5	E	18	0	23	2	0
5	F	6	0	8	0	0
6	A	8	0	12	10	0
7	A	367	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	315	0	0	1	0
7	C	316	0	0	2	0
7	D	283	0	0	2	0
7	E	308	0	0	2	0
7	F	266	0	0	0	0
All	All	16472	0	14187	55	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 2.

All (55) 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:A:138:TRP:HE1	6:A:306:TRS:H22	1.11	1.08
1:A:153:ARG:HH11	6:A:306:TRS:H31	1.17	1.06
1:A:153:ARG:HE	6:A:306:TRS:H11	1.39	0.85
1:A:138:TRP:NE1	6:A:306:TRS:H22	1.96	0.73
5:B:304:GOL:H12	7:B:420:HOH:O	1.88	0.73
1:C:288:ARG:NH2	7:C:402:HOH:O	2.24	0.70
5:A:308:GOL:H11	7:A:612:HOH:O	1.91	0.68
1:A:288:ARG:NH2	7:A:401:HOH:O	2.27	0.66
1:A:153:ARG:NH1	6:A:306:TRS:H31	2.02	0.65
1:A:184:GLU:HG3	7:A:592:HOH:O	1.99	0.62
1:C:99:GLU:HB3	1:C:124[A]:LYS:HD3	1.84	0.58
1:C:124[A]:LYS:N	1:C:124[A]:LYS:HD2	2.19	0.58
1:D:186:MET:HG3	4:D:304:PG4:H41	1.91	0.51
1:F:17:VAL:HG13	1:F:90:ALA:HB3	1.93	0.50
1:A:153:ARG:HE	6:A:306:TRS:C1	2.15	0.50
1:A:138:TRP:HE1	6:A:306:TRS:C2	2.03	0.49
1:A:122:ARG:NH1	7:A:404:HOH:O	2.35	0.48
1:D:15[B]:VAL:HG11	1:D:94:ALA:CB	2.43	0.48
1:A:153:ARG:HB3	6:A:306:TRS:O1	2.14	0.47
1:B:254:ARG:HG3	1:D:257:GLU:HG3	1.96	0.47
1:D:15[B]:VAL:HG11	1:D:94:ALA:HB1	1.96	0.47
1:B:142:PRO:HG2	1:B:245:VAL:HG13	1.95	0.47
1:D:15[A]:VAL:HG21	1:D:94:ALA:HB1	1.97	0.47
4:D:304:PG4:H72	7:D:627:HOH:O	2.15	0.47
1:F:17:VAL:HG13	1:F:90:ALA:CB	2.45	0.46
1:A:15:VAL:HG21	1:A:94:ALA:HB1	1.97	0.46
1:F:33:THR:HG23	1:F:99:GLU:HG2	1.96	0.46
4:D:304:PG4:H61	4:D:304:PG4:H42	1.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:GLU:HG3	7:C:626:HOH:O	2.16	0.46
1:D:288:ARG:HG3	7:D:571:HOH:O	2.17	0.45
1:D:173[A]:LEU:HD21	1:D:189:TYR:CG	2.51	0.45
4:E:305:PG4:H51	7:E:650:HOH:O	2.17	0.44
1:A:124:LYS:NZ	7:A:413:HOH:O	2.51	0.44
1:A:193:PHE:CZ	1:A:202:LEU:HD21	2.53	0.44
1:B:104:ILE:HD12	1:B:109:SER:HA	2.01	0.43
1:D:17:VAL:HG13	1:D:90:ALA:CB	2.48	0.43
1:C:76:ASP:HB2	1:F:28:GLY:O	2.18	0.43
1:D:292:ALA:C	1:D:294:HIS:H	2.20	0.43
4:E:305:PG4:H52	4:E:305:PG4:H72	1.63	0.43
1:B:176:PHE:HB3	1:B:272:HIS:HB3	2.01	0.43
1:D:119:ASN:HB3	1:D:122:ARG:HD3	2.01	0.42
1:E:121:GLU:OE2	5:E:306:GOL:O3	2.37	0.42
1:F:173:LEU:HD21	1:F:189:TYR:CG	2.55	0.42
1:A:153:ARG:NE	6:A:306:TRS:H11	2.21	0.42
1:D:42:PRO:HD3	1:D:168:PHE:CE1	2.54	0.42
1:E:176:PHE:HB3	1:E:272:HIS:HB3	2.02	0.41
6:A:306:TRS:H12	7:A:535:HOH:O	2.19	0.41
1:E:184:GLU:H	1:E:184:GLU:CD	2.24	0.41
4:E:305:PG4:H32	7:E:650:HOH:O	2.19	0.41
1:D:15[B]:VAL:HG23	1:D:24:TYR:HE1	1.86	0.41
1:A:176:PHE:HB3	1:A:272:HIS:HB3	2.02	0.41
1:A:104:ILE:HB	1:A:109:SER:HA	2.02	0.41
1:C:14:TYR:HB3	1:C:21:ARG:CG	2.51	0.40
1:B:173:LEU:HB3	1:B:174:PRO:HD3	2.04	0.40
1:E:188:HIS:ND1	5:E:304:GOL:H2	2.36	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	298/299 (100%)	288 (97%)	10 (3%)	0	100	100
1	B	289/299 (97%)	279 (96%)	10 (4%)	0	100	100
1	C	293/299 (98%)	283 (97%)	10 (3%)	0	100	100
1	D	293/299 (98%)	282 (96%)	11 (4%)	0	100	100
1	E	289/299 (97%)	279 (96%)	10 (4%)	0	100	100
1	F	291/299 (97%)	282 (97%)	9 (3%)	0	100	100
All	All	1753/1794 (98%)	1693 (97%)	60 (3%)	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	262/261 (100%)	259 (99%)	3 (1%)	73	52
1	B	254/261 (97%)	253 (100%)	1 (0%)	91	82
1	C	257/261 (98%)	252 (98%)	5 (2%)	57	26
1	D	257/261 (98%)	254 (99%)	3 (1%)	71	47
1	E	254/261 (97%)	250 (98%)	4 (2%)	62	35
1	F	255/261 (98%)	252 (99%)	3 (1%)	71	47
All	All	1539/1566 (98%)	1520 (99%)	19 (1%)	71	47

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	PHE
1	A	168	PHE
1	A	225	TYR
1	B	168	PHE
1	C	95[A]	LEU
1	C	95[B]	LEU
1	C	144	PHE

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Mol	Chain	Res	Type
1	C	168	PHE
1	C	225	TYR
1	D	144	PHE
1	D	168	PHE
1	D	225	TYR
1	E	144	PHE
1	E	168	PHE
1	E	225	TYR
1	E	257	GLU
1	F	139	ASP
1	F	144	PHE
1	F	168	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	261	ASN

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 29 ligands modelled in this entry, 6 are monoatomic - leaving 23 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	SO4	B	302	-	4,4,4	0.41	0	6,6,6	0.31	0
5	GOL	E	303	-	5,5,5	0.82	0	5,5,5	1.31	1 (20%)
5	GOL	A	305	-	5,5,5	0.70	0	5,5,5	0.98	0
3	SO4	A	302	-	4,4,4	0.17	0	6,6,6	0.23	0
5	GOL	A	304	-	5,5,5	0.60	0	5,5,5	0.58	0
4	PG4	D	304	-	12,12,12	0.51	0	11,11,11	0.75	0
5	GOL	C	304	-	5,5,5	0.44	0	5,5,5	1.11	1 (20%)
4	PG4	E	305	-	12,12,12	0.57	0	11,11,11	0.65	0
3	SO4	D	302	-	4,4,4	0.38	0	6,6,6	0.31	0
3	SO4	C	302	-	4,4,4	0.46	0	6,6,6	0.48	0
3	SO4	C	303	-	4,4,4	0.09	0	6,6,6	0.26	0
4	PG4	A	303	-	12,12,12	0.61	0	11,11,11	0.47	0
5	GOL	D	305	-	5,5,5	0.63	0	5,5,5	0.94	0
5	GOL	B	303	-	5,5,5	1.08	0	5,5,5	2.42	4 (80%)
5	GOL	A	308	-	5,5,5	0.58	0	5,5,5	1.00	0
3	SO4	D	303	-	4,4,4	0.55	0	6,6,6	0.30	0
3	SO4	E	302	-	4,4,4	0.28	0	6,6,6	0.47	0
6	TRS	A	306	-	7,7,7	0.27	0	9,9,9	0.40	0
5	GOL	E	304	-	5,5,5	0.67	0	5,5,5	1.40	0
5	GOL	A	307	-	5,5,5	0.44	0	5,5,5	0.68	0
5	GOL	E	306	-	5,5,5	1.45	1 (20%)	5,5,5	3.11	2 (40%)
5	GOL	F	302	-	5,5,5	0.63	0	5,5,5	0.79	0
5	GOL	B	304	-	5,5,5	0.59	0	5,5,5	0.87	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
6	TRS	A	306	-	-	6/9/9/9	-
4	PG4	D	304	-	-	8/10/10/10	-
4	PG4	A	303	-	-	0/10/10/10	-
5	GOL	C	304	-	-	0/4/4/4	-
5	GOL	D	305	-	-	2/4/4/4	-
5	GOL	B	303	-	-	4/4/4/4	-
5	GOL	E	304	-	-	2/4/4/4	-
4	PG4	E	305	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	E	303	-	-	1/4/4/4	-
5	GOL	A	307	-	-	4/4/4/4	-
5	GOL	A	308	-	-	2/4/4/4	-
5	GOL	E	306	-	-	2/4/4/4	-
5	GOL	F	302	-	-	3/4/4/4	-
5	GOL	A	305	-	-	2/4/4/4	-
5	GOL	A	304	-	-	2/4/4/4	-
5	GOL	B	304	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	306	GOL	O3-C3	-3.09	1.29	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	306	GOL	C3-C2-C1	-6.14	87.83	111.70
5	B	303	GOL	C3-C2-C1	-3.31	98.84	111.70
5	B	303	GOL	O2-C2-C1	-2.83	96.68	109.12
5	E	303	GOL	C3-C2-C1	2.75	122.39	111.70
5	E	306	GOL	O1-C1-C2	-2.37	98.86	110.20
5	B	303	GOL	O2-C2-C3	2.21	118.84	109.12
5	B	303	GOL	O1-C1-C2	-2.06	100.31	110.20
5	C	304	GOL	C3-C2-C1	-2.06	103.71	111.70

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	304	GOL	O2-C2-C3-O3
5	A	307	GOL	O1-C1-C2-C3
5	A	307	GOL	C1-C2-C3-O3
5	A	308	GOL	C1-C2-C3-O3
5	A	308	GOL	O2-C2-C3-O3
5	B	303	GOL	O1-C1-C2-C3
5	D	305	GOL	O1-C1-C2-C3
5	E	306	GOL	C1-C2-C3-O3
6	A	306	TRS	C1-C-C3-O3
6	A	306	TRS	C2-C-C3-O3

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Mol	Chain	Res	Type	Atoms
6	A	306	TRS	N-C-C3-O3
4	D	304	PG4	C5-C6-O4-C7
4	D	304	PG4	O2-C3-C4-O3
4	D	304	PG4	O1-C1-C2-O2
4	D	304	PG4	O3-C5-C6-O4
5	A	304	GOL	C1-C2-C3-O3
5	A	305	GOL	O1-C1-C2-C3
5	B	303	GOL	C1-C2-C3-O3
5	E	303	GOL	O1-C1-C2-C3
5	E	304	GOL	C1-C2-C3-O3
5	F	302	GOL	O1-C1-C2-C3
5	A	307	GOL	O1-C1-C2-O2
5	A	307	GOL	O2-C2-C3-O3
5	B	303	GOL	O1-C1-C2-O2
5	B	303	GOL	O2-C2-C3-O3
5	D	305	GOL	O1-C1-C2-O2
4	E	305	PG4	C5-C6-O4-C7
4	D	304	PG4	C4-C3-O2-C2
4	D	304	PG4	C6-C5-O3-C4
5	E	306	GOL	O2-C2-C3-O3
4	E	305	PG4	C1-C2-O2-C3
4	D	304	PG4	C1-C2-O2-C3
5	A	305	GOL	O1-C1-C2-O2
5	E	304	GOL	O1-C1-C2-O2
5	F	302	GOL	O2-C2-C3-O3
6	A	306	TRS	C2-C-C1-O1
4	D	304	PG4	C8-C7-O4-C6
6	A	306	TRS	C3-C-C1-O1
4	E	305	PG4	O3-C5-C6-O4
4	E	305	PG4	O2-C3-C4-O3
6	A	306	TRS	N-C-C1-O1
5	F	302	GOL	C1-C2-C3-O3
4	E	305	PG4	C3-C4-O3-C5

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	304	PG4	3	0
4	E	305	PG4	3	0
5	A	308	GOL	1	0
6	A	306	TRS	10	0

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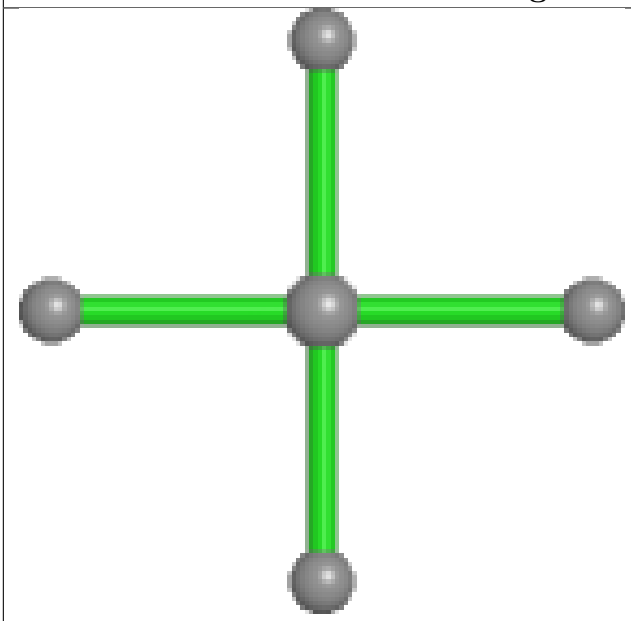
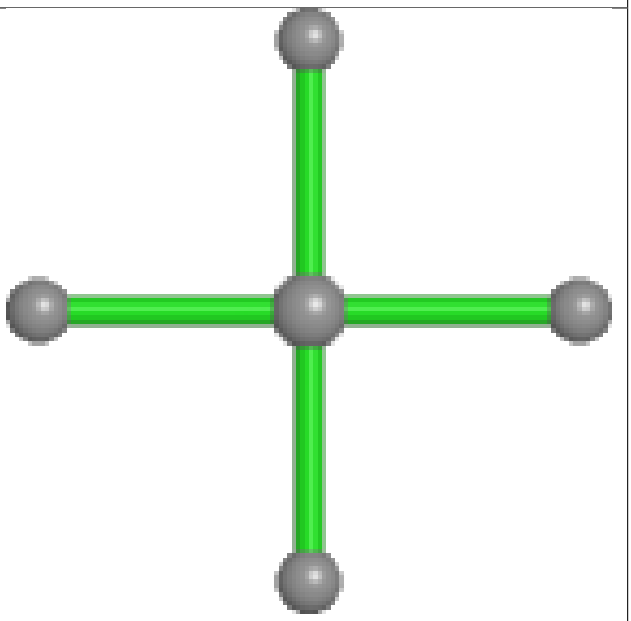
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	304	GOL	1	0
5	E	306	GOL	1	0
5	B	304	GOL	1	0

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

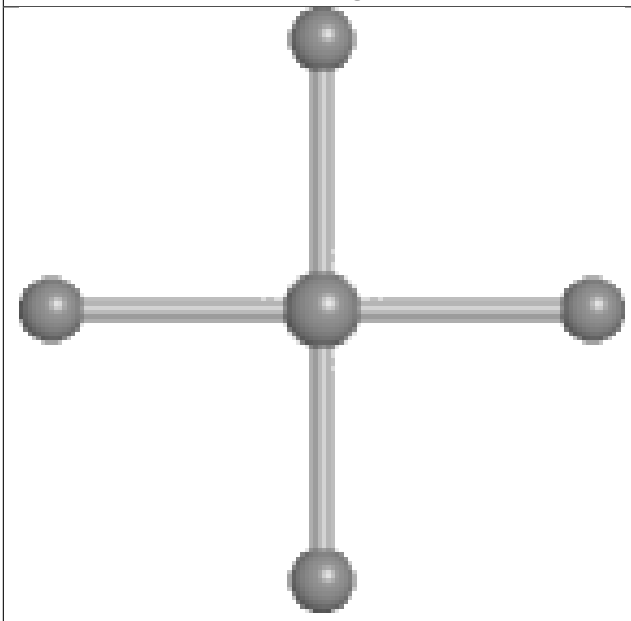
Ligand SO4 B 302



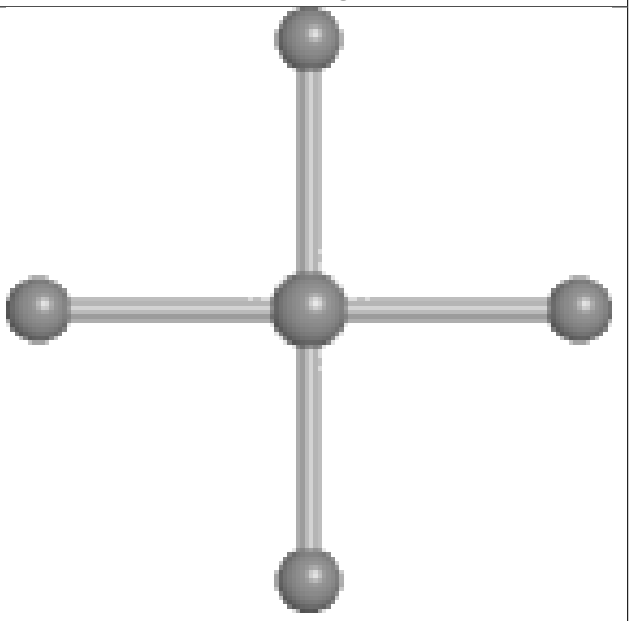
Bond lengths



Bond angles

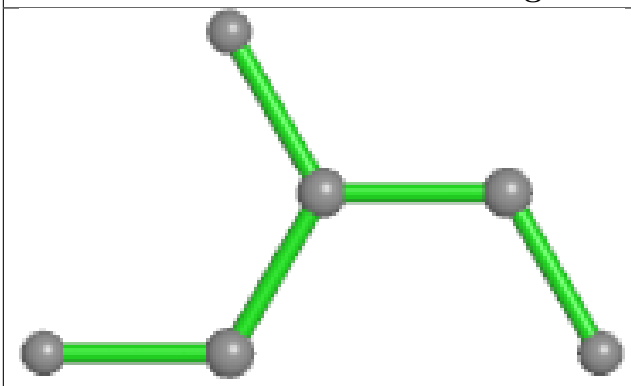


Torsions

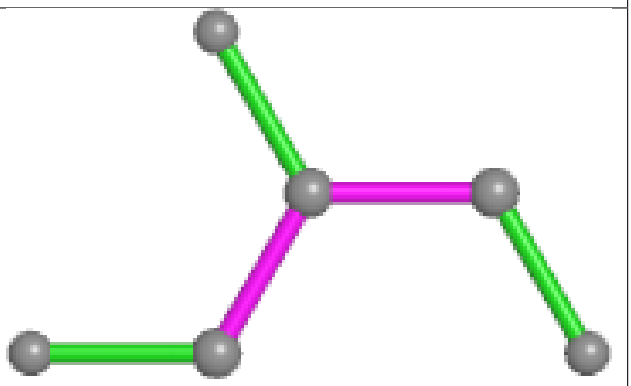


Rings

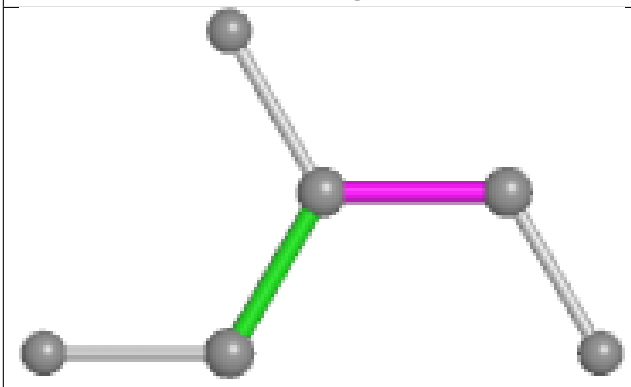
Ligand GOL E 303



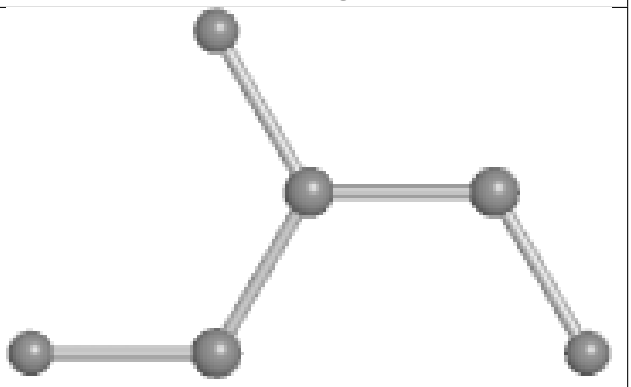
Bond lengths



Bond angles

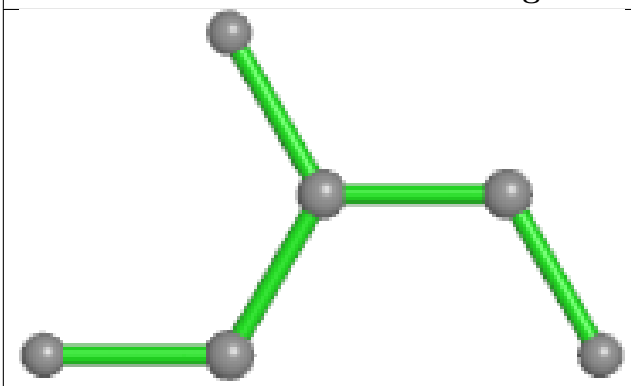


Torsions

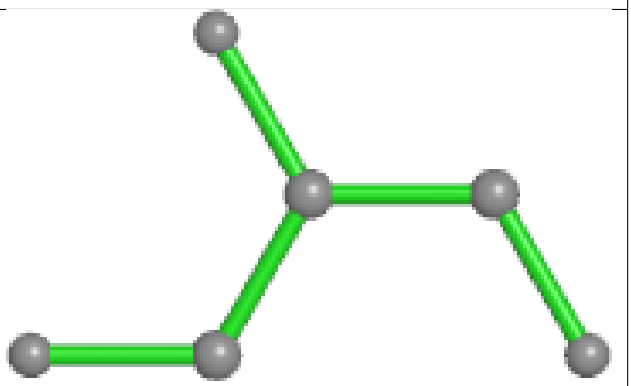


Rings

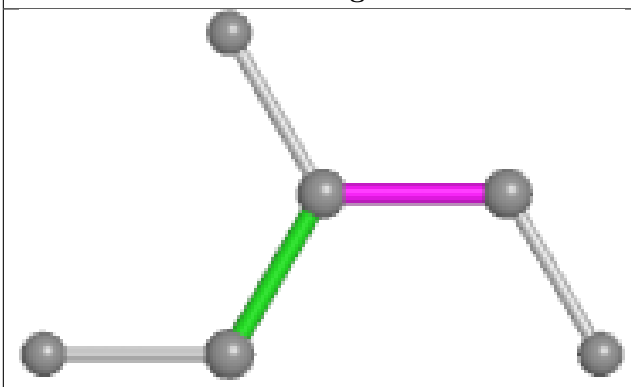
Ligand GOL A 305



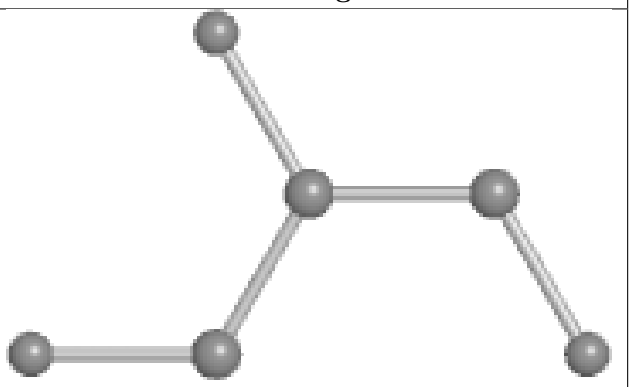
Bond lengths



Bond angles

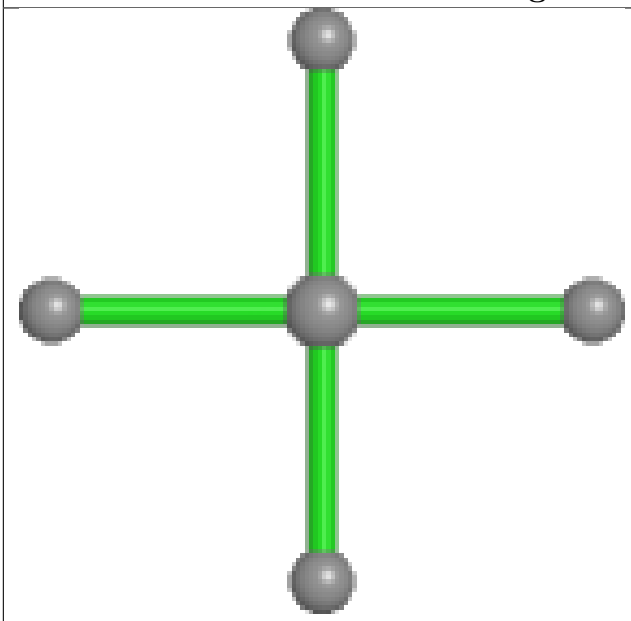


Torsions

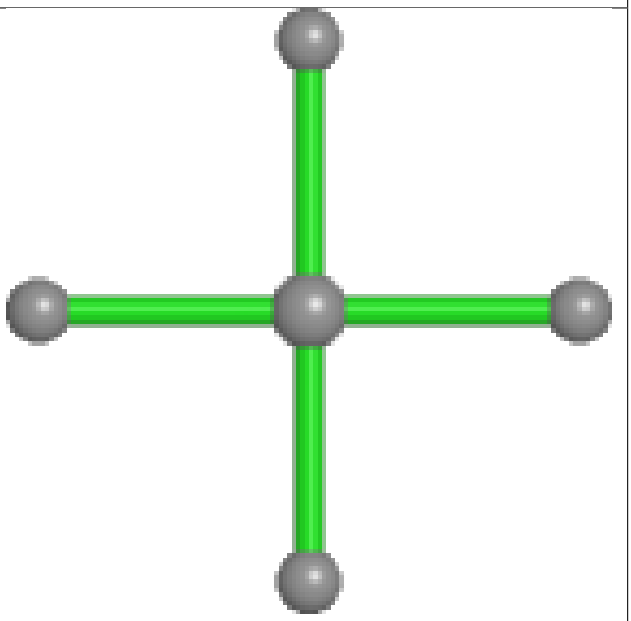


Rings

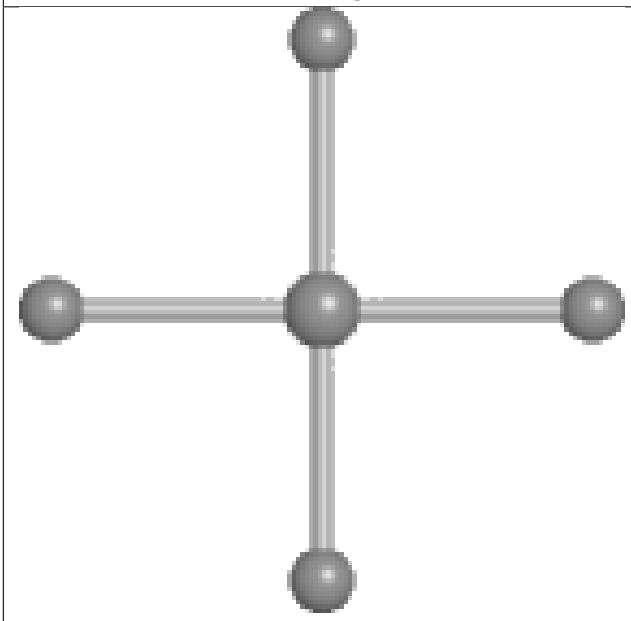
Ligand SO4 A 302



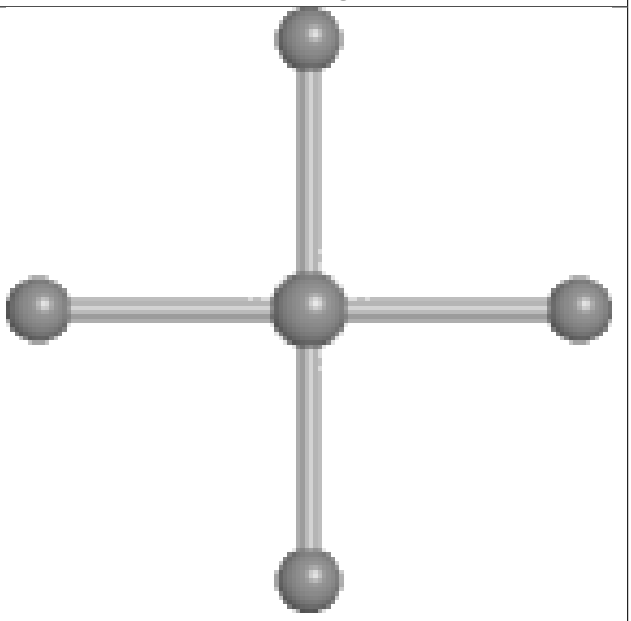
Bond lengths



Bond angles

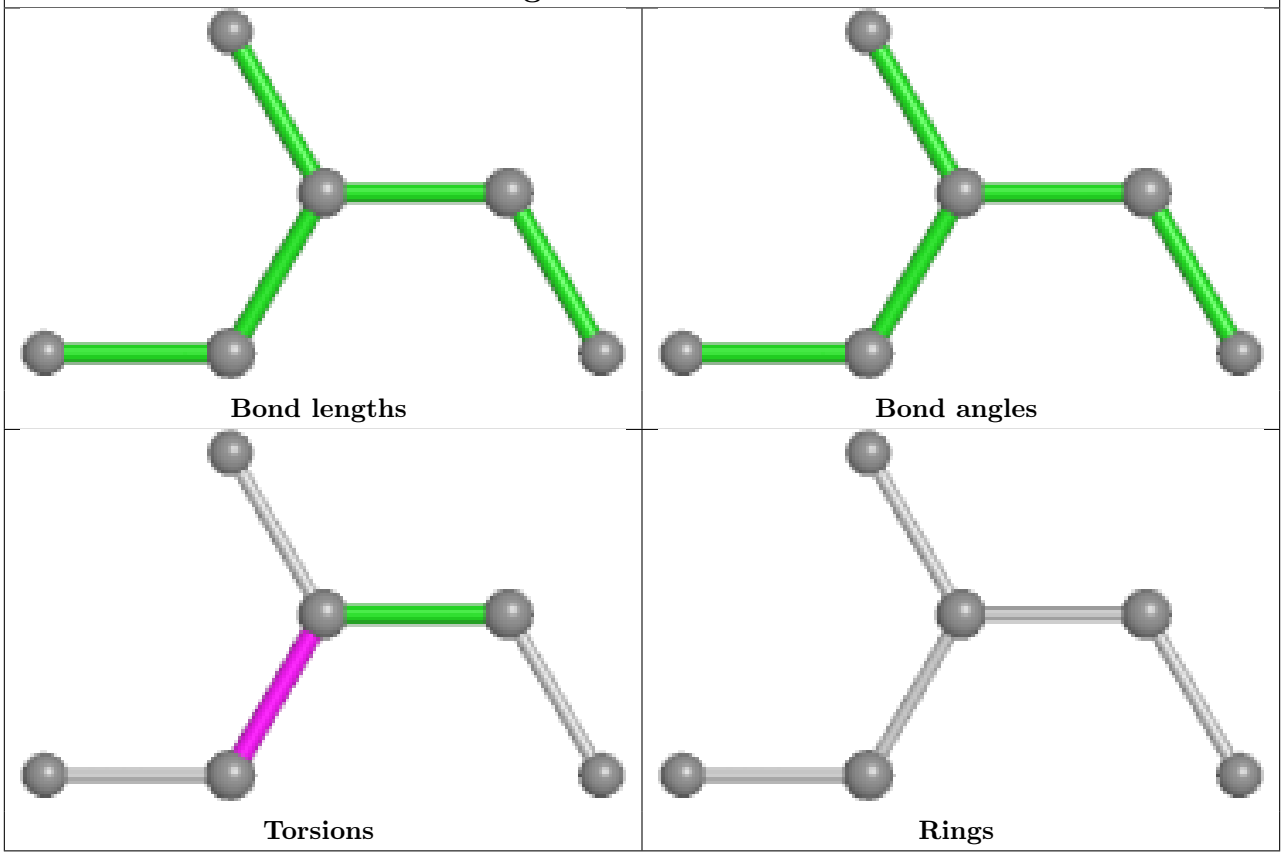


Torsions

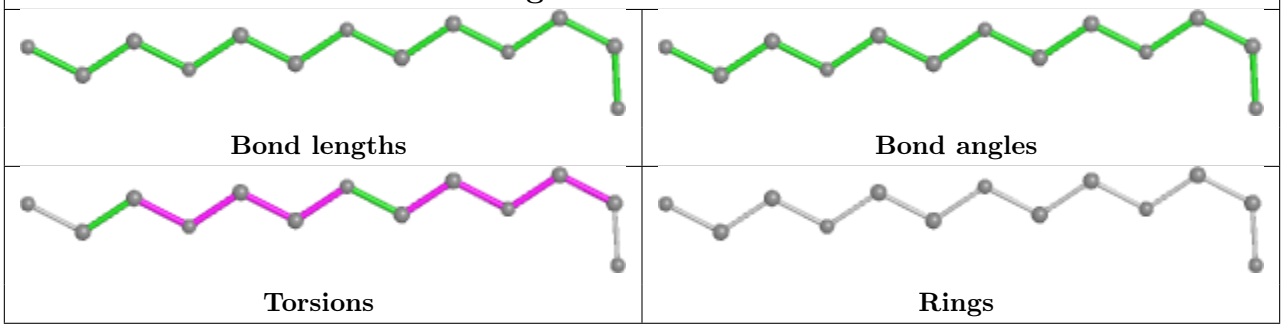


Rings

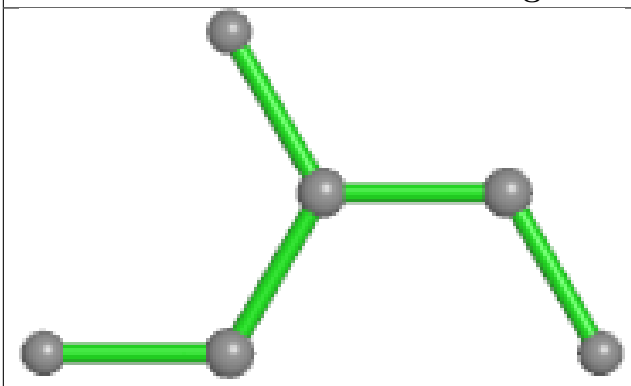
Ligand GOL A 304



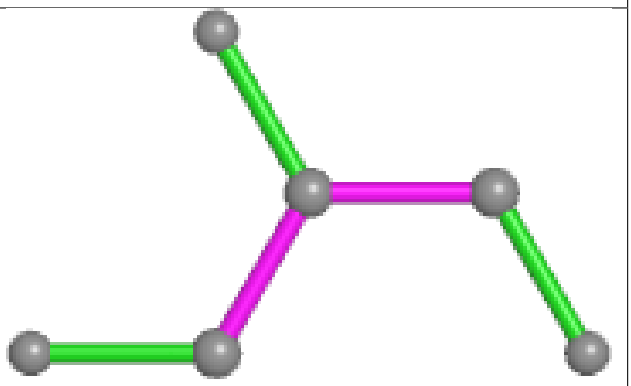
Ligand PG4 D 304



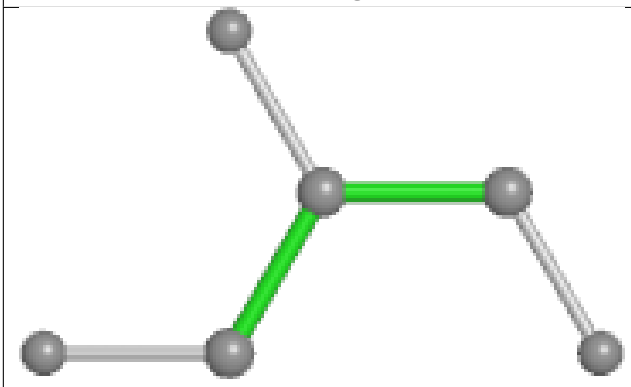
Ligand GOL C 304



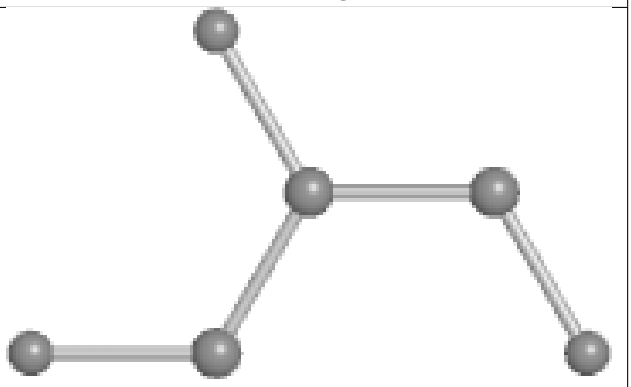
Bond lengths



Bond angles

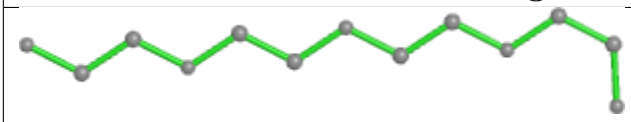


Torsions



Rings

Ligand PG4 E 305



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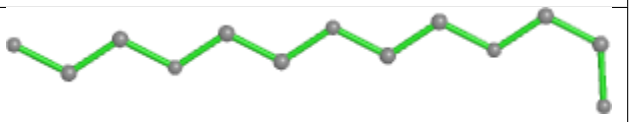
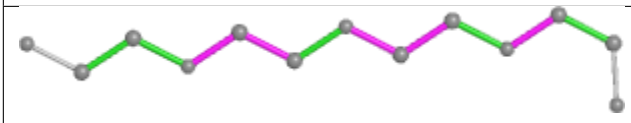


Bond angles



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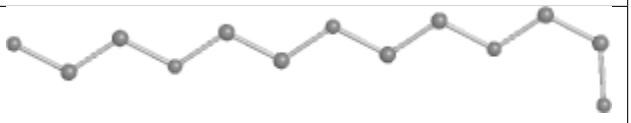
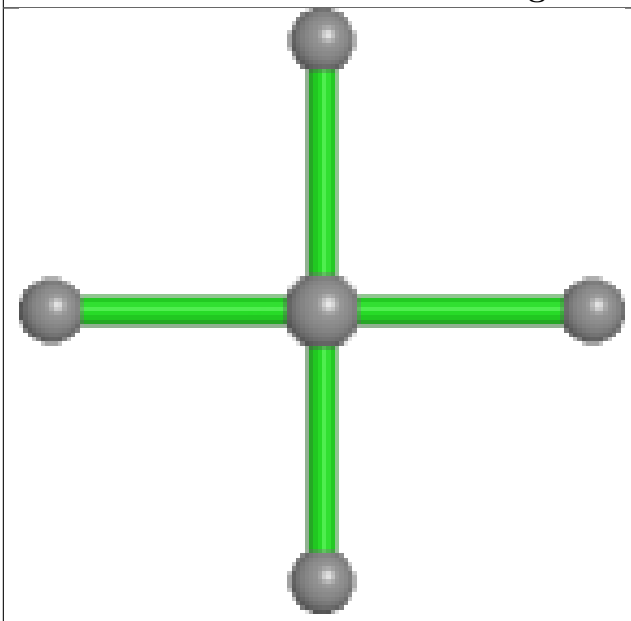


Rings

Ligand SO4 D 302



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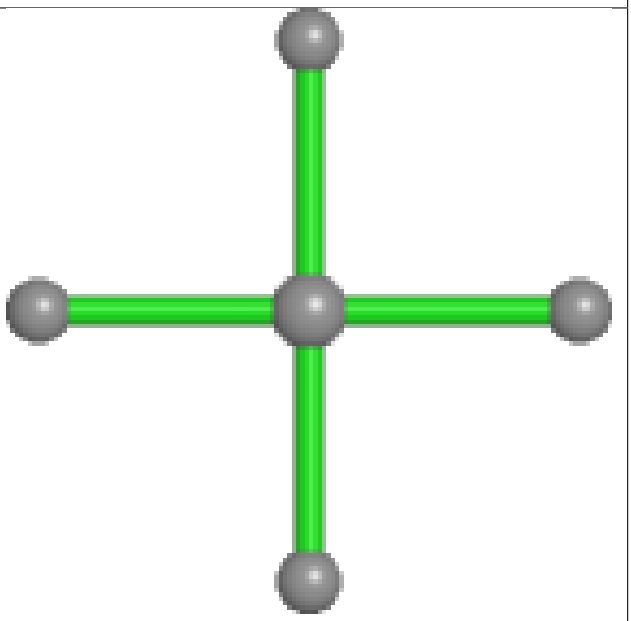
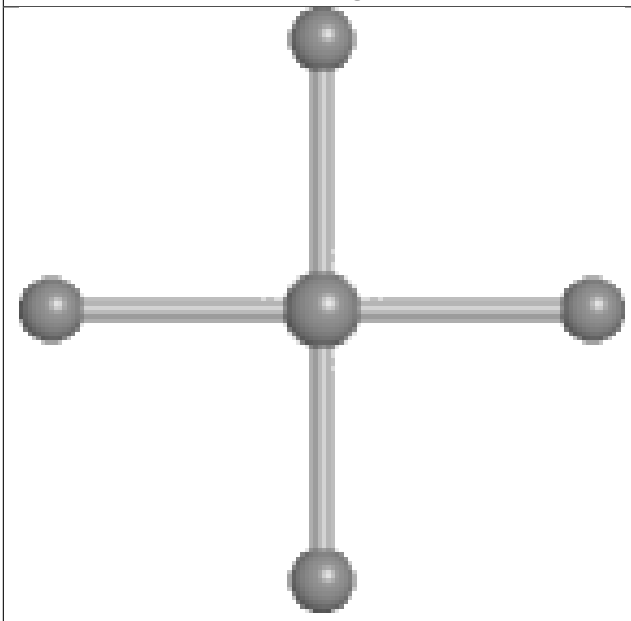
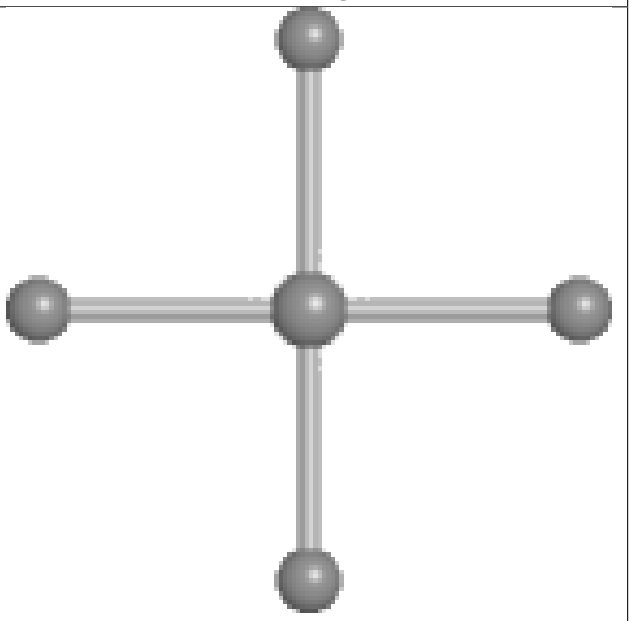


Bond angles

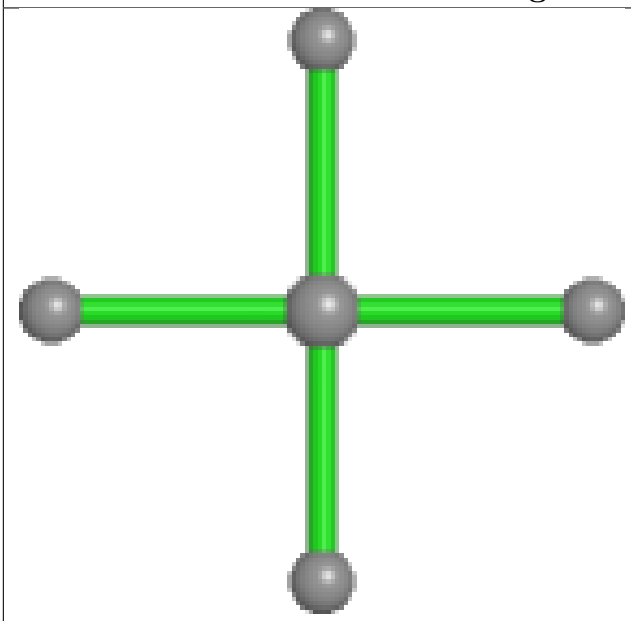


Torsions

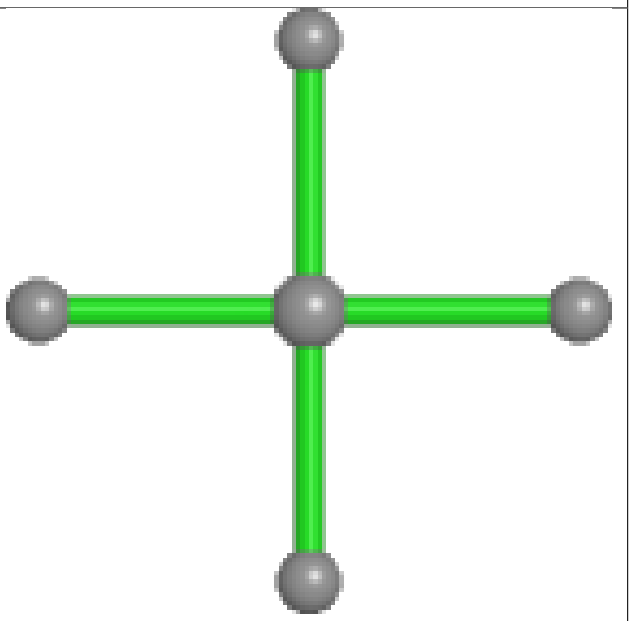


Rings

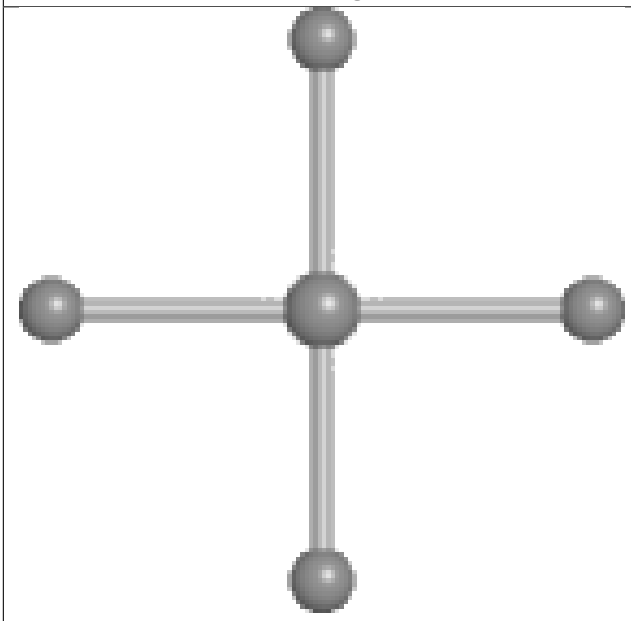
Ligand SO4 C 302



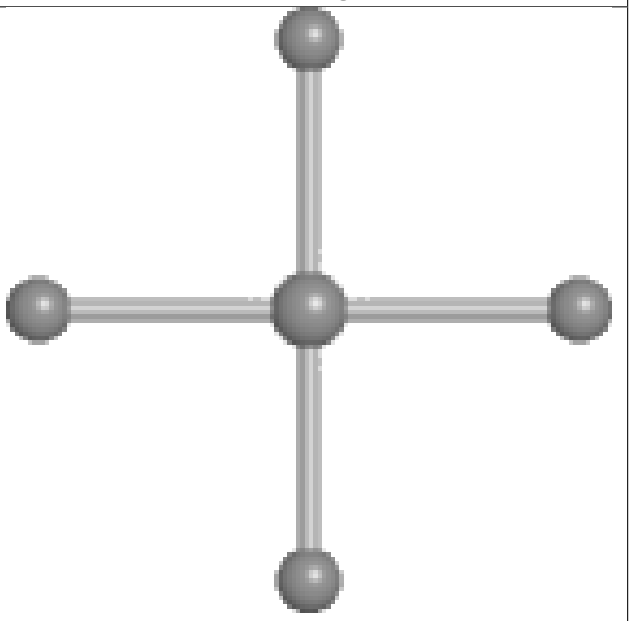
Bond lengths



Bond angles

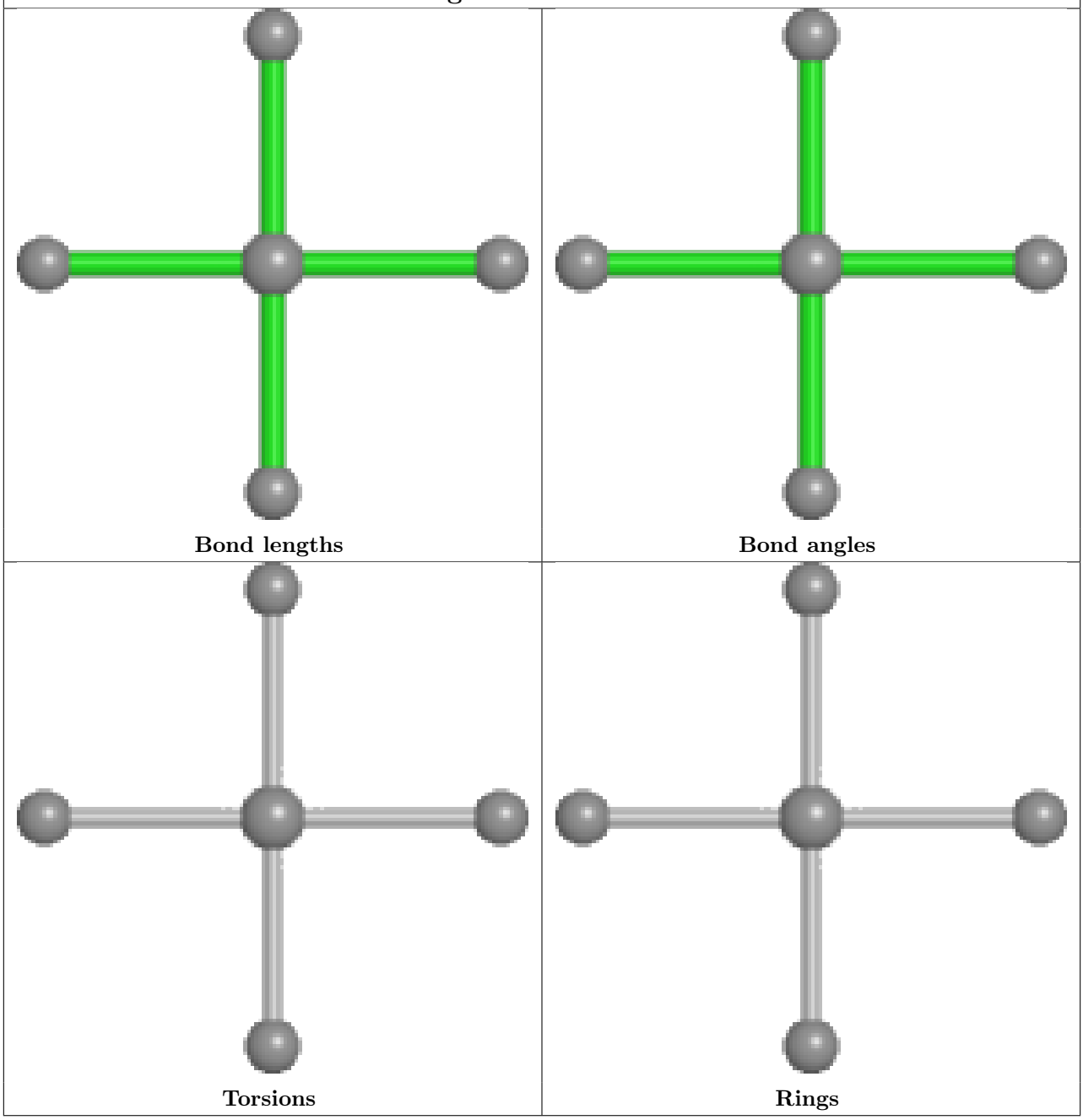


Torsions

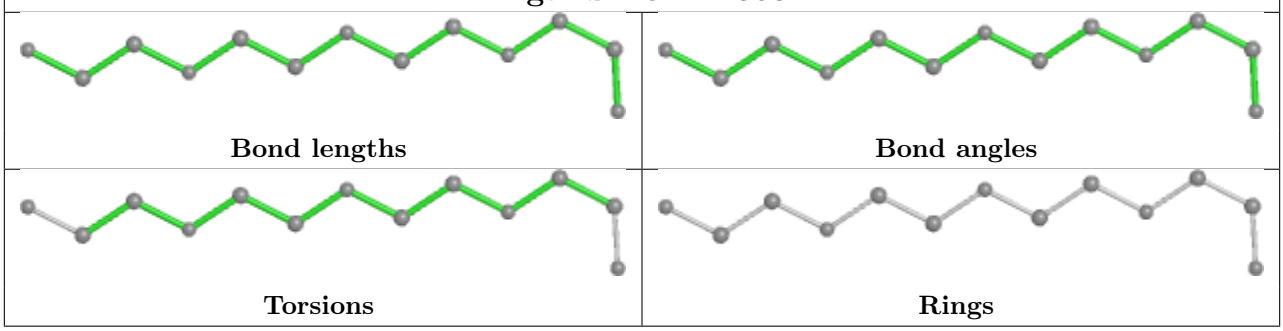


Rings

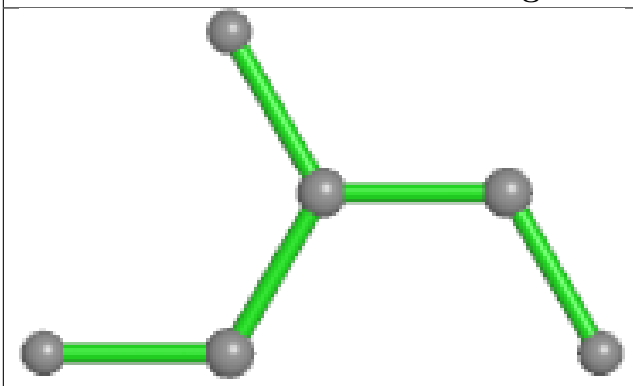
Ligand SO4 C 303



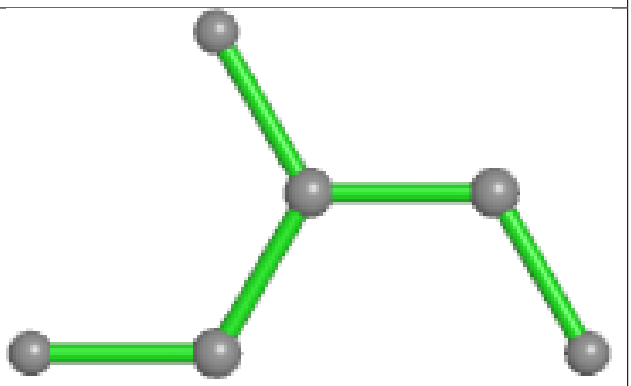
Ligand PG4 A 303



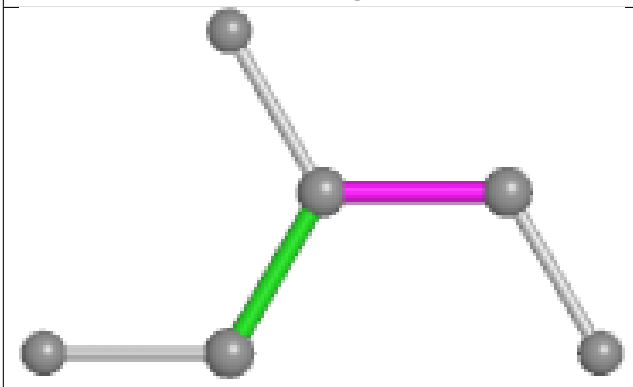
Ligand GOL D 305



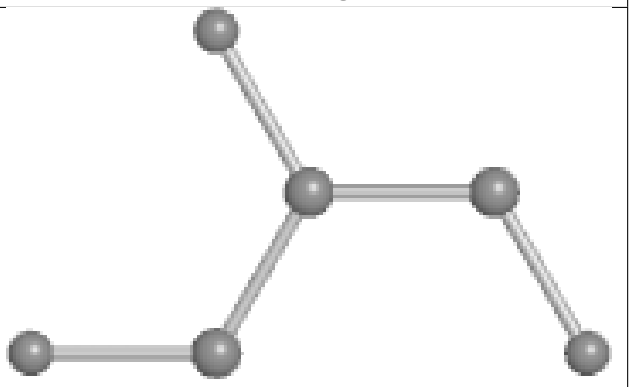
Bond lengths



Bond angles

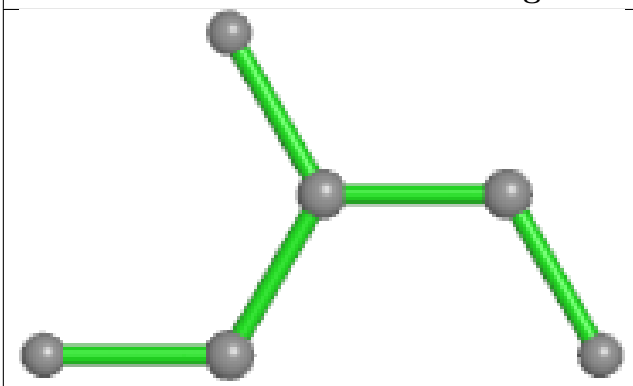


Torsions

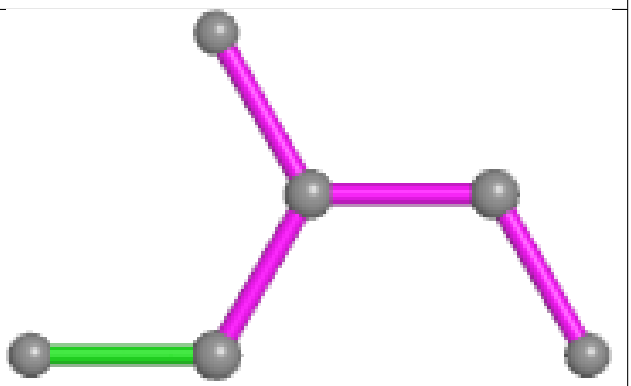


Rings

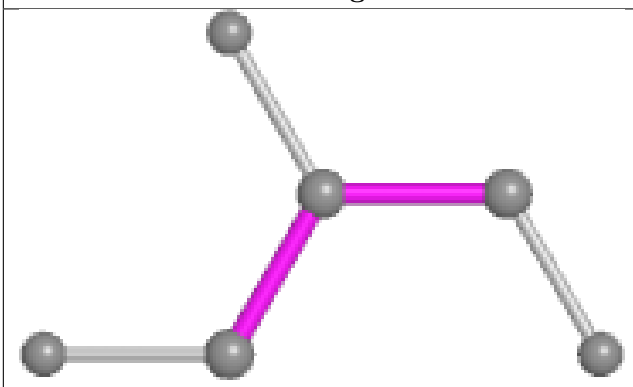
Ligand GOL B 303



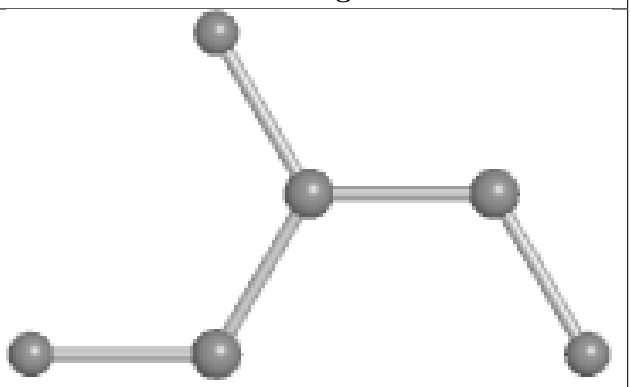
Bond lengths



Bond angles

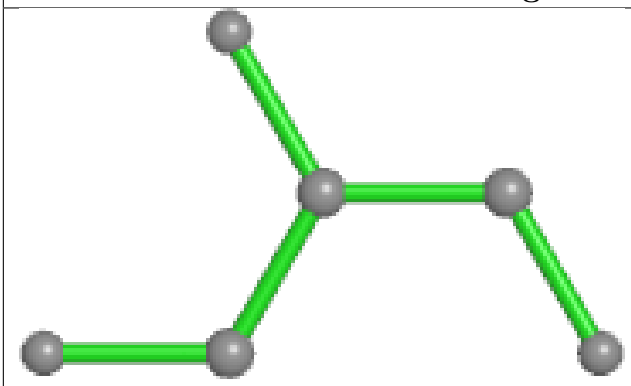


Torsions

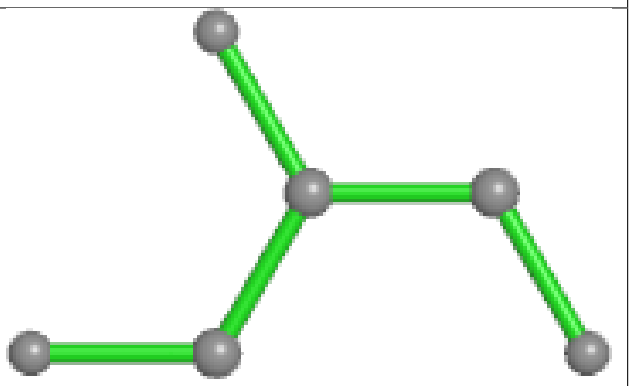


Rings

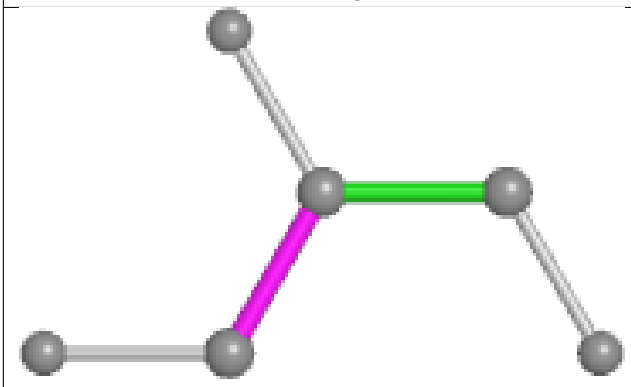
Ligand GOL A 308



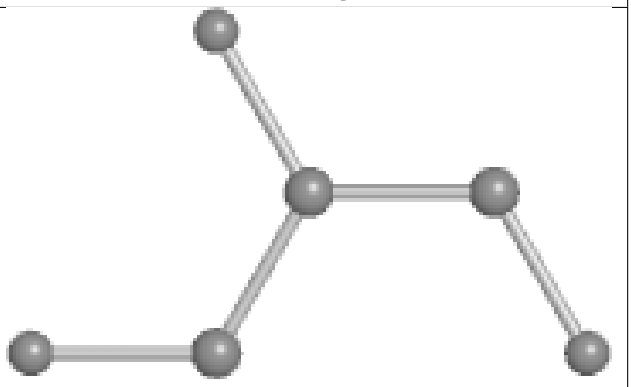
Bond lengths



Bond angles

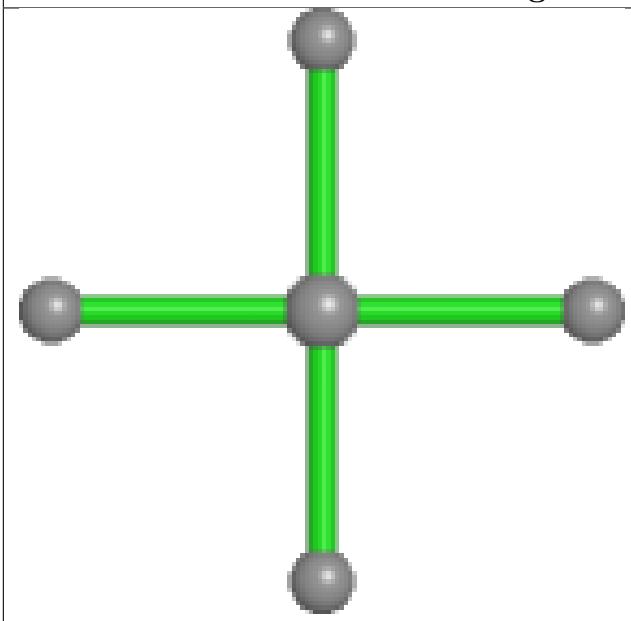


Torsions

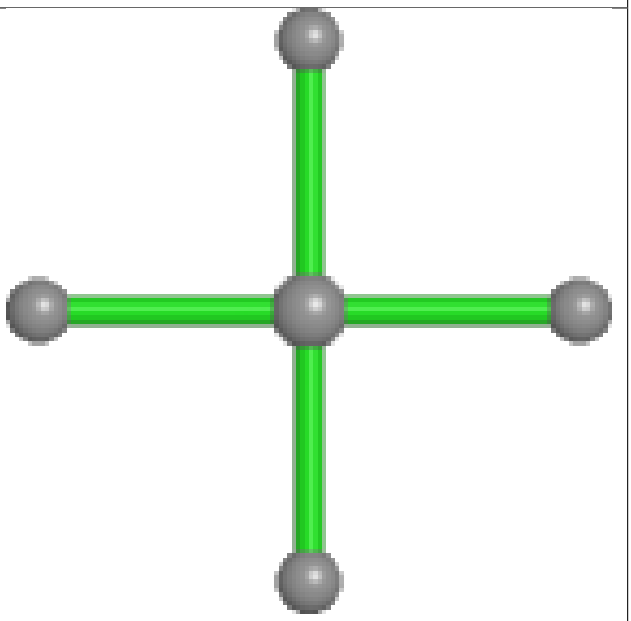


Rings

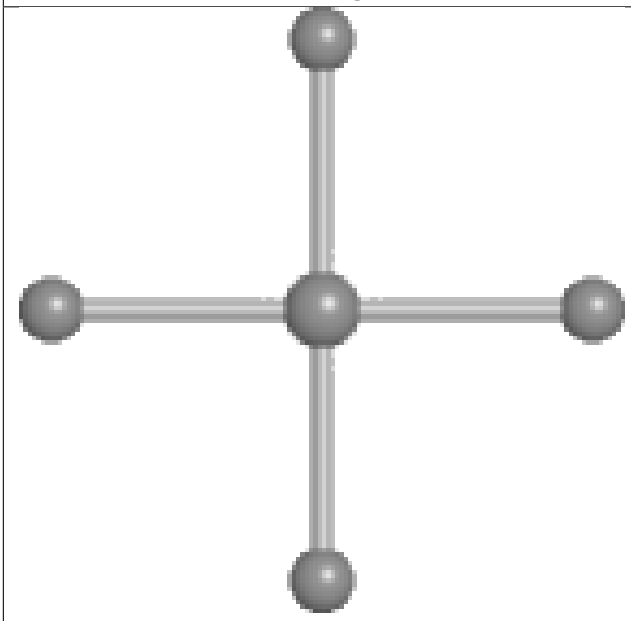
Ligand SO4 D 303



Bond lengths



Bond angles



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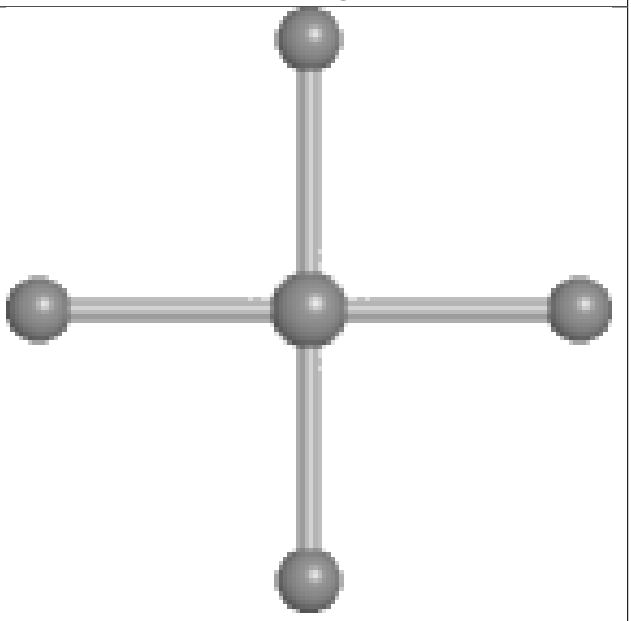
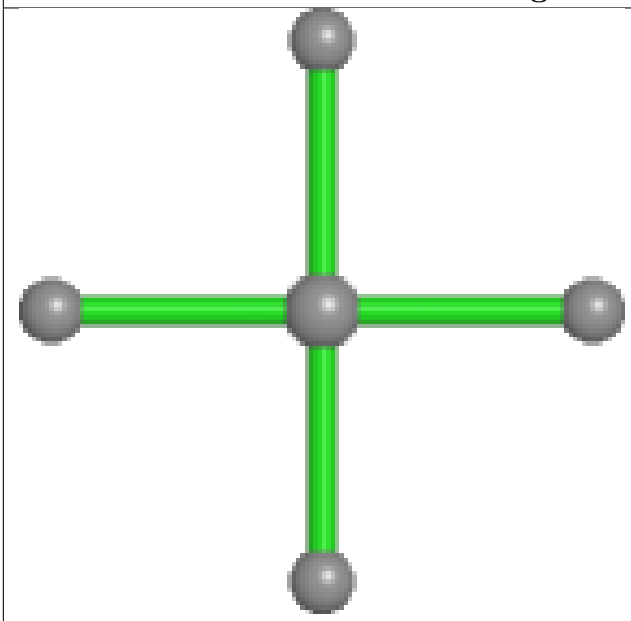
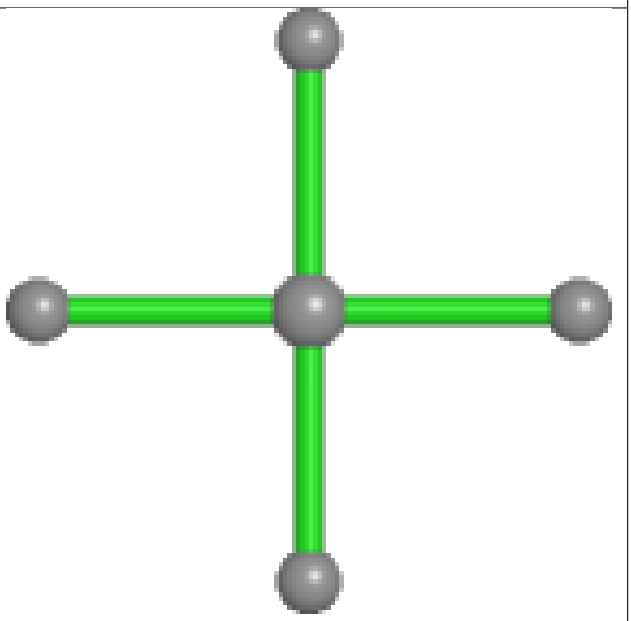


Rings

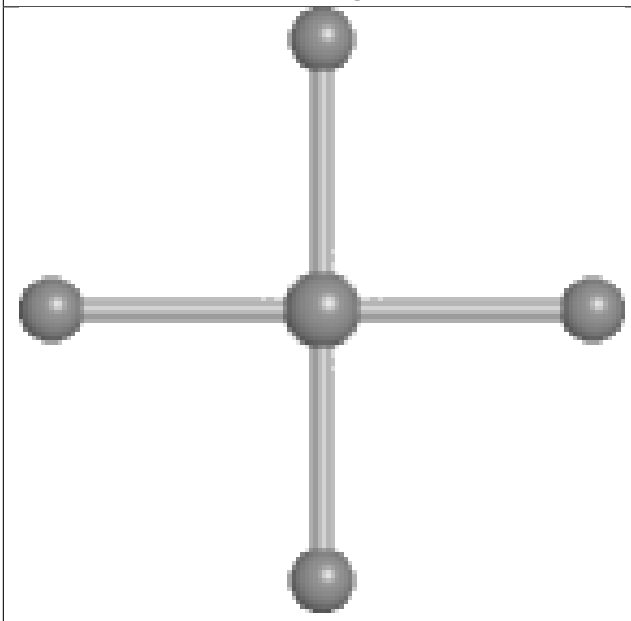
Ligand SO4 E 302



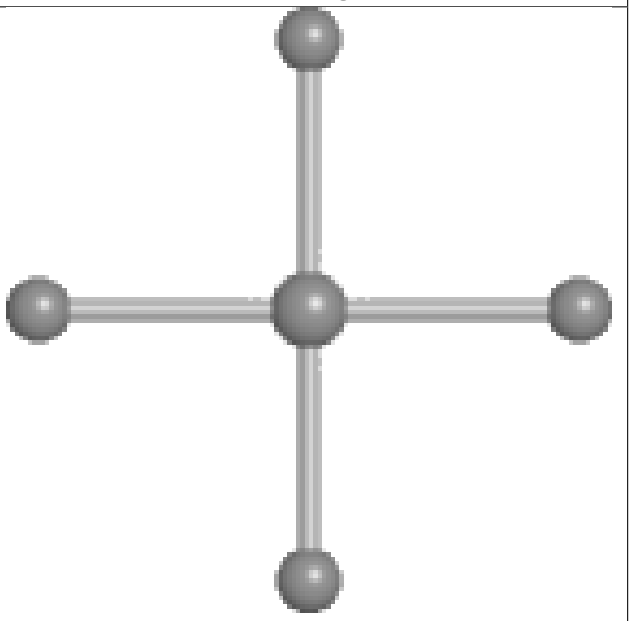
Bond lengths



Bond angles

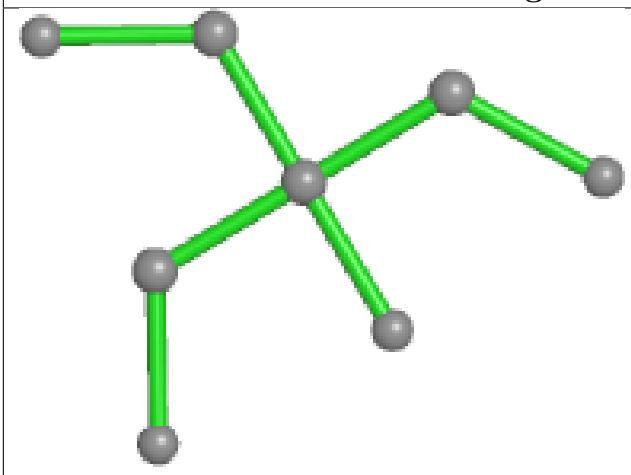


Torsions

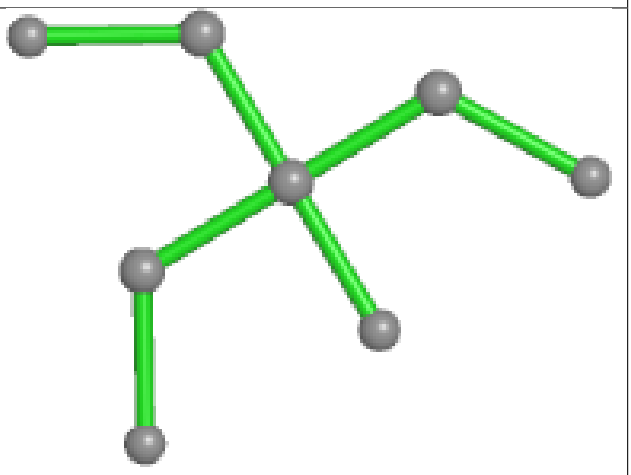


Rings

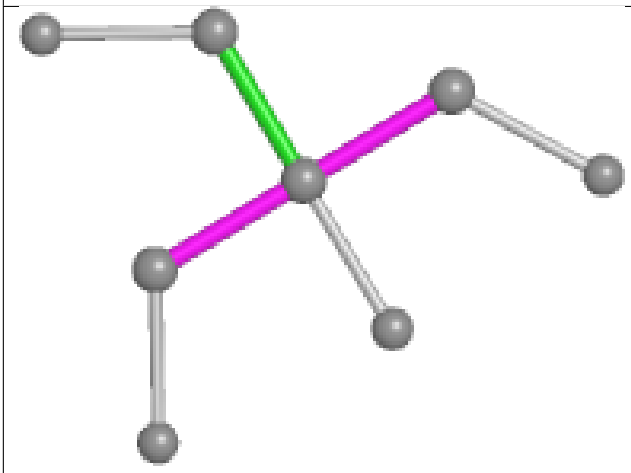
Ligand TRS A 306



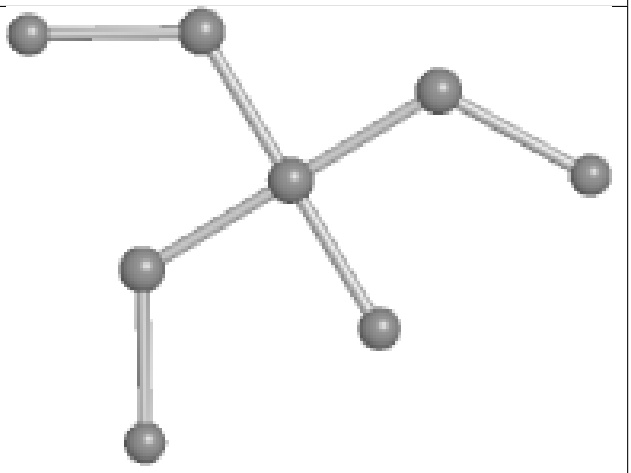
Bond lengths



Bond angles

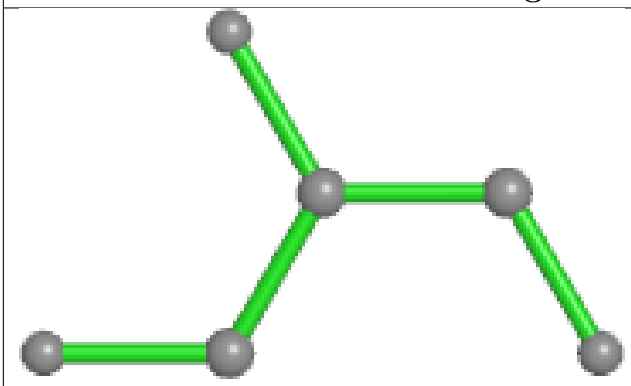


Torsions

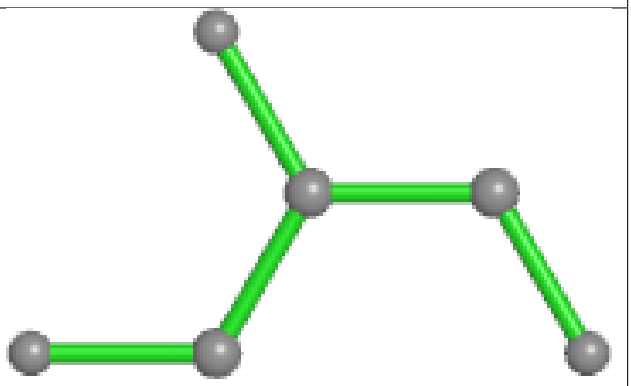


Rings

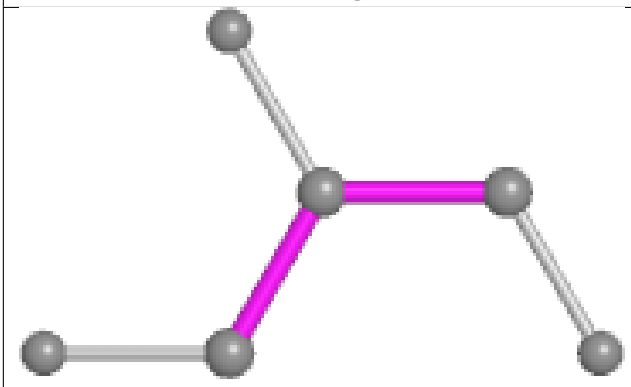
Ligand GOL E 304



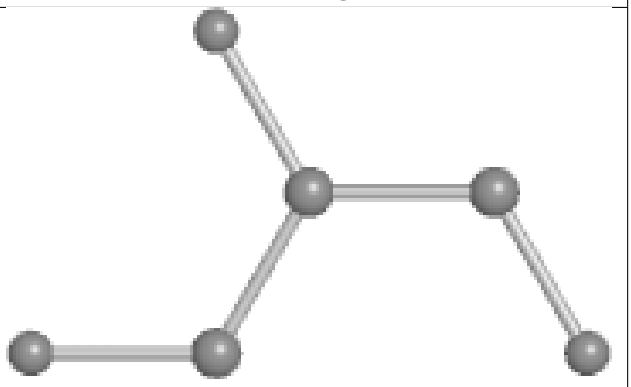
Bond lengths



Bond angles

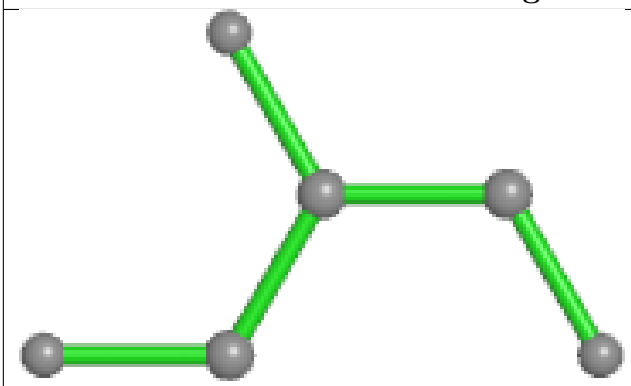


Torsions

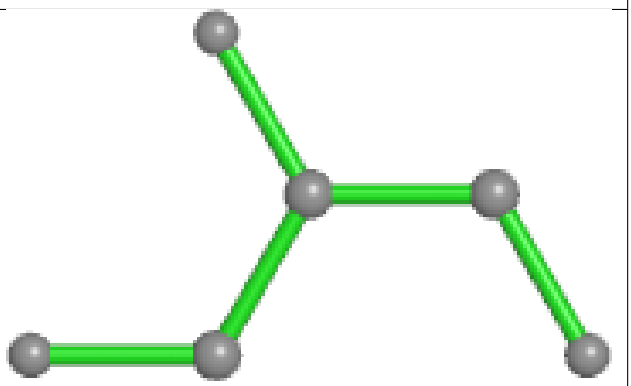


Rings

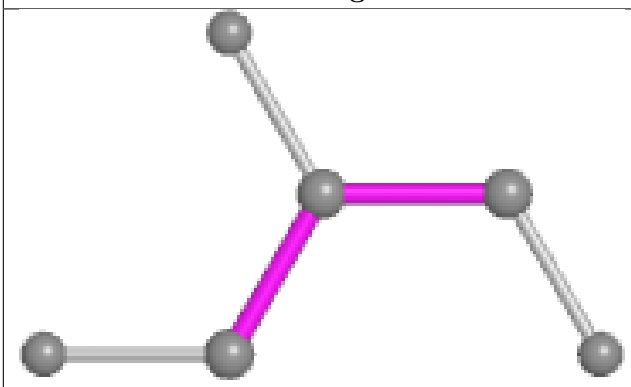
Ligand GOL A 307



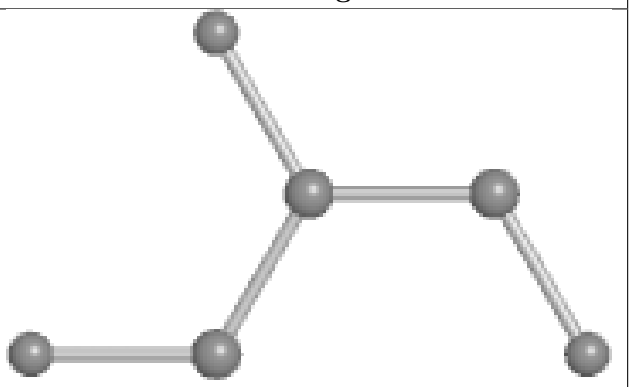
Bond lengths



Bond angles

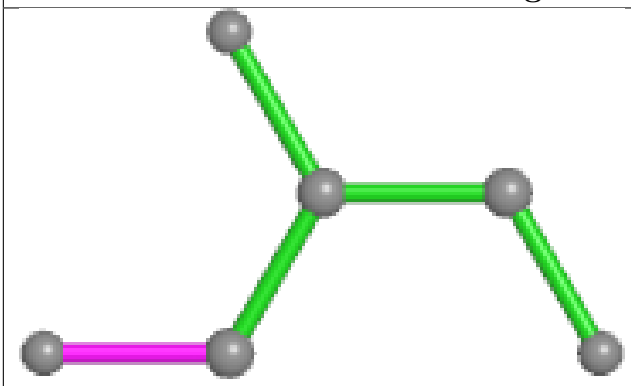


Torsions

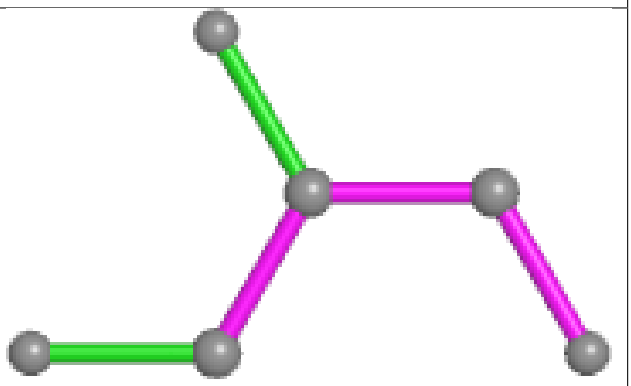


Rings

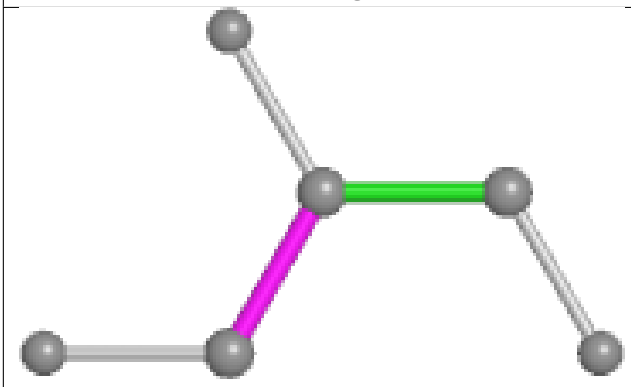
Ligand GOL E 306



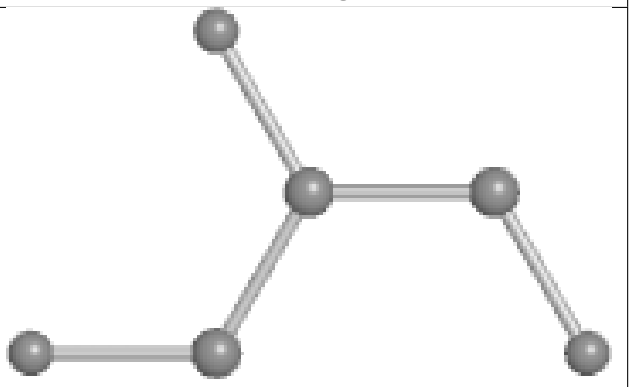
Bond lengths



Bond angles

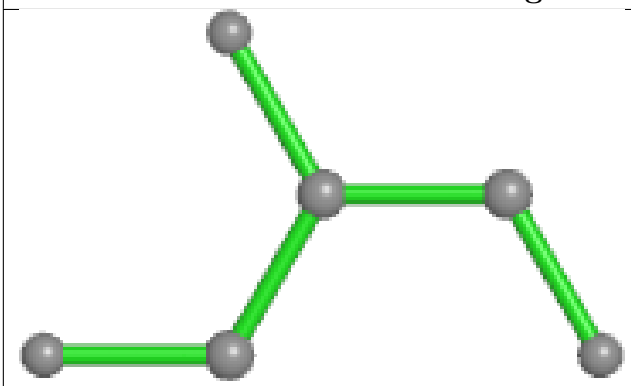


Torsions

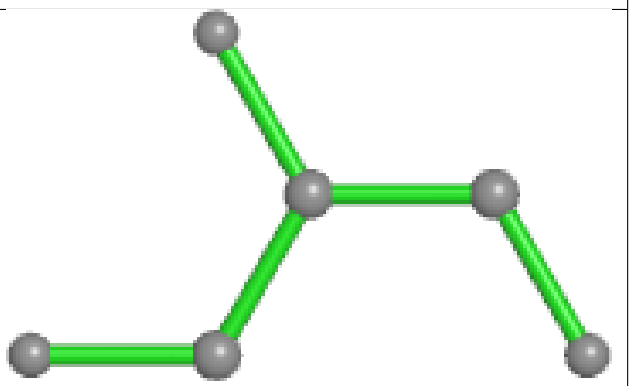


Rings

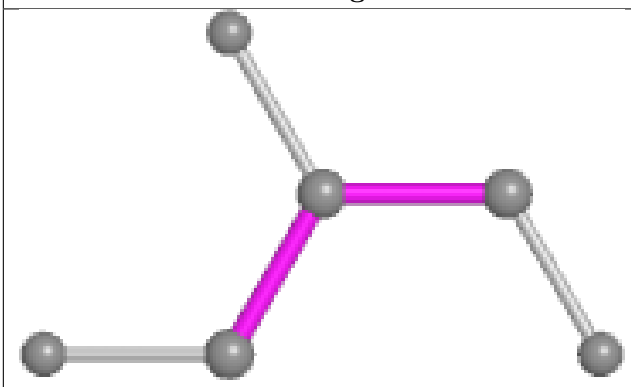
Ligand GOL F 302



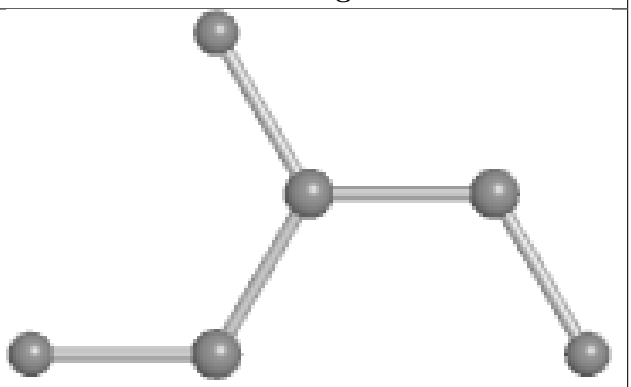
Bond lengths



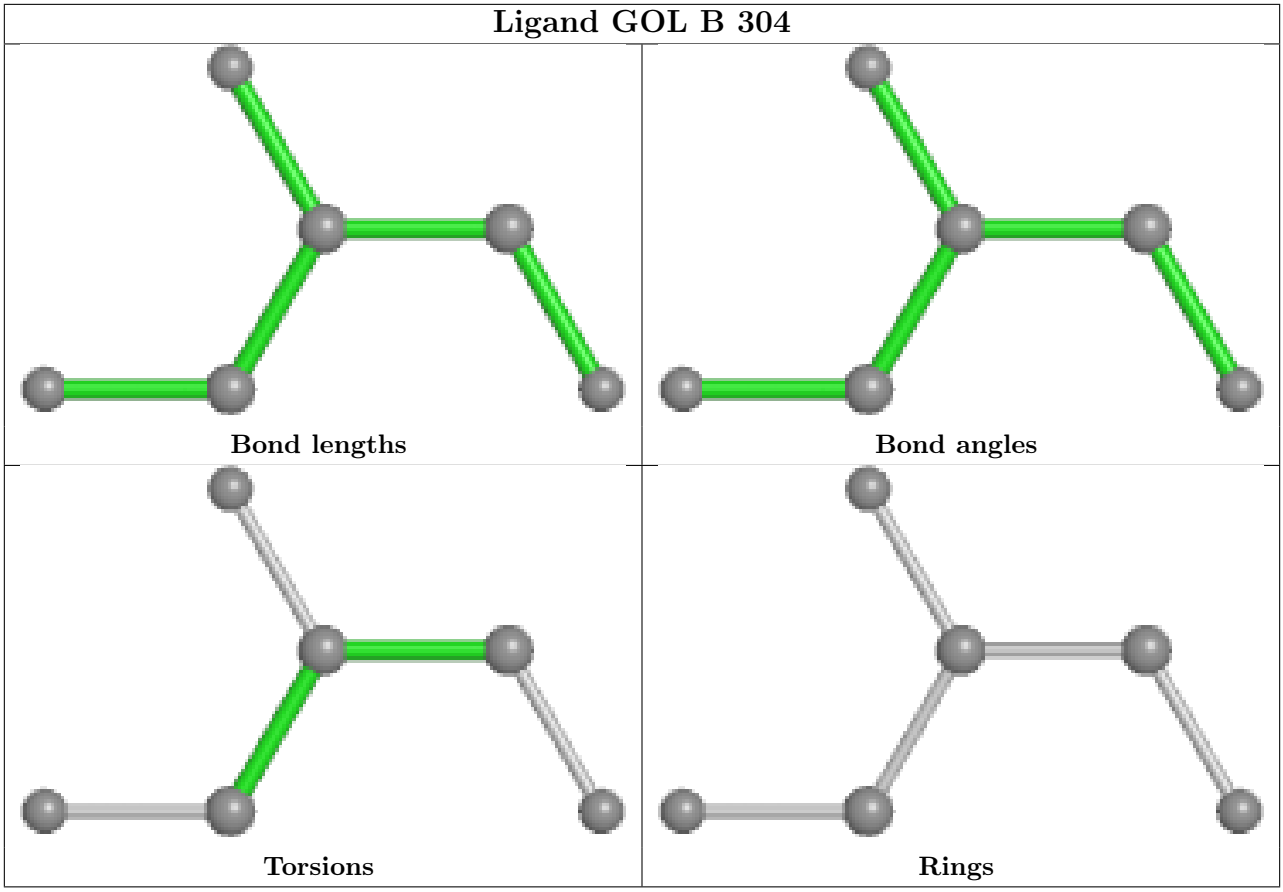
Bond angles



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	293/299 (97%)	-0.25	2 (0%)	87	90	11, 16, 27, 47	0
1	B	290/299 (96%)	-0.27	1 (0%)	94	95	11, 15, 24, 40	0
1	C	292/299 (97%)	-0.15	4 (1%)	75	79	11, 16, 28, 70	0
1	D	293/299 (97%)	-0.20	3 (1%)	82	85	11, 16, 29, 80	0
1	E	289/299 (96%)	-0.21	3 (1%)	82	85	11, 16, 28, 49	0
1	F	291/299 (97%)	-0.30	3 (1%)	82	85	10, 15, 23, 47	0
All	All	1748/1794 (97%)	-0.23	16 (0%)	84	87	10, 16, 28, 80	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	294	HIS	4.4
1	C	294	HIS	3.9
1	C	3	GLU	3.9
1	C	292	ALA	3.8
1	D	292	ALA	3.5
1	C	293	LEU	3.3
1	A	294	HIS	3.2
1	A	295	HIS	2.9
1	F	293	LEU	2.8
1	D	3	GLU	2.6
1	B	2	SER	2.4
1	F	292	ALA	2.4
1	E	3	GLU	2.3
1	F	3	GLU	2.3
1	E	165	TYR	2.3
1	E	144	PHE	2.1

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	A	305	6/6	0.45	0.19	43,44,45,46	0
5	GOL	A	307	6/6	0.62	0.28	45,45,46,47	0
5	GOL	E	303	6/6	0.73	0.17	37,38,40,41	0
5	GOL	B	304	6/6	0.75	0.16	41,41,41,43	0
4	PG4	D	304	13/13	0.75	0.27	40,43,48,49	0
5	GOL	E	304	6/6	0.78	0.16	39,42,45,47	0
6	TRS	A	306	8/8	0.78	0.22	17,28,33,34	0
5	GOL	A	308	6/6	0.79	0.19	41,48,49,50	0
5	GOL	F	302	6/6	0.80	0.14	34,40,42,42	0
3	SO4	C	303	5/5	0.82	0.18	75,75,75,75	0
4	PG4	E	305	13/13	0.82	0.19	21,26,33,36	0
3	SO4	D	303	5/5	0.85	0.24	34,37,39,39	0
5	GOL	C	304	6/6	0.85	0.17	22,27,30,30	0
5	GOL	E	306	6/6	0.89	0.17	25,29,31,33	0
4	PG4	A	303	13/13	0.89	0.16	24,28,33,35	0
5	GOL	D	305	6/6	0.89	0.14	19,28,31,32	0
5	GOL	A	304	6/6	0.92	0.25	22,35,38,40	0
5	GOL	B	303	6/6	0.93	0.18	24,31,34,34	0
3	SO4	A	302	5/5	0.94	0.16	78,78,78,78	0
3	SO4	E	302	5/5	0.94	0.10	23,25,27,28	5
3	SO4	C	302	5/5	0.97	0.12	24,29,30,31	0
3	SO4	B	302	5/5	0.98	0.10	21,25,26,28	0
3	SO4	D	302	5/5	0.98	0.08	17,19,22,24	0
2	CL	C	301	1/1	0.99	0.05	15,15,15,15	0
2	CL	B	301	1/1	0.99	0.07	15,15,15,15	0
2	CL	F	301	1/1	1.00	0.07	14,14,14,14	0
2	CL	A	301	1/1	1.00	0.05	15,15,15,15	0

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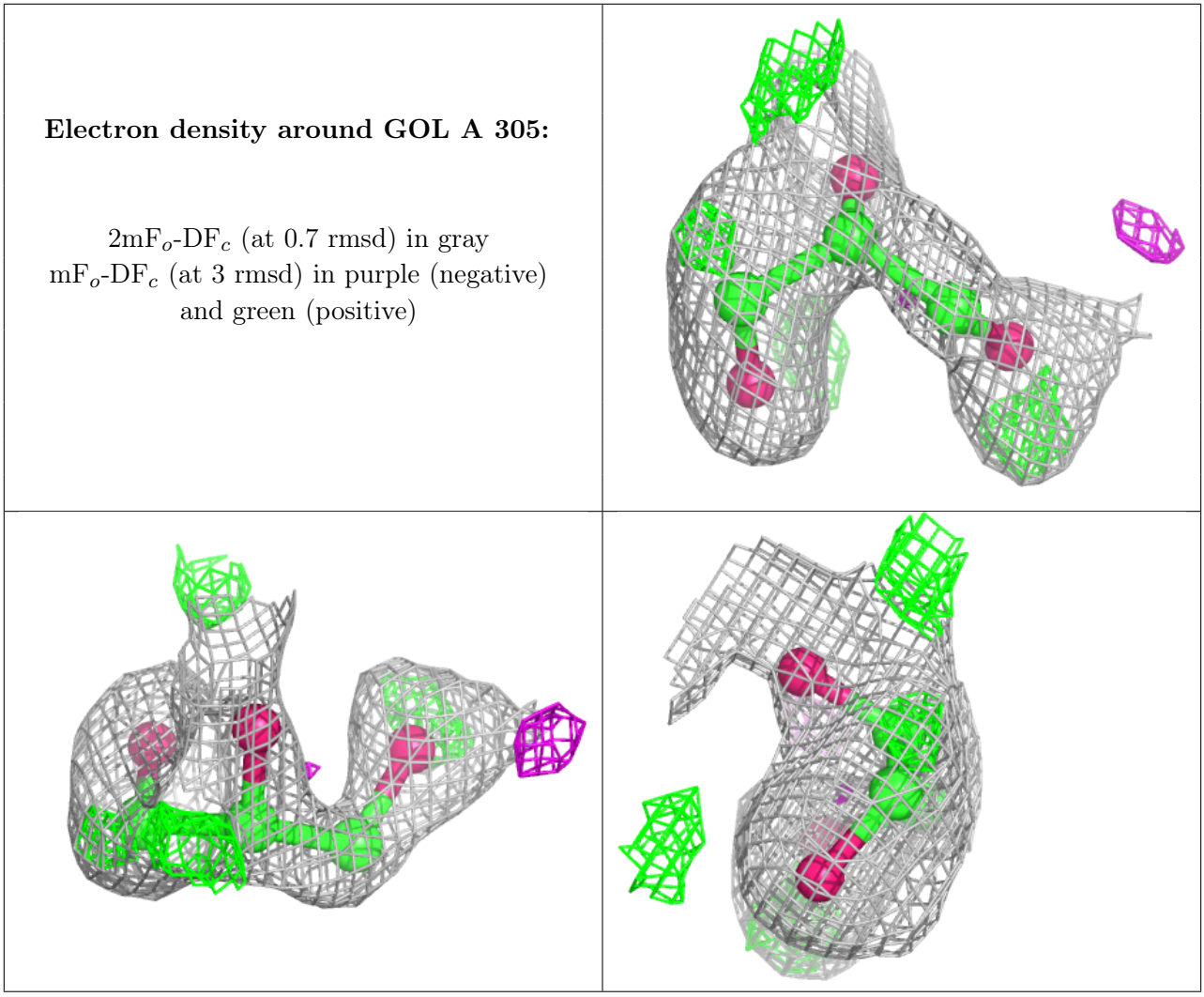
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	D	301	1/1	1.00	0.05	16,16,16,16	0
2	CL	E	301	1/1	1.00	0.05	17,17,17,17	0

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.

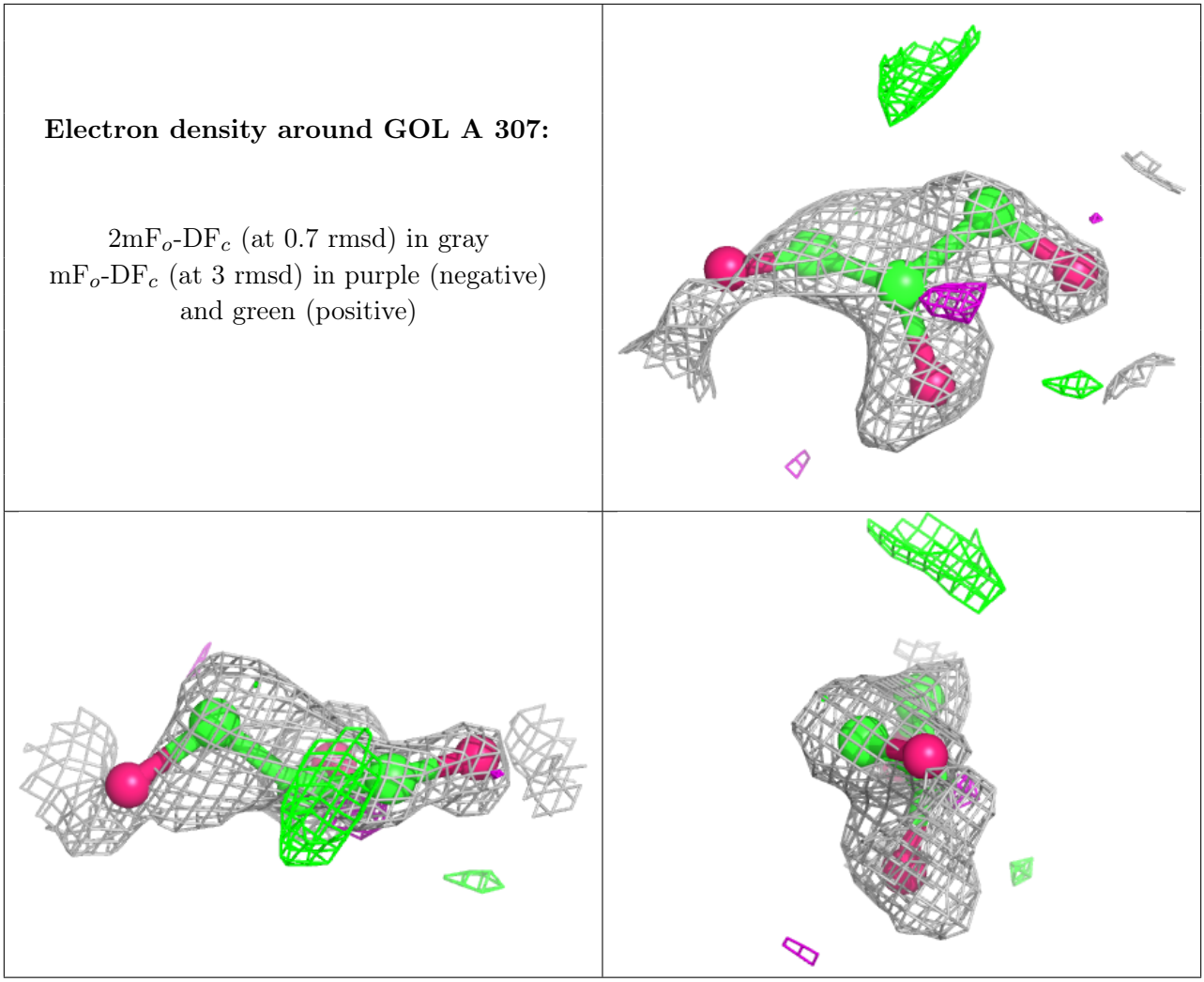
Electron density around GOL A 305:

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



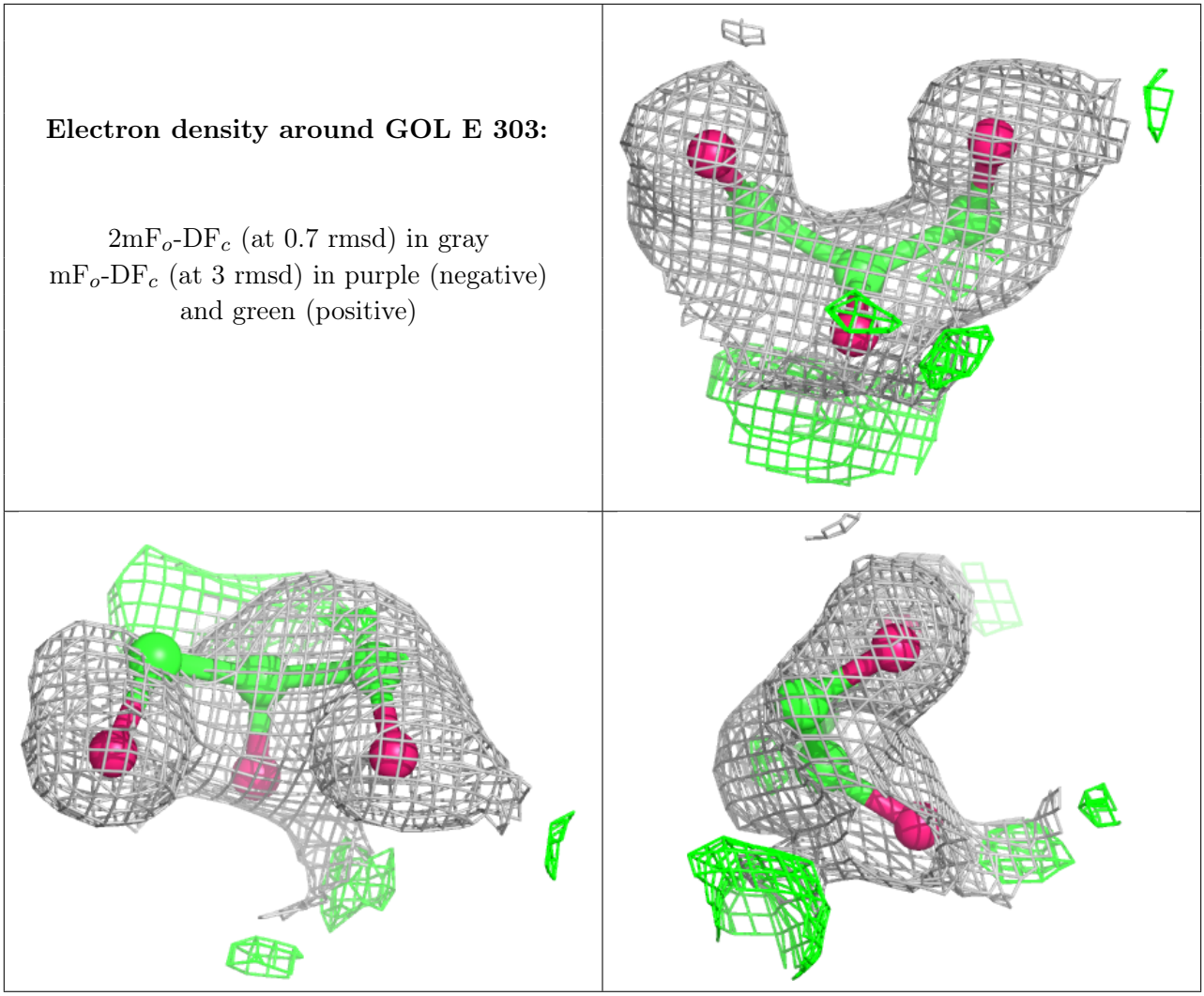
Electron density around GOL A 307:

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



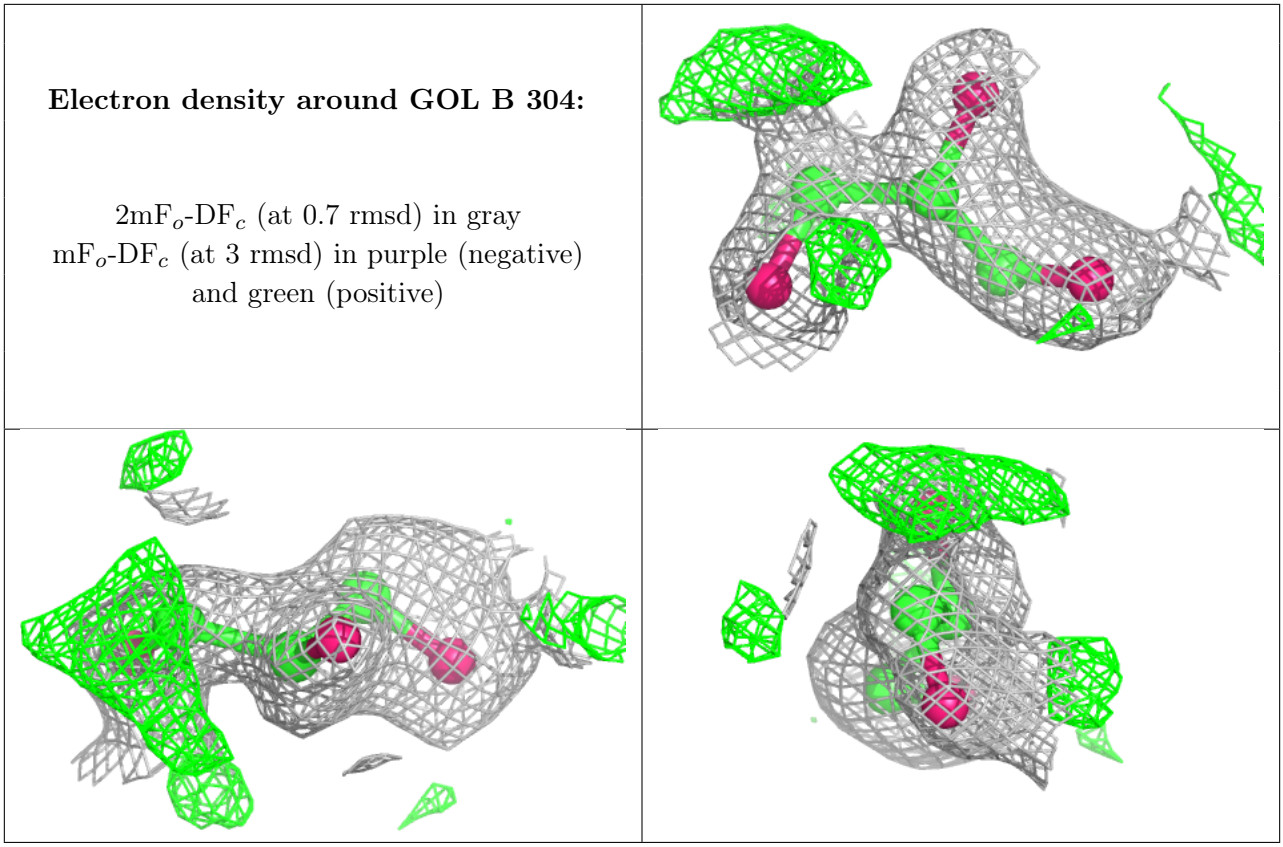
Electron density around GOL E 303:

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



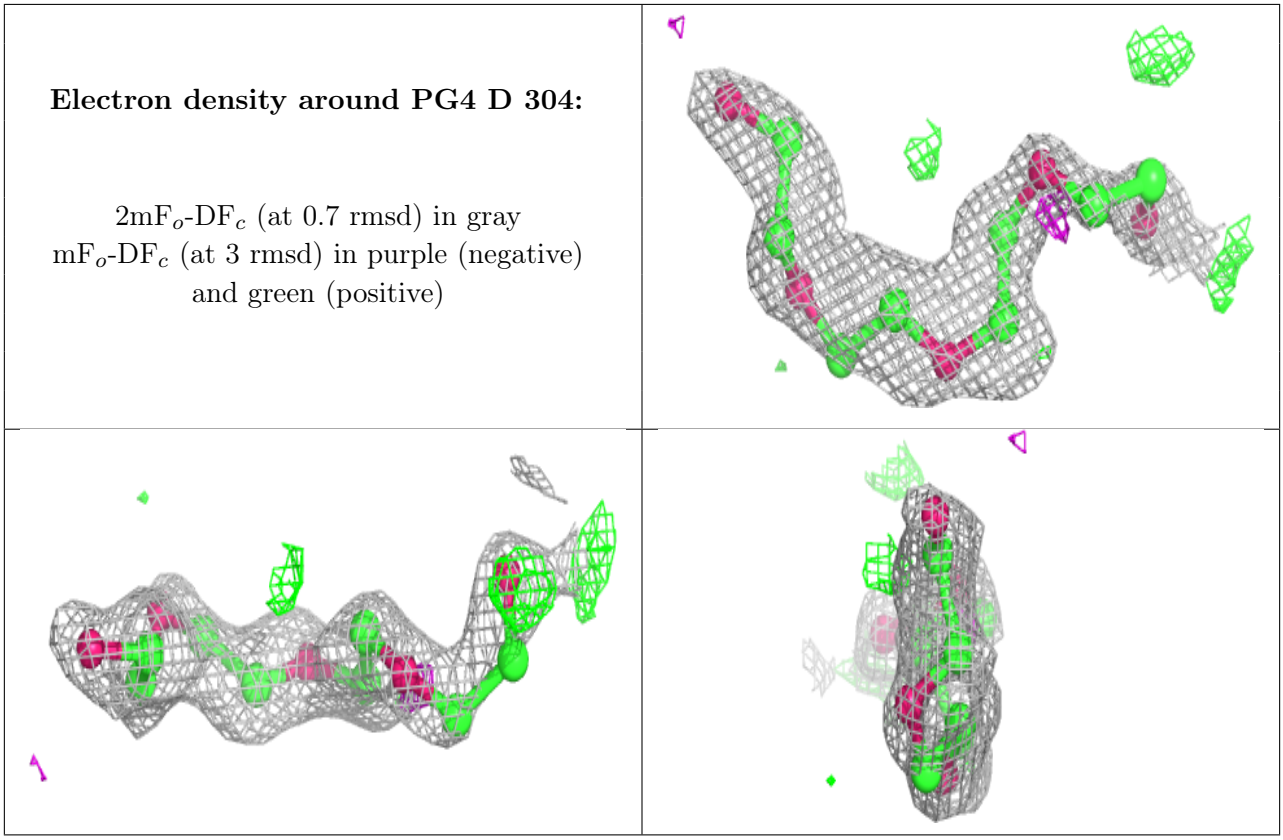
Electron density around GOL B 304:

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



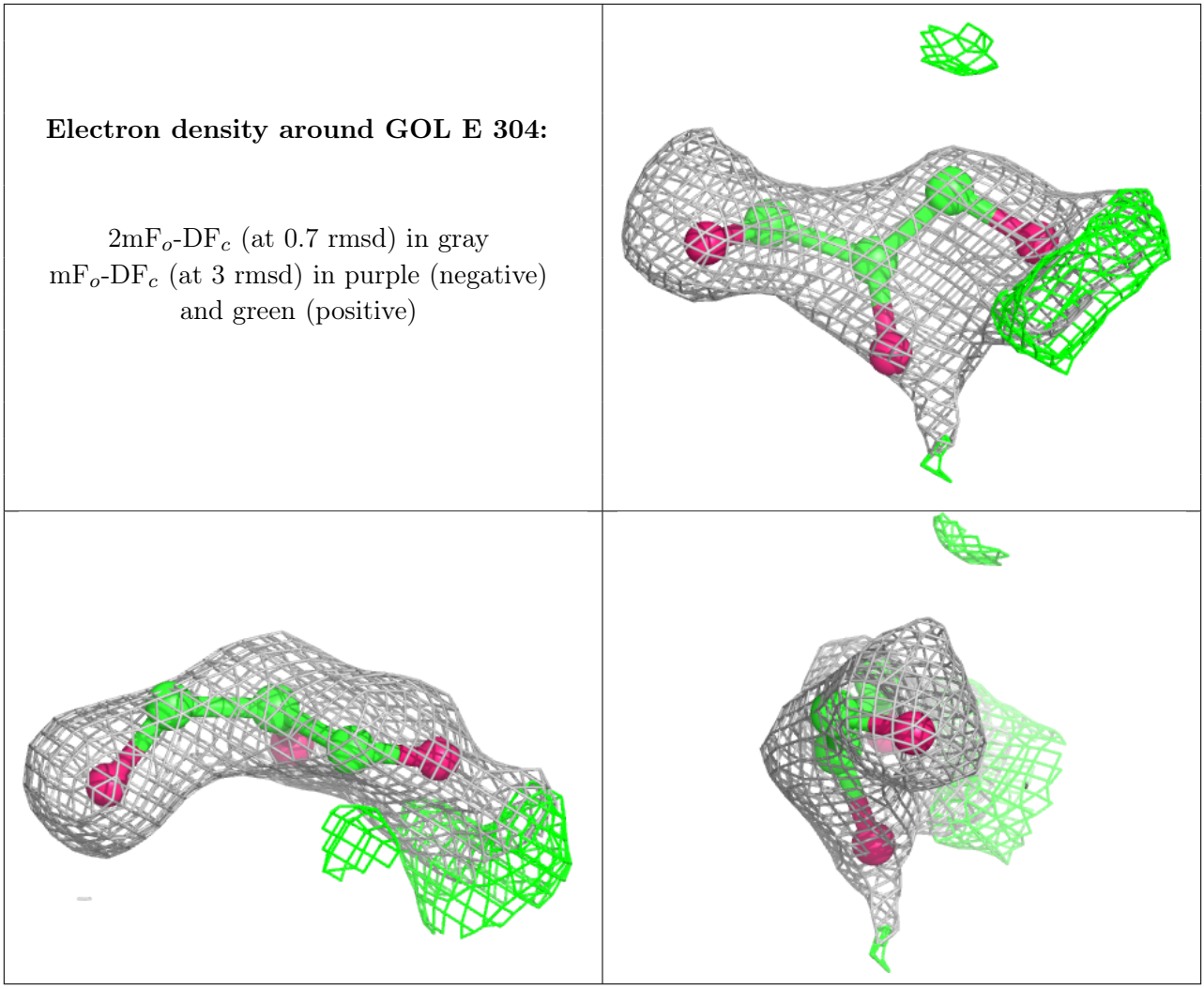
Electron density around PG4 D 304:

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



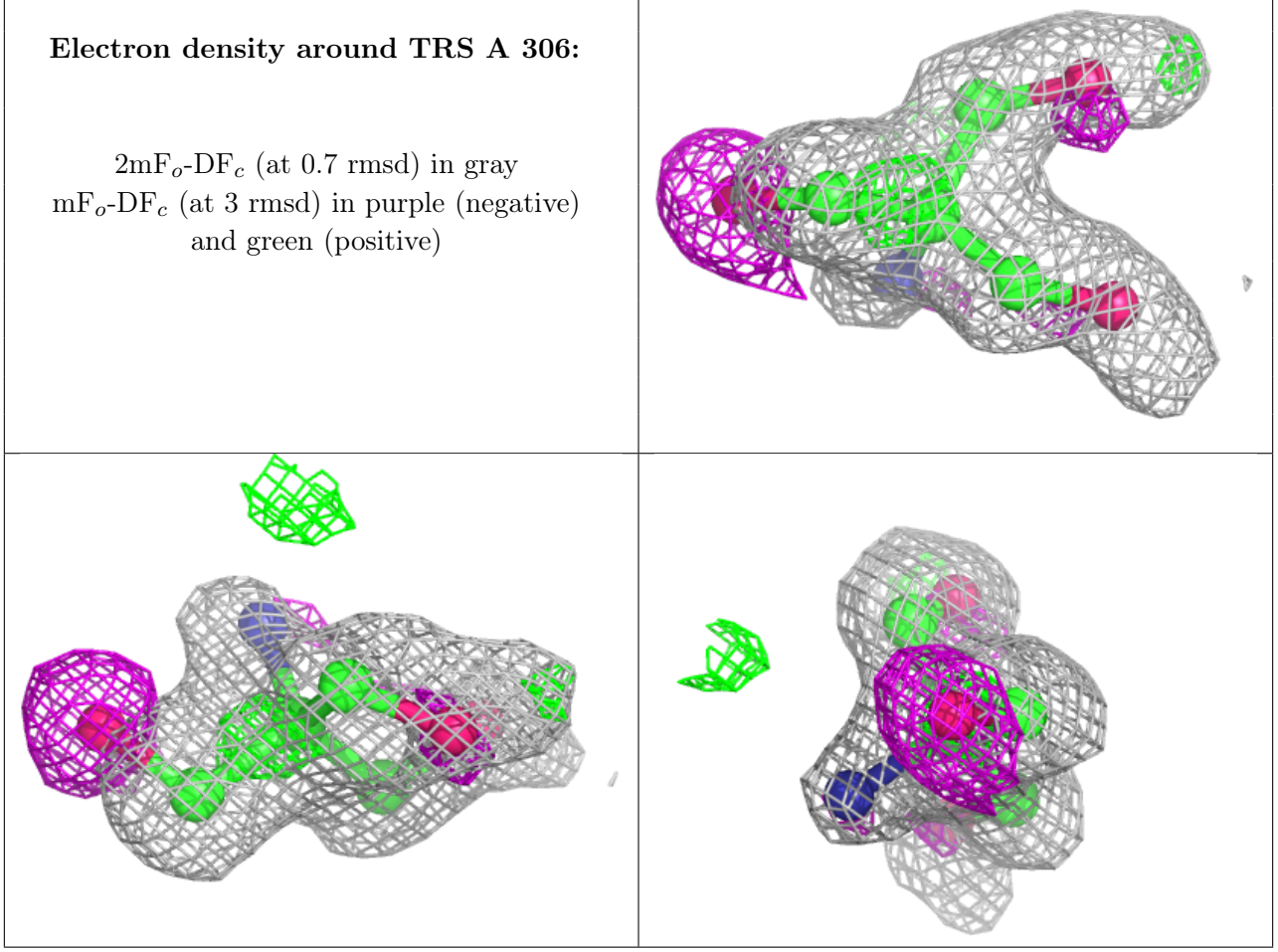
Electron density around GOL E 304:

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



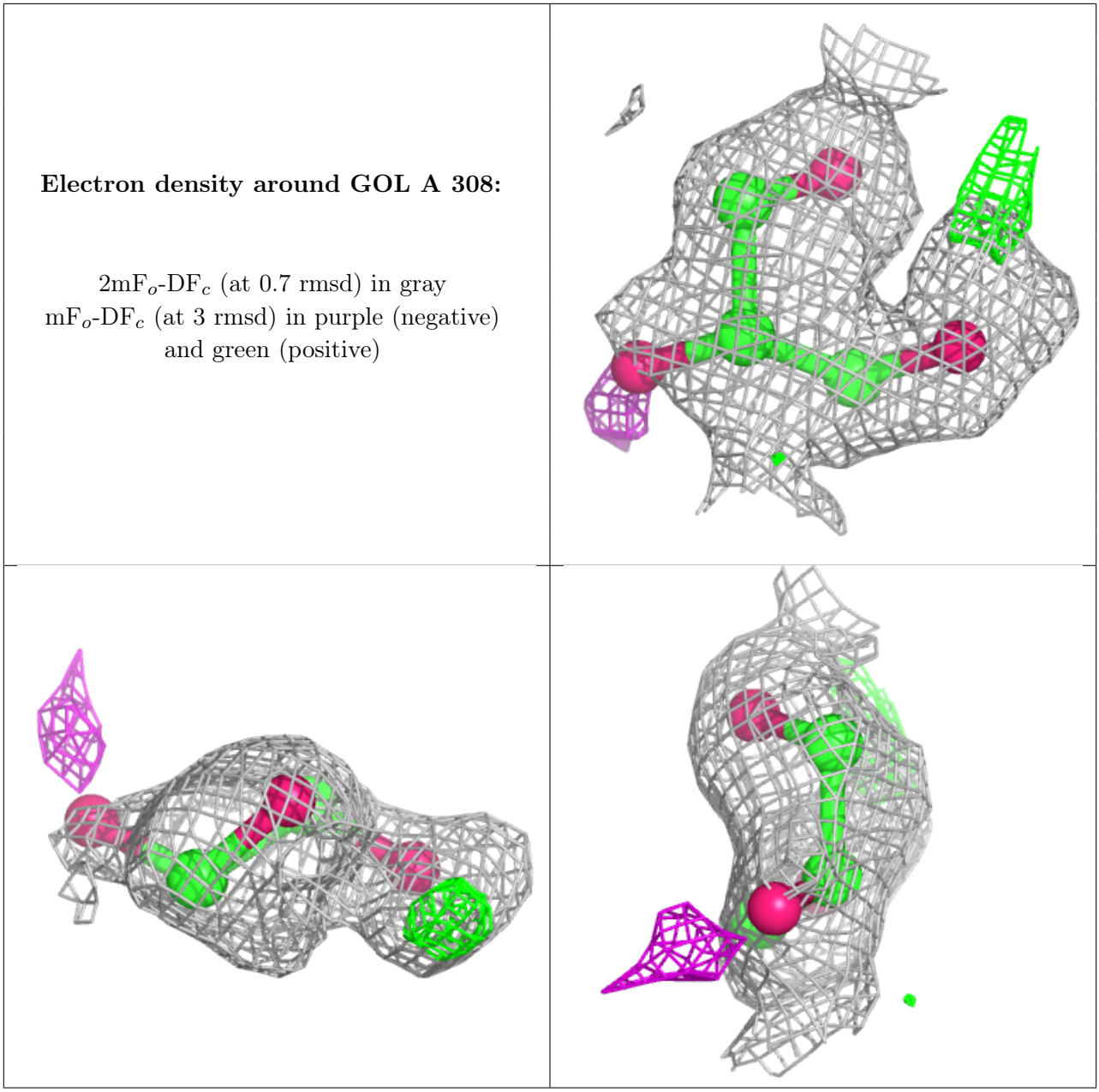
Electron density around TRS A 306:

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



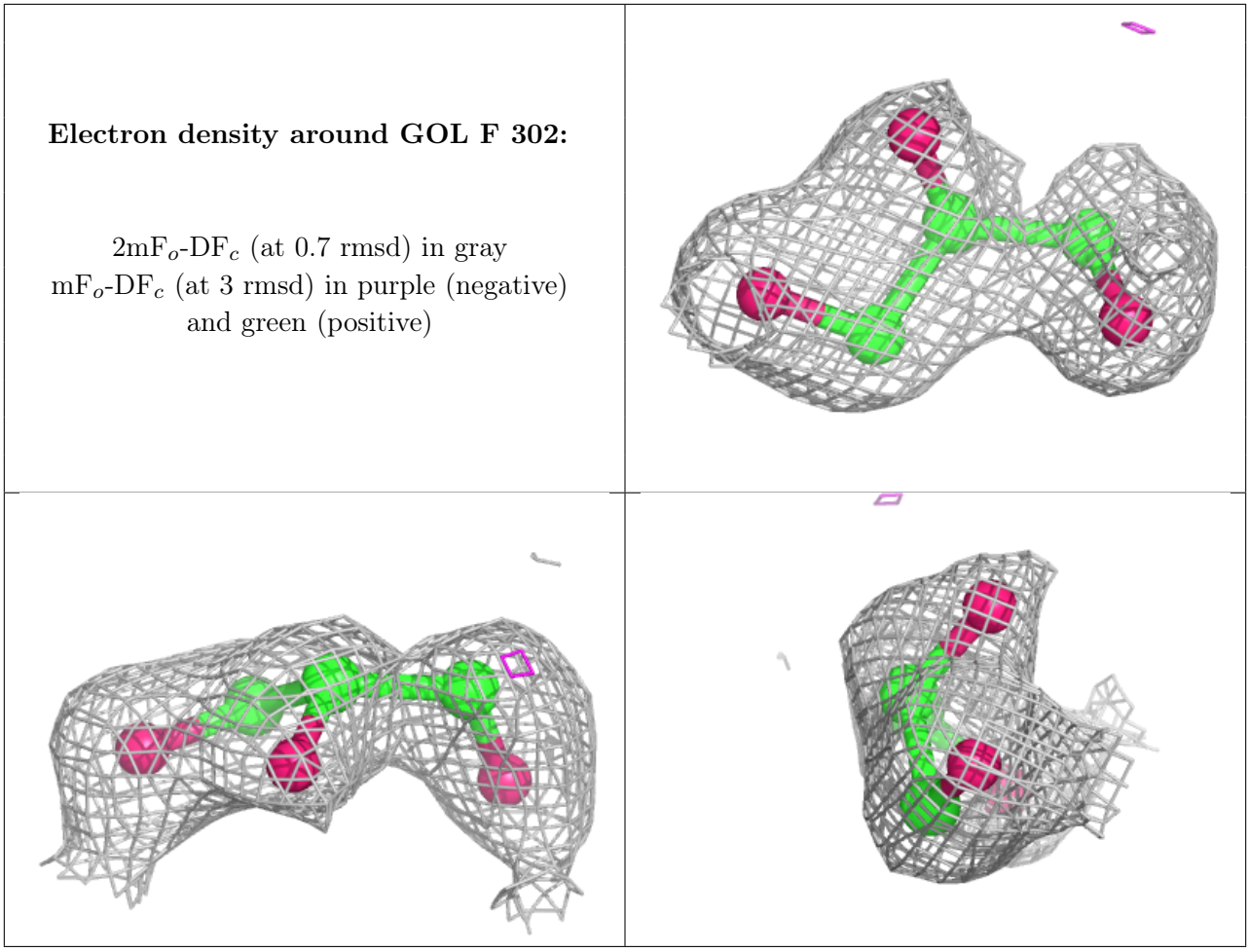
Electron density around GOL A 308:

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



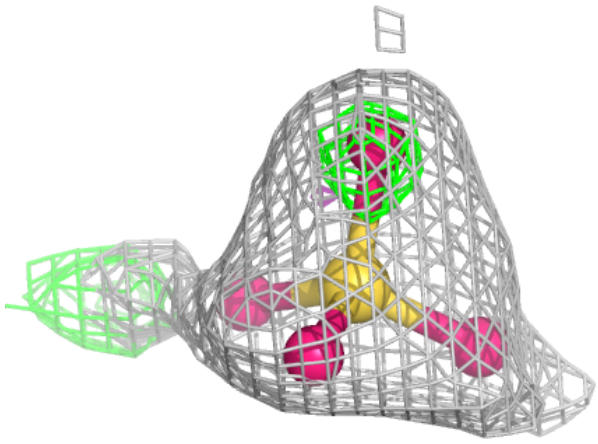
Electron density around GOL F 302:

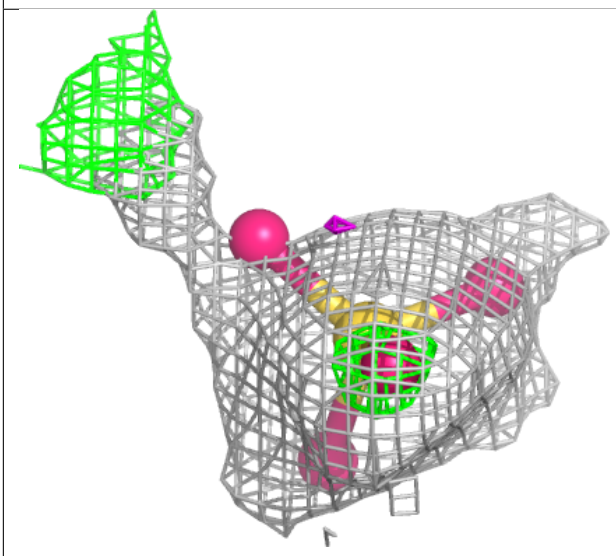
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

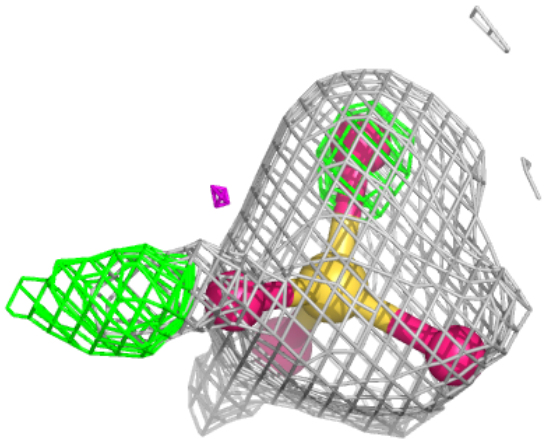


Electron density around SO4 C 303:

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

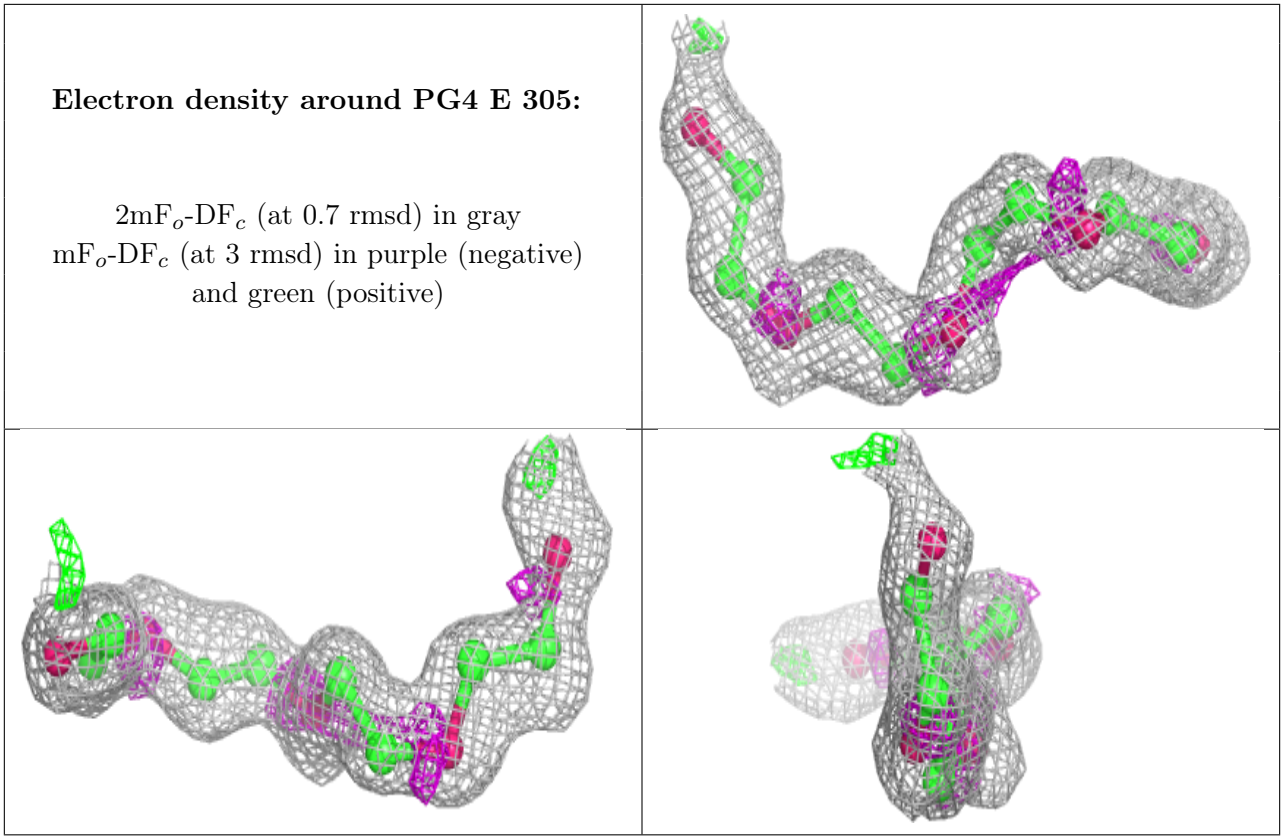






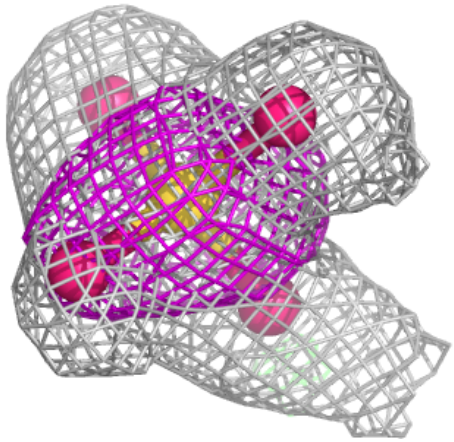
Electron density around PG4 E 305:

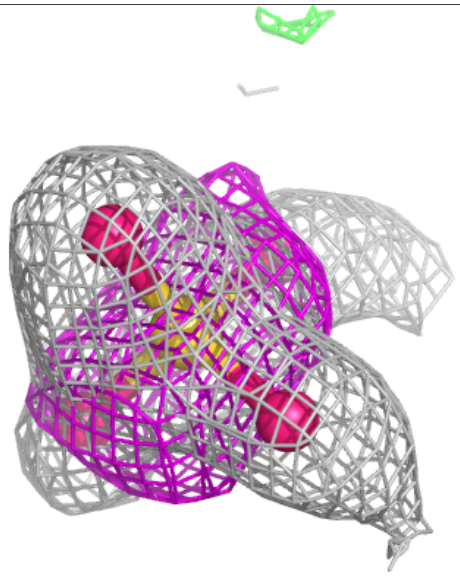
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

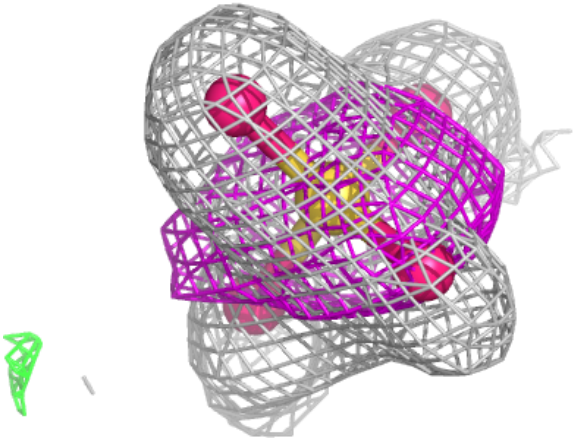


Electron density around SO4 D 303:

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

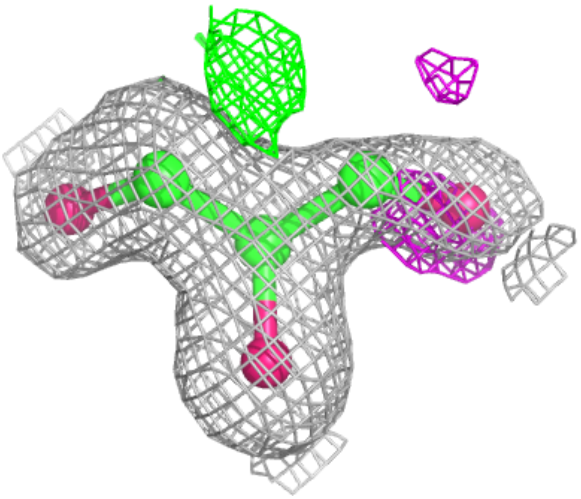


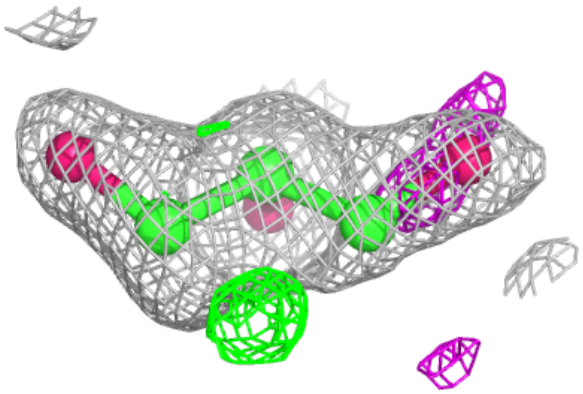


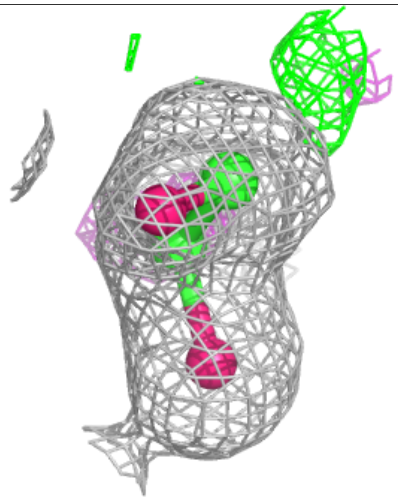


Electron density around GOL C 304:

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

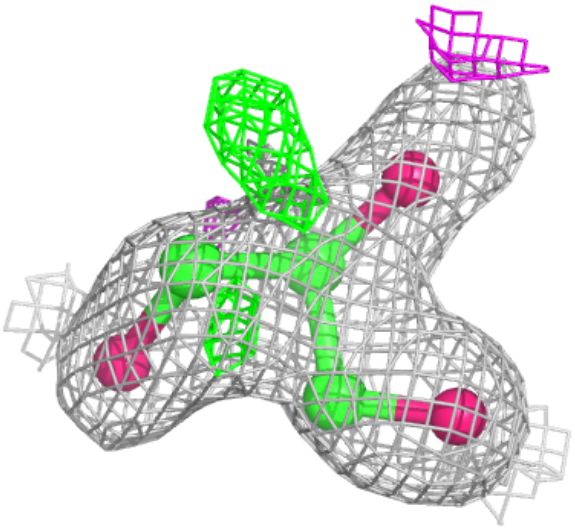


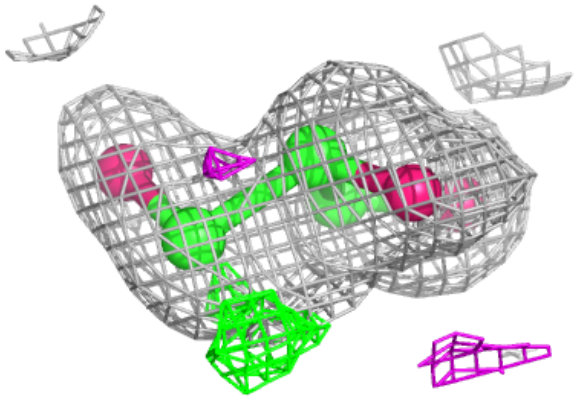


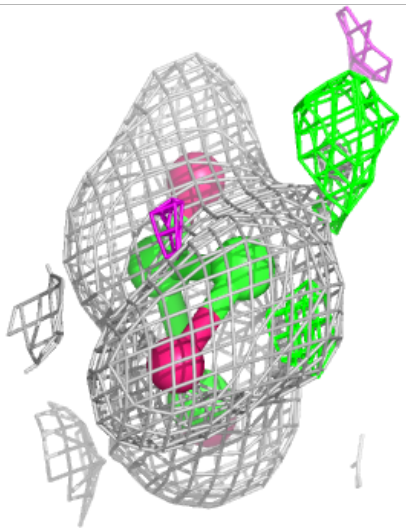


Electron density around GOL E 306:

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

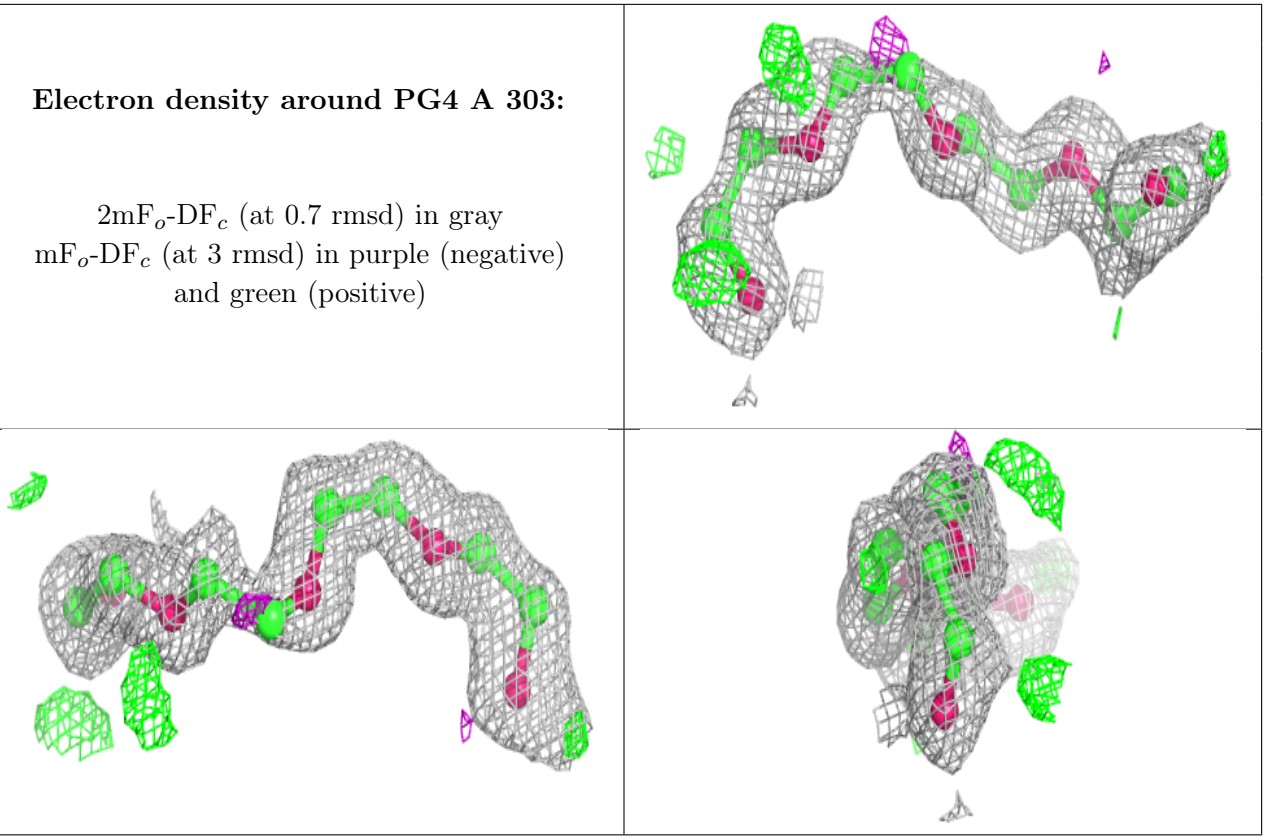






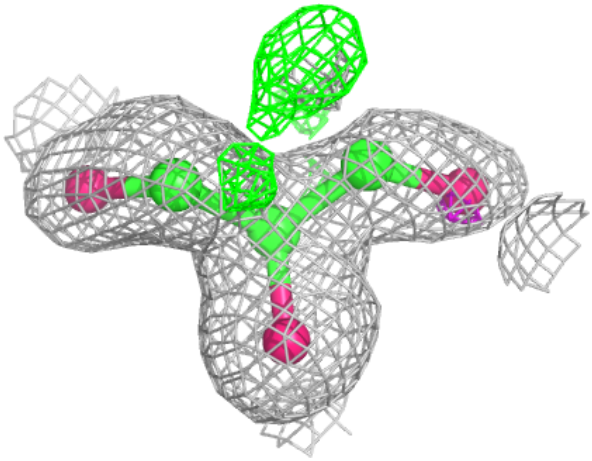
Electron density around PG4 A 303:

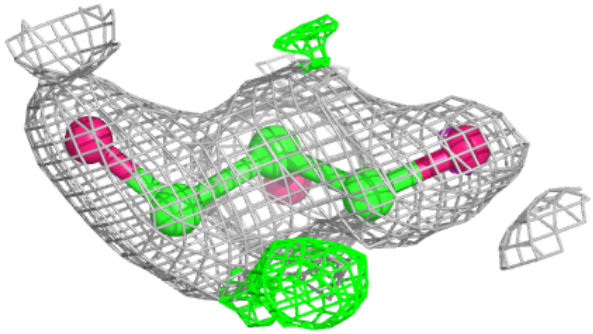
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

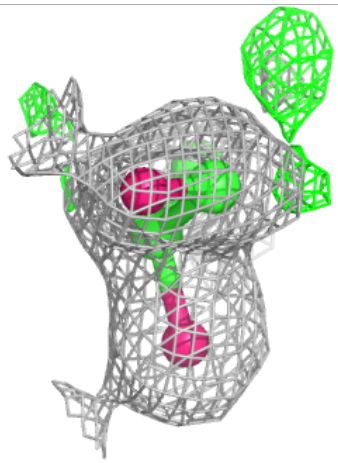


Electron density around GOL D 305:

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

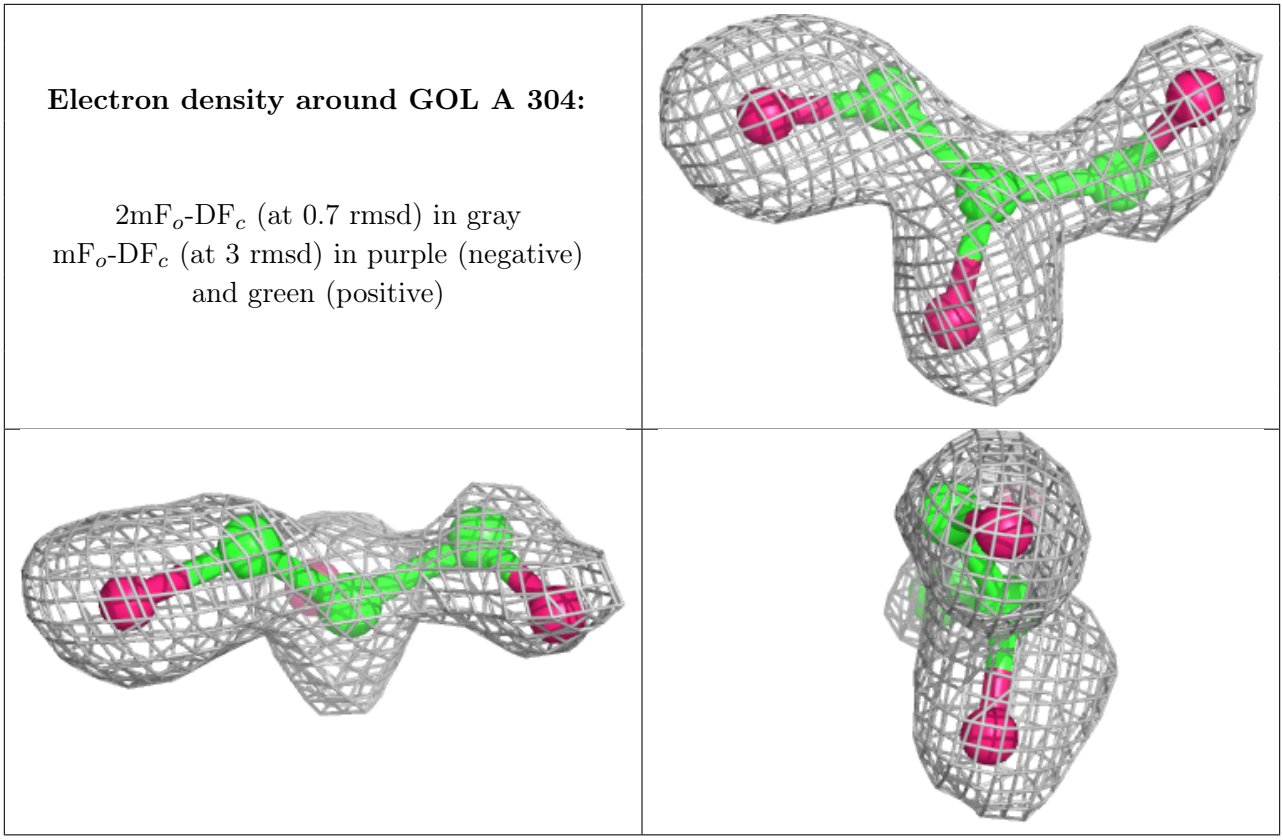






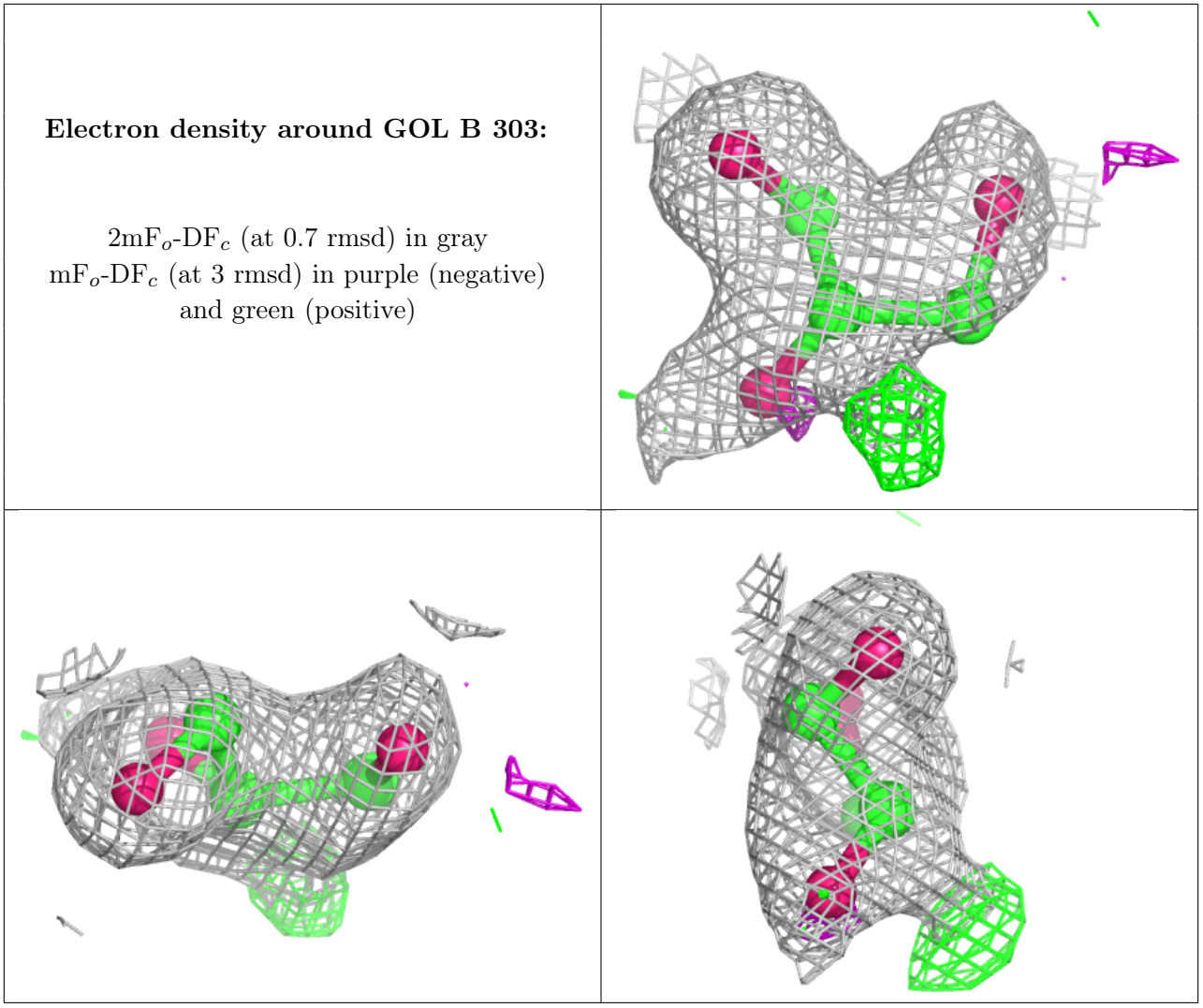
Electron density around GOL A 304:

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



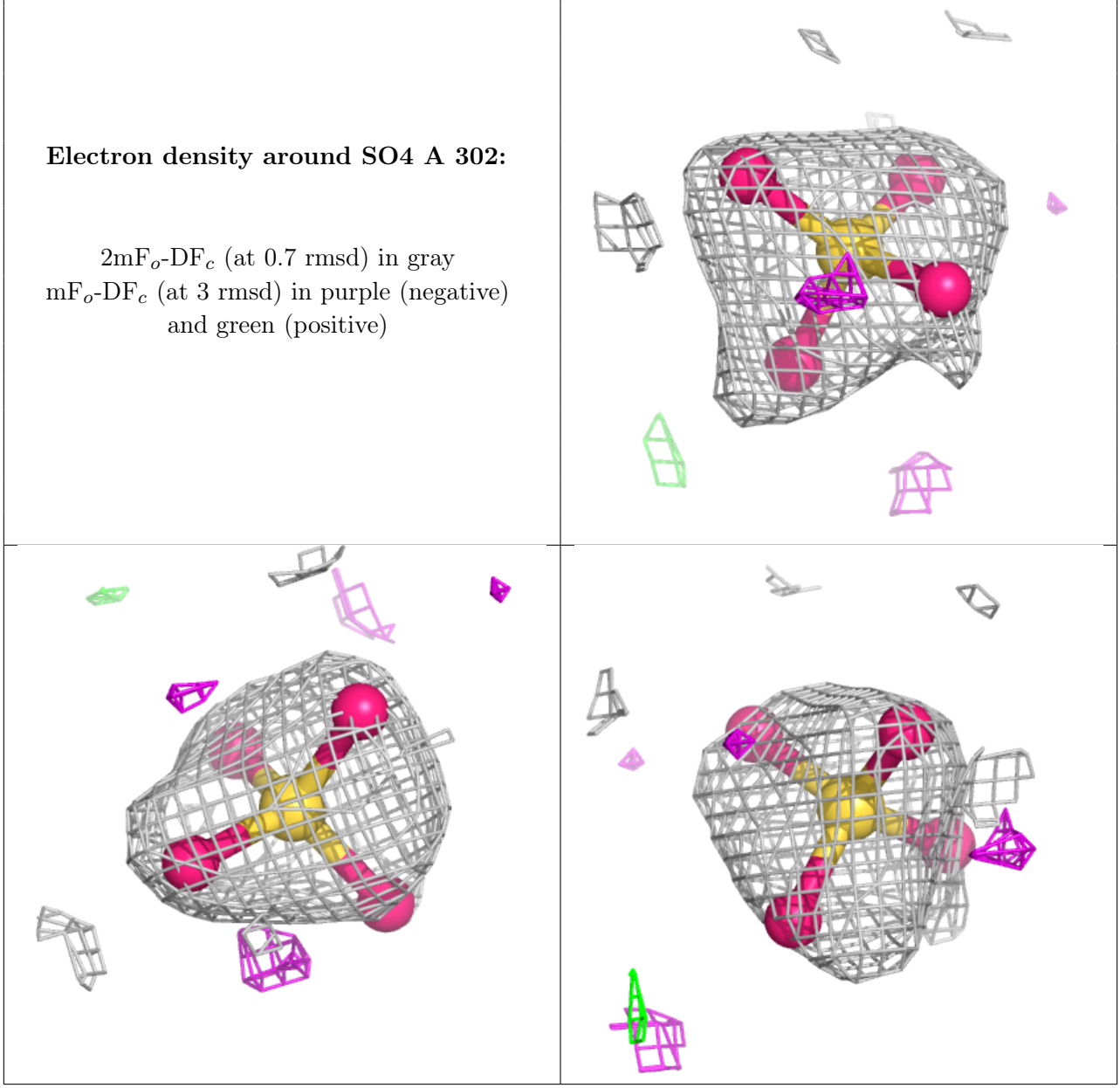
Electron density around GOL B 303:

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



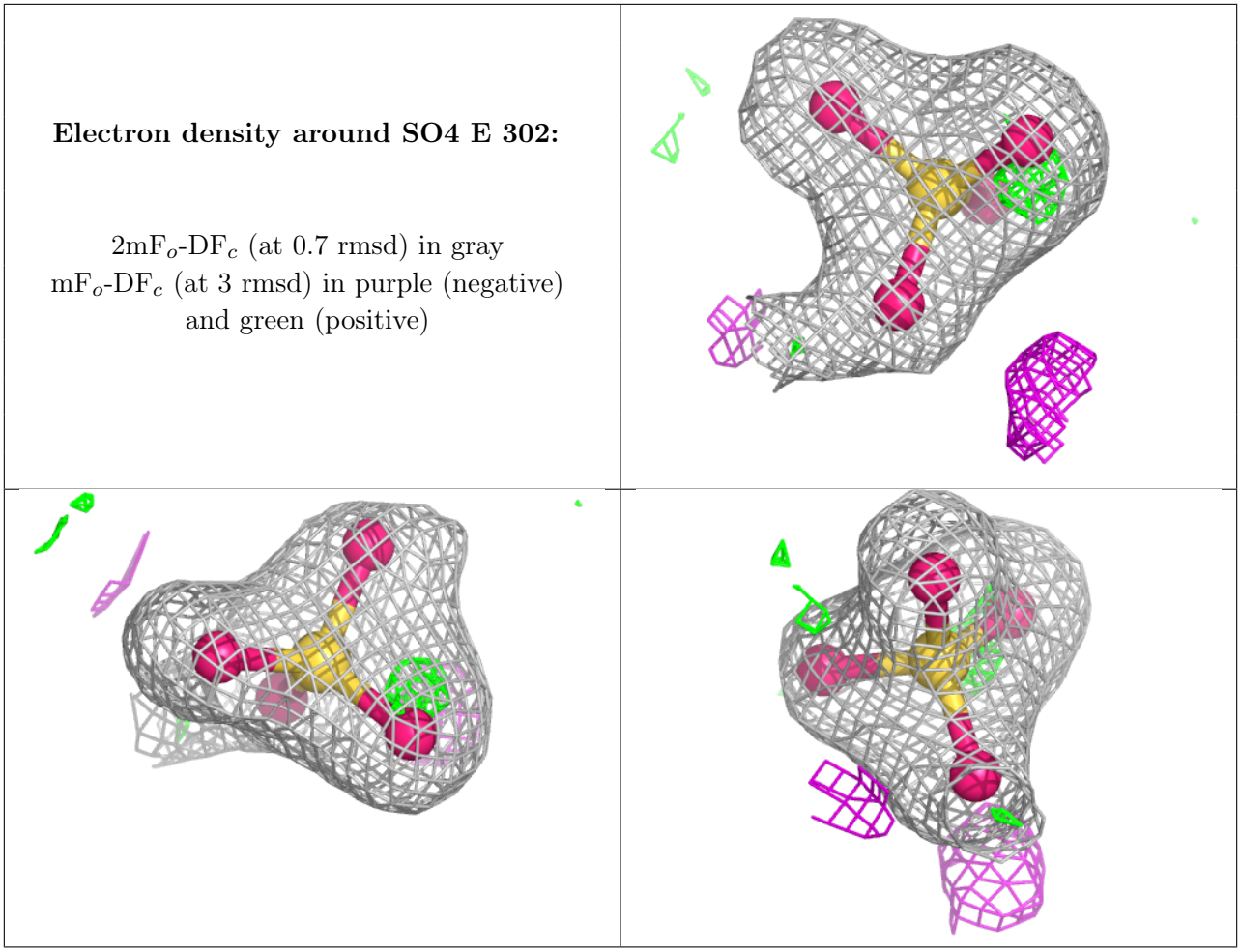
Electron density around SO4 A 302:

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



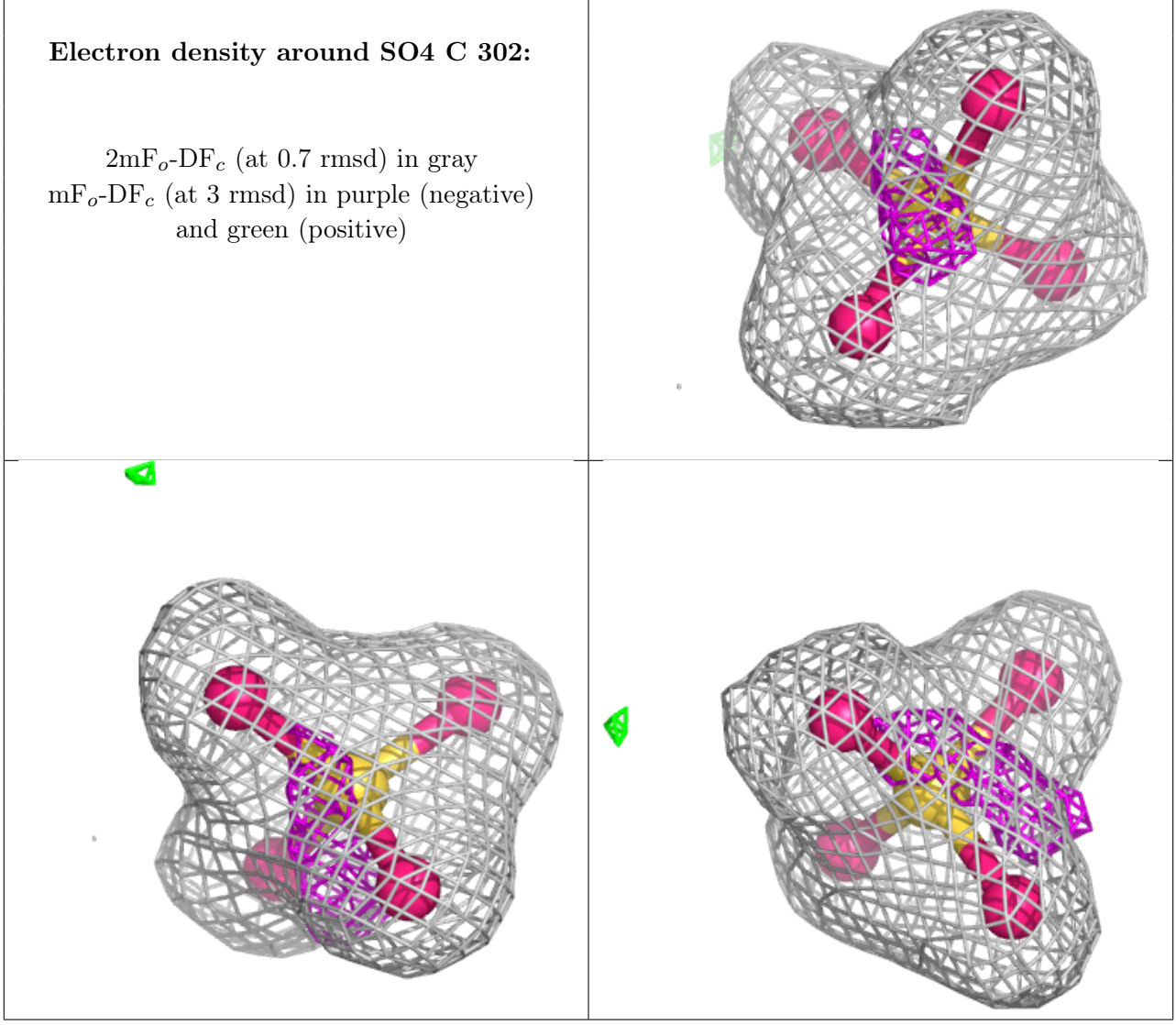
Electron density around SO4 E 302:

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



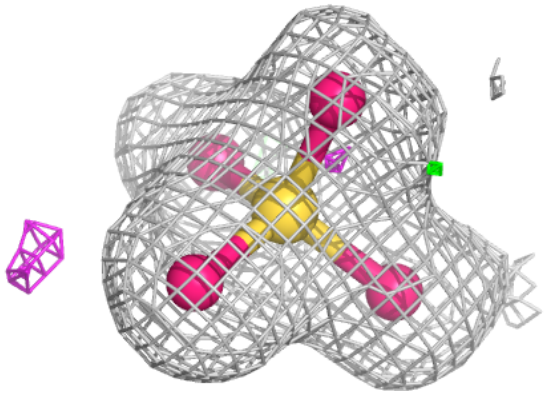
Electron density around SO4 C 302:

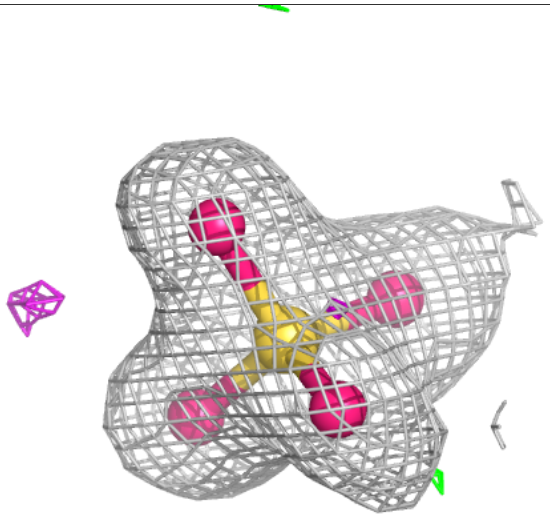
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

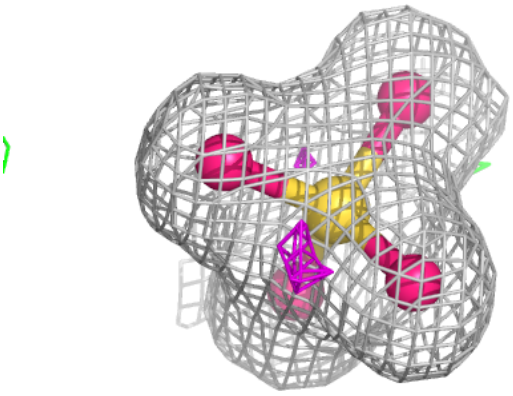


Electron density around SO4 B 302:

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

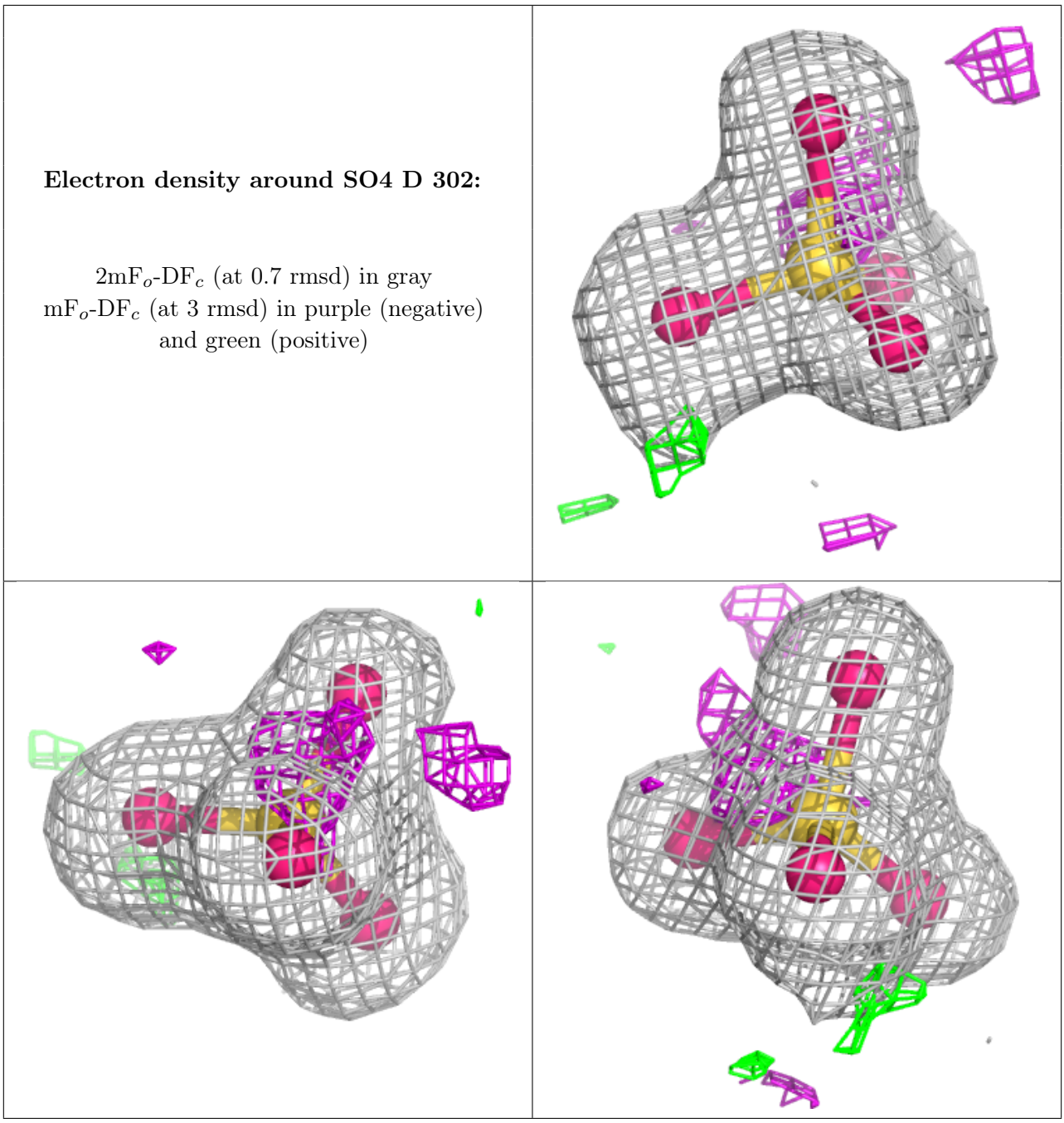






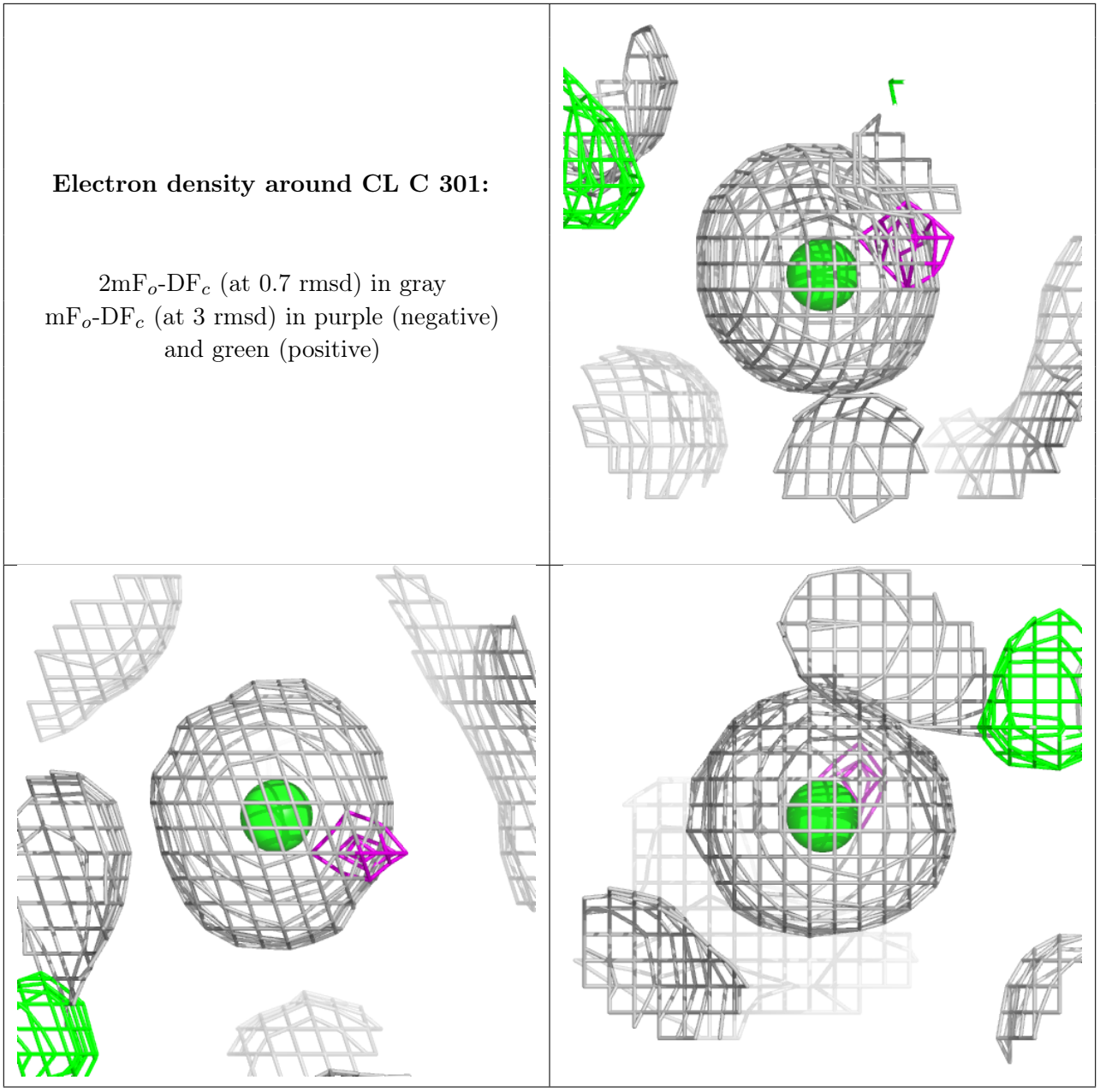
Electron density around SO4 D 302:

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



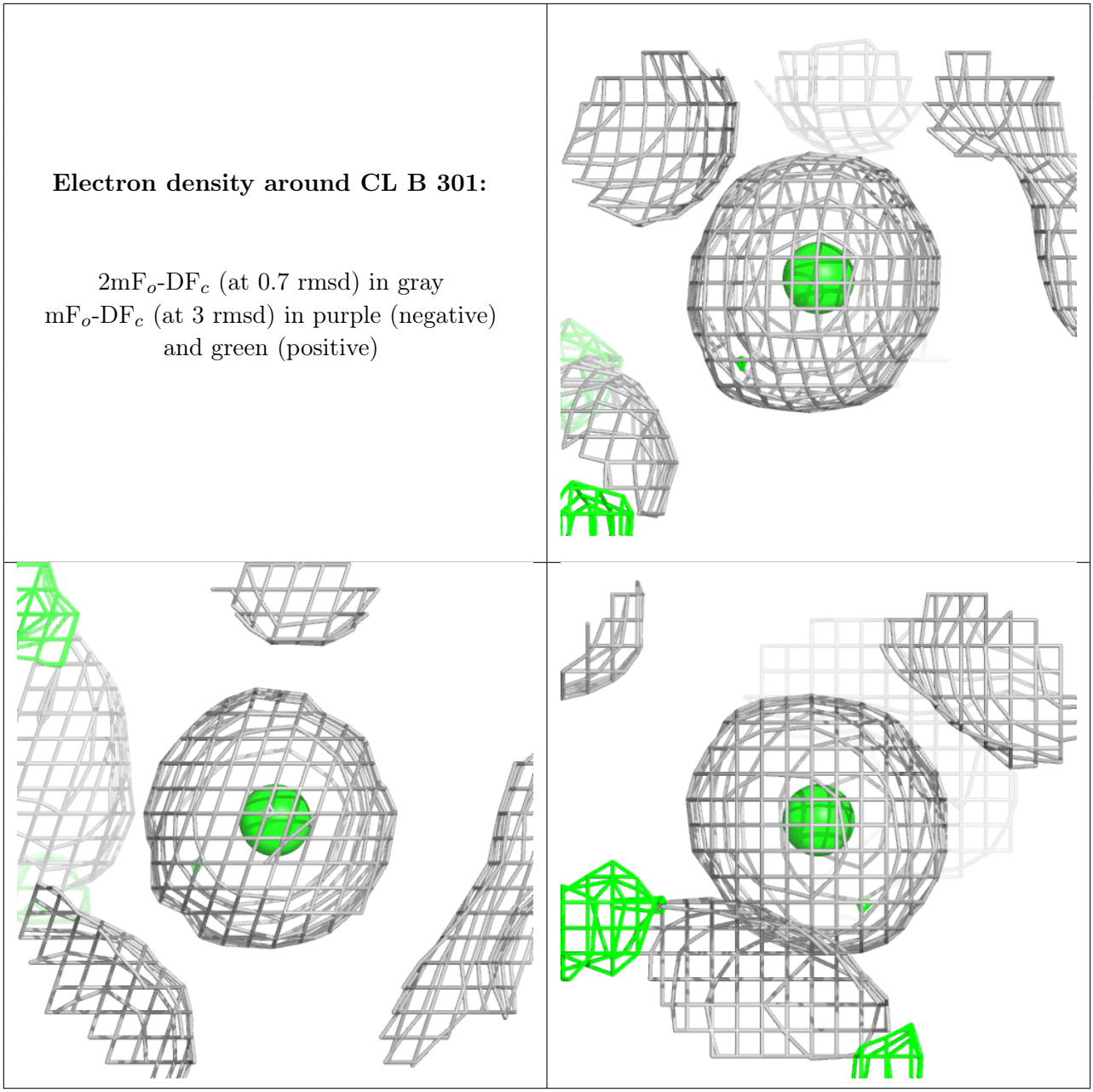
Electron density around CL C 301:

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



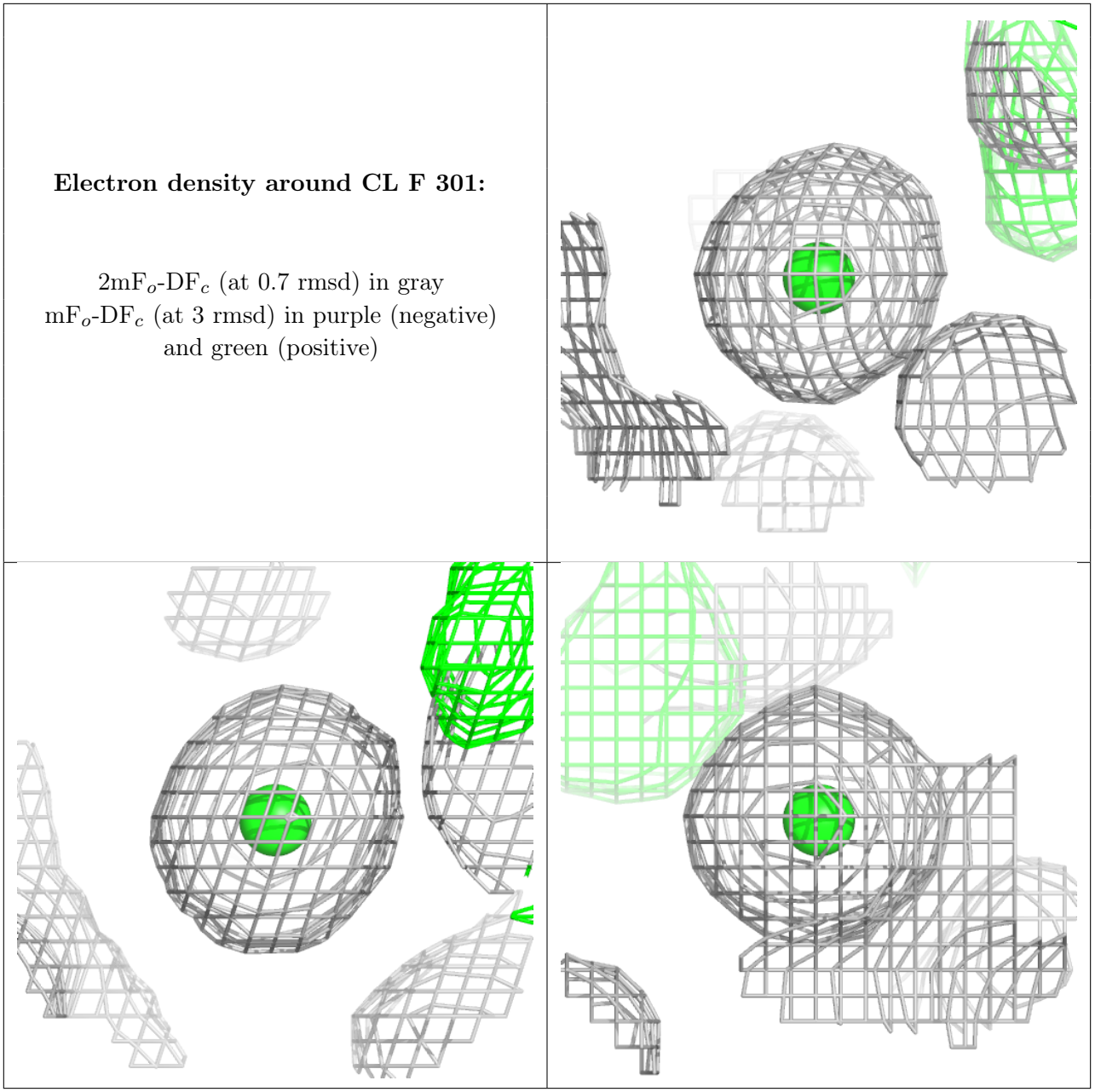
Electron density around CL B 301:

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



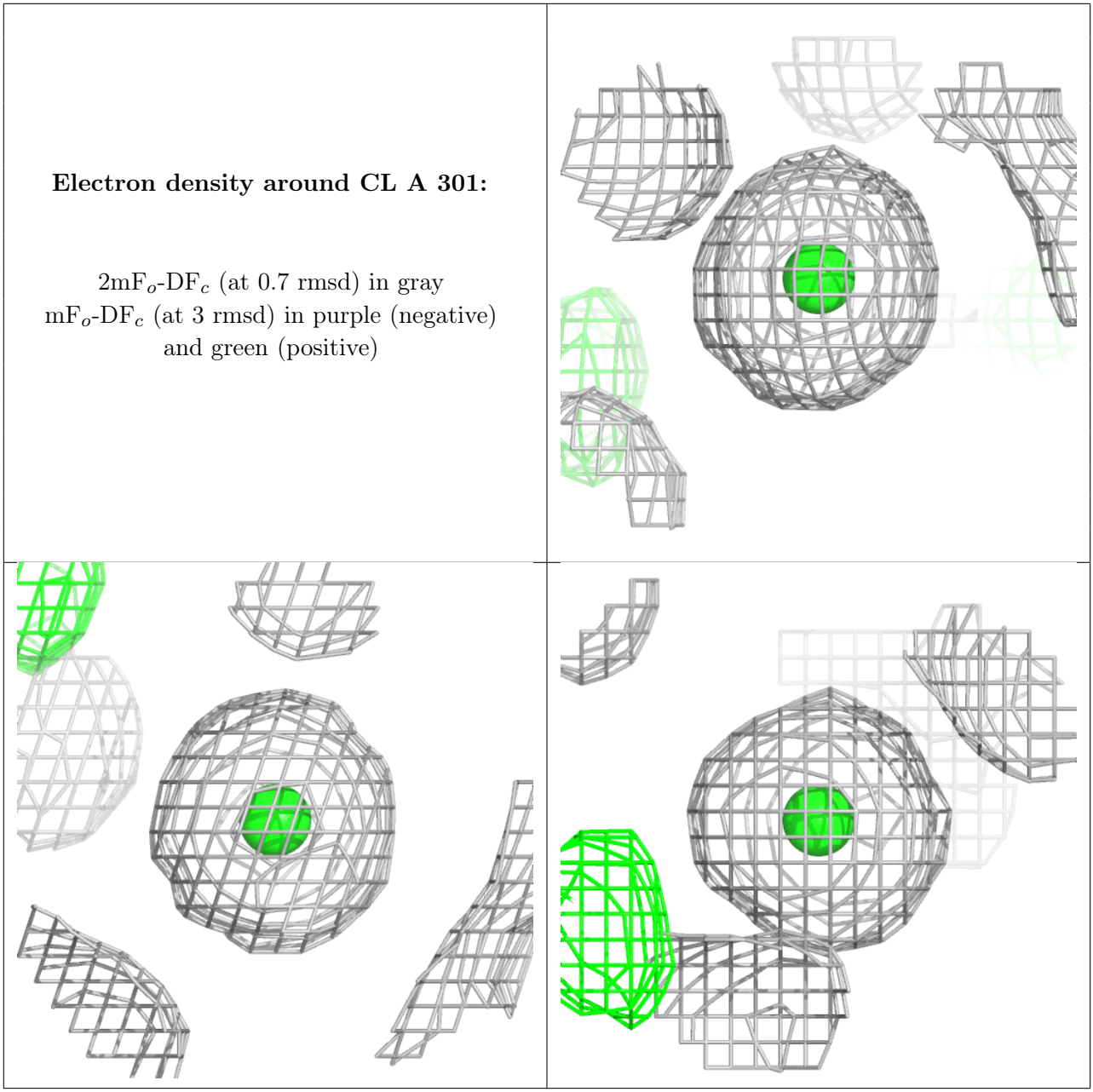
Electron density around CL F 301:

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



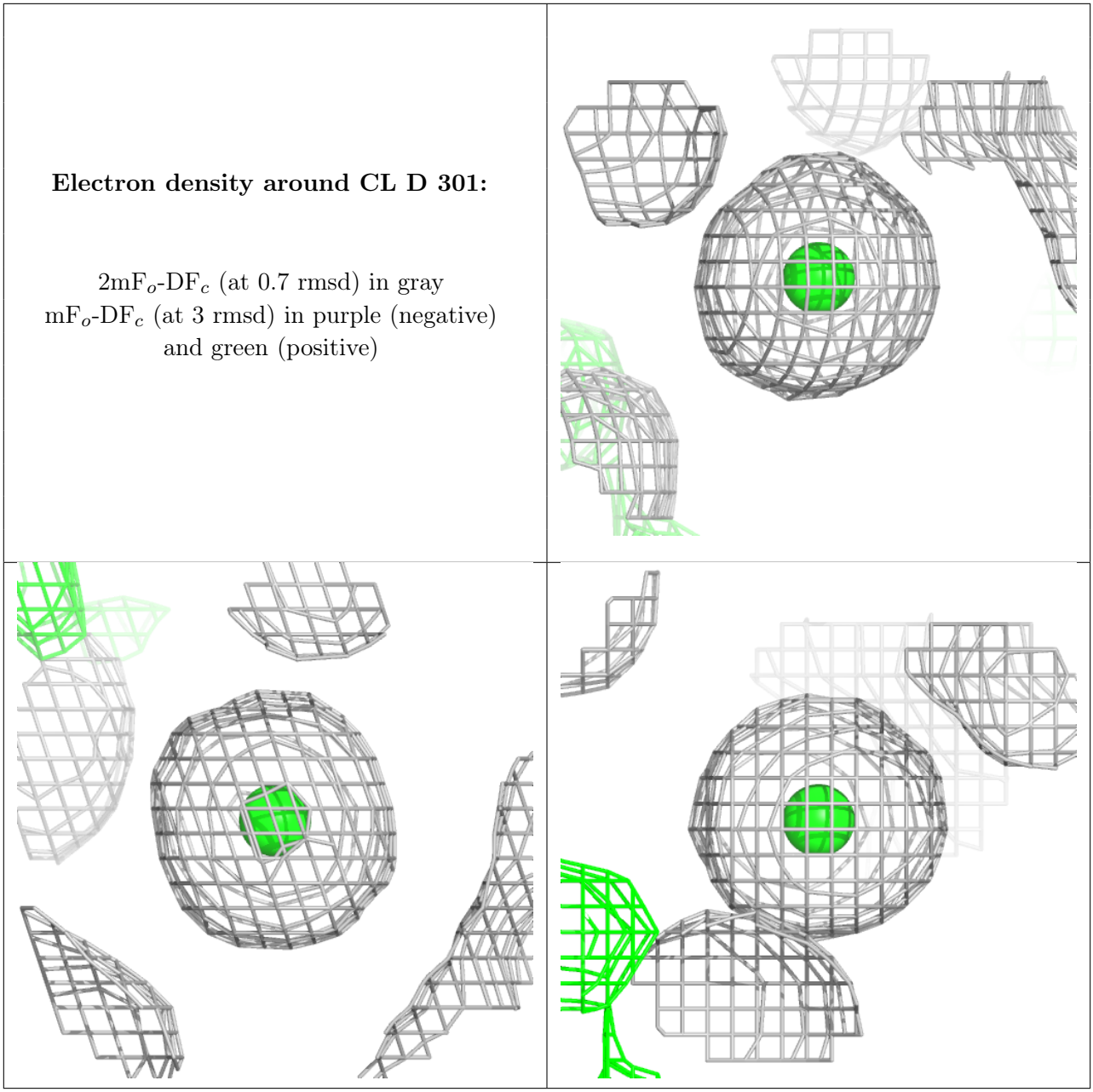
Electron density around CL A 301:

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



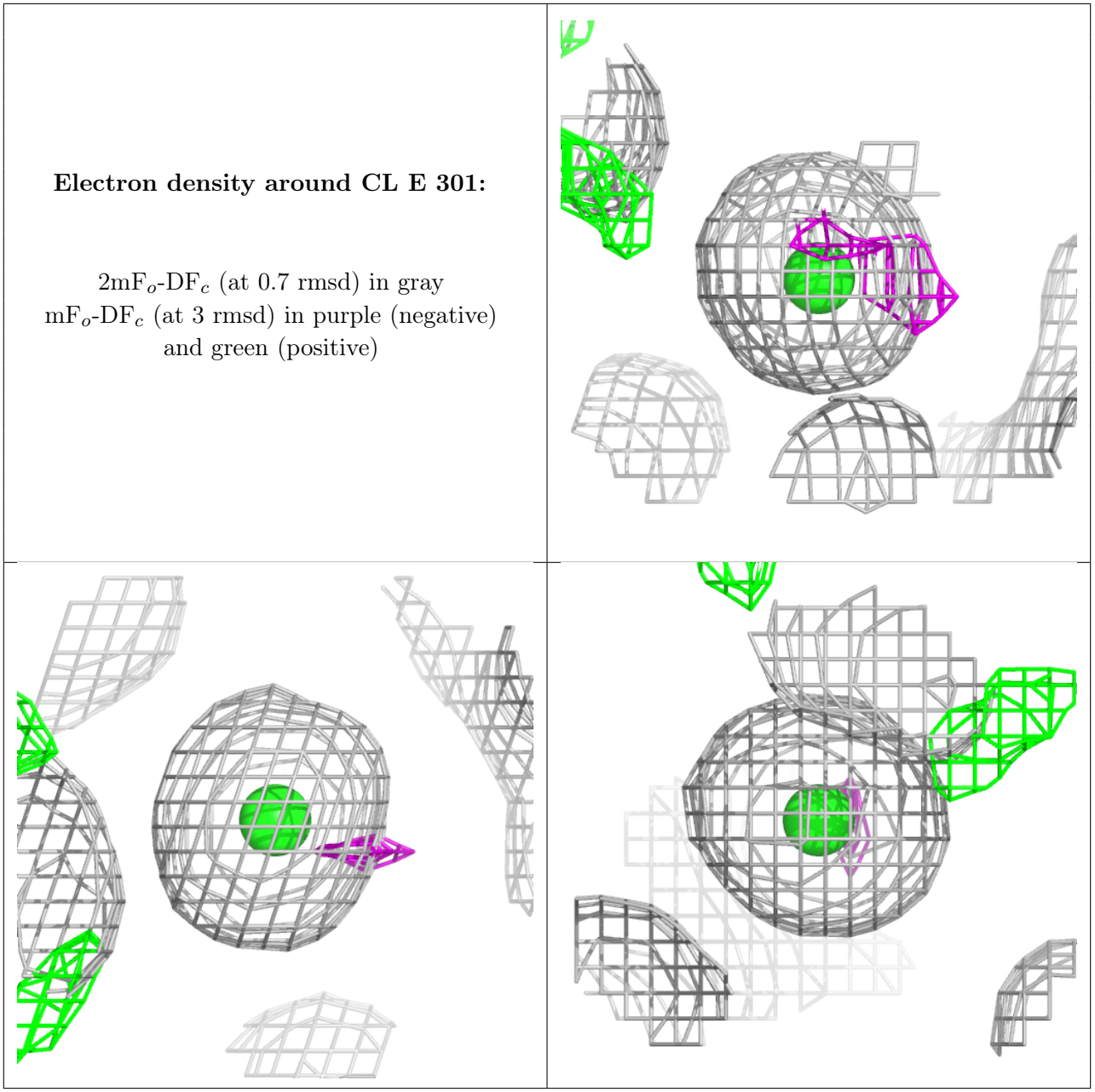
Electron density around CL D 301:

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



Electron density around CL E 301:

$2mF_o$-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.