Full wwPDB X-ray Structure Validation Report (i)

Mar 15, 2026 – 12:40 AM UTC

PDB ID	:	8IOO / pdb_00008ioo
Title	:	Crystal structure of Deinococcus radiodurans RecJ-like protein in complex with Mg2+
Authors	:	Cheng, K.
Deposited on	:	2023-03-13
Resolution	:	2.00 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:

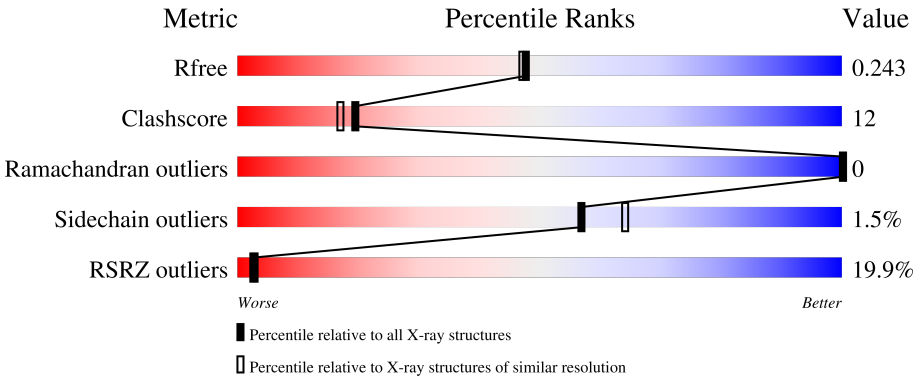
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	338	14% 81% 15% ·
1	B	338	35% 72% 22% · ·
1	C	338	9% 86% 11% · ·

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7766 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.

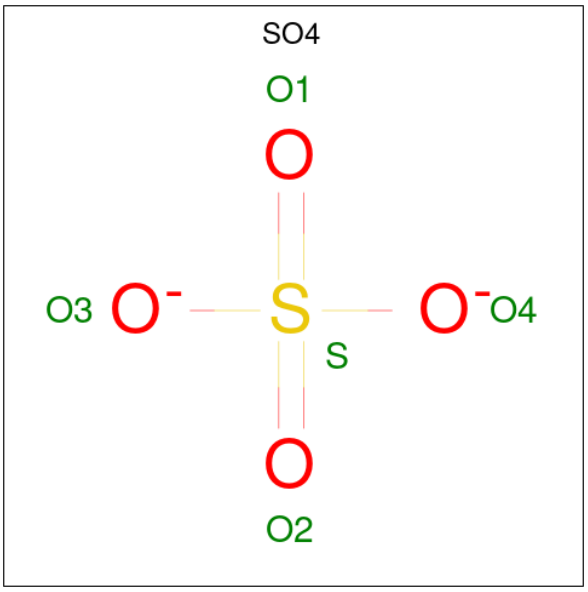
- Molecule 1 is a protein called RecJ-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2437	1522	442	464	9			
1	B	325	Total	C	N	O	S	0	0	0
			2423	1513	440	461	9			
1	C	327	Total	C	N	O	S	0	0	0
			2435	1521	442	463	9			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: 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	A	1	Total O S 5 4 1	0	0
3	B	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

- Molecule 4 is water.

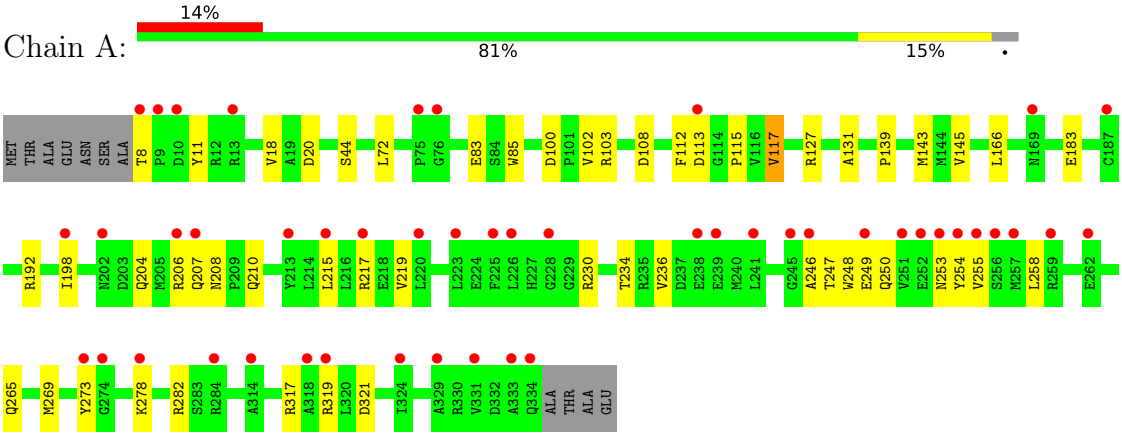
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	144	Total O 144 144	0	0
4	B	134	Total O 134 134	0	0
4	C	162	Total O 162 162	0	0

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.

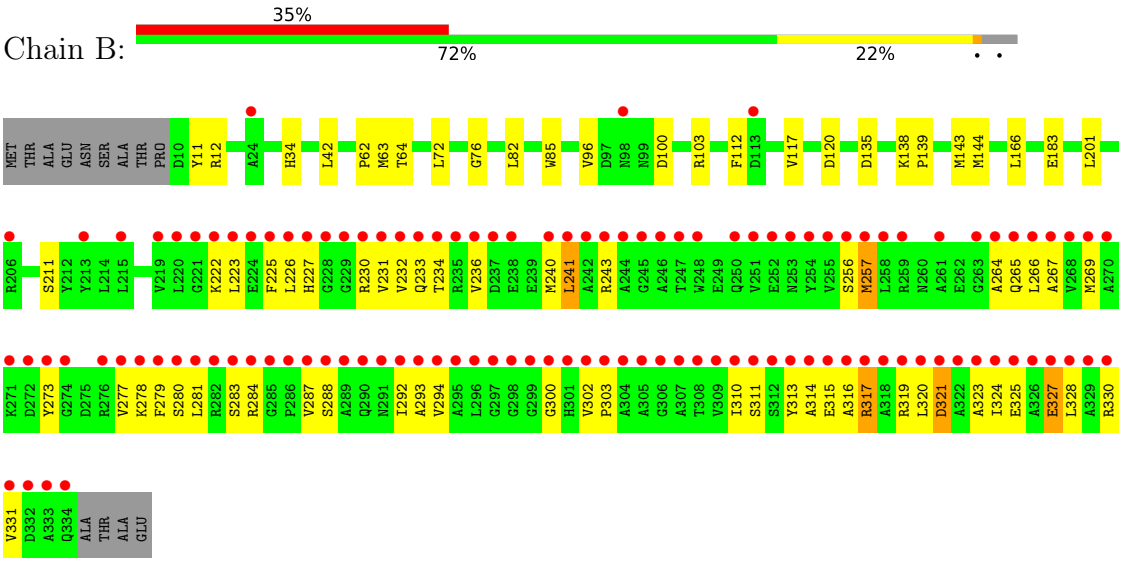
• Molecule 1: RecJ-like protein

Chain A:



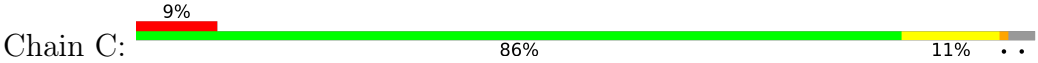
• Molecule 1: RecJ-like protein

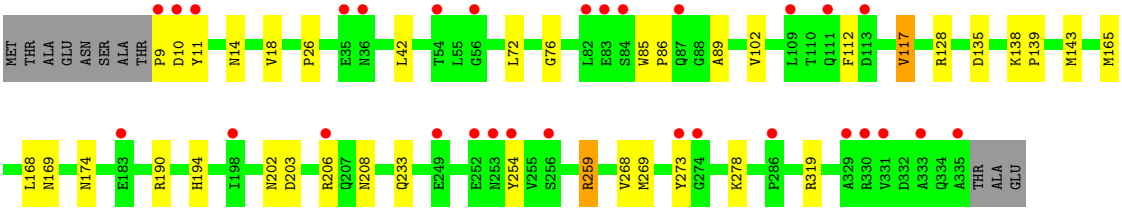
Chain B:



• Molecule 1: RecJ-like protein

Chain C:




MET THR ALA GLU ASN SER ALA THR P9 D10 Y11 N14 V18 P26 E35 N36 L42 T54 L55 G56 L72 G76 L82 E83 S84 W85 P86 Q87 G88 A89 V102 L109 T110 Q111 F112 D113 V117 R128 D135 K138 P139 M143 M165
L168 N169 N174 E183 R190 H194 I198 N202 D203 R206 Q207 N208 Q233 E249 E252 N253 Y254 V255 S256 R259 V268 M269 Y273 G274 K278 P286 R319 A329 R330 V331 D332 A333 Q334 A335 THR ALA GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	152.90Å 124.84Å 80.92Å 90.00° 92.72° 90.00°	Depositor
Resolution (Å)	42.04 – 2.00 42.04 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.04-2.00) 99.5 (42.04-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.228 , 0.244 0.229 , 0.243	Depositor DCC
R_{free} test set	5273 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7766	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: MG, SO4

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	0.47	0/2485	0.75	1/3390 (0.0%)
1	B	0.60	0/2470	0.86	1/3368 (0.0%)
1	C	0.49	1/2483 (0.0%)	0.74	1/3386 (0.0%)
All	All	0.52	1/7438 (0.0%)	0.78	3/10144 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	26	PRO	N-CD	-6.59	1.38	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	273	TYR	N-CA-C	-7.88	99.91	110.55
1	A	273	TYR	N-CA-C	-7.36	98.62	110.32
1	B	300	GLY	N-CA-C	5.36	117.27	110.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	ARG	Sidechain
1	B	317	ARG	Sidechain
1	C	128	ARG	Sidechain
1	C	190	ARG	Sidechain
1	C	259	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2437	0	2406	62	0
1	B	2423	0	2392	83	0
1	C	2435	0	2405	28	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
4	A	144	0	0	36	1
4	B	134	0	0	28	0
4	C	162	0	0	12	2
All	All	7766	0	7203	169	2

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 12.

All (169) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:SER:HB2	4:B:505:HOH:O	1.11	1.25
1:B:292:ILE:HG12	4:B:506:HOH:O	1.10	1.25
1:A:207:GLN:N	4:A:501:HOH:O	1.80	1.13
1:A:207:GLN:C	4:A:501:HOH:O	1.88	1.12
1:A:103:ARG:HG3	4:A:507:HOH:O	1.49	1.12
1:A:254:TYR:N	4:A:502:HOH:O	1.80	1.11
1:C:208:ASN:ND2	4:C:502:HOH:O	1.84	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:GLN:NE2	4:A:503:HOH:O	1.90	1.04
1:A:207:GLN:CA	4:A:501:HOH:O	2.06	1.01
1:B:281:LEU:HG	4:B:510:HOH:O	1.61	1.00
1:C:319:ARG:NH2	4:C:505:HOH:O	1.92	0.99
1:B:257:MET:N	4:B:504:HOH:O	1.94	0.98
1:C:174:ASN:OD1	4:C:501:HOH:O	1.83	0.97
1:A:230:ARG:HD2	4:A:503:HOH:O	1.61	0.96
1:A:103:ARG:CG	4:A:507:HOH:O	2.08	0.96
1:B:231:VAL:HG22	1:B:266:LEU:HB3	1.47	0.96
1:A:249:GLU:OE1	1:A:249:GLU:N	2.00	0.95
1:B:302:VAL:HG13	1:B:303:PRO:HD3	1.48	0.94
1:B:281:LEU:HD21	1:B:320:LEU:HD11	1.48	0.94
1:A:206:ARG:C	4:A:501:HOH:O	2.06	0.92
1:B:284:ARG:O	4:B:501:HOH:O	1.85	0.92
1:A:208:ASN:N	4:A:501:HOH:O	1.95	0.91
1:A:20:ASP:OD2	4:A:505:HOH:O	1.86	0.91
1:A:282:ARG:NH2	4:A:508:HOH:O	2.02	0.90
1:B:100:ASP:OD2	4:B:503:HOH:O	1.90	0.89
1:A:317:ARG:NE	4:A:504:HOH:O	1.83	0.89
1:B:280:SER:C	4:B:510:HOH:O	2.15	0.87
1:A:204:GLN:OE1	4:A:506:HOH:O	1.92	0.85
1:A:319:ARG:NH1	4:A:509:HOH:O	2.02	0.85
1:B:265:GLN:O	4:B:505:HOH:O	1.94	0.85
1:B:323:ALA:O	4:B:506:HOH:O	1.95	0.85
1:C:202:ASN:HB3	1:C:206:ARG:NH2	1.94	0.83
1:B:64:THR:OG1	4:B:507:HOH:O	1.96	0.83
1:B:281:LEU:CA	4:B:510:HOH:O	2.26	0.83
1:A:100:ASP:CG	4:A:507:HOH:O	2.21	0.82
1:B:293:ALA:HB1	4:B:511:HOH:O	1.80	0.82
1:A:321:ASP:OD1	4:A:504:HOH:O	1.96	0.82
1:B:230:ARG:NH1	1:B:265:GLN:OE1	2.13	0.81
1:C:203:ASP:OD2	4:C:506:HOH:O	1.98	0.81
1:A:100:ASP:OD2	4:A:507:HOH:O	1.97	0.81
1:B:234:THR:HG23	1:B:269:MET:HE3	1.63	0.81
1:C:14:ASN:OD1	4:C:507:HOH:O	1.98	0.80
1:A:139:PRO:HD2	1:A:143:MET:SD	2.22	0.80
1:A:253:ASN:CG	4:A:513:HOH:O	2.26	0.79
1:A:321:ASP:CG	4:A:504:HOH:O	2.26	0.78
1:B:293:ALA:O	4:B:509:HOH:O	2.02	0.77
1:B:222:LYS:HG2	1:B:240:MET:HE1	1.66	0.76
1:A:72:LEU:HD22	1:A:166:LEU:HD22	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LEU:HA	4:B:510:HOH:O	1.85	0.74
1:A:230:ARG:CD	4:A:503:HOH:O	2.21	0.74
1:B:236:VAL:CG1	1:B:241:LEU:HD21	2.18	0.74
1:A:278:LYS:HE2	4:A:515:HOH:O	1.88	0.73
1:C:135:ASP:OD2	1:C:138:LYS:HE2	1.87	0.73
1:A:100:ASP:OD1	4:A:507:HOH:O	2.06	0.73
1:A:247:THR:H	1:A:250:GLN:HE21	1.36	0.73
1:B:234:THR:HG23	1:B:269:MET:CE	2.18	0.72
1:B:42:LEU:HD12	1:B:63:MET:SD	2.31	0.70
1:B:280:SER:O	4:B:510:HOH:O	2.08	0.69
1:B:311:SER:HB3	1:B:315:GLU:HG3	1.73	0.69
1:A:253:ASN:ND2	4:A:513:HOH:O	2.24	0.69
1:B:103:ARG:NH2	4:B:512:HOH:O	2.24	0.68
1:A:236:VAL:HG23	1:A:269:MET:HE1	1.73	0.68
1:A:103:ARG:HB2	4:A:507:HOH:O	1.94	0.67
1:A:247:THR:H	1:A:250:GLN:NE2	1.92	0.67
1:C:202:ASN:HB3	1:C:206:ARG:HH22	1.59	0.66
1:B:292:ILE:HG23	1:B:323:ALA:HB1	1.76	0.66
1:B:256:SER:OG	4:B:504:HOH:O	2.12	0.66
4:A:567:HOH:O	1:C:194:HIS:HD2	1.78	0.65
1:A:83:GLU:OE2	4:A:510:HOH:O	2.13	0.65
1:B:120:ASP:O	1:B:144:MET:HE1	1.97	0.64
1:A:230:ARG:NH1	4:A:503:HOH:O	1.83	0.63
1:B:230:ARG:HA	1:B:264:ALA:HA	1.81	0.62
1:A:143:MET:HE1	1:A:183:GLU:HG3	1.81	0.62
1:B:302:VAL:CG1	1:B:303:PRO:HD3	2.26	0.62
1:A:247:THR:HB	1:A:249:GLU:OE1	1.99	0.62
1:B:292:ILE:HG23	1:B:323:ALA:CB	2.32	0.59
1:B:323:ALA:HB1	4:B:506:HOH:O	2.00	0.59
1:A:192:ARG:CZ	1:A:198:ILE:HG22	2.32	0.59
1:B:294:VAL:HG22	4:B:509:HOH:O	2.03	0.59
1:B:315:GLU:O	1:B:319:ARG:HG2	2.03	0.59
1:C:102:VAL:HG12	4:C:510:HOH:O	2.02	0.58
1:B:223:LEU:C	1:B:223:LEU:HD23	2.28	0.58
1:B:265:GLN:HG2	4:B:501:HOH:O	2.03	0.58
1:B:281:LEU:N	4:B:510:HOH:O	2.28	0.57
1:A:210:GLN:HG2	1:B:225:PHE:CD2	2.40	0.57
1:B:236:VAL:HG11	1:B:241:LEU:HD21	1.87	0.56
1:B:327:GLU:O	1:B:331:VAL:HG23	2.05	0.56
1:B:279:PHE:CE1	1:B:320:LEU:HD22	2.40	0.55
1:B:12:ARG:NH1	4:B:516:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:TRP:CE2	1:C:112:PHE:HB2	2.42	0.55
1:A:113:ASP:HA	4:A:524:HOH:O	2.06	0.55
1:B:227:HIS:HD2	1:B:231:VAL:HG21	1.71	0.54
1:B:293:ALA:O	4:B:511:HOH:O	2.18	0.54
1:B:311:SER:CB	1:B:315:GLU:HG3	2.38	0.53
1:B:143:MET:HE1	1:B:183:GLU:HG2	1.91	0.52
1:C:76:GLY:N	4:C:504:HOH:O	1.89	0.52
1:C:139:PRO:HD2	1:C:143:MET:SD	2.49	0.52
1:A:44:SER:HB3	1:A:145:VAL:HG21	1.92	0.52
1:A:246:ALA:HA	1:A:250:GLN:HE22	1.75	0.52
1:B:34:HIS:HB3	1:B:96:VAL:HB	1.92	0.52
1:C:11:TYR:CZ	1:C:138:LYS:HE3	2.45	0.51
1:B:222:LYS:CG	1:B:240:MET:HE1	2.38	0.51
1:B:323:ALA:C	4:B:506:HOH:O	2.48	0.51
1:A:210:GLN:HG2	1:B:225:PHE:CE2	2.45	0.51
1:B:277:VAL:HG21	1:B:316:ALA:HB3	1.93	0.51
1:C:206:ARG:NH1	4:C:514:HOH:O	2.43	0.51
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.76	0.51
1:B:62:PRO:HG3	1:B:82:LEU:HG	1.93	0.51
1:B:313:TYR:O	1:B:314:ALA:C	2.54	0.50
1:A:255:VAL:N	4:A:502:HOH:O	2.33	0.50
1:A:85:TRP:CE2	1:A:112:PHE:HB2	2.47	0.50
1:C:233:GLN:HG2	1:C:268:VAL:HB	1.94	0.50
1:A:215:LEU:HD22	1:A:246:ALA:CB	2.41	0.50
1:A:103:ARG:CB	4:A:507:HOH:O	2.40	0.50
1:B:279:PHE:CE2	1:B:320:LEU:HD13	2.47	0.50
1:B:223:LEU:HD21	1:B:225:PHE:CE2	2.48	0.49
1:C:42:LEU:CD2	1:C:72:LEU:HD23	2.43	0.49
1:C:259:ARG:NH2	4:C:517:HOH:O	2.46	0.48
1:B:233:GLN:HE22	1:B:317:ARG:HG3	1.78	0.48
1:A:247:THR:N	1:A:250:GLN:HE21	2.09	0.48
1:B:227:HIS:HB2	1:B:231:VAL:HB	1.95	0.48
1:B:273:TYR:OH	4:B:508:HOH:O	2.00	0.48
1:B:85:TRP:CE2	1:B:112:PHE:HB2	2.50	0.47
1:B:227:HIS:CD2	1:B:231:VAL:HG21	2.49	0.47
1:B:292:ILE:HD11	1:B:327:GLU:HB2	1.97	0.47
1:A:215:LEU:HD22	1:A:246:ALA:HB1	1.97	0.47
1:B:278:LYS:NZ	1:B:279:PHE:O	2.29	0.47
1:A:8:THR:HG23	1:A:11:TYR:H	1.79	0.47
1:B:278:LYS:HD2	1:B:278:LYS:C	2.39	0.47
1:C:76:GLY:CA	4:C:504:HOH:O	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LYS:HD3	4:C:503:HOH:O	2.15	0.46
1:A:210:GLN:HE21	1:B:225:PHE:HB3	1.80	0.46
1:B:42:LEU:HD23	1:B:72:LEU:HD23	1.97	0.46
1:C:169:ASN:OD1	4:C:508:HOH:O	2.21	0.46
1:B:72:LEU:HD22	1:B:166:LEU:HD22	1.99	0.45
1:A:210:GLN:HE21	1:B:225:PHE:CB	2.29	0.45
1:B:222:LYS:HD3	1:B:222:LYS:HA	1.80	0.45
1:B:135:ASP:OD2	1:B:138:LYS:HE2	2.17	0.45
1:C:254:TYR:HB2	1:C:269:MET:HE3	1.99	0.45
1:A:117:VAL:HG22	1:A:131:ALA:HB3	1.99	0.45
1:A:234:THR:HG22	1:A:258:LEU:HD11	1.98	0.44
1:B:325:GLU:O	1:B:328:LEU:HB3	2.17	0.44
1:B:288:SER:O	1:B:327:GLU:HG3	2.17	0.44
1:C:18:VAL:HG13	1:C:117:VAL:CG1	2.47	0.44
1:A:8:THR:CG2	1:A:11:TYR:H	2.31	0.44
1:B:287:VAL:HG22	1:B:331:VAL:HG21	1.99	0.44
1:A:248:TRP:N	1:A:249:GLU:OE1	2.51	0.44
1:A:102:VAL:HG12	4:A:547:HOH:O	2.18	0.43
1:C:86:PRO:HG2	1:C:89:ALA:HB2	2.00	0.43
1:B:243:ARG:HH11	1:B:243:ARG:HG3	1.84	0.43
1:A:219:VAL:HG22	1:A:236:VAL:CG2	2.49	0.42
1:B:321:ASP:HA	1:B:324:ILE:HD12	2.01	0.42
1:B:76:GLY:N	4:B:502:HOH:O	1.86	0.42
1:C:9:PRO:HB2	1:C:10:ASP:H	1.63	0.42
1:A:321:ASP:OD2	4:A:504:HOH:O	2.21	0.41
1:B:232:VAL:HG12	1:B:267:ALA:HA	2.01	0.41
1:A:115:PRO:HG3	4:A:641:HOH:O	2.20	0.41
1:C:143:MET:HG3	1:C:168:LEU:CD1	2.50	0.41
1:A:18:VAL:HG13	1:A:117:VAL:CG1	2.50	0.41
1:B:201:LEU:HD23	1:B:201:LEU:HA	1.85	0.41
1:B:139:PRO:HD2	1:B:143:MET:SD	2.61	0.41
1:B:279:PHE:CD2	1:B:320:LEU:HD13	2.56	0.41
1:B:11:TYR:CZ	1:B:138:LYS:HE3	2.56	0.41
1:C:42:LEU:HD23	1:C:72:LEU:HD23	2.03	0.41
1:A:317:ARG:CD	4:A:504:HOH:O	2.49	0.40
1:C:165:MET:HE2	1:C:165:MET:HB2	1.95	0.40
1:A:108:ASP:OD2	4:A:512:HOH:O	2.21	0.40
1:B:257:MET:CB	4:B:504:HOH:O	2.69	0.40
1:B:257:MET:HB3	4:B:504:HOH:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:620:HOH:O	4:C:589:HOH:O[4_556]	1.89	0.31
4:C:628:HOH:O	4:C:651:HOH:O[2_556]	2.15	0.05

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	325/338 (96%)	318 (98%)	7 (2%)	0	100	100
1	B	323/338 (96%)	301 (93%)	22 (7%)	0	100	100
1	C	325/338 (96%)	320 (98%)	5 (2%)	0	100	100
All	All	973/1014 (96%)	939 (96%)	34 (4%)	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	248/255 (97%)	247 (100%)	1 (0%)	84	89
1	B	246/255 (96%)	237 (96%)	9 (4%)	30	30
1	C	247/255 (97%)	246 (100%)	1 (0%)	84	89
All	All	741/765 (97%)	730 (98%)	11 (2%)	57	64

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	VAL
1	B	117	VAL
1	B	211	SER
1	B	226	LEU
1	B	241	LEU
1	B	257	MET
1	B	310	ILE
1	B	321	ASP
1	B	327	GLU
1	B	330	ARG
1	C	117	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	B	174	ASN
1	B	202	ASN
1	B	210	GLN
1	B	227	HIS
1	B	233	GLN
1	B	253	ASN
1	C	111	GLN
1	C	169	ASN
1	C	194	HIS
1	C	202	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	A	403	-	4,4,4	0.38	0	6,6,6	0.10	0
3	SO4	C	403	-	4,4,4	0.45	0	6,6,6	0.10	0
3	SO4	B	403	-	4,4,4	0.43	0	6,6,6	0.09	0
3	SO4	B	404	-	4,4,4	0.40	0	6,6,6	0.10	0
3	SO4	A	404	-	4,4,4	0.43	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

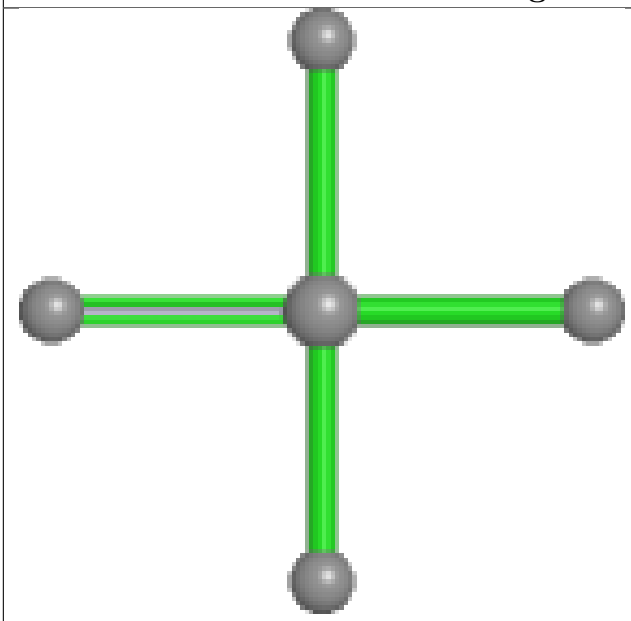
There are no torsion outliers.

There are no ring outliers.

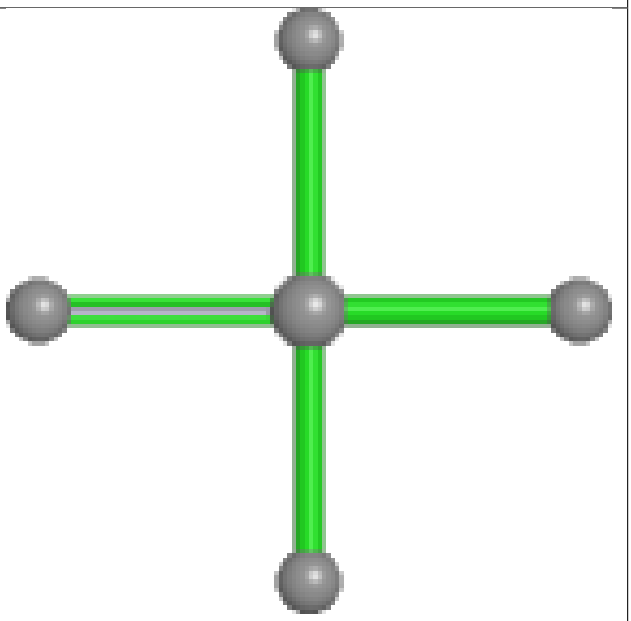
No monomer is involved in short contacts.

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

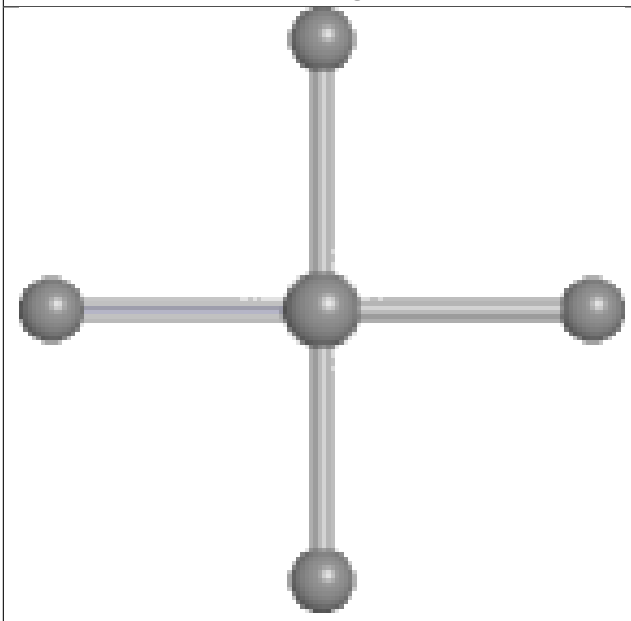
Ligand SO4 A 403



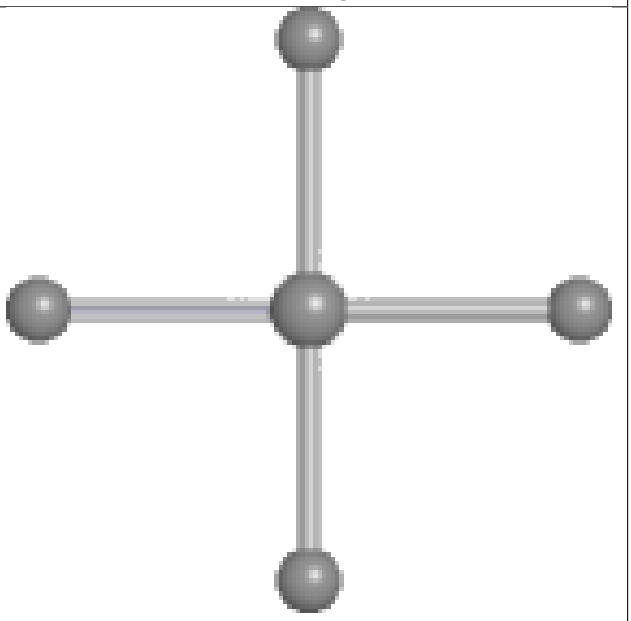
Bond lengths



Bond angles

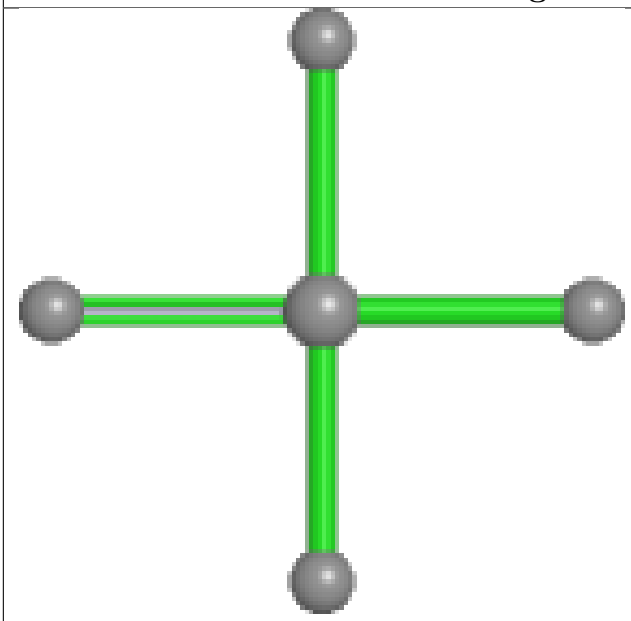


Torsions

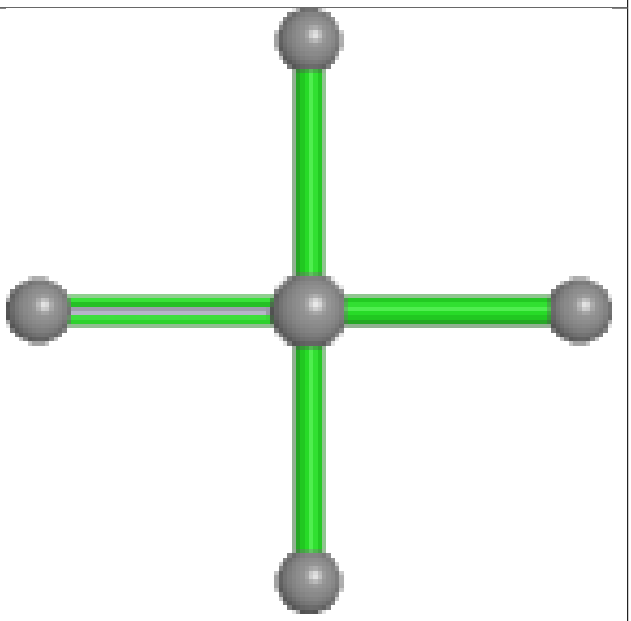


Rings

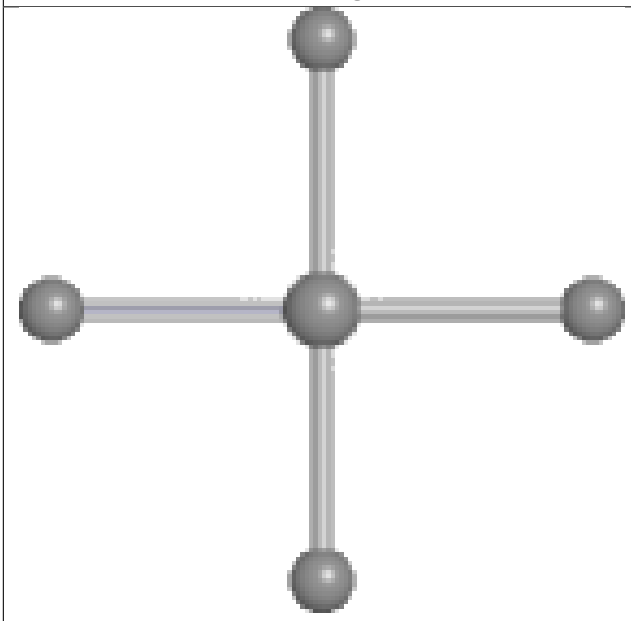
Ligand SO4 C 403



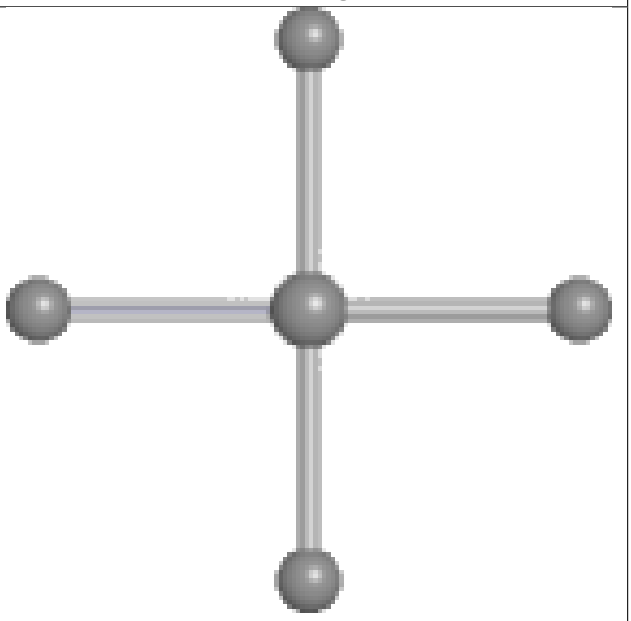
Bond lengths



Bond angles

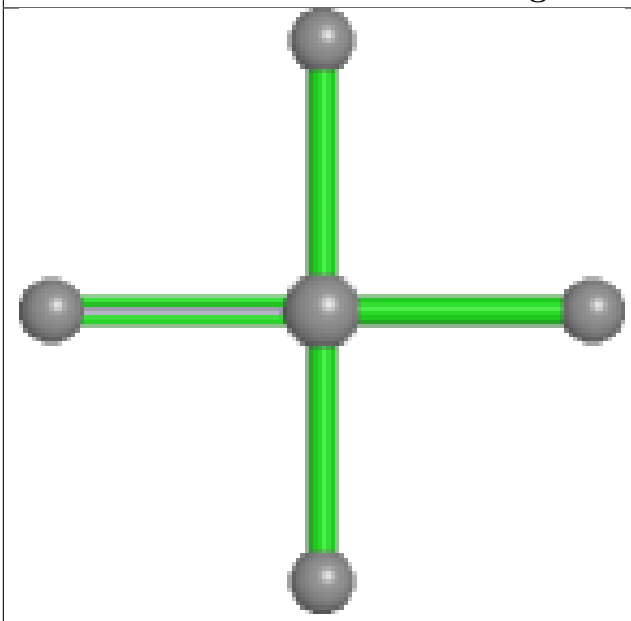


Torsions

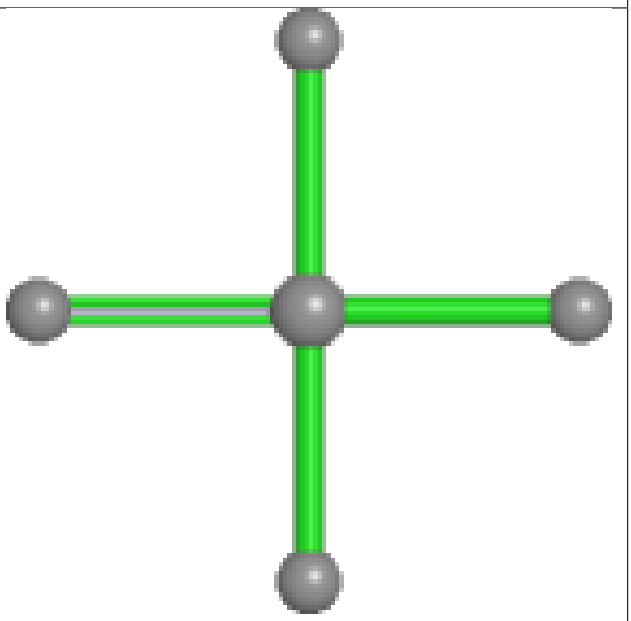


Rings

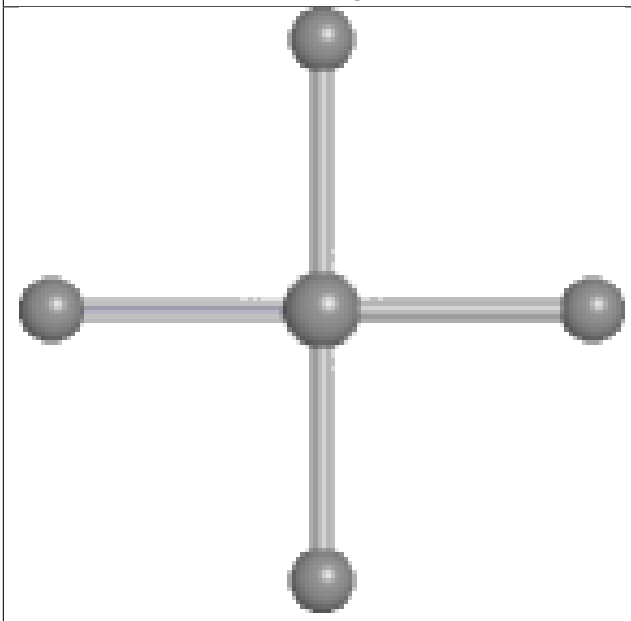
Ligand SO4 B 403



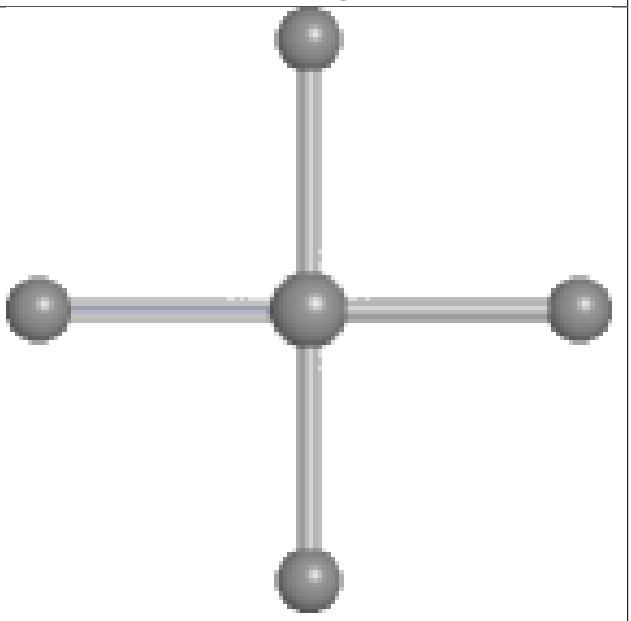
Bond lengths



Bond angles

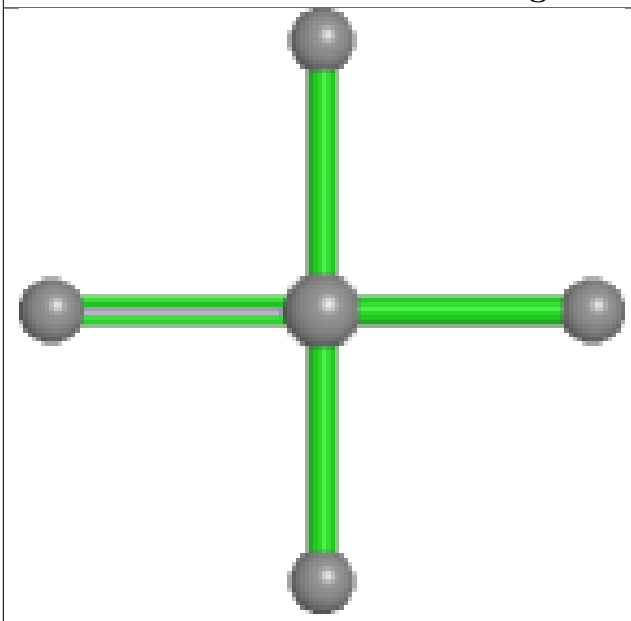


Torsions

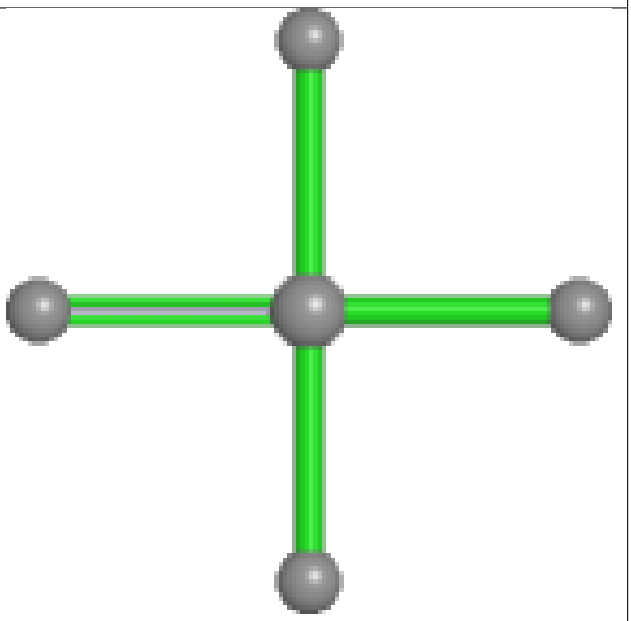


Rings

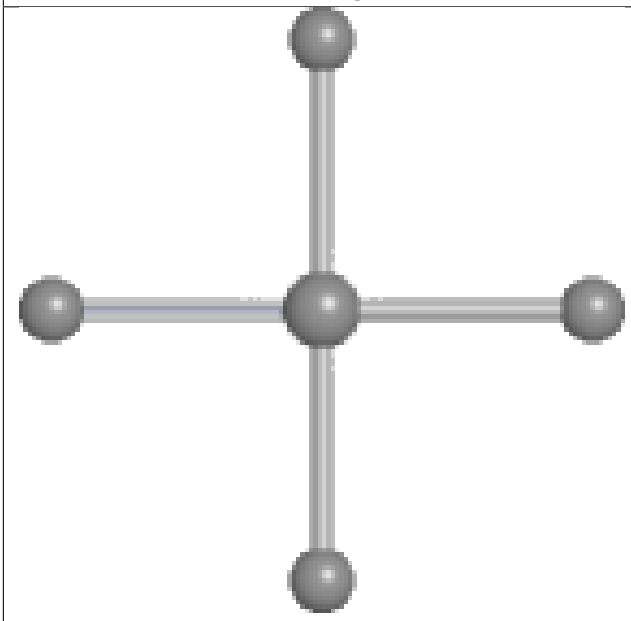
Ligand SO4 B 404



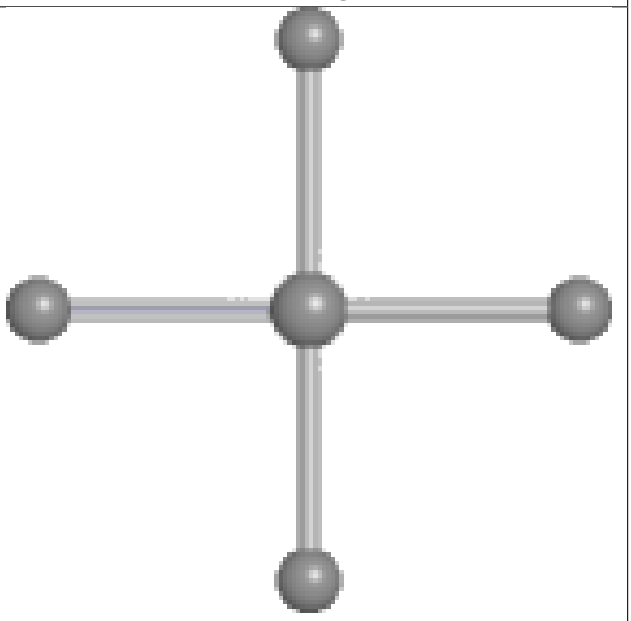
Bond lengths



Bond angles

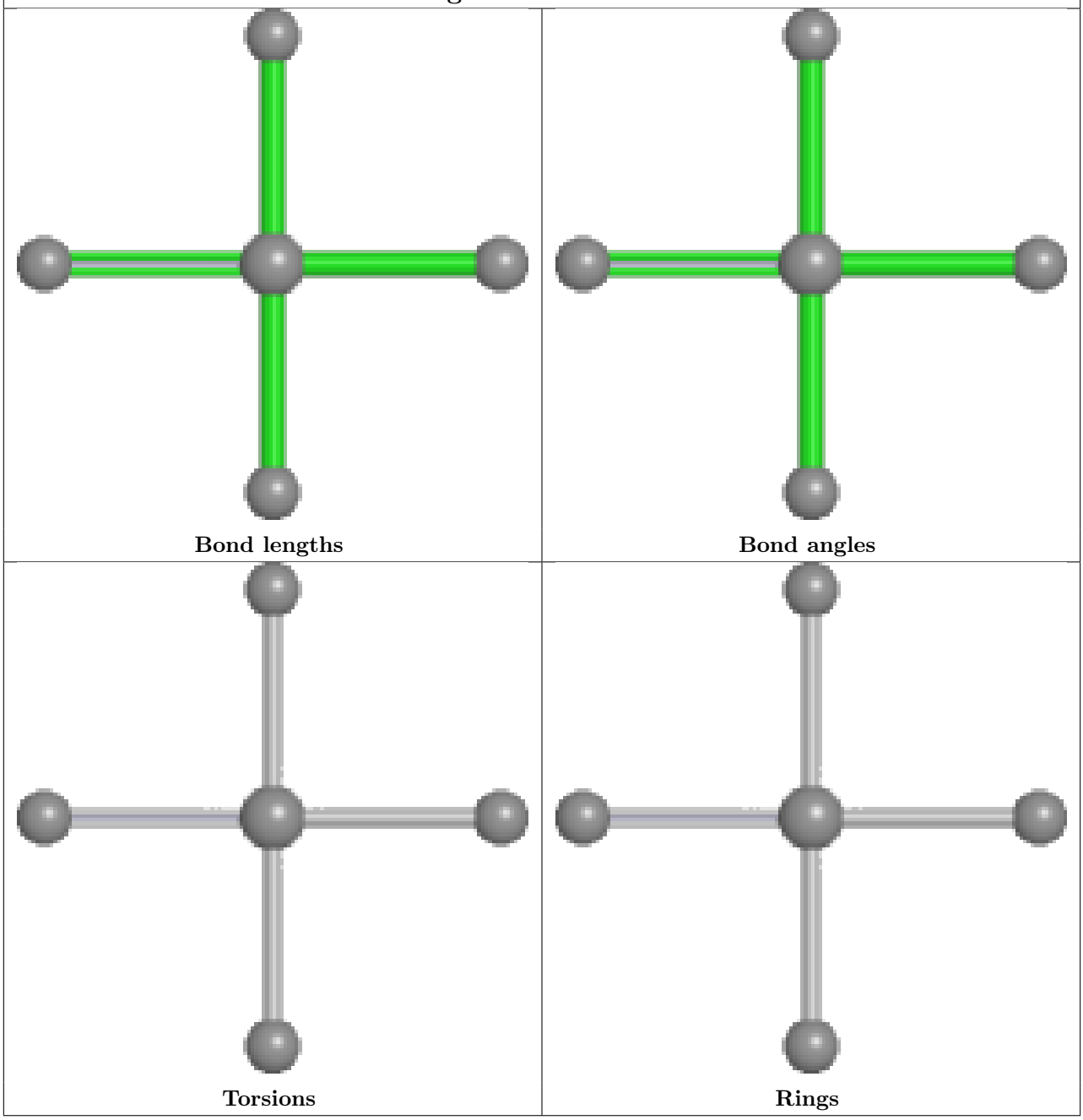


Torsions



Rings

Ligand SO4 A 404



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	327/338 (96%)	0.98	48 (14%) 6 5	26, 45, 71, 83	0
1	B	325/338 (96%)	2.08	117 (36%) 1 1	28, 45, 124, 146	0
1	C	327/338 (96%)	0.73	30 (9%) 14 13	30, 41, 60, 75	0
All	All	979/1014 (96%)	1.26	195 (19%) 3 2	26, 44, 113, 146	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	ALA	11.4
1	B	333	ALA	10.8
1	B	286	PRO	9.1
1	B	281	LEU	8.8
1	B	331	VAL	8.8
1	B	296	LEU	8.4
1	B	294	VAL	8.3
1	B	304	ALA	8.2
1	B	226	LEU	7.7
1	B	302	VAL	7.6
1	B	324	ILE	7.5
1	B	328	LEU	7.4
1	B	318	ALA	7.4
1	B	292	ILE	7.3
1	B	310	ILE	7.3
1	B	316	ALA	7.2
1	B	293	ALA	7.2
1	B	266	LEU	7.2
1	B	320	LEU	7.2
1	B	309	VAL	7.1
1	B	332	ASP	7.1
1	B	323	ALA	7.0
1	B	307	ALA	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	313	TYR	6.7
1	B	330	ARG	6.7
1	B	322	ALA	6.7
1	B	277	VAL	6.7
1	B	231	VAL	6.6
1	B	236	VAL	6.6
1	B	255	VAL	6.6
1	B	314	ALA	6.5
1	B	303	PRO	6.3
1	C	9	PRO	6.3
1	B	232	VAL	6.2
1	B	267	ALA	5.9
1	B	287	VAL	5.9
1	B	280	SER	5.9
1	B	248	TRP	5.8
1	B	268	VAL	5.8
1	C	335	ALA	5.7
1	B	334	GLN	5.6
1	B	279	PHE	5.6
1	B	295	ALA	5.6
1	B	300	GLY	5.5
1	A	9	PRO	5.4
1	B	305	ALA	5.3
1	A	255	VAL	5.3
1	B	278	LYS	5.2
1	A	253	ASN	5.2
1	B	227	HIS	5.2
1	B	282	ARG	5.2
1	B	288	SER	5.2
1	B	283	SER	5.1
1	B	326	ALA	5.1
1	B	273	TYR	5.1
1	B	289	ALA	5.0
1	B	234	THR	4.7
1	B	229	GLY	4.7
1	A	8	THR	4.7
1	B	317	ARG	4.6
1	B	269	MET	4.5
1	B	306	GLY	4.5
1	B	284	ARG	4.5
1	B	233	GLN	4.5
1	B	285	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	299	GLY	4.4
1	A	228	GLY	4.4
1	B	311	SER	4.2
1	C	254	TYR	4.2
1	B	270	ALA	4.2
1	B	258	LEU	4.1
1	A	252	GLU	4.1
1	B	264	ALA	4.1
1	B	271	LYS	4.0
1	B	308	THR	3.9
1	B	276	ARG	3.9
1	B	274	GLY	3.9
1	B	257	MET	3.9
1	B	241	LEU	3.9
1	B	301	HIS	3.8
1	B	261	ALA	3.8
1	B	251	VAL	3.8
1	A	273	TYR	3.8
1	C	113	ASP	3.8
1	B	224	GLU	3.8
1	A	249	GLU	3.7
1	B	263	GLY	3.7
1	C	83	GLU	3.6
1	C	333	ALA	3.6
1	B	223	LEU	3.6
1	B	222	LYS	3.6
1	B	225	PHE	3.6
1	B	291	ASN	3.6
1	A	329	ALA	3.6
1	B	228	GLY	3.6
1	B	256	SER	3.5
1	A	251	VAL	3.5
1	C	253	ASN	3.5
1	B	297	GLY	3.4
1	B	272	ASP	3.4
1	A	206	ARG	3.4
1	A	223	LEU	3.4
1	B	327	GLU	3.3
1	B	230	ARG	3.2
1	B	243	ARG	3.2
1	B	246	ALA	3.2
1	B	319	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	226	LEU	3.1
1	A	187	CYS	3.1
1	B	247	THR	3.1
1	C	183	GLU	3.0
1	C	249	GLU	3.0
1	B	235	ARG	3.0
1	B	315	GLU	3.0
1	B	298	GLY	2.9
1	A	334	GLN	2.9
1	B	265	GLN	2.9
1	A	256	SER	2.9
1	B	206	ARG	2.9
1	B	254	TYR	2.9
1	B	312	SER	2.8
1	A	257	MET	2.8
1	B	242	ALA	2.8
1	B	98	ASN	2.8
1	B	290	GLN	2.8
1	B	321	ASP	2.8
1	C	273	TYR	2.8
1	C	206	ARG	2.7
1	A	333	ALA	2.7
1	A	220	LEU	2.7
1	A	76	GLY	2.7
1	A	225	PHE	2.7
1	A	284	ARG	2.7
1	B	220	LEU	2.7
1	C	198	ILE	2.7
1	C	87	GLN	2.6
1	C	274	GLY	2.6
1	C	329	ALA	2.6
1	A	254	TYR	2.6
1	A	75	PRO	2.6
1	B	219	VAL	2.6
1	A	245	GLY	2.6
1	B	24	ALA	2.5
1	A	239	GLU	2.5
1	B	221	GLY	2.5
1	A	259	ARG	2.5
1	B	113	ASP	2.4
1	A	246	ALA	2.4
1	B	240	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	36	ASN	2.4
1	A	213	TYR	2.4
1	C	11	TYR	2.4
1	A	324	ILE	2.4
1	C	256	SER	2.4
1	B	259	ARG	2.4
1	A	238	GLU	2.4
1	C	252	GLU	2.4
1	A	10	ASP	2.4
1	B	325	GLU	2.3
1	A	113	ASP	2.3
1	A	314	ALA	2.3
1	C	10	ASP	2.3
1	A	331	VAL	2.3
1	B	253	ASN	2.3
1	B	244	ALA	2.3
1	A	278	LYS	2.3
1	C	331	VAL	2.3
1	A	319	ARG	2.3
1	A	274	GLY	2.3
1	B	252	GLU	2.2
1	A	241	LEU	2.2
1	A	215	LEU	2.2
1	B	215	LEU	2.2
1	C	111	GLN	2.2
1	A	202	ASN	2.2
1	A	198	ILE	2.2
1	B	238	GLU	2.2
1	A	318	ALA	2.2
1	C	82	LEU	2.2
1	C	84	SER	2.2
1	B	213	TYR	2.2
1	A	169	ASN	2.2
1	C	54	THR	2.2
1	A	207	GLN	2.1
1	C	56	GLY	2.1
1	B	237	ASP	2.1
1	A	13	ARG	2.1
1	A	217	ARG	2.1
1	C	330	ARG	2.1
1	A	262	GLU	2.1
1	C	35	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	250	GLN	2.1
1	B	245	GLY	2.1
1	C	109	LEU	2.0
1	C	286	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

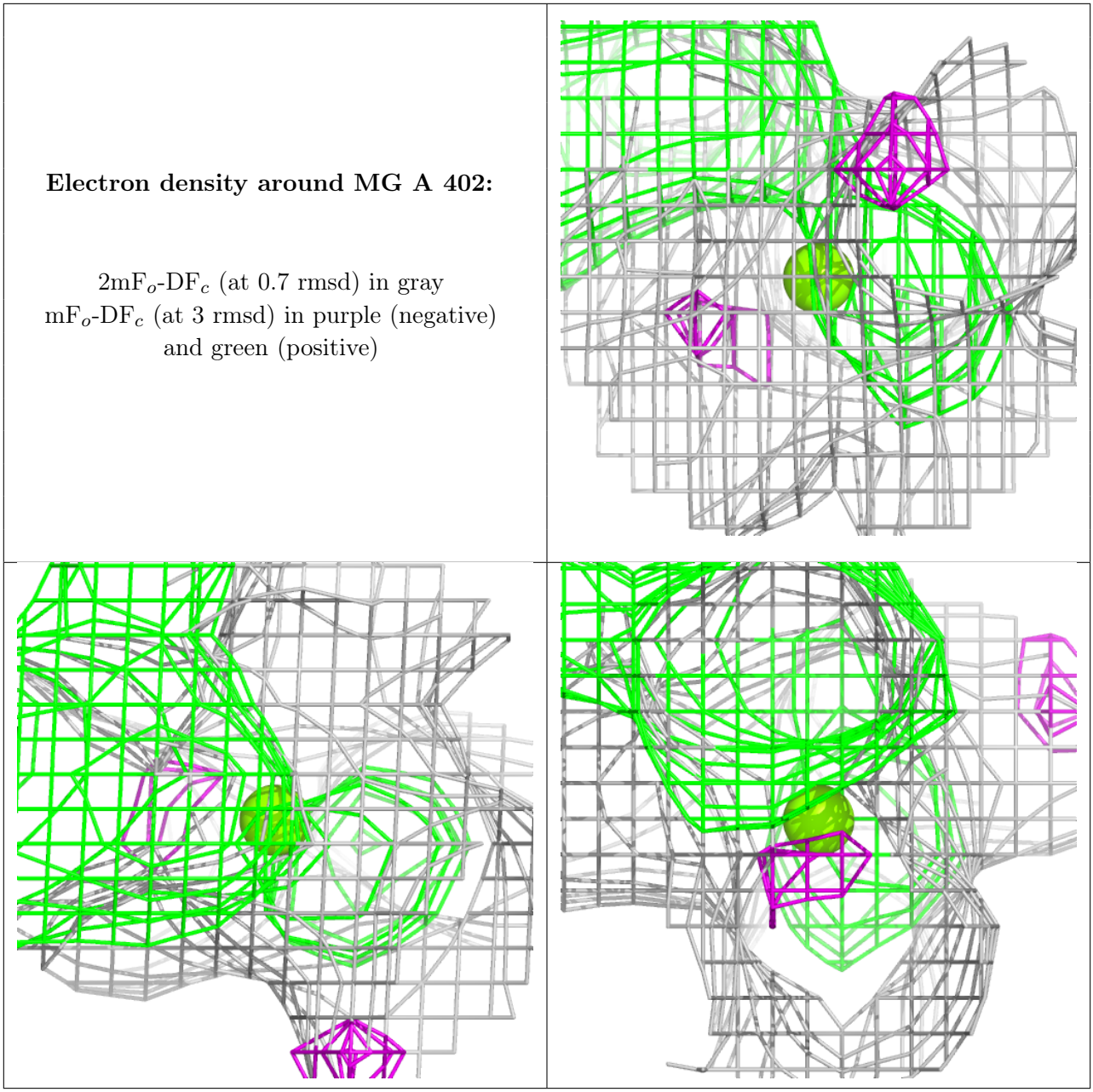
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MG	A	402	1/1	0.82	0.16	39,39,39,39	0
3	SO4	A	403	5/5	0.94	0.29	34,35,35,35	0
2	MG	C	401	1/1	0.95	0.16	25,25,25,25	0
3	SO4	B	404	5/5	0.95	0.27	31,31,31,31	0
3	SO4	A	404	5/5	0.96	0.20	32,32,32,33	0
3	SO4	C	403	5/5	0.96	0.16	31,32,32,32	0
2	MG	B	402	1/1	0.97	0.07	36,36,36,36	0
2	MG	B	401	1/1	0.97	0.12	23,23,23,23	0
3	SO4	B	403	5/5	0.98	0.17	30,30,30,30	0
2	MG	A	401	1/1	0.98	0.26	29,29,29,29	0
2	MG	C	402	1/1	0.98	0.05	34,34,34,34	0

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

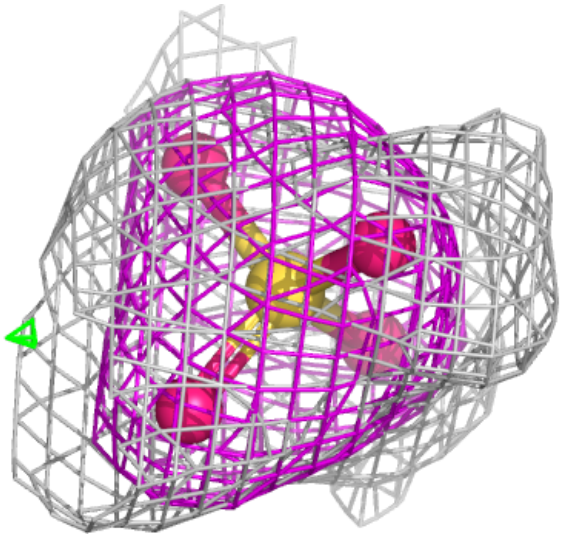
Electron density around MG A 402:

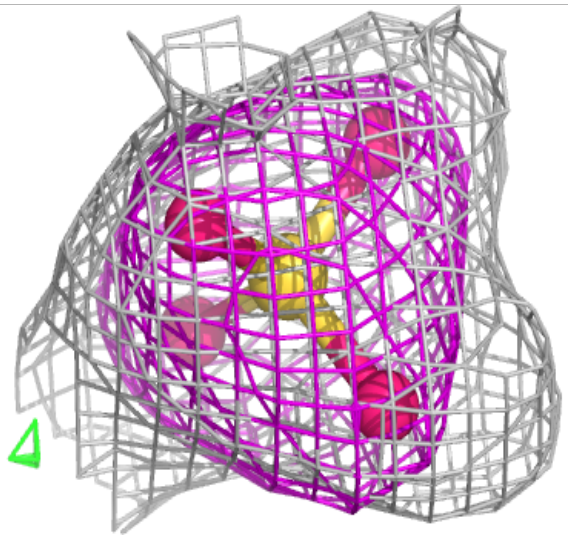
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

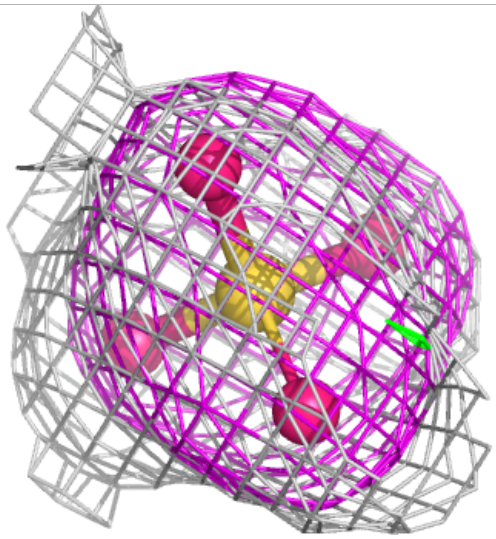


Electron density around SO4 A 403:

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

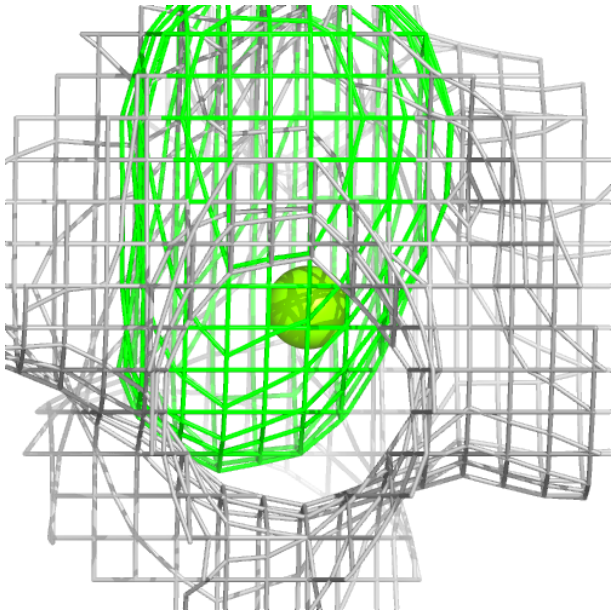


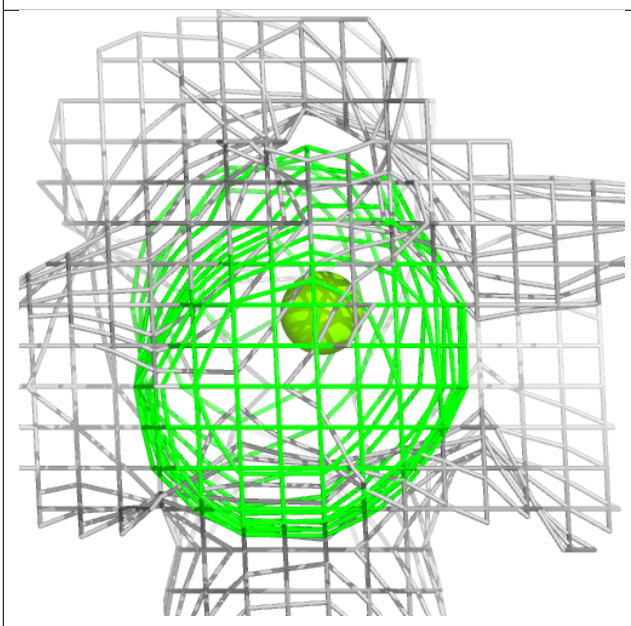


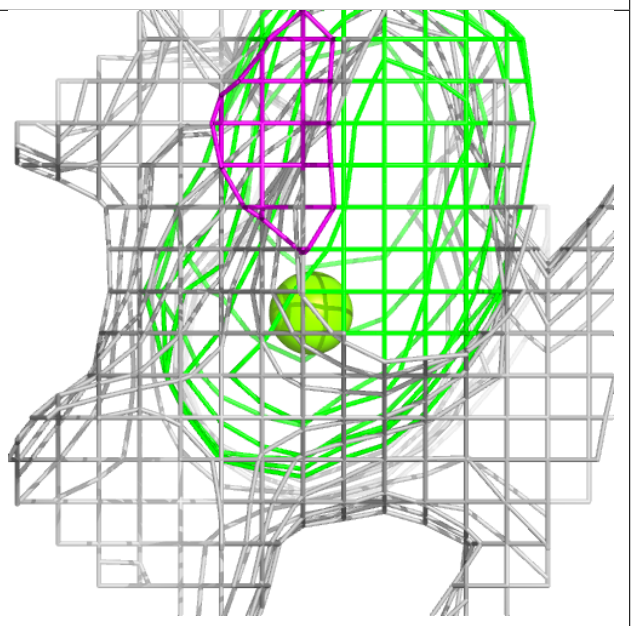


Electron density around MG C 401:

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

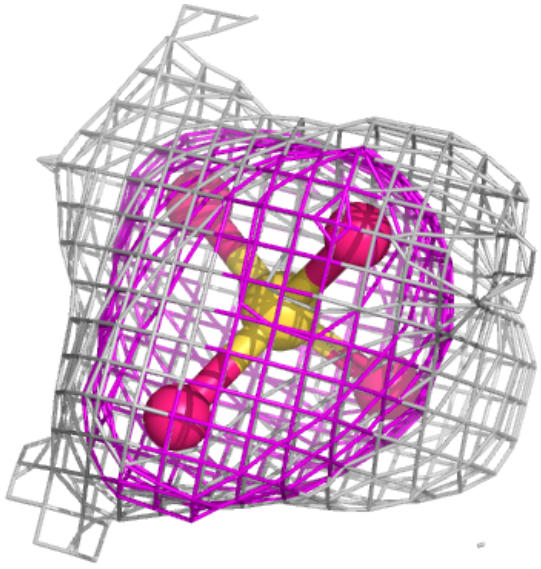


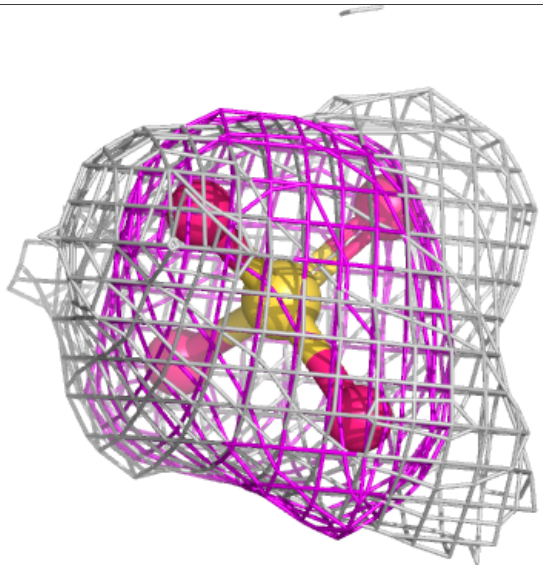


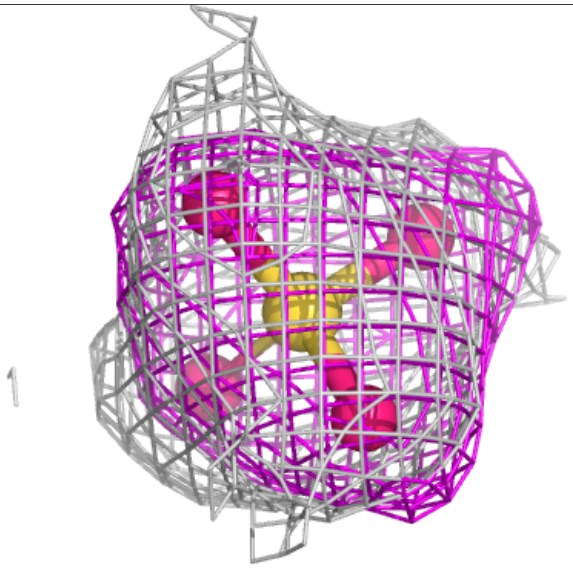


Electron density around SO4 B 404:

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

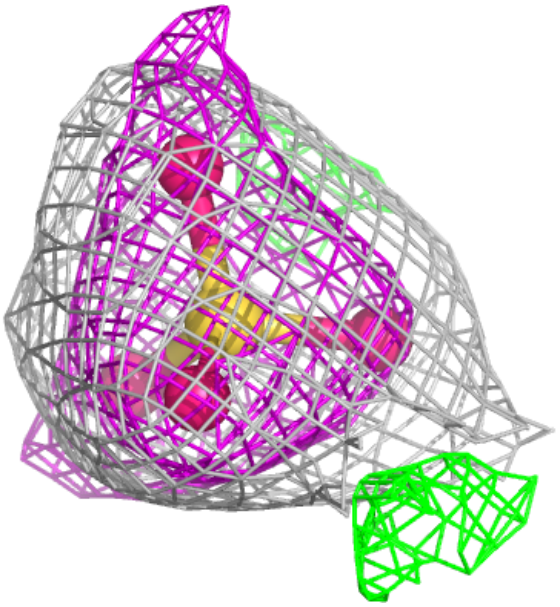


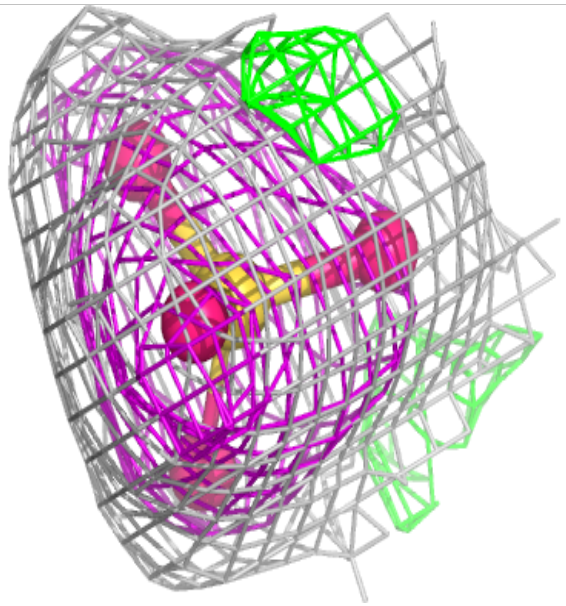


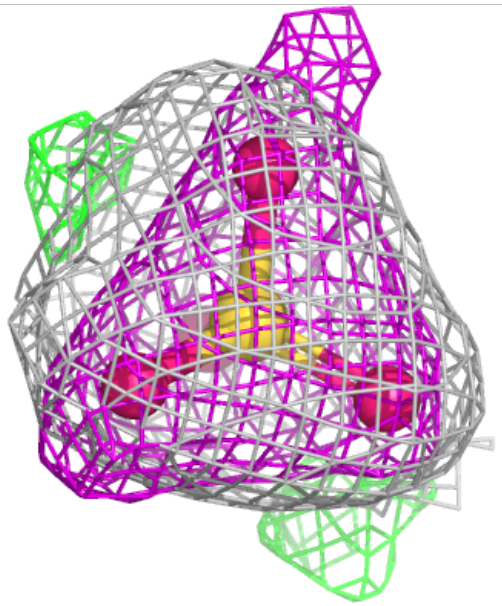


Electron density around SO4 A 404:

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

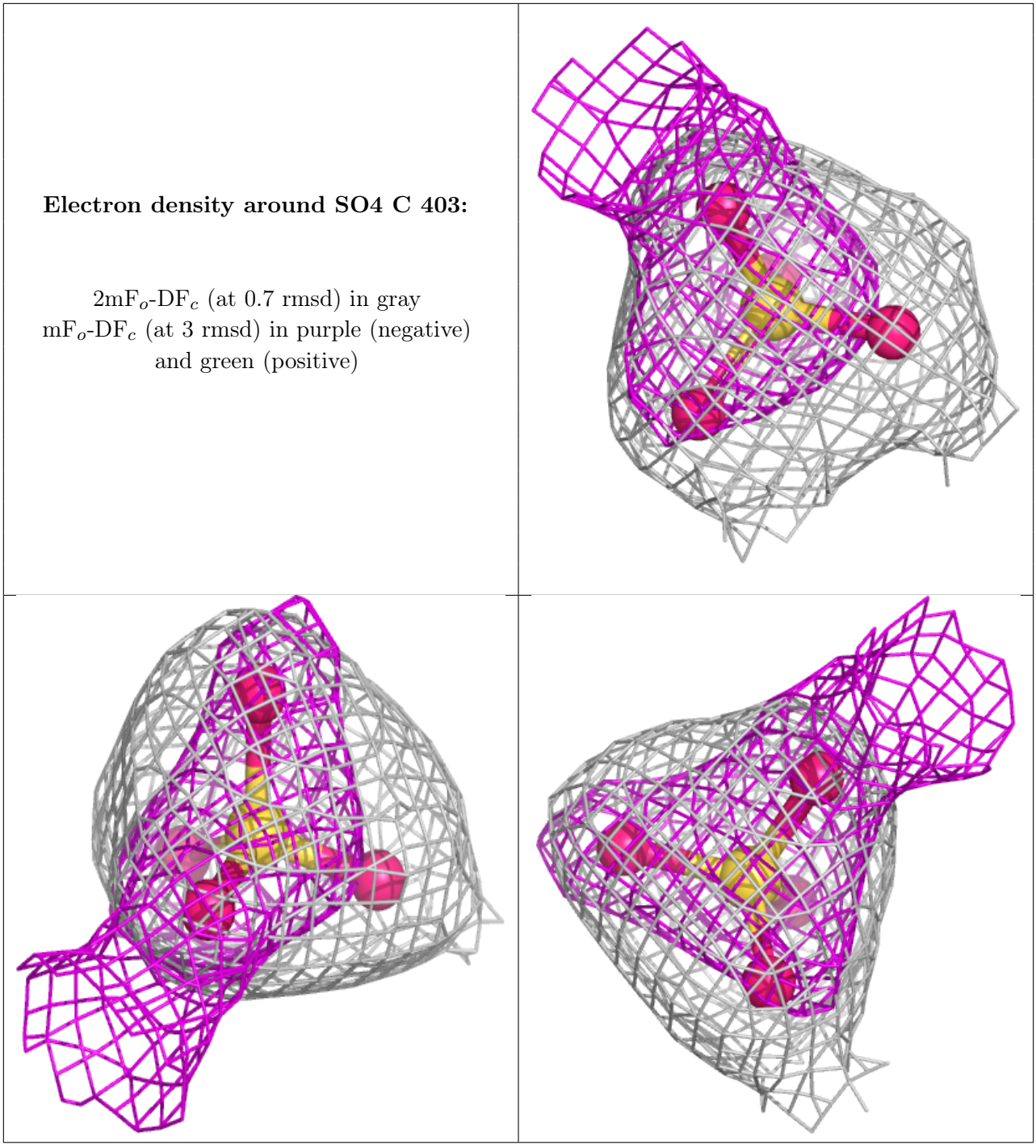






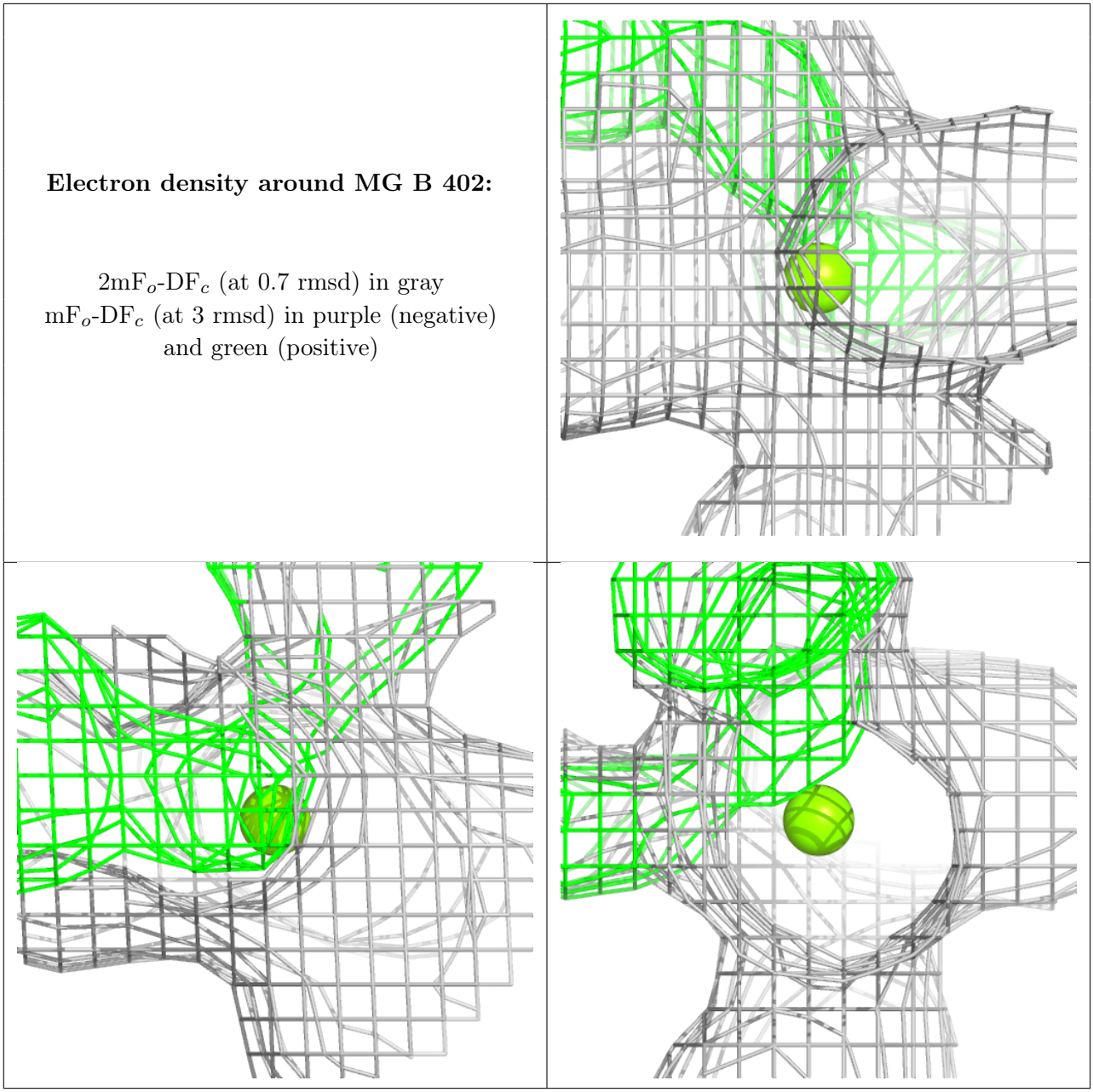
Electron density around SO4 C 403:

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



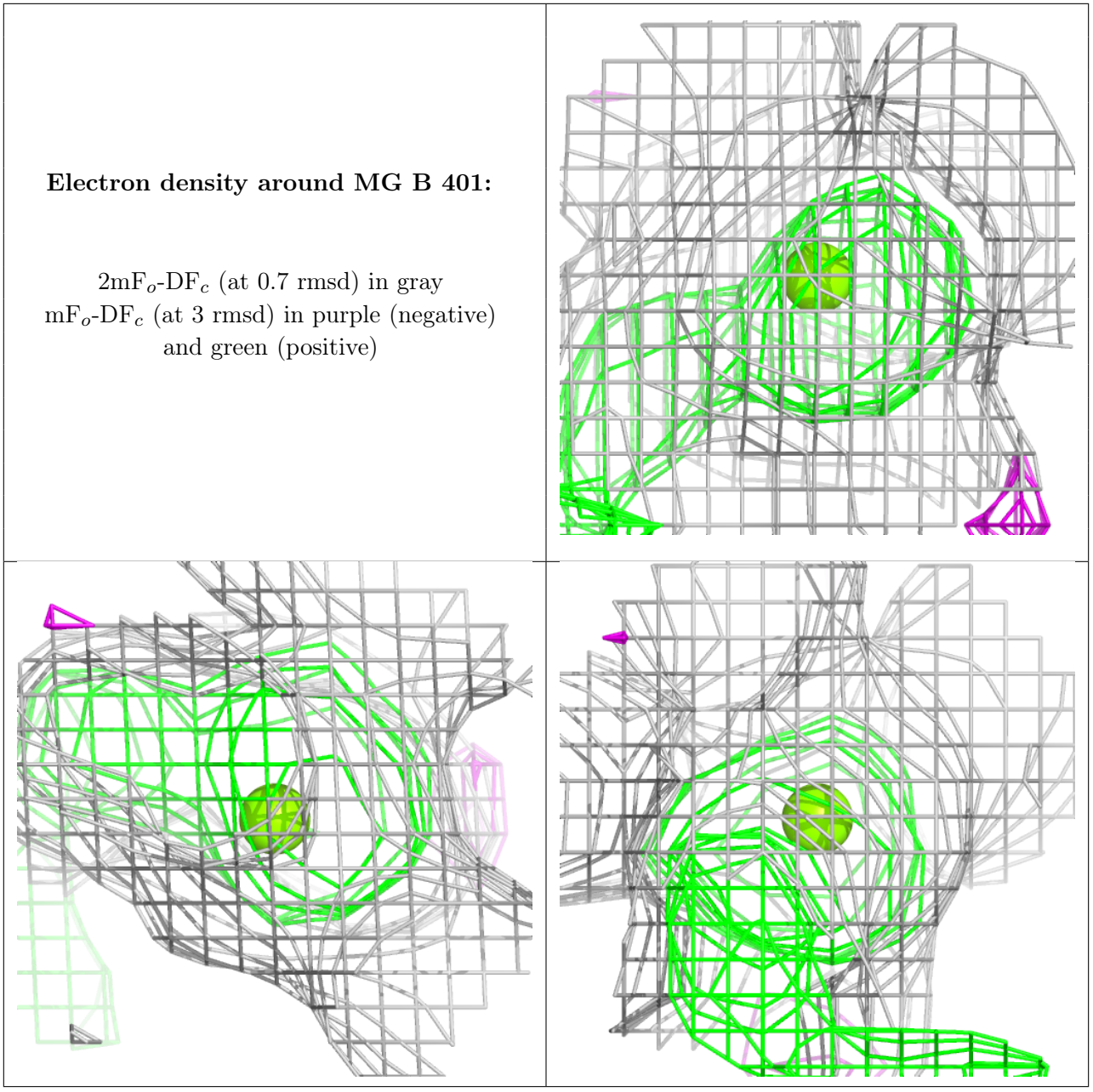
Electron density around MG B 402:

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



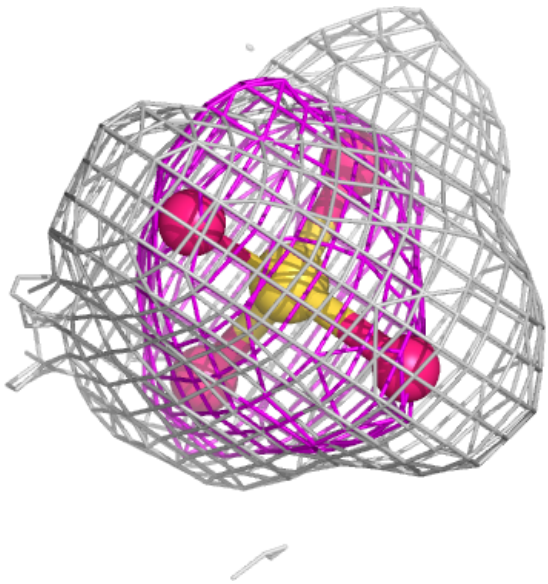
Electron density around MG B 401:

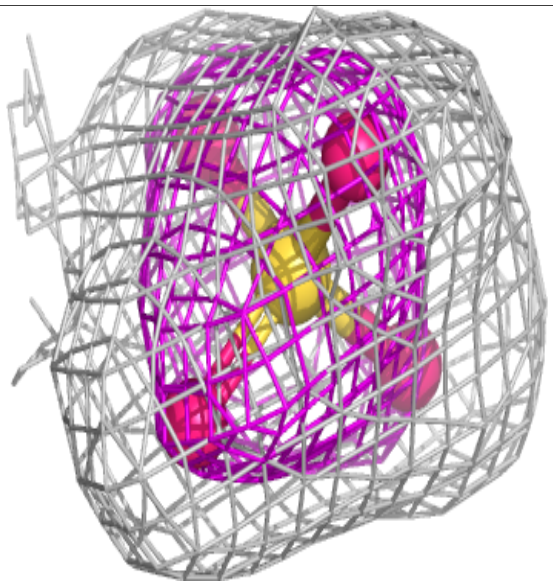
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

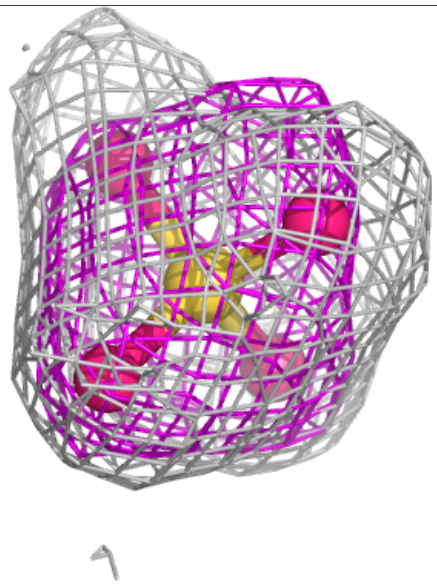


Electron density around SO4 B 403:

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

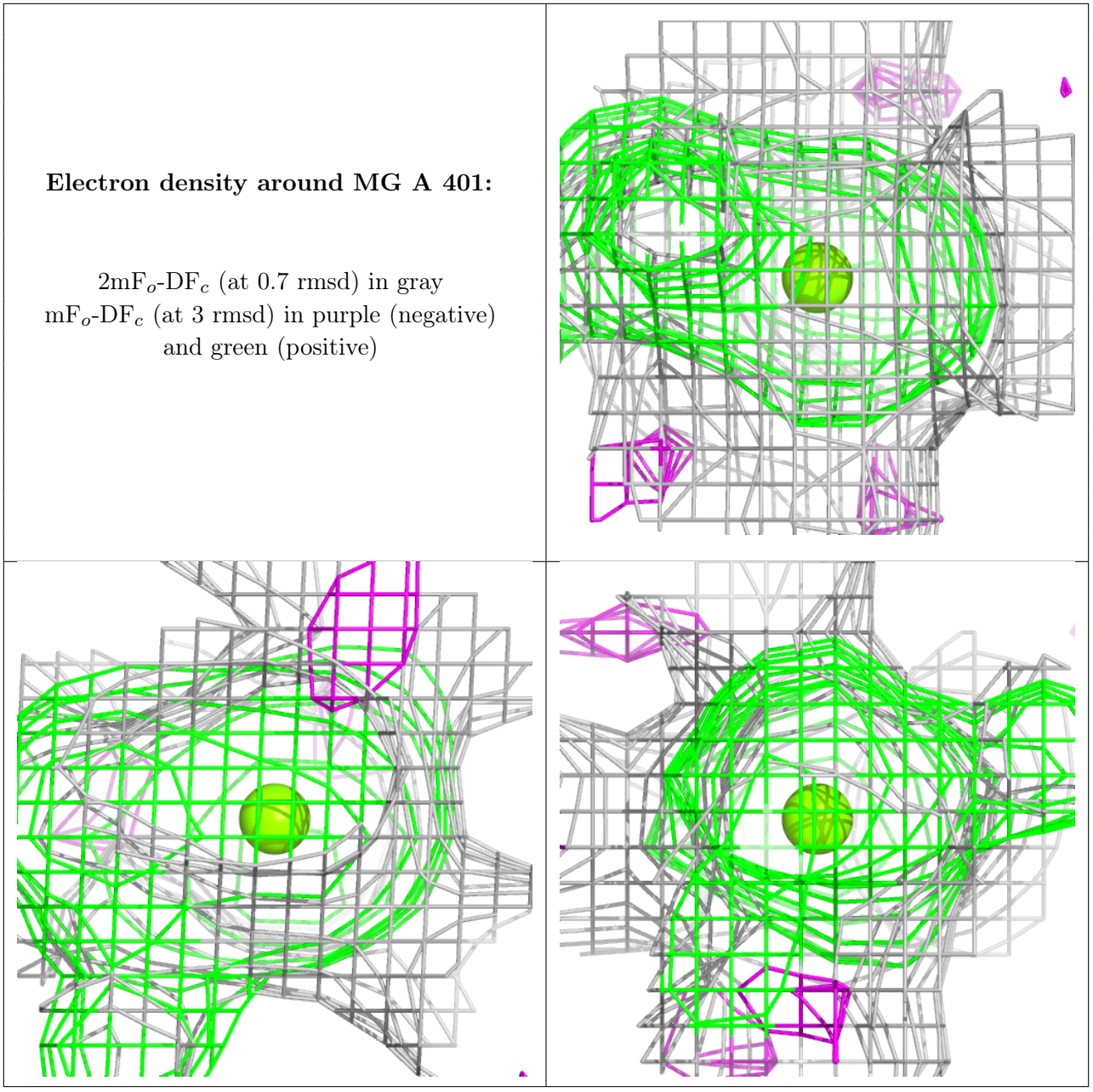






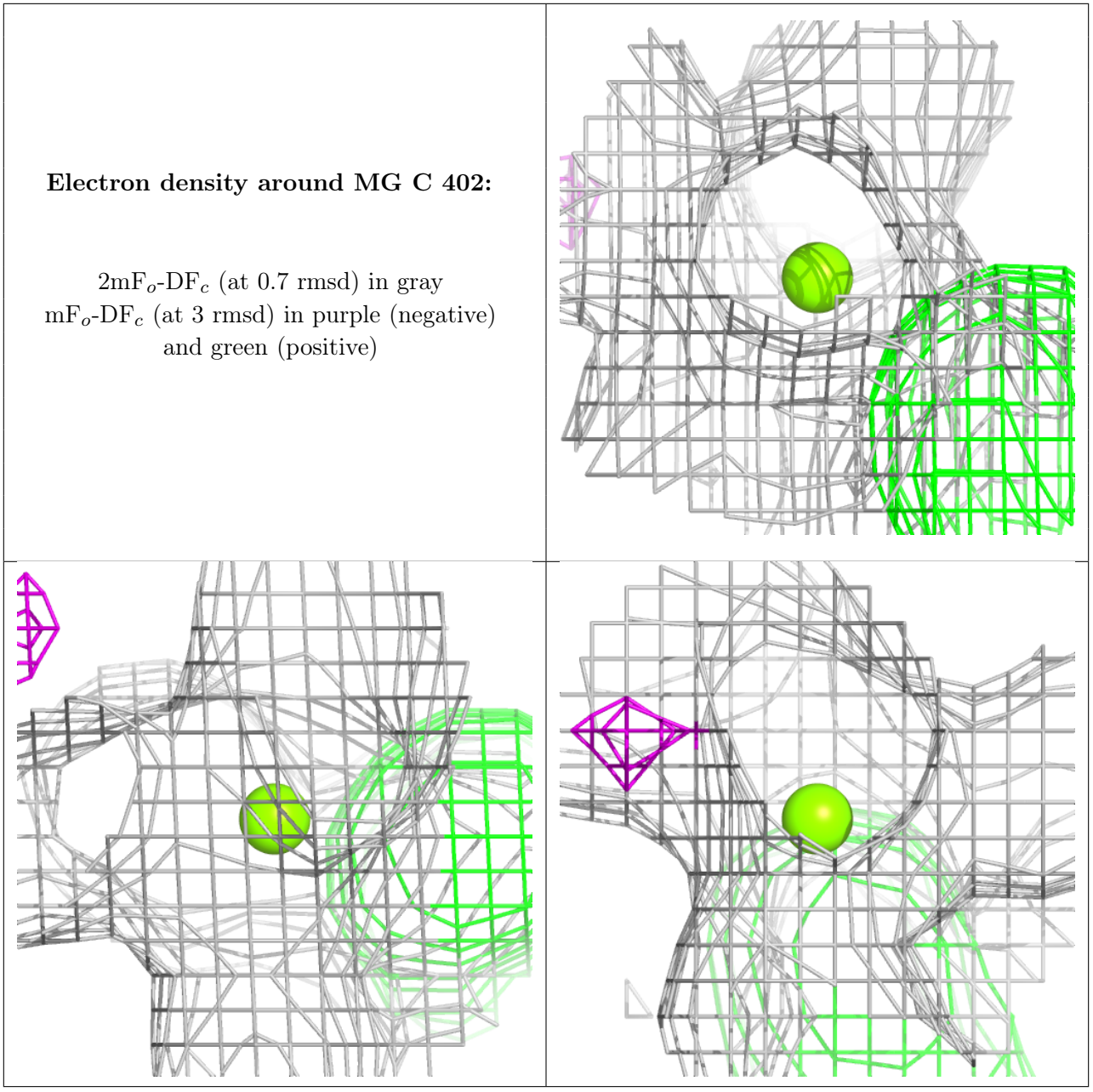
Electron density around MG A 401:

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



Electron density around MG C 402:

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



6.5 Other polymers

There are no such residues in this entry.