Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2026 – 01:15 pm GMT

PDB ID	:	9SUZ / pdb_00009suz
Title	:	gamma carbonic anhydrase LreCA from Limosilactobacillus reuteri in space group P212121
Authors	:	Angeli, A.; Ferraroni, M.
Deposited on	:	2025-09-30
Resolution	:	1.26 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:

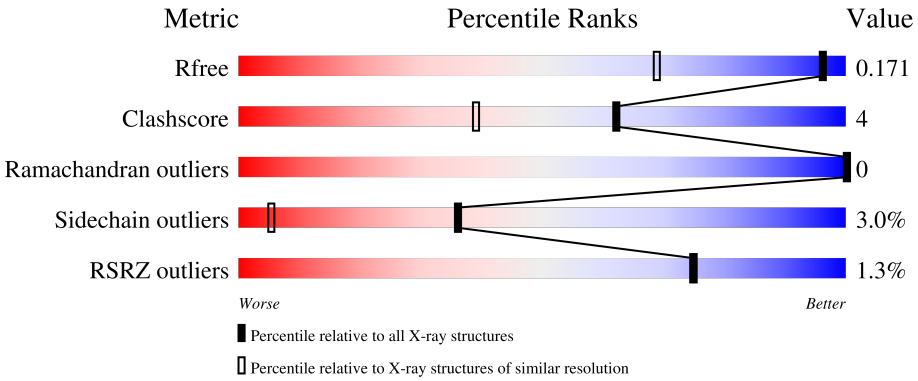
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.26 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	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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	AAA	179	89% 9% .
1	BBB	179	88% 10% .
1	CCC	179	4% 87% 12% .

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
3	NA	CCC	205	-	-	X	-

2 Entry composition

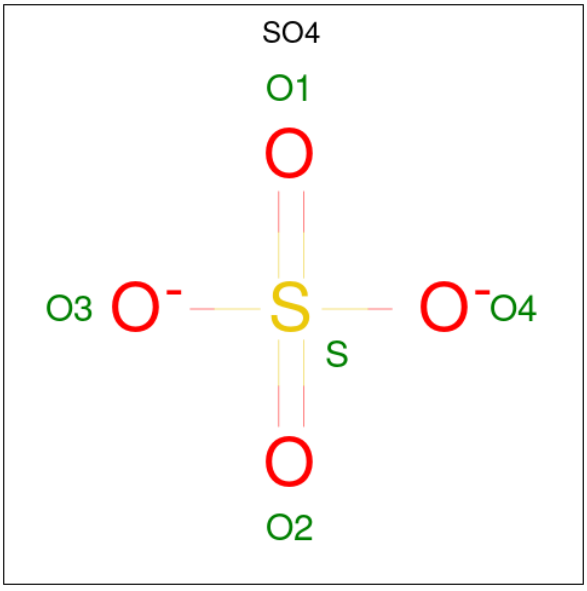
There are 6 unique types of molecules in this entry. The entry contains 4516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 gamma carbonic anhydrase LreCA from Limosilactobacillus reuteri.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	179	Total	C	N	O	S	8	6	0
			1382	875	244	254	9			
1	BBB	179	Total	C	N	O	S	8	7	0
			1388	878	246	256	8			
1	CCC	179	Total	C	N	O	S	8	3	0
			1366	863	242	252	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	O	S		0	0
			5	4	1			
2	AAA	1	Total	O	S		0	0
			5	4	1			

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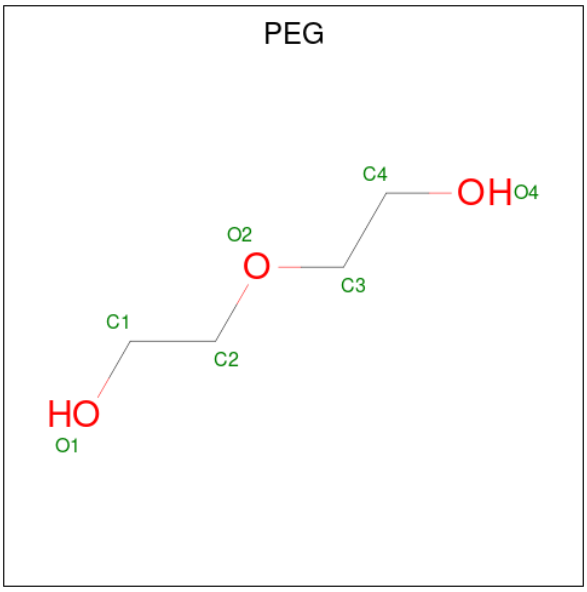
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	BBB	1	Total O S 5 4 1	0	0
2	BBB	1	Total O S 5 4 1	0	0
2	BBB	1	Total O S 5 4 1	0	0
2	CCC	1	Total O S 5 4 1	0	0
2	CCC	1	Total O S 5 4 1	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Na 1 1	0	0
3	BBB	1	Total Na 1 1	0	0
3	CCC	1	Total Na 1 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	BBB	1	Total C O 7 4 3	0	0
4	CCC	1	Total C O 7 4 3	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	BBB	2	Total Zn 2 2	0	0
5	CCC	1	Total Zn 1 1	0	0

- Molecule 6 is water.

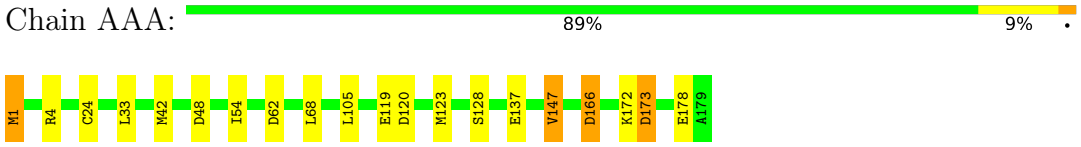
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	115	Total O 115 115	0	0
6	BBB	112	Total O 112 112	0	0
6	CCC	98	Total O 98 98	0	0

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.

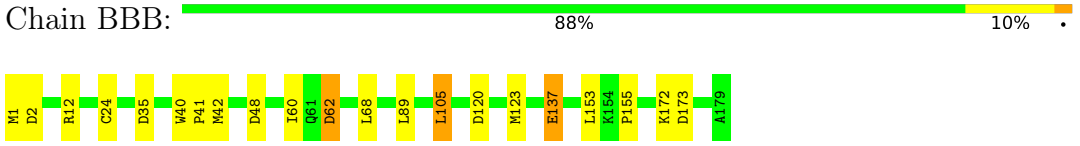
• Molecule 1: gamma carbonic anhydrase LreCA from Limosilactobacillus reuteri

Chain AAA:



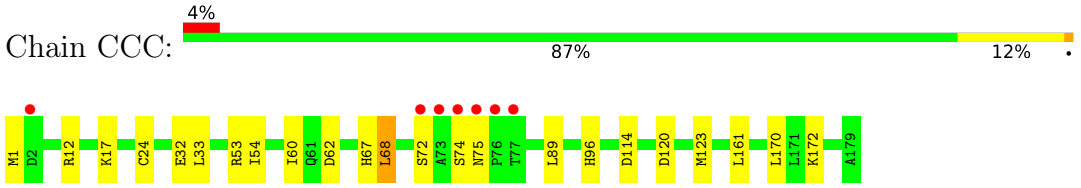
• Molecule 1: gamma carbonic anhydrase LreCA from Limosilactobacillus reuteri

Chain BBB:



• Molecule 1: gamma carbonic anhydrase LreCA from Limosilactobacillus reuteri

Chain CCC:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.82Å 90.78Å 117.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.26 50.00 – 1.26	Depositor EDS
% Data completeness (in resolution range)	90.8 (50.00-1.26) 91.9 (50.00-1.26)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.26Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.135 , 0.170 0.135 , 0.171	Depositor DCC
R_{free} test set	6725 reflections (4.46%)	wwPDB-VP
Wilson B-factor (Å^2)	16.0	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	4516	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SO4, ZN, PEG

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	AAA	1.18	4/1423 (0.3%)	1.27	8/1926 (0.4%)
1	BBB	1.04	0/1432	1.14	10/1939 (0.5%)
1	CCC	1.36	4/1398 (0.3%)	1.22	5/1894 (0.3%)
All	All	1.20	8/4253 (0.2%)	1.21	23/5759 (0.4%)

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	AAA	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	1	MET	C-N	28.47	1.72	1.33
1	AAA	1	MET	C-N	-13.72	1.14	1.33
1	AAA	166	ASP	CG-OD2	6.23	1.37	1.25
1	AAA	178	GLU	C-O	-5.96	1.16	1.24
1	CCC	12	ARG	N-CA	5.76	1.50	1.45
1	CCC	96	HIS	CE1-NE2	5.63	1.38	1.32
1	CCC	170	LEU	C-O	5.59	1.30	1.24
1	AAA	137	GLU	CD-OE1	5.07	1.34	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	1	MET	O-C-N	-10.78	105.76	123.00
1	CCC	1	MET	CA-C-N	-9.77	105.18	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	1	MET	C-N-CA	-9.77	105.18	121.39
1	AAA	166	ASP	CA-CB-CG	9.09	121.69	112.60
1	AAA	48	ASP	CA-CB-CG	8.03	120.63	112.60
1	AAA	1	MET	CA-C-N	7.43	135.74	121.54
1	AAA	1	MET	C-N-CA	7.43	135.74	121.54
1	BBB	120	ASP	CA-CB-CG	6.83	119.43	112.60
1	BBB	1	MET	CA-C-N	6.42	132.04	123.05
1	BBB	1	MET	C-N-CA	6.42	132.04	123.05
1	CCC	120	ASP	CA-CB-CG	6.18	118.78	112.60
1	CCC	96	HIS	CE1-NE2-CD2	-6.05	102.94	109.00
1	BBB	35	ASP	CA-CB-CG	5.98	118.58	112.60
1	BBB	48	ASP	CA-CB-CG	5.91	118.51	112.60
1	AAA	173	ASP	CA-CB-CG	5.70	118.30	112.60
1	AAA	120	ASP	CA-CB-CG	5.61	118.21	112.60
1	BBB	2	ASP	CA-CB-CG	5.53	118.13	112.60
1	BBB	137	GLU	CB-CG-CD	-5.46	103.31	112.60
1	AAA	4	ARG	CB-CA-C	-5.39	101.85	110.79
1	CCC	96	HIS	CG-CD2-NE2	5.32	112.52	107.20
1	BBB	62	ASP	CA-CB-CG	5.27	117.87	112.60
1	BBB	12	ARG	CG-CD-NE	-5.16	100.65	112.00
1	BBB	2	ASP	CB-CA-C	5.07	118.51	110.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	1	MET	Mainchain

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	AAA	1382	0	1441	11	0
1	BBB	1388	0	1447	12	0
1	CCC	1366	0	1414	13	0
2	AAA	10	0	0	0	0
2	BBB	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CCC	10	0	0	1	0
3	AAA	1	0	0	1	0
3	BBB	1	0	0	1	0
3	CCC	1	0	0	2	0
4	BBB	7	0	10	2	0
4	CCC	7	0	10	0	0
5	BBB	2	0	0	0	0
5	CCC	1	0	0	0	0
6	AAA	115	0	0	6	0
6	BBB	112	0	0	4	0
6	CCC	98	0	0	4	0
All	All	4516	0	4322	35	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 4.

All (35) 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:AAA:173:ASP:OD1	6:AAA:301:HOH:O	1.91	0.88
1:BBB:123:MET:CE	6:BBB:358:HOH:O	2.21	0.87
1:BBB:123:MET:HE1	6:BBB:358:HOH:O	1.73	0.86
1:BBB:155:PRO:HD3	4:BBB:204:PEG:H42	1.59	0.84
1:CCC:114:ASP:OD2	6:CCC:302:HOH:O	1.98	0.82
1:CCC:24:CYS:SG	3:CCC:205:NA:NA	1.98	0.76
1:AAA:123:MET:CE	6:AAA:364:HOH:O	2.35	0.74
1:AAA:123:MET:HE1	6:AAA:364:HOH:O	1.87	0.73
1:AAA:119:GLU:OE1	6:AAA:302:HOH:O	2.07	0.72
1:BBB:24:CYS:SG	3:BBB:207:NA:NA	2.04	0.70
1:AAA:24:CYS:SG	3:AAA:203:NA:NA	2.06	0.69
1:AAA:173:ASP:HA	6:AAA:301:HOH:O	2.00	0.60
1:CCC:17:LYS:NZ	2:CCC:202:SO4:O3	2.29	0.58
1:BBB:123:MET:HE2	6:BBB:358:HOH:O	1.95	0.57
1:CCC:72:SER:HB3	6:CCC:363:HOH:O	2.05	0.56
1:CCC:74:SER:OG	1:CCC:75[B]:ASN:OD1	2.25	0.55
1:CCC:60:ILE:HD12	1:CCC:89:LEU:HD12	1.90	0.51
1:CCC:33:LEU:CD2	1:CCC:54:ILE:HD12	2.40	0.51
1:AAA:33:LEU:CD2	1:AAA:54:ILE:HD12	2.41	0.50
1:AAA:123:MET:HE2	6:AAA:364:HOH:O	2.04	0.50
1:BBB:137:GLU:HG3	6:BBB:320:HOH:O	2.15	0.47
1:CCC:75[B]:ASN:CB	6:CCC:307:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:60:ILE:HD12	1:BBB:89:LEU:HD12	1.99	0.45
1:AAA:166:ASP:OD2	1:BBB:173:ASP:OD2	2.34	0.44
1:CCC:75[B]:ASN:CG	6:CCC:307:HOH:O	2.60	0.44
1:CCC:67:HIS:CG	1:CCC:68:LEU:H	2.35	0.44
1:BBB:40:TRP:HB3	1:BBB:41:PRO:HD2	1.98	0.44
1:CCC:123[B]:MET:HG2	1:CCC:161:LEU:HD21	2.00	0.43
1:AAA:128:SER:HB3	1:AAA:147:VAL:HG13	2.01	0.43
1:CCC:32:GLU:HB2	1:CCC:53:ARG:HD3	2.00	0.43
1:CCC:24:CYS:HG	3:CCC:205:NA:NA	1.57	0.42
1:BBB:153:LEU:O	4:BBB:204:PEG:H31	2.20	0.42

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	AAA	183/179 (102%)	178 (97%)	5 (3%)	0	100	100
1	BBB	184/179 (103%)	180 (98%)	4 (2%)	0	100	100
1	CCC	180/179 (101%)	177 (98%)	3 (2%)	0	100	100
All	All	547/537 (102%)	535 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	151/145 (104%)	145 (96%)	6 (4%)	28 2
1	BBB	152/145 (105%)	145 (95%)	7 (5%)	24 2
1	CCC	148/145 (102%)	145 (98%)	3 (2%)	48 12
All	All	451/435 (104%)	435 (96%)	16 (4%)	36 3

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	42[A]	MET
1	AAA	42[B]	MET
1	AAA	62	ASP
1	AAA	68	LEU
1	AAA	147	VAL
1	AAA	172	LYS
1	BBB	42[A]	MET
1	BBB	42[B]	MET
1	BBB	62	ASP
1	BBB	68	LEU
1	BBB	105[A]	LEU
1	BBB	105[B]	LEU
1	BBB	172	LYS
1	CCC	62	ASP
1	CCC	68	LEU
1	CCC	172	LYS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
2	SO4	BBB	202	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	AAA	201	-	4,4,4	0.37	0	6,6,6	0.27	0
2	SO4	CCC	202	-	4,4,4	0.45	0	6,6,6	0.15	0
2	SO4	BBB	203	5	4,4,4	0.29	0	6,6,6	0.54	0
2	SO4	BBB	201	-	4,4,4	0.83	0	6,6,6	0.46	0
2	SO4	CCC	201	-	4,4,4	0.35	0	6,6,6	0.15	0
4	PEG	BBB	204	-	6,6,6	0.62	0	5,5,5	0.45	0
4	PEG	CCC	203	-	6,6,6	0.51	0	5,5,5	0.47	0
2	SO4	AAA	202	-	4,4,4	0.23	0	6,6,6	0.12	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
4	PEG	BBB	204	-	-	2/4/4/4	-
4	PEG	CCC	203	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	CCC	203	PEG	O1-C1-C2-O2
4	CCC	203	PEG	O2-C3-C4-O4
4	BBB	204	PEG	C4-C3-O2-C2
4	BBB	204	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
4	CCC	203	PEG	C1-C2-O2-C3

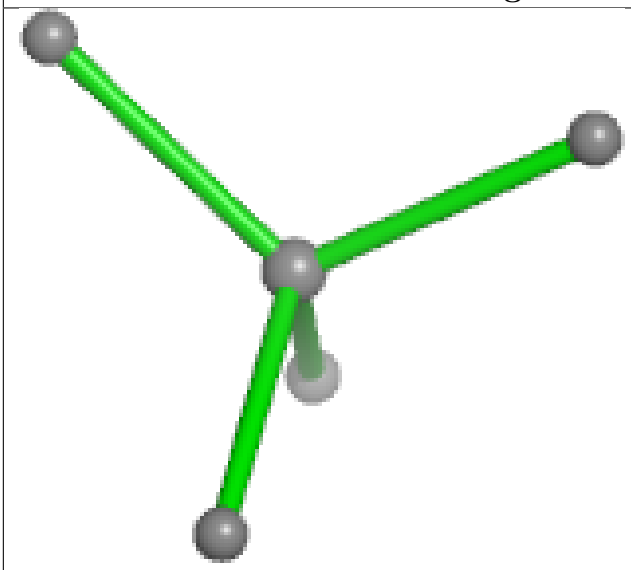
There are no ring outliers.

2 monomers are involved in 3 short contacts:

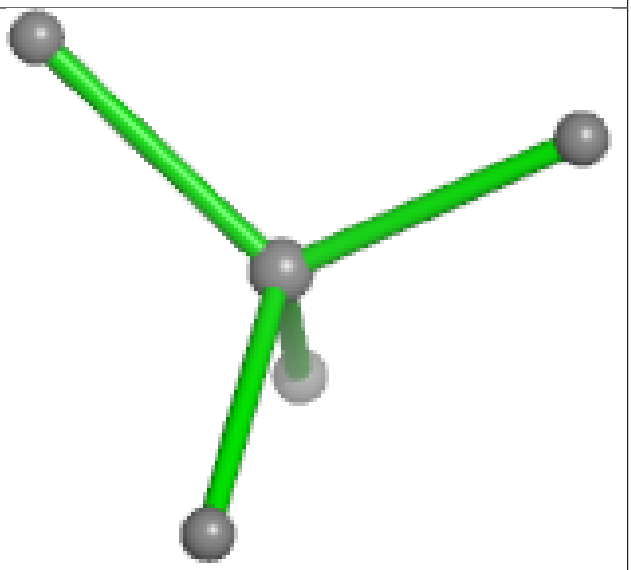
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	CCC	202	SO4	1	0
4	BBB	204	PEG	2	0

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.

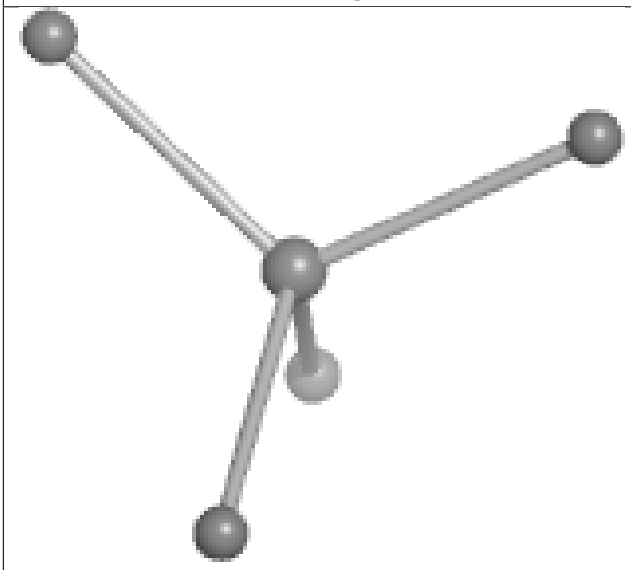
Ligand SO4 BBB 202



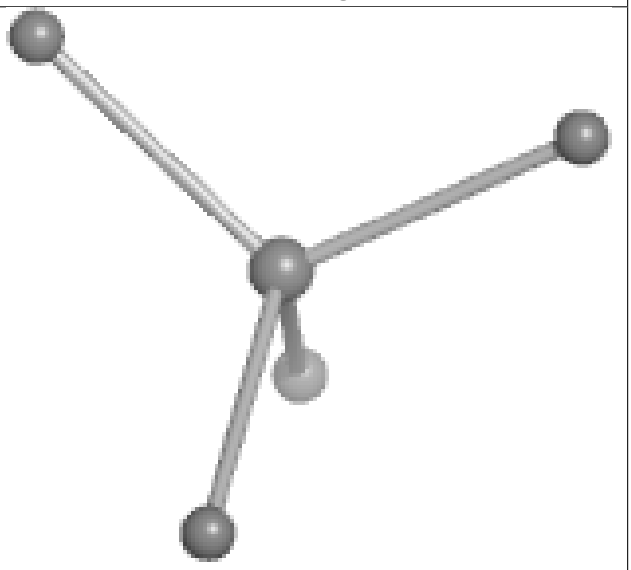
Bond lengths



Bond angles

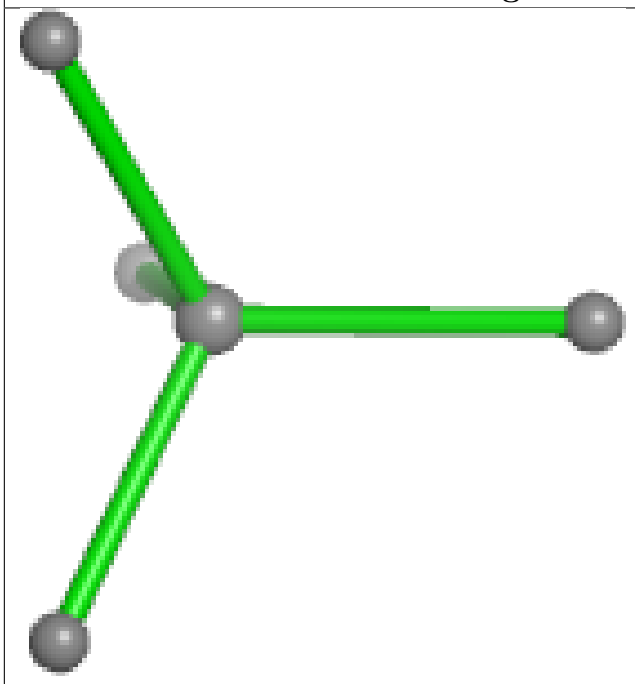


Torsions

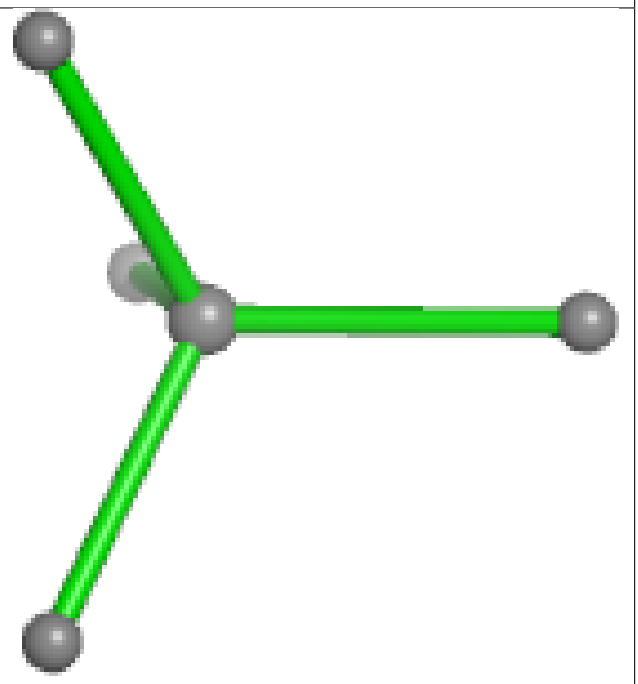


Rings

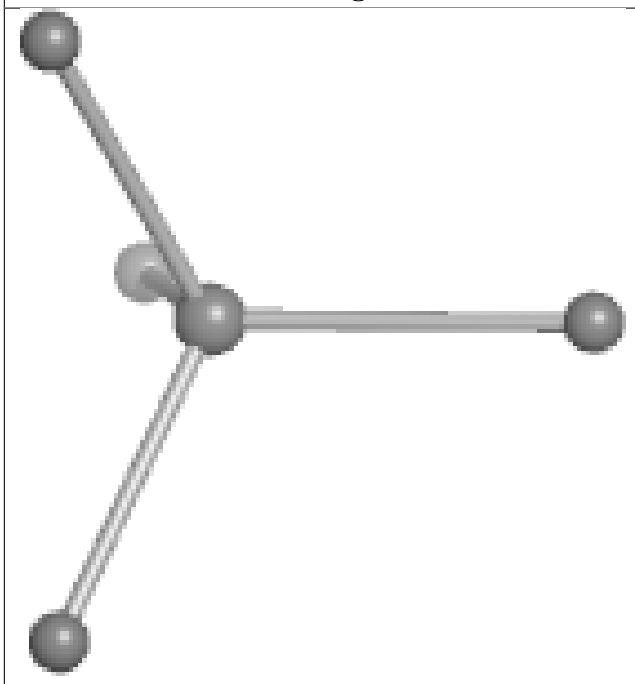
Ligand SO4 AAA 201



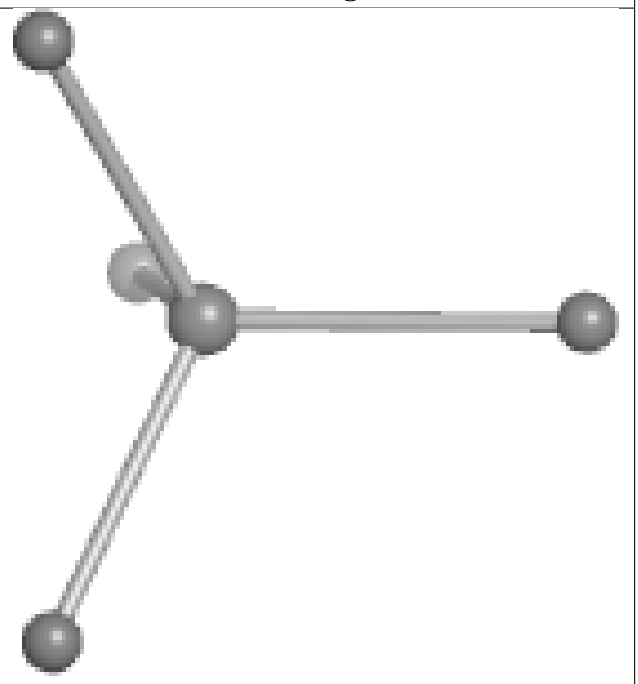
Bond lengths



Bond angles

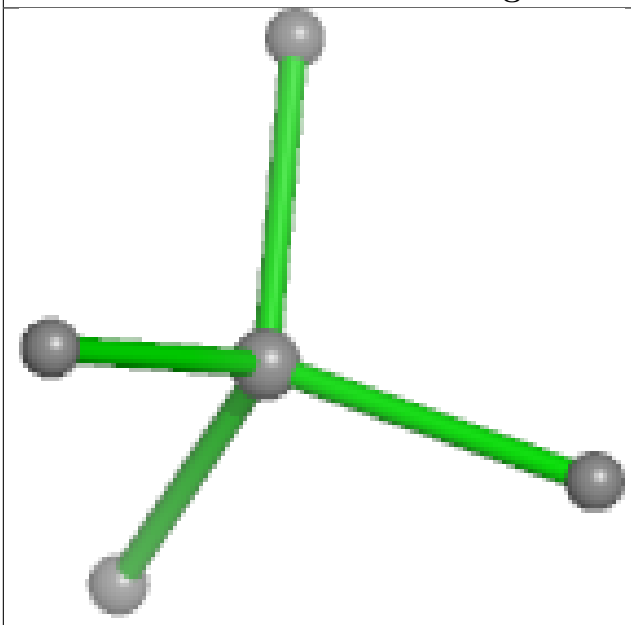


Torsions

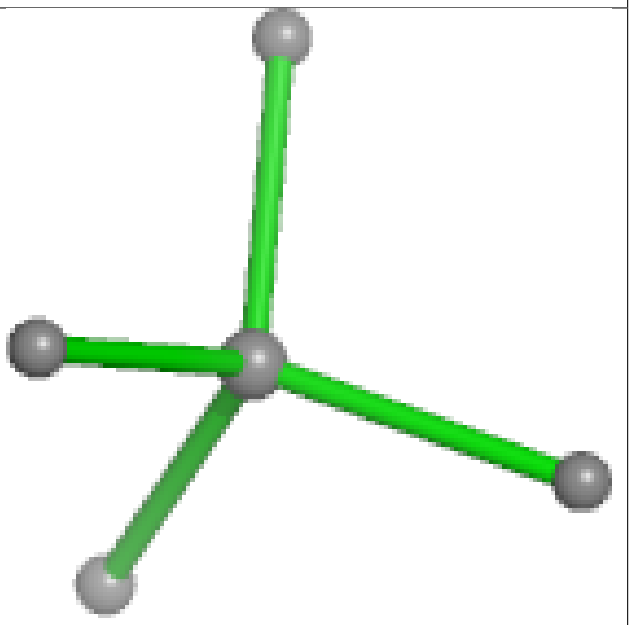


Rings

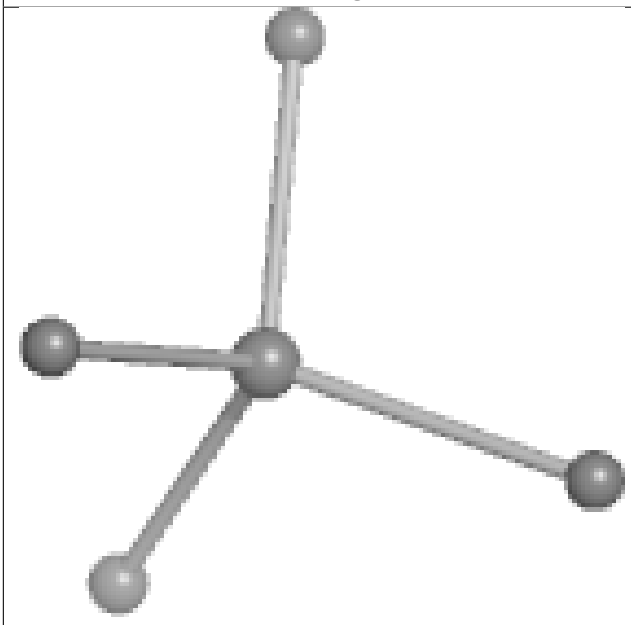
Ligand SO4 CCC 202



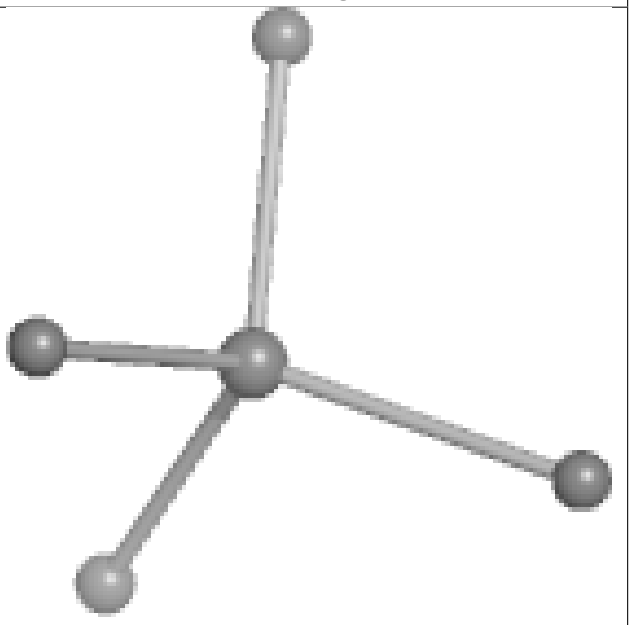
Bond lengths



Bond angles

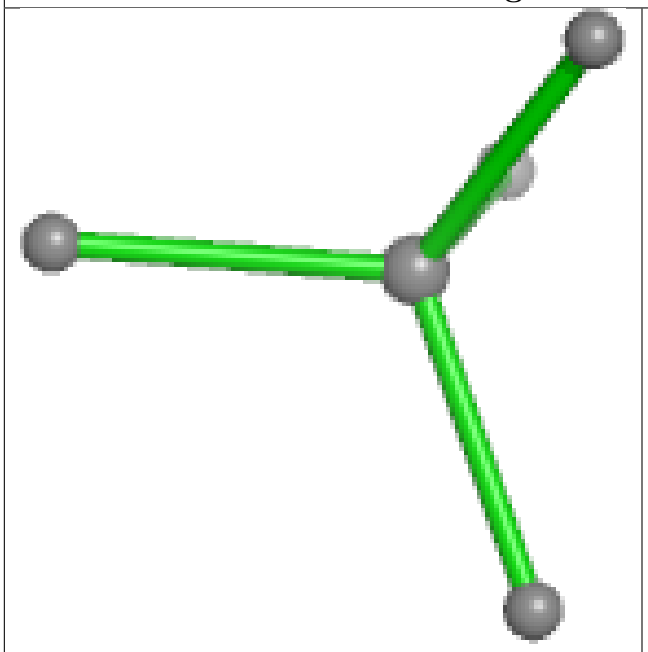


Torsions

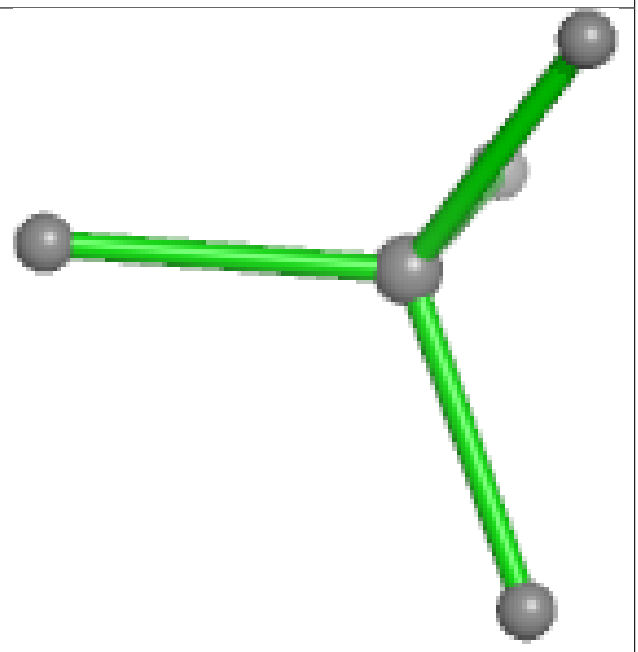


Rings

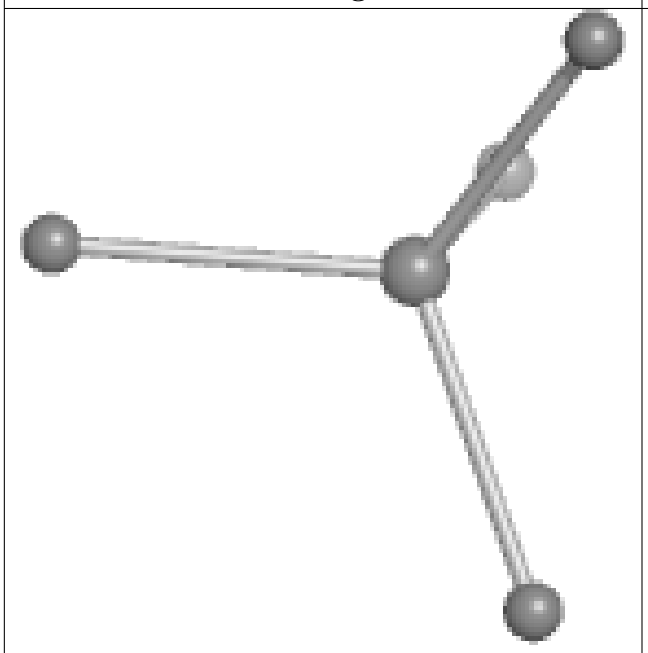
Ligand SO4 BBB 203



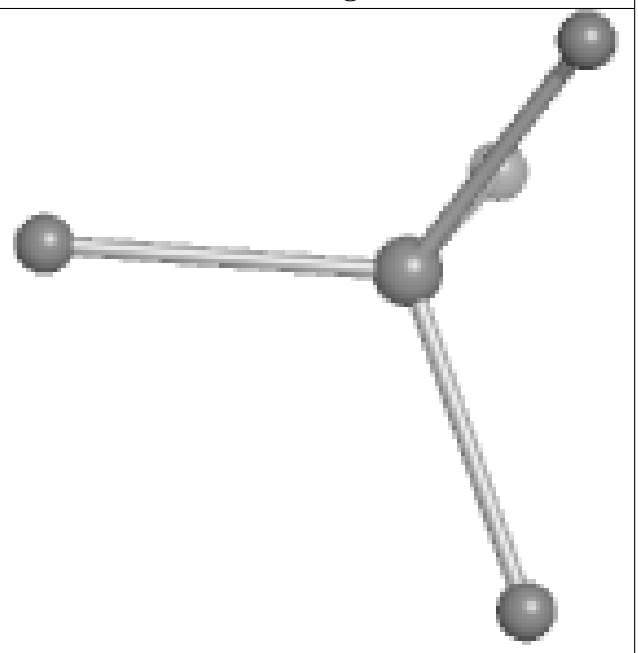
Bond lengths



Bond angles

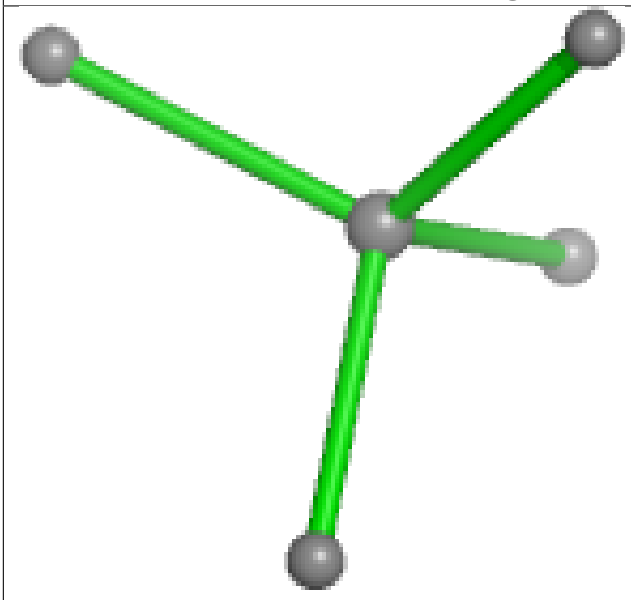


Torsions

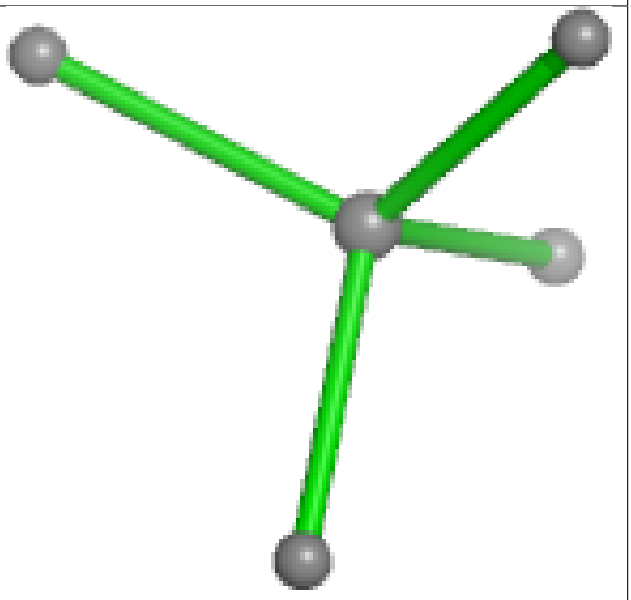


Rings

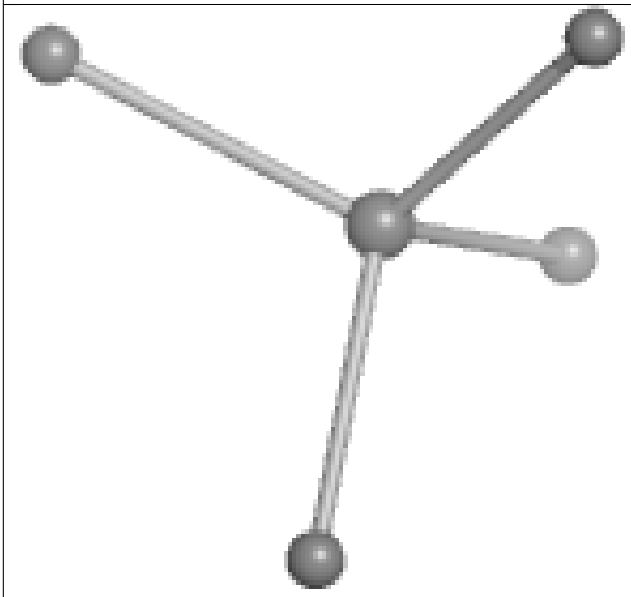
Ligand SO4 BBB 201



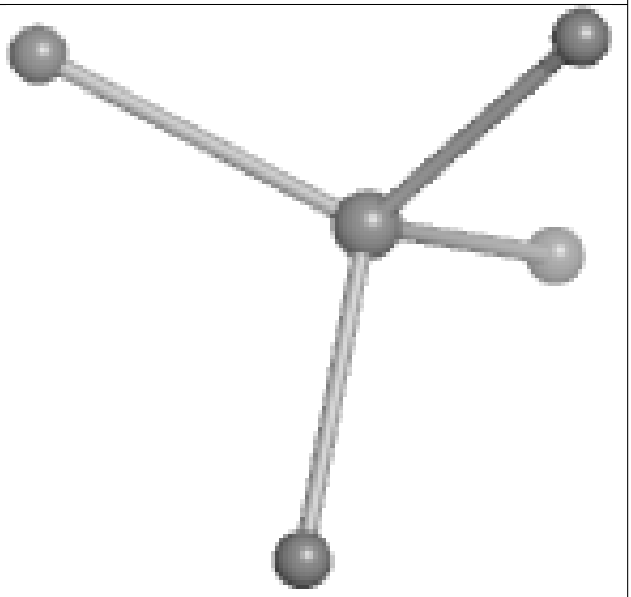
Bond lengths



Bond angles

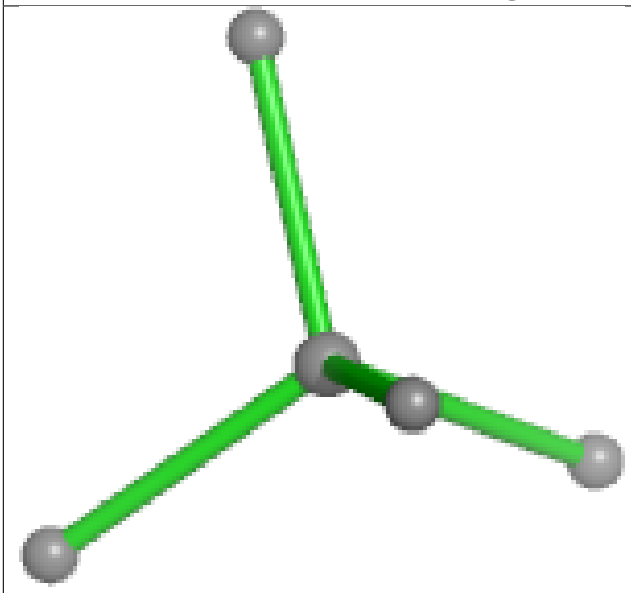


Torsions

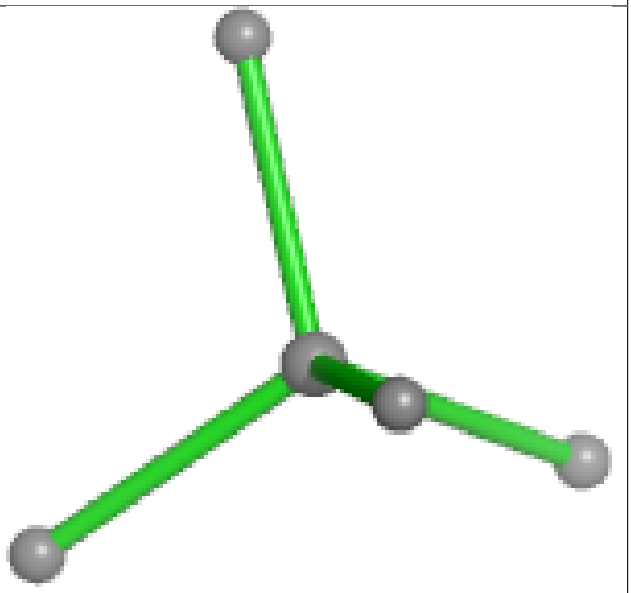


Rings

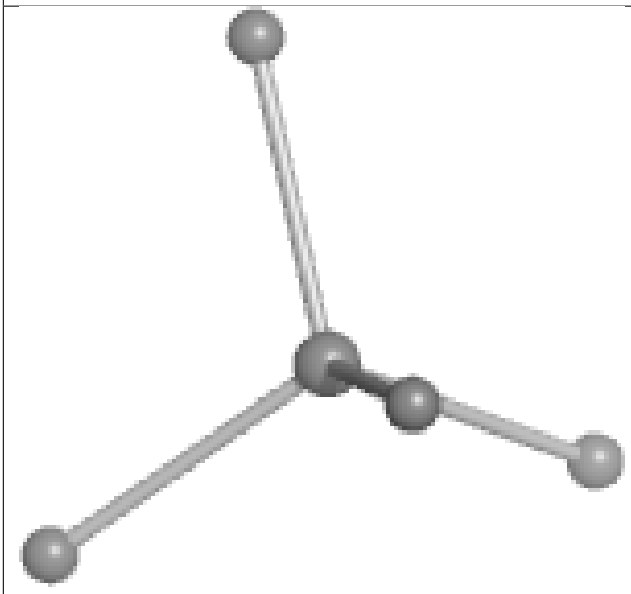
Ligand SO4 CCC 201



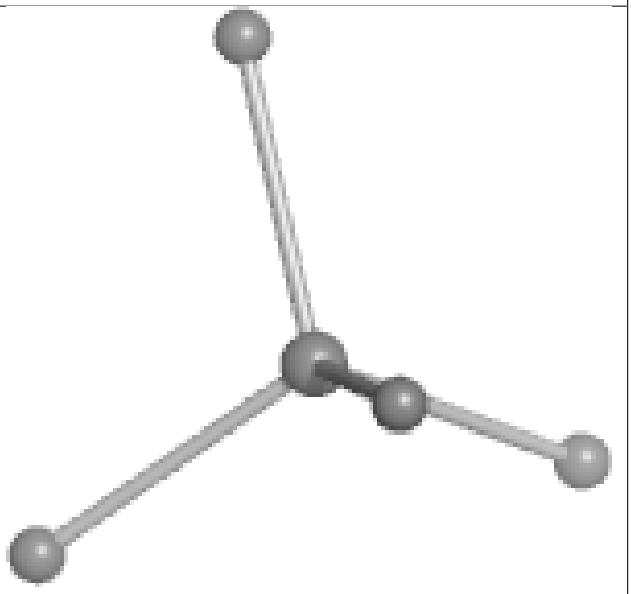
Bond lengths



Bond angles

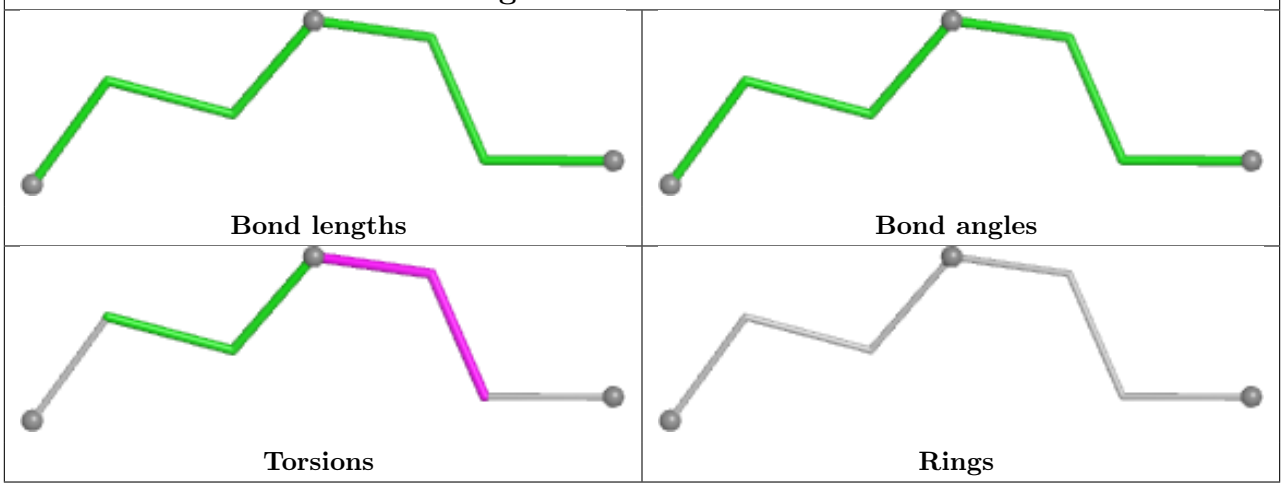


Torsions

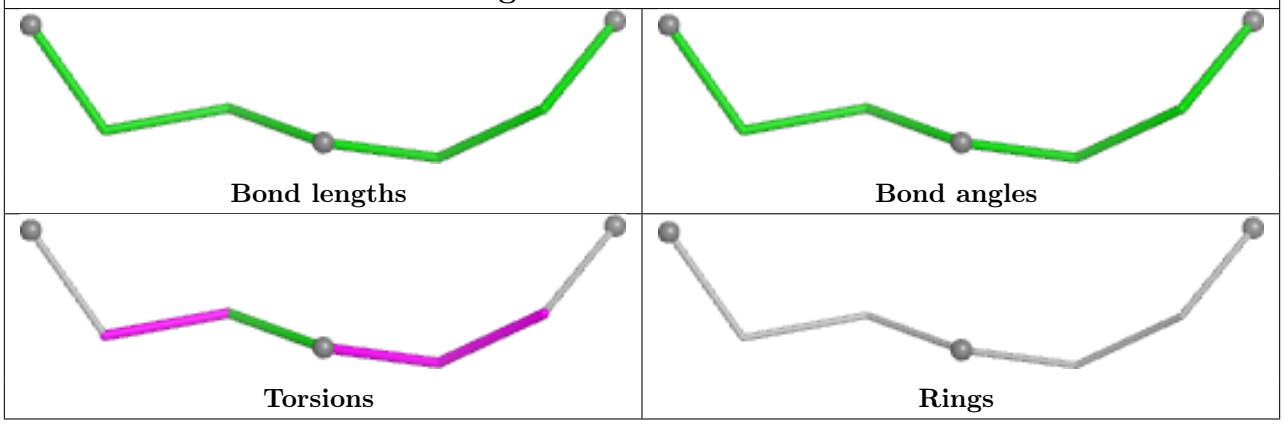


Rings

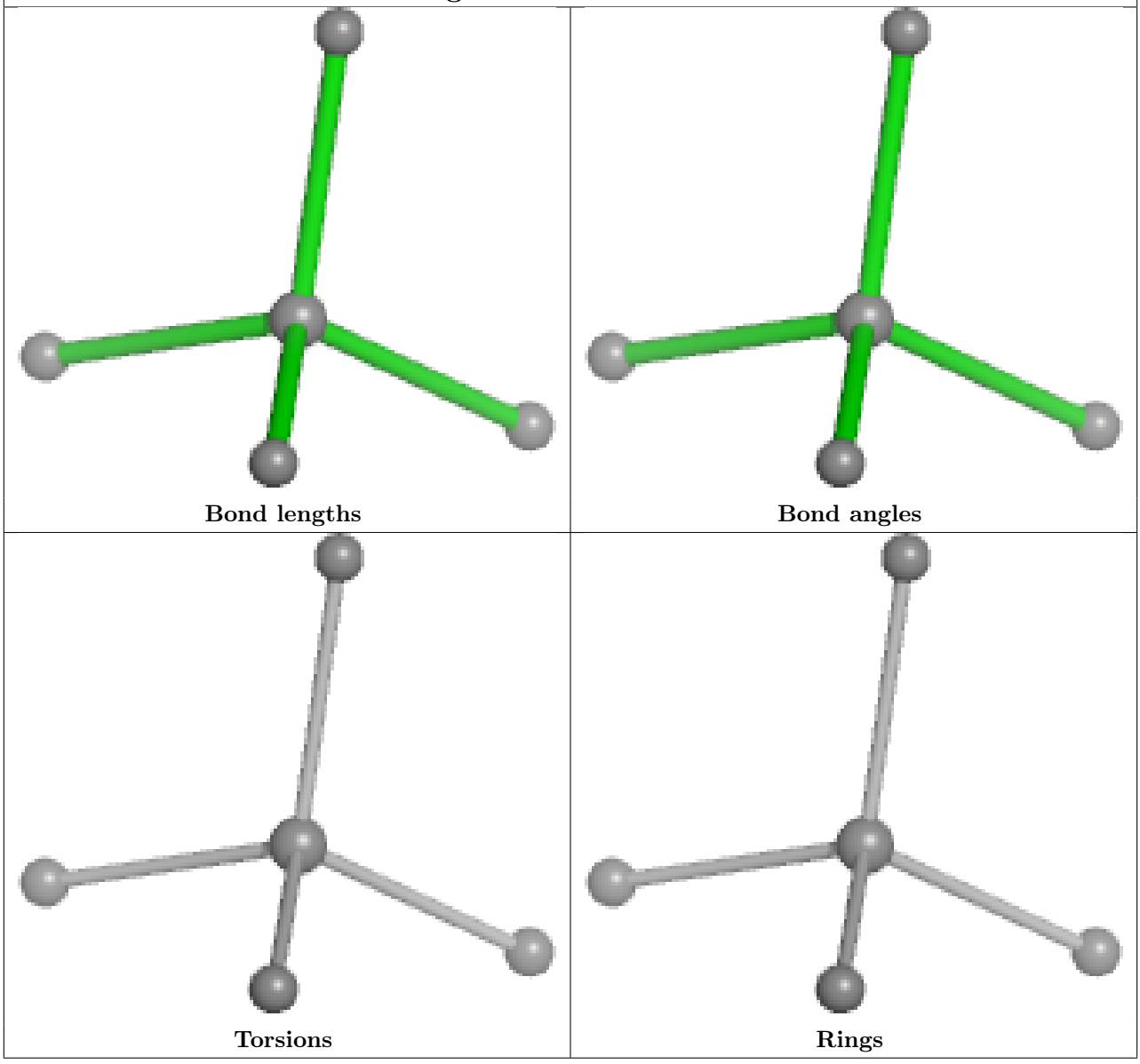
Ligand PEG BBB 204



Ligand PEG CCC 203



Ligand SO4 AAA 202



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	CCC	1
1	AAA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CCC	1:MET	C	2:ASP	N	1.72
1	AAA	1:MET	C	2:ASP	N	1.14

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	AAA	178/179 (99%)	-0.21	0	100	100	10, 17, 35, 59	6 (3%)
1	BBB	178/179 (99%)	-0.21	0	100	100	9, 17, 32, 49	7 (3%)
1	CCC	178/179 (99%)	0.06	7 (3%)	43	45	9, 19, 44, 72	3 (1%)
All	All	534/537 (99%)	-0.12	7 (1%)	75	75	9, 17, 38, 72	16 (2%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	76	PRO	4.2
1	CCC	73	ALA	3.4
1	CCC	74	SER	3.2
1	CCC	2	ASP	3.0
1	CCC	72	SER	2.7
1	CCC	77	THR	2.7
1	CCC	75[A]	ASN	2.3

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

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

6.3 Carbohydrates

There are no 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,

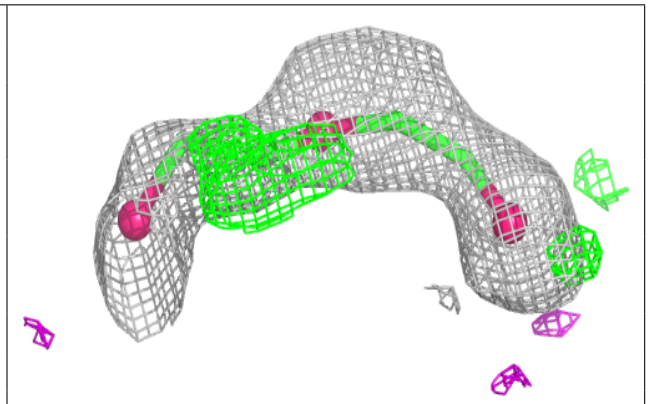
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

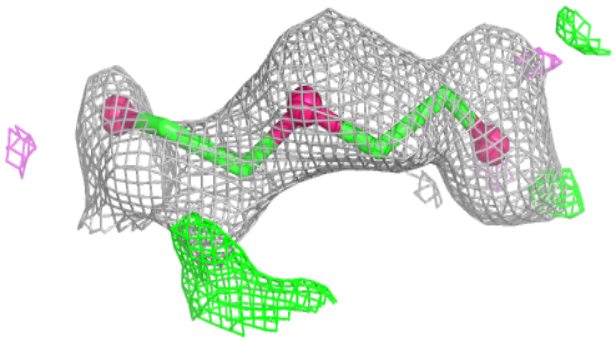
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PEG	CCC	203	7/7	0.86	0.17	33,49,59,61	0
4	PEG	BBB	204	7/7	0.87	0.12	30,39,51,59	0
2	SO4	AAA	202	5/5	0.89	0.14	28,30,31,37	5
2	SO4	CCC	201	5/5	0.89	0.09	45,56,67,82	0
2	SO4	BBB	202	5/5	0.90	0.10	37,61,72,79	0
2	SO4	AAA	201	5/5	0.91	0.10	28,51,60,67	0
2	SO4	BBB	201	5/5	0.93	0.10	29,36,42,43	0
2	SO4	BBB	203	5/5	0.94	0.10	9,16,22,23	5
2	SO4	CCC	202	5/5	0.94	0.09	32,36,44,50	5
3	NA	BBB	207	1/1	0.98	0.04	29,29,29,29	0
3	NA	AAA	203	1/1	0.99	0.03	27,27,27,27	0
3	NA	CCC	205	1/1	0.99	0.04	30,30,30,30	0
5	ZN	BBB	205	1/1	1.00	0.02	15,15,15,15	0
5	ZN	BBB	206	1/1	1.00	0.01	15,15,15,15	0
5	ZN	CCC	204	1/1	1.00	0.02	15,15,15,15	0

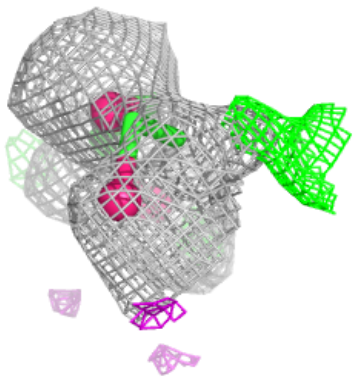
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEG CCC 203:

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

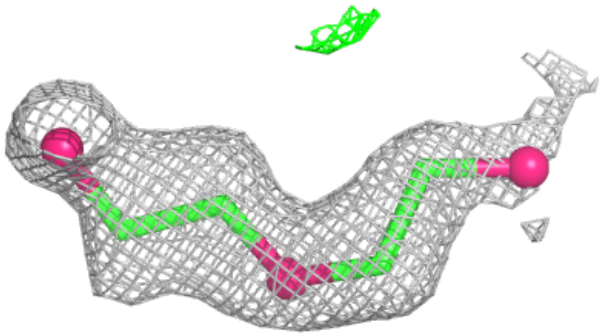


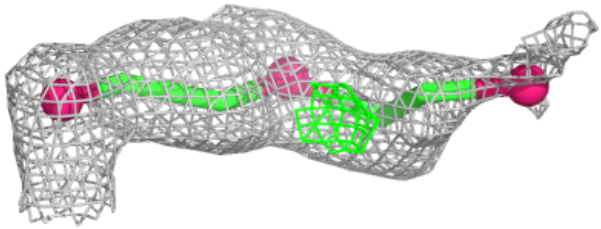


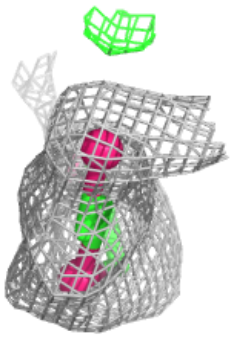


Electron density around PEG BBB 204:

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

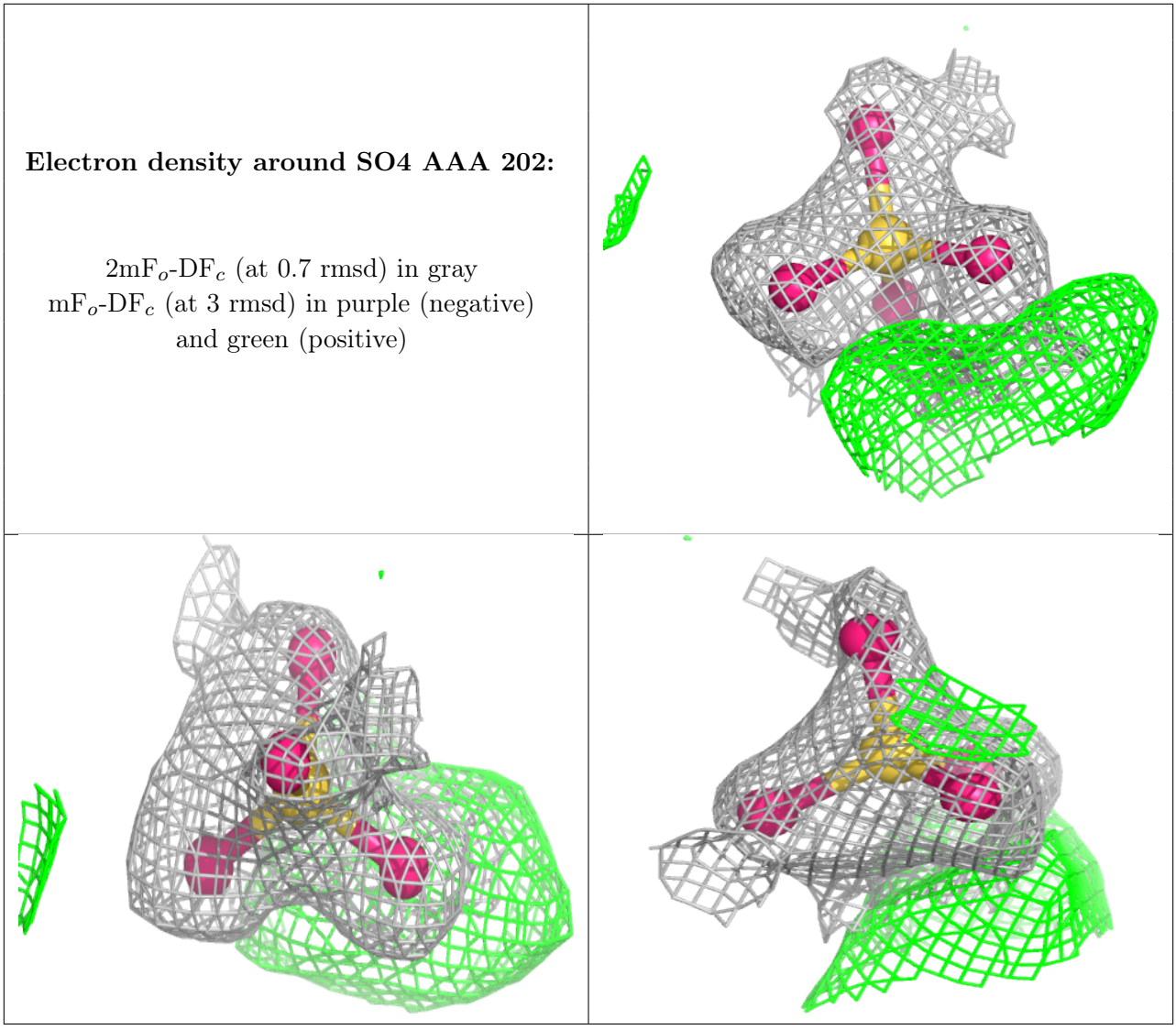






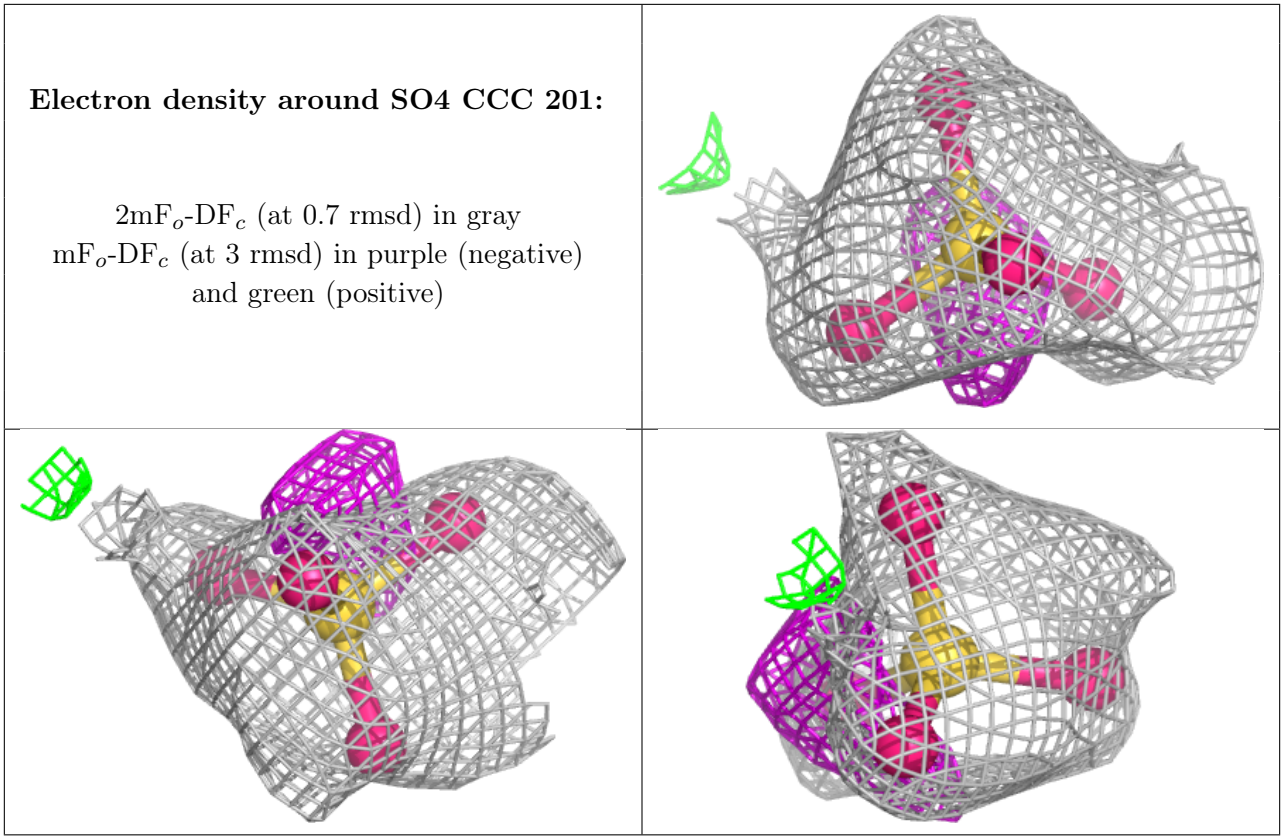
Electron density around SO4 AAA 202:

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



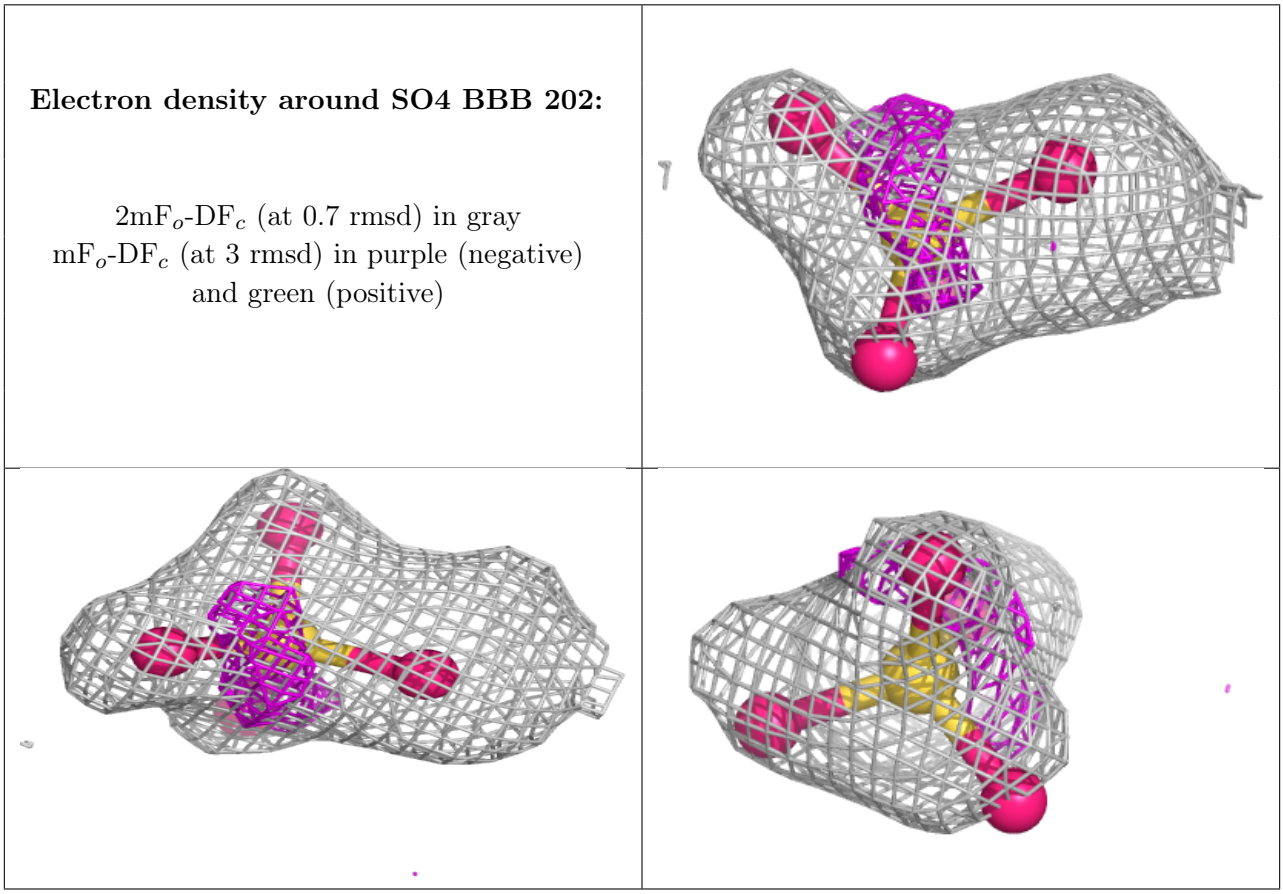
Electron density around SO4 CCC 201:

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



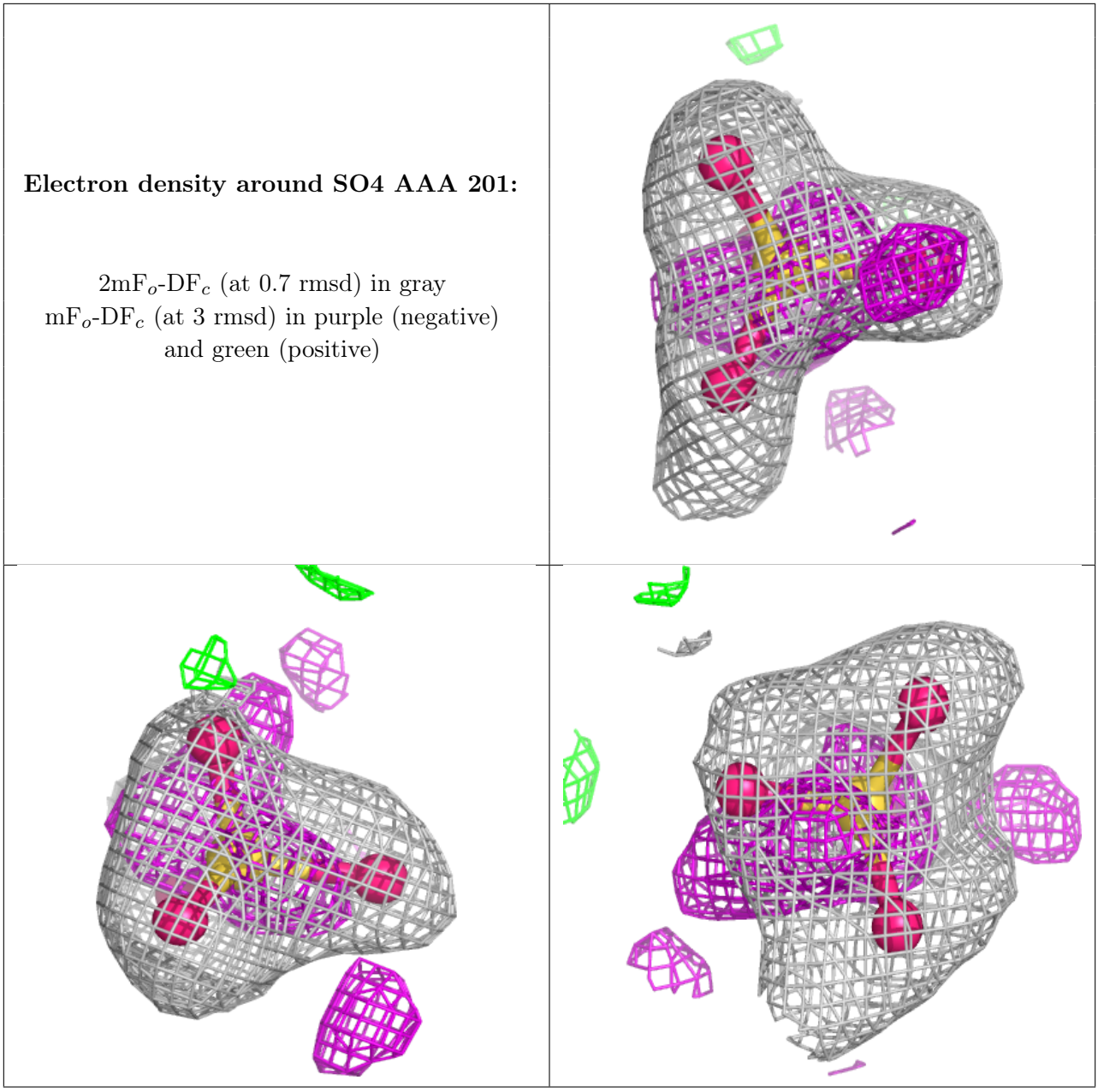
Electron density around SO4 BBB 202:

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



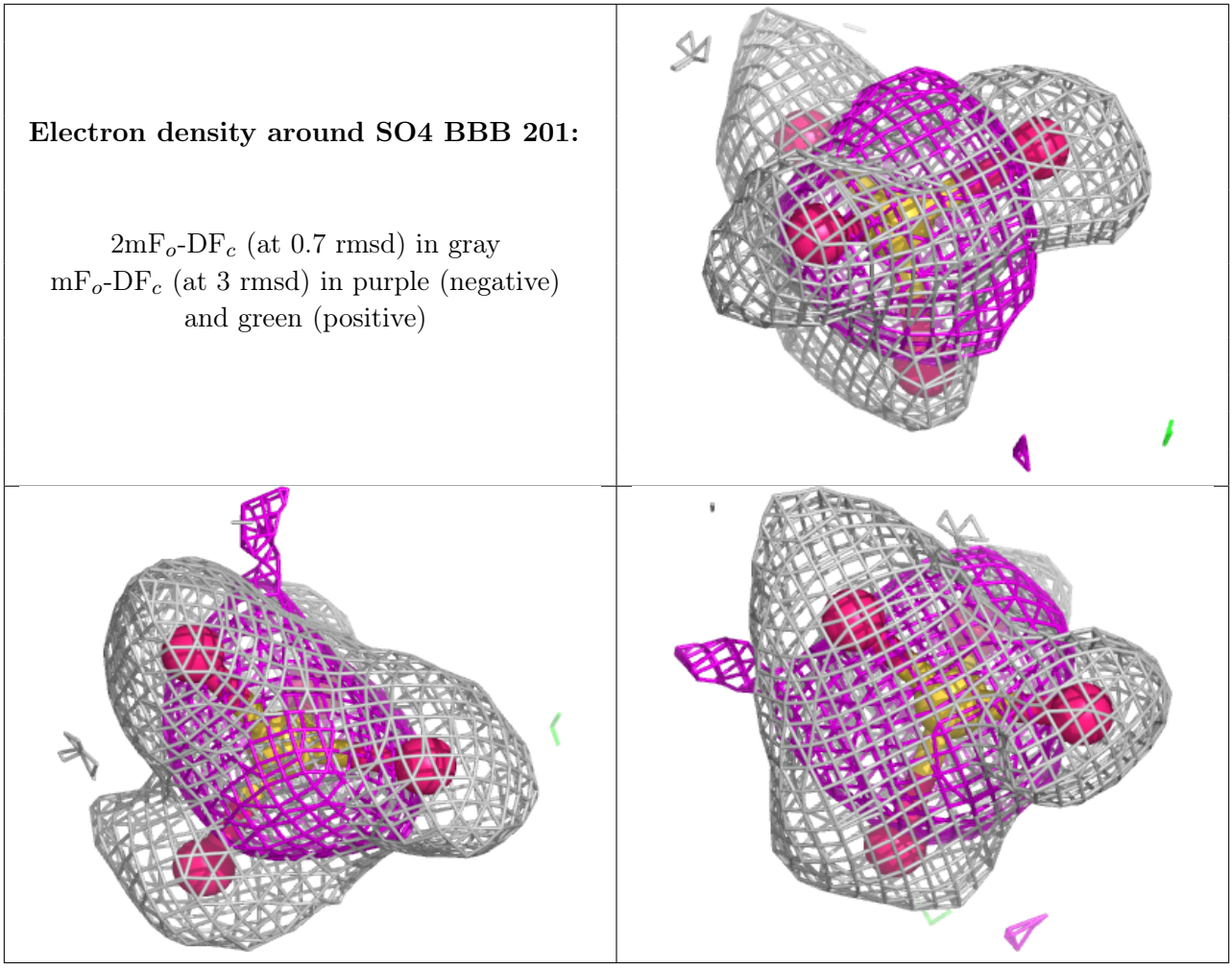
Electron density around SO4 AAA 201:

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



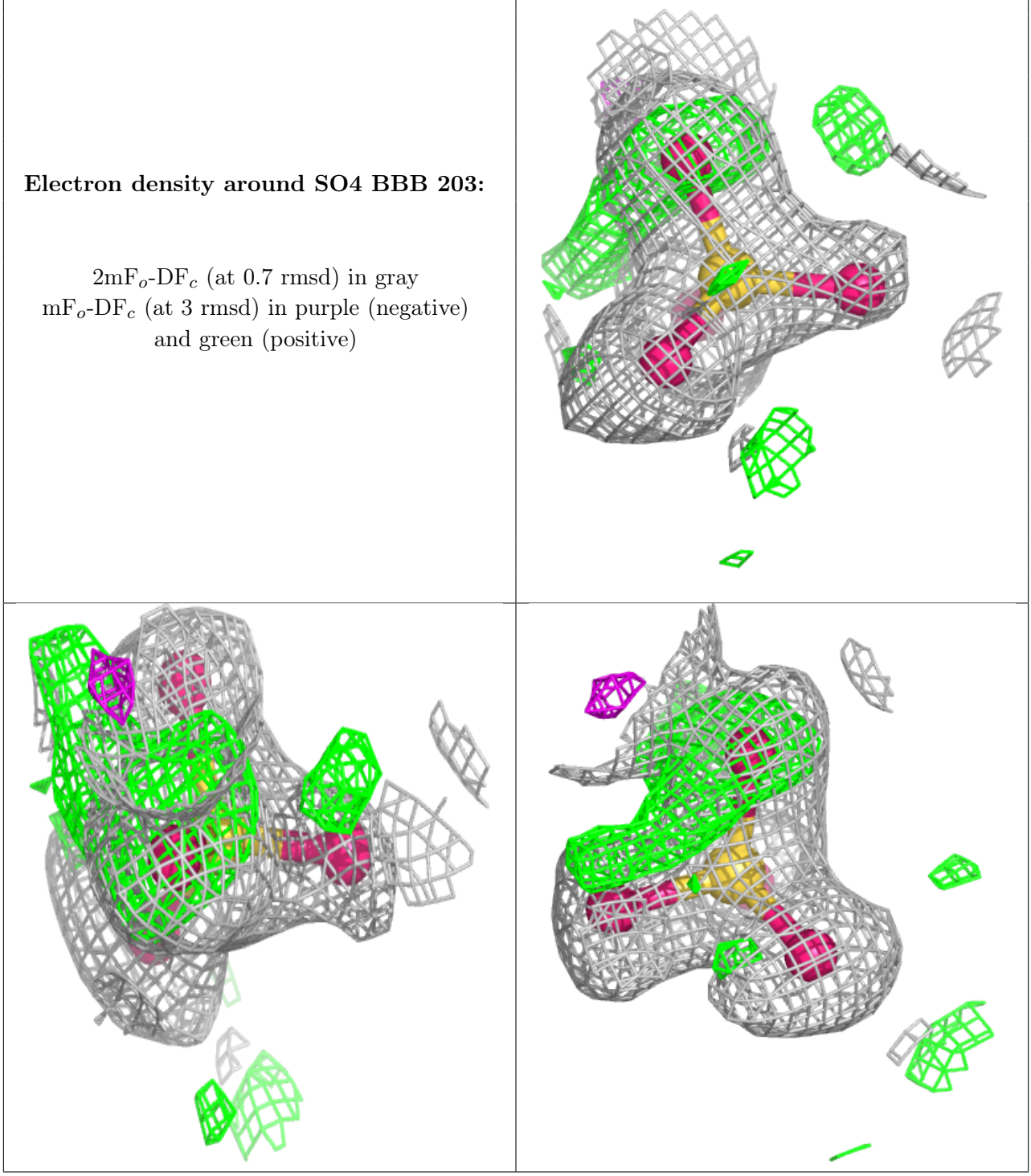
Electron density around SO4 BBB 201:

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



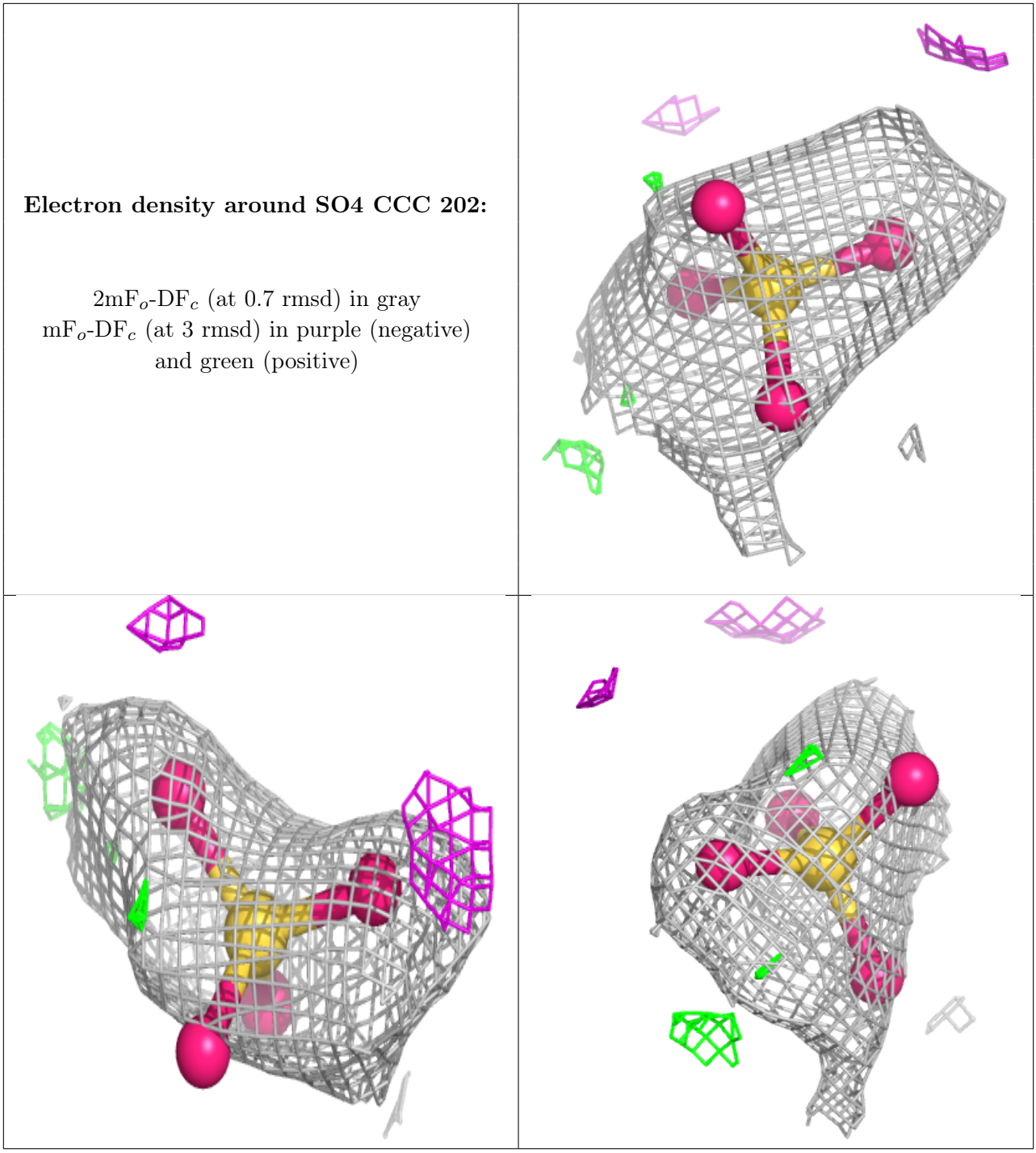
Electron density around SO4 BBB 203:

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



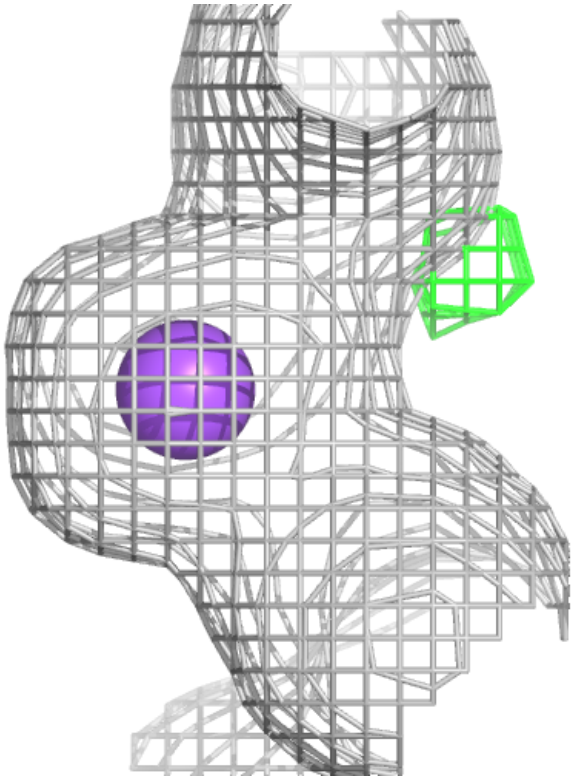
Electron density around SO4 CCC 202:

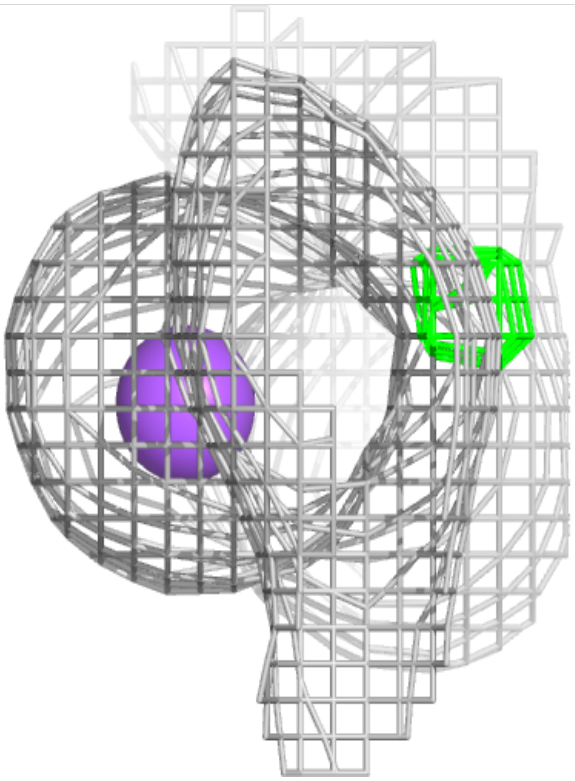
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

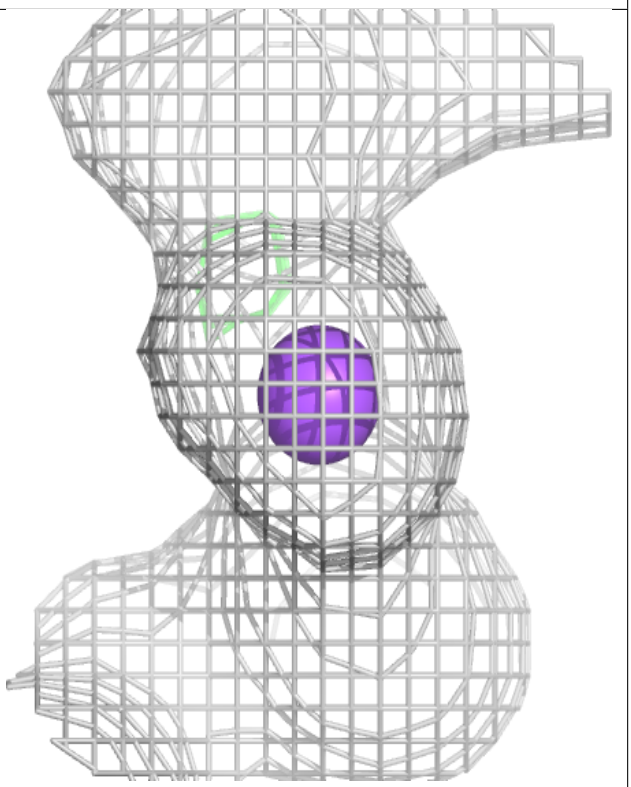


Electron density around NA BBB 207:

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

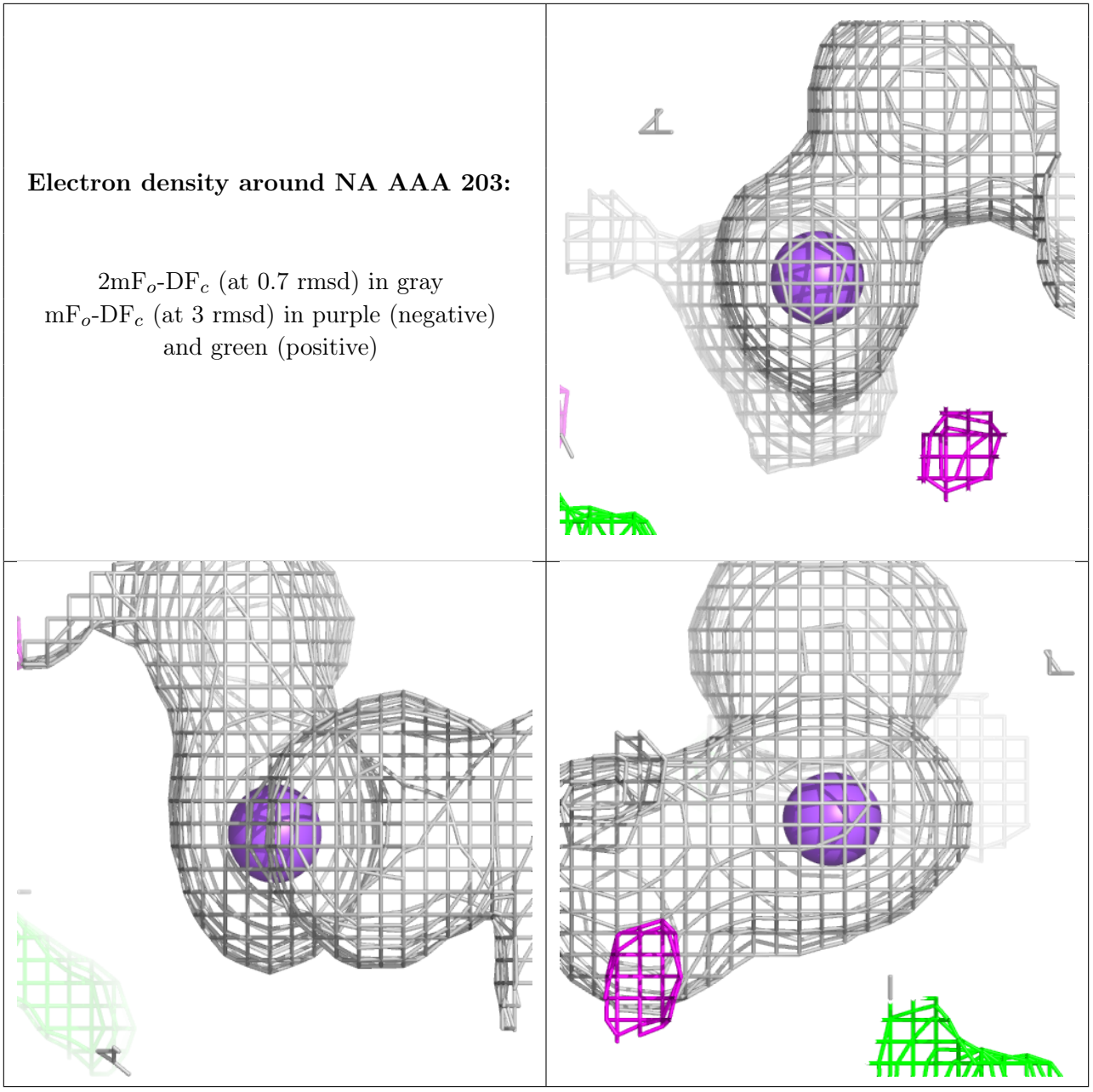






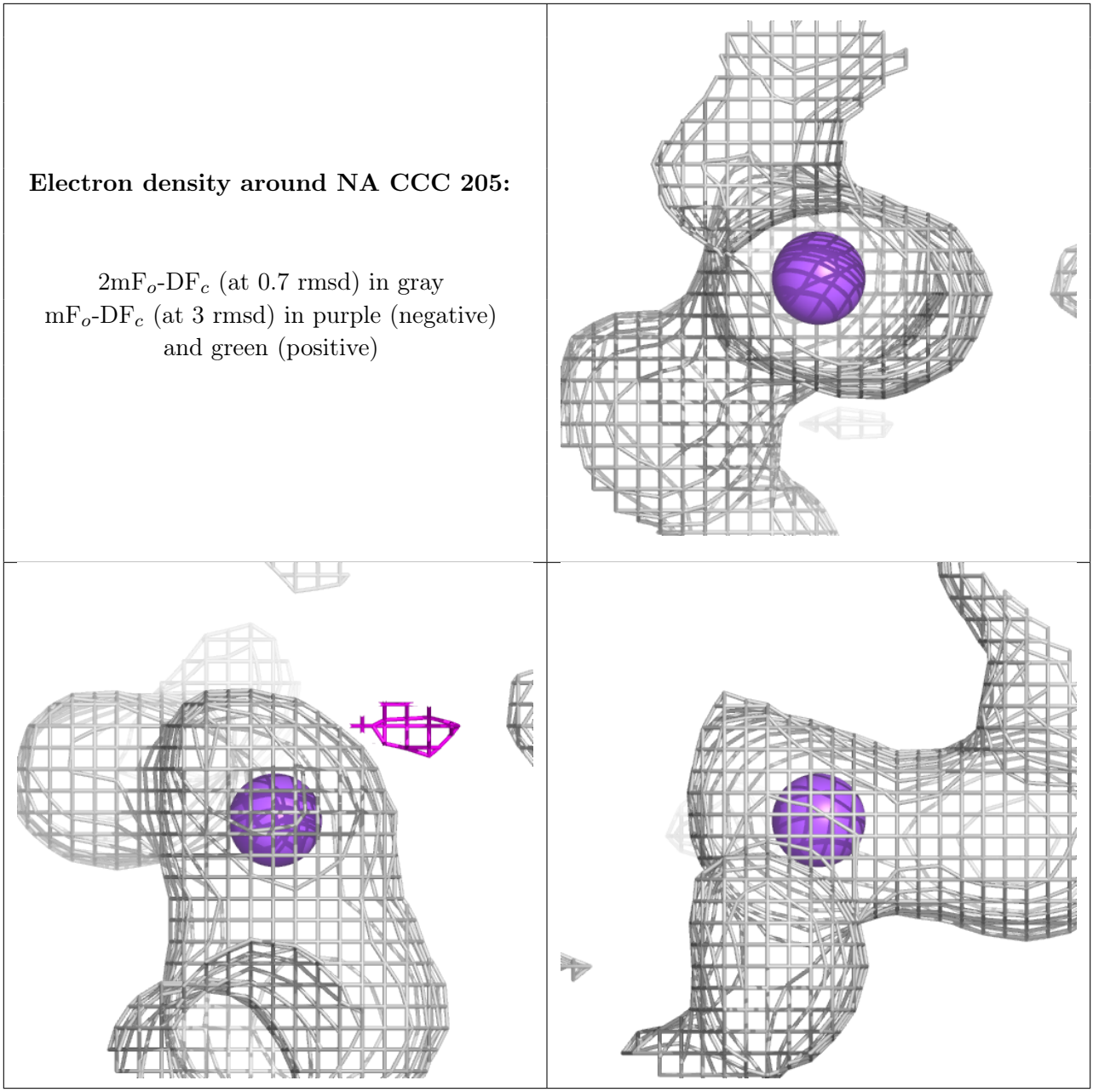
Electron density around NA AAA 203:

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



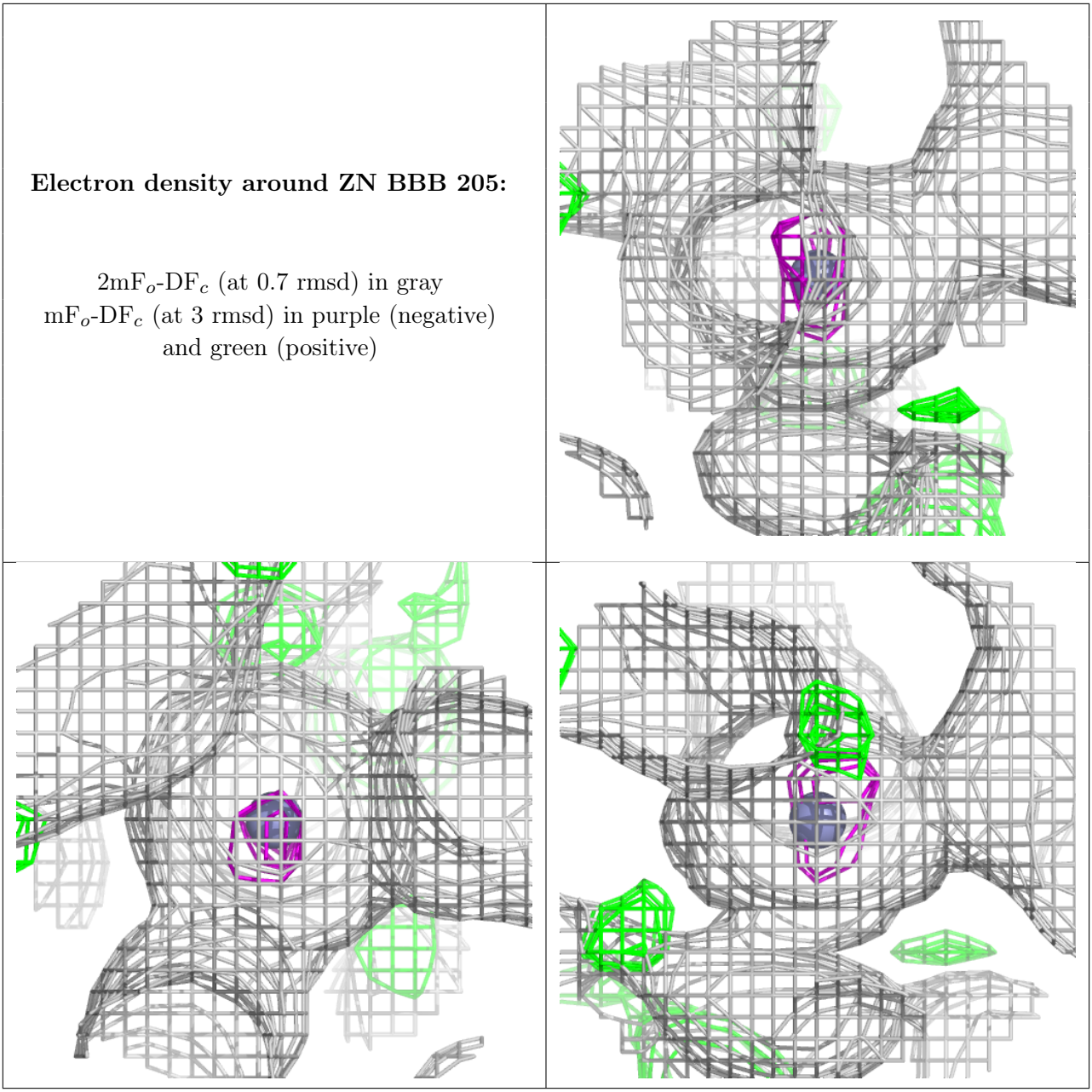
Electron density around NA CCC 205:

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



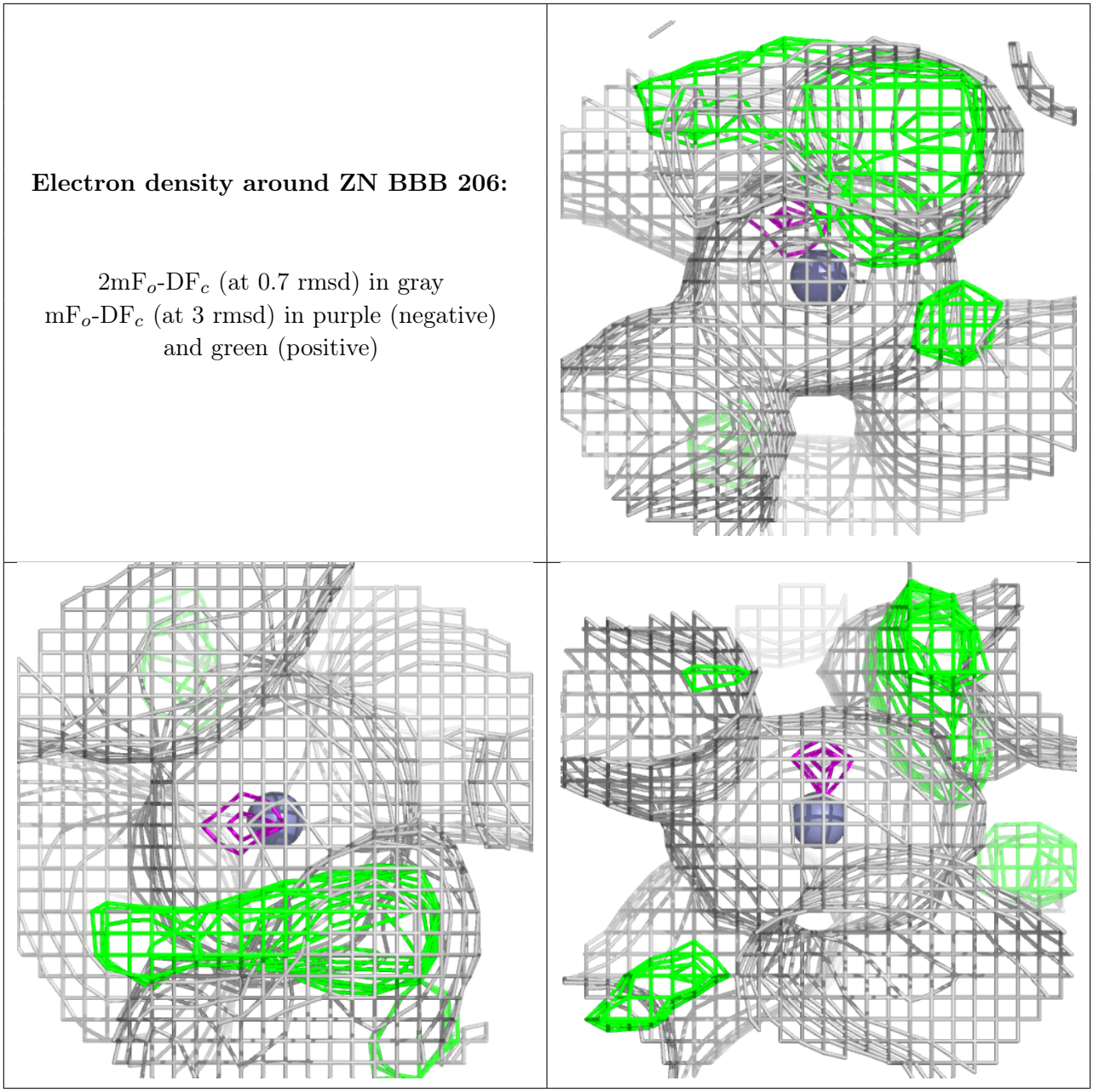
Electron density around ZN BBB 205:

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



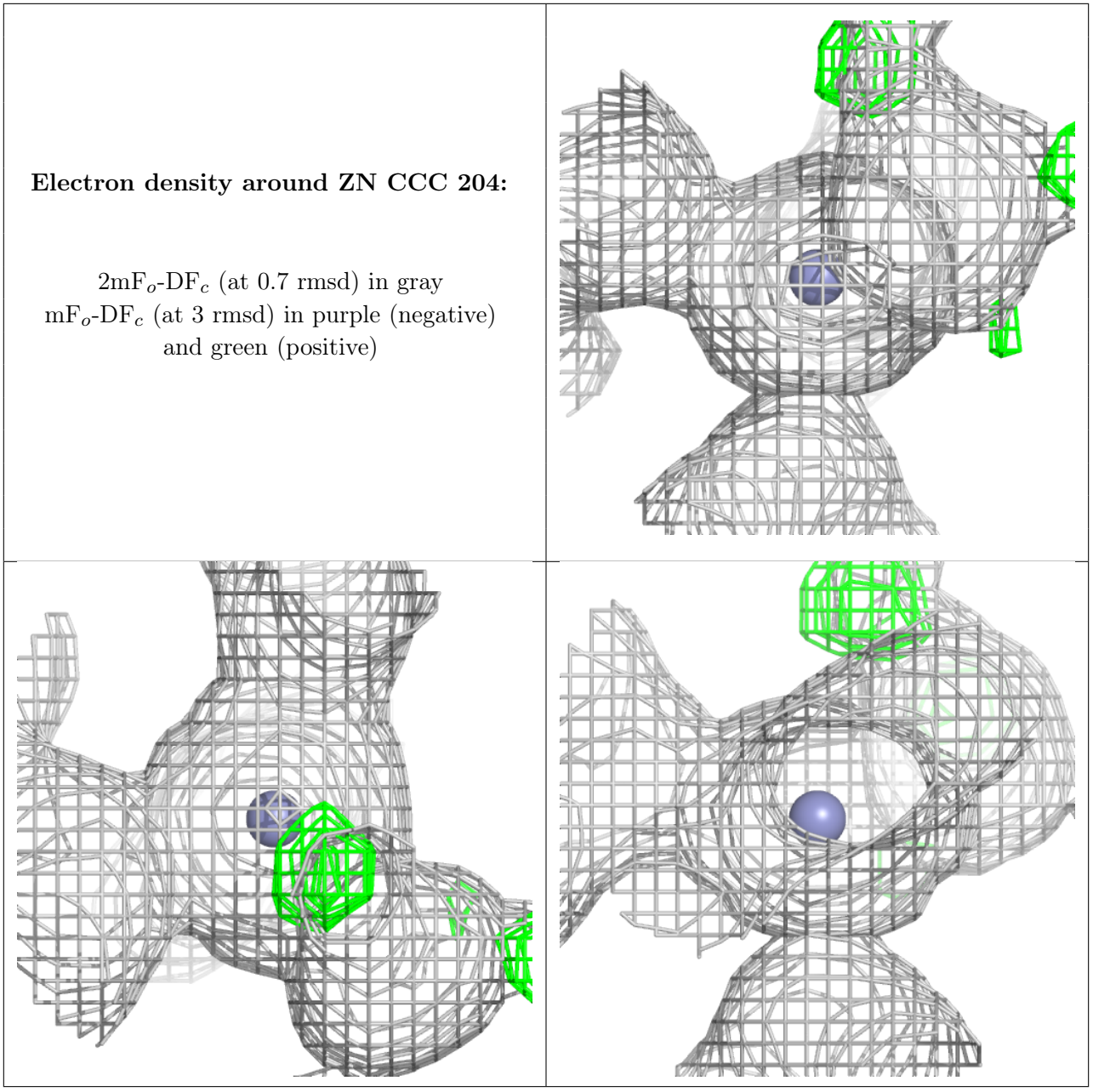
Electron density around ZN BBB 206:

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



Electron density around ZN CCC 204:

$2mF_o$-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.