Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 11:06 am GMT

PDB ID	:	6SJI
Title	:	The structure of thiocyanate dehydrogenase from Thioalkalivibrio paradoxus mutant with His 482 replaced by Gln
Authors	:	Polyakov, K.M.; Tikhonova, T.V.; Rakitina, T.V.; Osipov, E.; Popov, V.O.
Deposited on	:	2019-08-13
Resolution	:	1.80 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 ⓘ symbol.

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

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

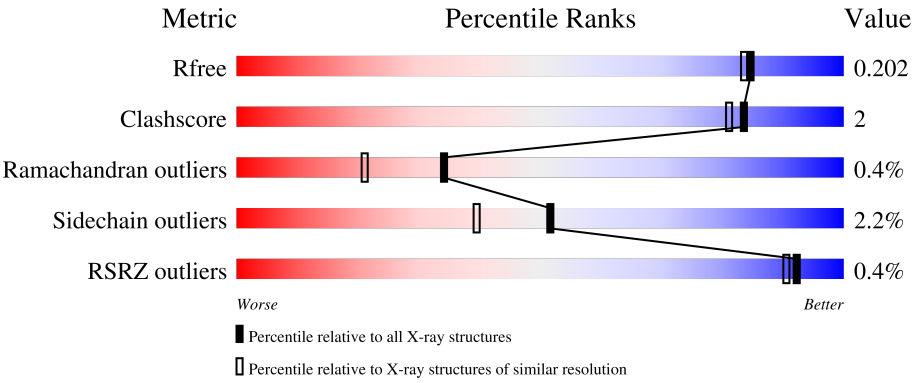
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	470	91% 8%
1	B	470	92% 7%
1	J	470	87% 12%
1	K	470	% 91% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15854 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 thiocyanate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	6	0
			3679	2346	614	699	20			
1	B	467	Total	C	N	O	S	0	4	0
			3651	2329	607	697	18			
1	J	467	Total	C	N	O	S	0	6	0
			3660	2338	607	696	19			
1	K	467	Total	C	N	O	S	0	4	0
			3657	2334	610	695	18			

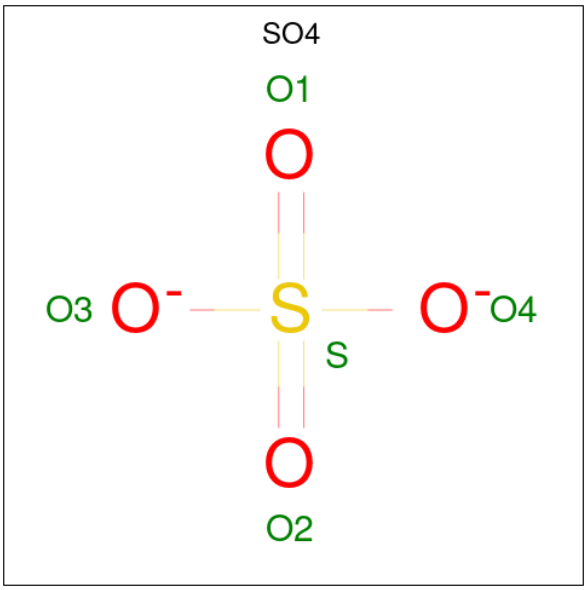
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ALA	-	expression tag	UNP W0DP94
A	80	MET	-	expression tag	UNP W0DP94
A	81	GLY	-	expression tag	UNP W0DP94
A	482	GLN	HIS	conflict	UNP W0DP94
B	79	ALA	-	expression tag	UNP W0DP94
B	80	MET	-	expression tag	UNP W0DP94
B	81	GLY	-	expression tag	UNP W0DP94
B	482	GLN	HIS	conflict	UNP W0DP94
J	79	ALA	-	expression tag	UNP W0DP94
J	80	MET	-	expression tag	UNP W0DP94
J	81	GLY	-	expression tag	UNP W0DP94
J	482	GLN	HIS	conflict	UNP W0DP94
K	79	ALA	-	expression tag	UNP W0DP94
K	80	MET	-	expression tag	UNP W0DP94
K	81	GLY	-	expression tag	UNP W0DP94
K	482	GLN	HIS	conflict	UNP W0DP94

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	J	2	Total Cu 2 2	0	0
2	K	3	Total Cu 3 3	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	A	1	Total O S 5 4 1	0	0
3	K	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	298	Total O 298 298	0	0
4	B	314	Total O 314 314	0	0

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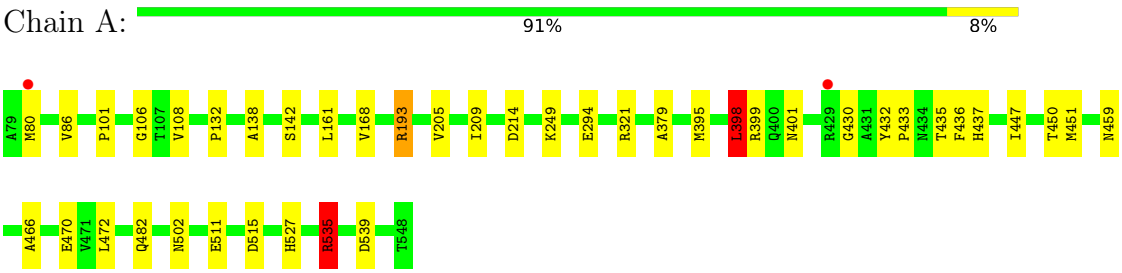
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	284	Total O 284 284	0	0
4	K	287	Total O 287 287	0	0

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.

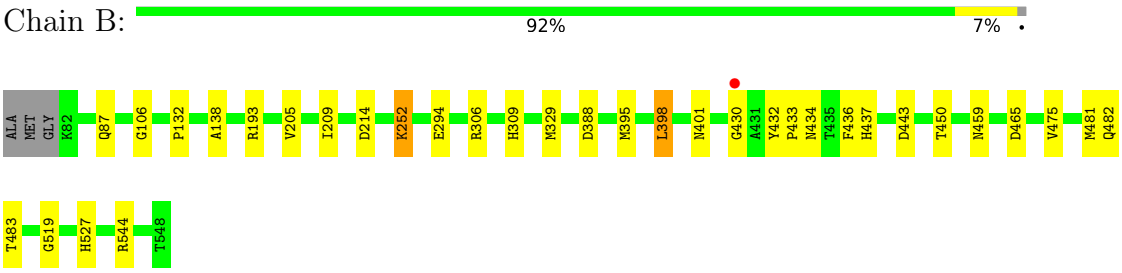
- Molecule 1: thiocyanate dehydrogenase

Chain A:



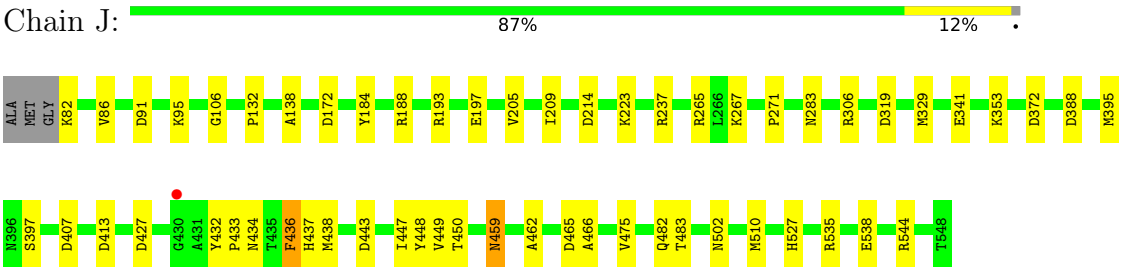
- Molecule 1: thiocyanate dehydrogenase

Chain B:



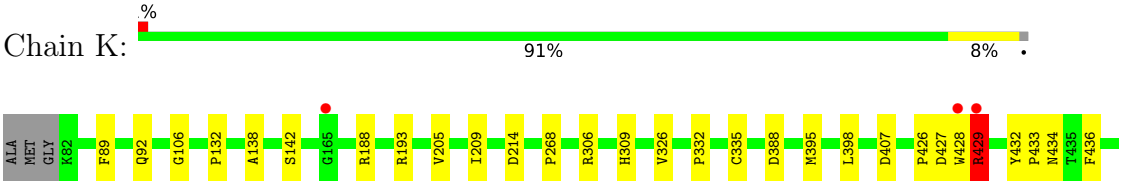
- Molecule 1: thiocyanate dehydrogenase

Chain J:



- Molecule 1: thiocyanate dehydrogenase

Chain K:




D443
T450
M459
D465
M481
Q482
G519
H527
R536
T548

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.08Å 160.41Å 90.88Å 90.00° 98.11° 90.00°	Depositor
Resolution (Å)	89.97 – 1.80 89.97 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (89.97-1.80) 96.3 (89.97-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0158 2016/10/03	Depositor
R, R_{free}	0.159 , 0.198 0.164 , 0.202	Depositor DCC
R_{free} test set	8761 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15854	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, 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	1.00	0/3808	1.02	13/5193 (0.3%)
1	B	1.03	0/3773	0.97	10/5148 (0.2%)
1	J	1.00	2/3789 (0.1%)	1.04	20/5169 (0.4%)
1	K	1.04	0/3778	1.01	10/5155 (0.2%)
All	All	1.02	2/15148 (0.0%)	1.01	53/20665 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	538	GLU	CD-OE1	6.42	1.32	1.25
1	J	184	TYR	CG-CD1	5.58	1.46	1.39

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	193	ARG	NE-CZ-NH1	13.37	126.98	120.30
1	K	535	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	A	535	ARG	NE-CZ-NH1	-9.88	115.36	120.30
1	J	214	ASP	CB-CG-OD1	9.26	126.64	118.30
1	B	388	ASP	CB-CG-OD1	8.84	126.25	118.30
1	K	188	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	K	443	ASP	CB-CG-OD1	8.25	125.73	118.30
1	J	193	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	535	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	A	398	LEU	CA-CB-CG	7.50	132.55	115.30
1	A	399	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	K	429	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	J	407	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	443	ASP	CB-CG-OD1	6.59	124.23	118.30
1	K	214	ASP	CB-CG-OD1	6.56	124.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	399	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	J	544	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	J	319	ASP	CB-CG-OD1	6.47	124.13	118.30
1	J	544	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	A	214	ASP	CB-CG-OD1	6.36	124.03	118.30
1	J	319	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	472	LEU	CA-CB-CG	6.33	129.86	115.30
1	J	306	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	193[A]	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	A	193[B]	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	J	443	ASP	CB-CG-OD1	6.07	123.76	118.30
1	J	188	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	J	407	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	A	398	LEU	CB-CG-CD2	-6.00	100.80	111.00
1	J	388	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	465	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	B	465	ASP	CB-CG-OD1	5.88	123.60	118.30
1	J	535	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	B	214	ASP	CB-CG-OD1	5.68	123.41	118.30
1	J	329	MET	CG-SD-CE	-5.65	91.15	100.20
1	J	413	ASP	CB-CG-OD1	5.65	123.39	118.30
1	J	535	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	K	465	ASP	CB-CG-OD1	5.59	123.33	118.30
1	J	465	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	544	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	K	193	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	B	544	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	K	193	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	B	193	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	K	388	ASP	CB-CG-OD1	5.27	123.05	118.30
1	A	539	ASP	CB-CG-OD1	5.27	123.04	118.30
1	J	91	ASP	CB-CG-OD1	5.18	122.96	118.30
1	K	407	ASP	CB-CG-OD1	5.11	122.89	118.30
1	B	306	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	A	321	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	J	237	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	329	MET	CB-CG-SD	-5.05	97.25	112.40
1	A	535	ARG	CG-CD-NE	-5.03	101.23	111.80

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	3679	0	3566	18	0
1	B	3651	0	3531	19	0
1	J	3660	0	3545	19	0
1	K	3657	0	3541	15	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	J	2	0	0	0	0
2	K	3	0	0	0	0
3	A	10	0	0	0	0
3	K	5	0	0	0	0
4	A	298	0	0	1	0
4	B	314	0	0	1	0
4	J	284	0	0	1	0
4	K	287	0	0	2	0
All	All	15854	0	14183	69	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 (69) 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:J:197[B]:GLU:OE2	4:J:701:HOH:O	1.58	1.19
1:A:435:THR:HG22	1:A:451[A]:MET:HE1	1.49	0.93
1:A:294:GLU:HB2	1:A:398:LEU:HD21	1.51	0.90
1:J:434:ASN:HD22	1:J:436:PHE:HD1	1.26	0.81
1:J:450:THR:HG21	1:J:482:GLN:O	1.82	0.80
1:A:435:THR:CG2	1:A:451[A]:MET:HE1	2.16	0.75
1:A:450[B]:THR:HG21	1:A:482:GLN:O	1.89	0.73
1:B:450[A]:THR:HG21	1:B:482:GLN:O	1.91	0.70
1:K:306[B]:ARG:HG3	1:K:306[B]:ARG:HH11	1.63	0.62
1:K:450:THR:HG21	1:K:482:GLN:O	1.97	0.62
1:B:294:GLU:HB2	1:B:398:LEU:CD2	2.28	0.62
1:B:437:HIS:HB2	1:B:450[A]:THR:CG2	2.31	0.60
1:A:401[A]:ASN:ND2	1:A:430:GLY:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ALA:HB3	1:A:398:LEU:HG	1.83	0.59
1:J:434:ASN:ND2	1:J:436:PHE:HD1	1.97	0.59
1:K:535:ARG:HD3	4:K:781:HOH:O	2.02	0.58
1:A:294:GLU:HB2	1:A:398:LEU:CD2	2.31	0.57
1:A:86:VAL:HG12	1:B:519:GLY:HA3	1.86	0.56
1:K:426:PRO:O	1:K:429:ARG:HD3	2.06	0.56
1:K:106:GLY:HA2	1:K:132:PRO:O	2.07	0.55
1:A:436:PHE:HD2	1:A:437:HIS:CD2	2.25	0.55
1:B:434:ASN:HD22	1:B:436:PHE:HD1	1.54	0.54
1:B:437:HIS:HB2	1:B:450[A]:THR:HG21	1.89	0.53
1:J:265:ARG:HD2	1:J:267:LYS:HE2	1.91	0.53
1:J:449[A]:VAL:HG23	1:J:462:ALA:HB3	1.91	0.53
1:B:294:GLU:HB2	1:B:398:LEU:HD23	1.90	0.52
1:J:459:ASN:HD22	1:J:459:ASN:N	2.08	0.52
1:J:436:PHE:HD2	1:J:437:HIS:CD2	2.28	0.51
1:A:101:PRO:HA	1:A:108[B]:VAL:HG22	1.94	0.49
1:A:106:GLY:HA2	1:A:132:PRO:O	2.13	0.49
1:A:432:TYR:HA	1:A:433:PRO:C	2.33	0.49
1:J:436:PHE:CD2	1:J:437:HIS:CD2	3.01	0.48
1:K:459:ASN:HD22	1:K:481:MET:H	1.62	0.48
1:B:436:PHE:HD2	1:B:437:HIS:CD2	2.32	0.47
1:J:432:TYR:HA	1:J:433:PRO:C	2.33	0.47
1:B:138:ALA:HB1	1:B:209:ILE:HG12	1.96	0.47
1:B:459:ASN:HD22	1:B:481:MET:H	1.61	0.47
1:K:434:ASN:HB3	1:K:436:PHE:CZ	2.50	0.47
1:B:252:LYS:HE2	1:B:252:LYS:HB3	1.72	0.46
1:A:447:ILE:HG13	1:A:466:ALA:HB2	1.97	0.46
1:B:401:ASN:HB2	1:B:430:GLY:O	2.16	0.46
1:B:432:TYR:HA	1:B:433:PRO:C	2.34	0.46
4:A:723:HOH:O	1:B:87:GLN:HB2	2.14	0.46
1:B:436:PHE:CD2	1:B:437:HIS:CD2	3.04	0.45
1:J:449[A]:VAL:CG2	1:J:462:ALA:HB3	2.45	0.45
1:J:138:ALA:HB1	1:J:209:ILE:HG12	1.99	0.45
1:K:306[B]:ARG:HG3	1:K:306[B]:ARG:NH1	2.30	0.45
1:A:138:ALA:HB1	1:A:209:ILE:HG12	1.97	0.45
1:B:106:GLY:HA2	1:B:132:PRO:O	2.18	0.44
1:A:436:PHE:CD2	1:A:437:HIS:CD2	3.04	0.44
1:K:138:ALA:HB1	1:K:209:ILE:HG12	2.00	0.43
1:J:106:GLY:HA2	1:J:132:PRO:O	2.18	0.43
1:B:437:HIS:HB2	1:B:450[A]:THR:HG23	1.99	0.43
1:A:511:GLU:O	1:A:515:ASP:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:89:PHE:O	1:K:92:GLN:HG2	2.18	0.42
1:J:95:LYS:HA	1:J:95:LYS:HD2	1.79	0.42
1:B:450[B]:THR:HG23	1:B:481:MET:CG	2.49	0.42
1:J:475:VAL:HG21	1:J:510:MET:CE	2.49	0.42
1:B:309:HIS:CE1	4:B:796:HOH:O	2.73	0.41
1:J:86:VAL:HG12	1:K:519:GLY:HA3	2.02	0.41
1:K:309:HIS:CD2	4:K:726:HOH:O	2.72	0.41
1:A:161:LEU:HG	1:A:168:VAL:HG21	2.01	0.41
1:J:447:ILE:HG13	1:J:466:ALA:HB2	2.02	0.41
1:K:142:SER:O	1:K:535:ARG:HA	2.21	0.41
1:J:223:LYS:HG2	1:J:283:ASN:HD22	1.86	0.41
1:K:432:TYR:HB3	1:K:433:PRO:HA	2.03	0.41
1:A:142:SER:O	1:A:535:ARG:HA	2.22	0.40
1:J:438:MET:HA	1:J:448:TYR:O	2.22	0.40
1:K:326:VAL:CG1	1:K:335:CYS:HB3	2.50	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	474/470 (101%)	446 (94%)	26 (6%)	2 (0%)	34	21
1	B	469/470 (100%)	439 (94%)	29 (6%)	1 (0%)	47	33
1	J	471/470 (100%)	445 (94%)	25 (5%)	1 (0%)	47	33
1	K	469/470 (100%)	443 (94%)	22 (5%)	4 (1%)	17	6
All	All	1883/1880 (100%)	1773 (94%)	102 (5%)	8 (0%)	34	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	MET
1	K	398	LEU
1	K	428	TRP
1	K	205	VAL
1	K	427	ASP
1	A	205	VAL
1	B	205	VAL
1	J	205	VAL

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	399/393 (102%)	389 (98%)	10 (2%)	47 34
1	B	396/393 (101%)	390 (98%)	6 (2%)	65 56
1	J	398/393 (101%)	384 (96%)	14 (4%)	36 21
1	K	396/393 (101%)	391 (99%)	5 (1%)	69 62
All	All	1589/1572 (101%)	1554 (98%)	35 (2%)	52 39

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193[A]	ARG
1	A	193[B]	ARG
1	A	249	LYS
1	A	395	MET
1	A	398	LEU
1	A	459	ASN
1	A	470	GLU
1	A	502	ASN
1	A	527	HIS
1	A	535	ARG
1	B	252	LYS
1	B	395	MET
1	B	398	LEU
1	B	475	VAL

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Mol	Chain	Res	Type
1	B	483	THR
1	B	527	HIS
1	J	82	LYS
1	J	172	ASP
1	J	271	PRO
1	J	341	GLU
1	J	353	LYS
1	J	372	ASP
1	J	395	MET
1	J	397	SER
1	J	427	ASP
1	J	436	PHE
1	J	459	ASN
1	J	483	THR
1	J	502	ASN
1	J	527	HIS
1	K	268	PRO
1	K	332	PRO
1	K	395	MET
1	K	429	ARG
1	K	527	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	ASN
1	A	502	ASN
1	B	313	ASN
1	B	434	ASN
1	B	459	ASN
1	J	283	ASN
1	J	390	GLN
1	J	502	ASN
1	K	126	ASN
1	K	313	ASN
1	K	342	ASN
1	K	434	ASN
1	K	459	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 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	603	-	4,4,4	0.30	0	6,6,6	0.74	0
3	SO4	A	604	-	4,4,4	0.27	0	6,6,6	0.28	0
3	SO4	K	604	-	4,4,4	0.13	0	6,6,6	0.53	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

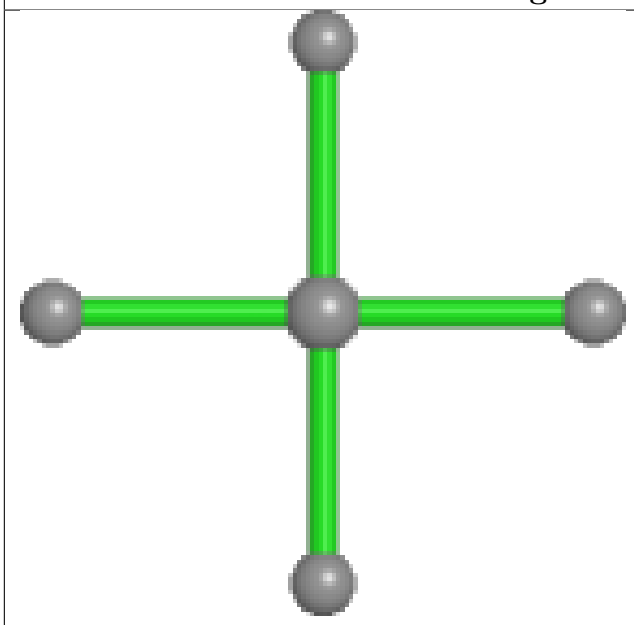
There are no ring outliers.

No monomer is involved in short contacts.

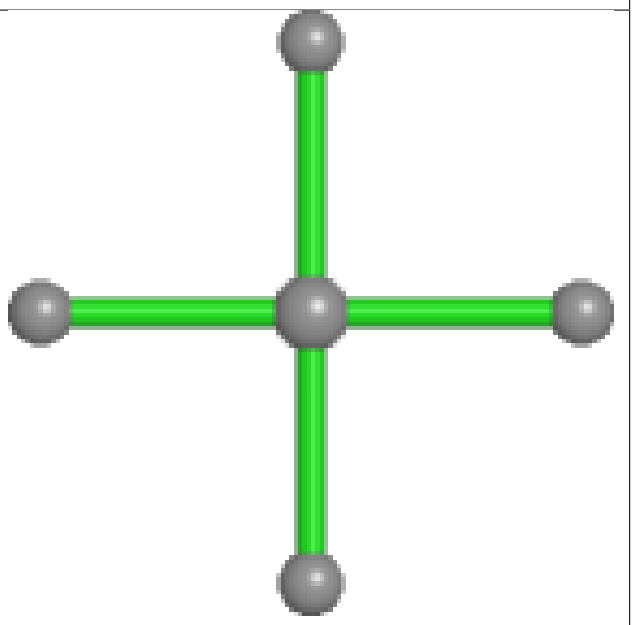
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

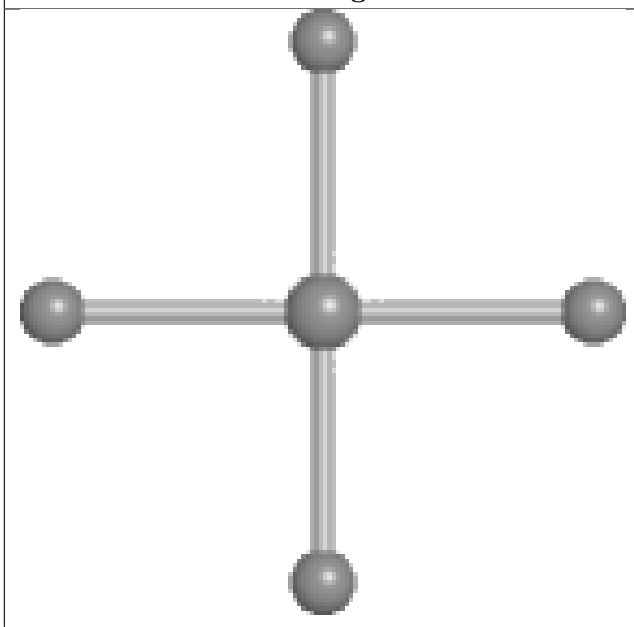
Ligand SO4 A 603



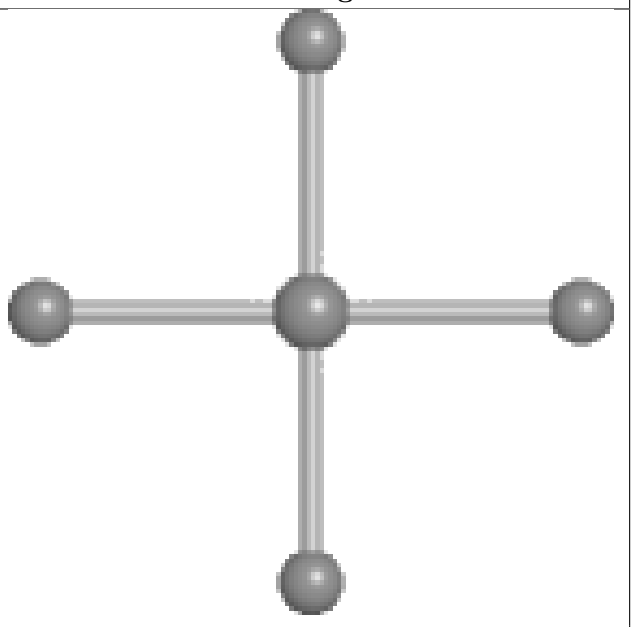
Bond lengths



Bond angles

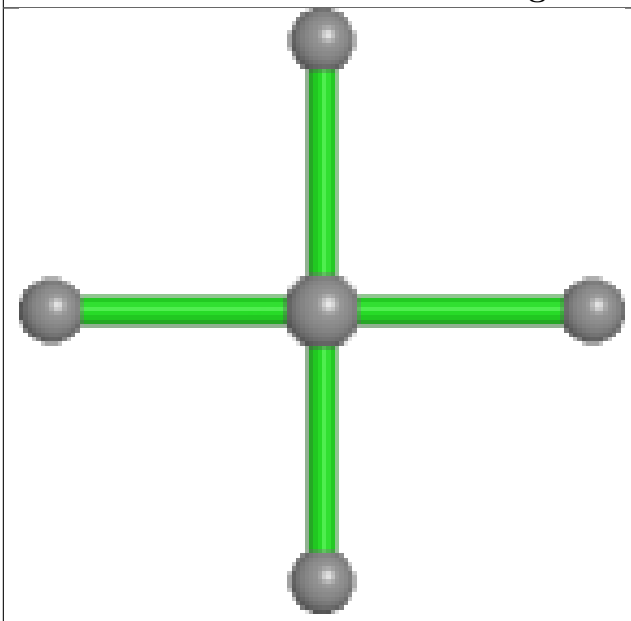


Torsions

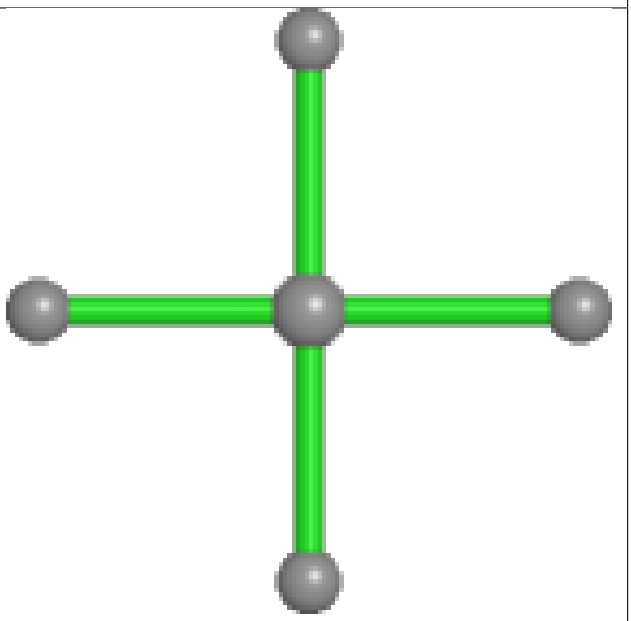


Rings

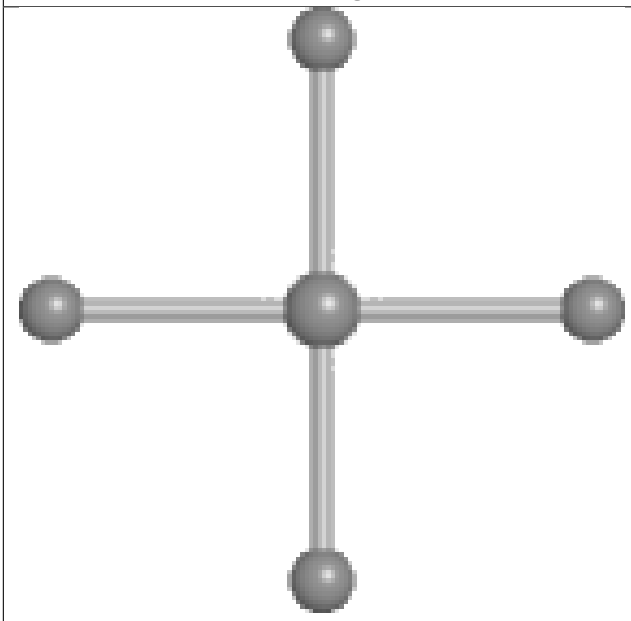
Ligand SO4 A 604



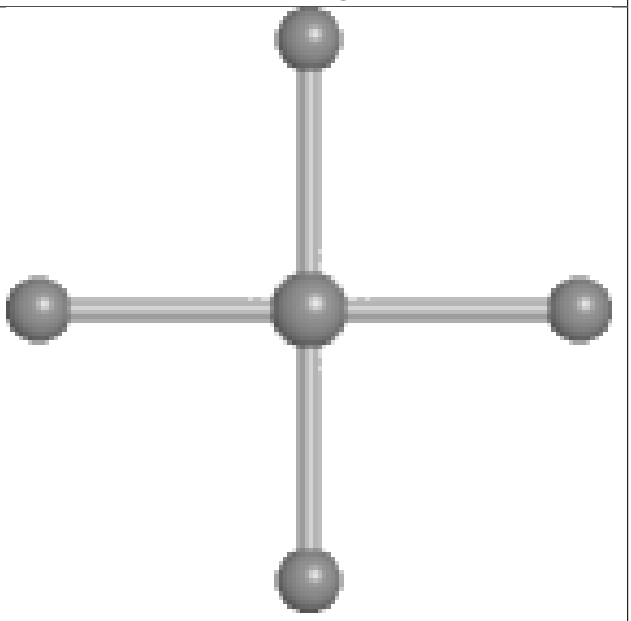
Bond lengths



Bond angles

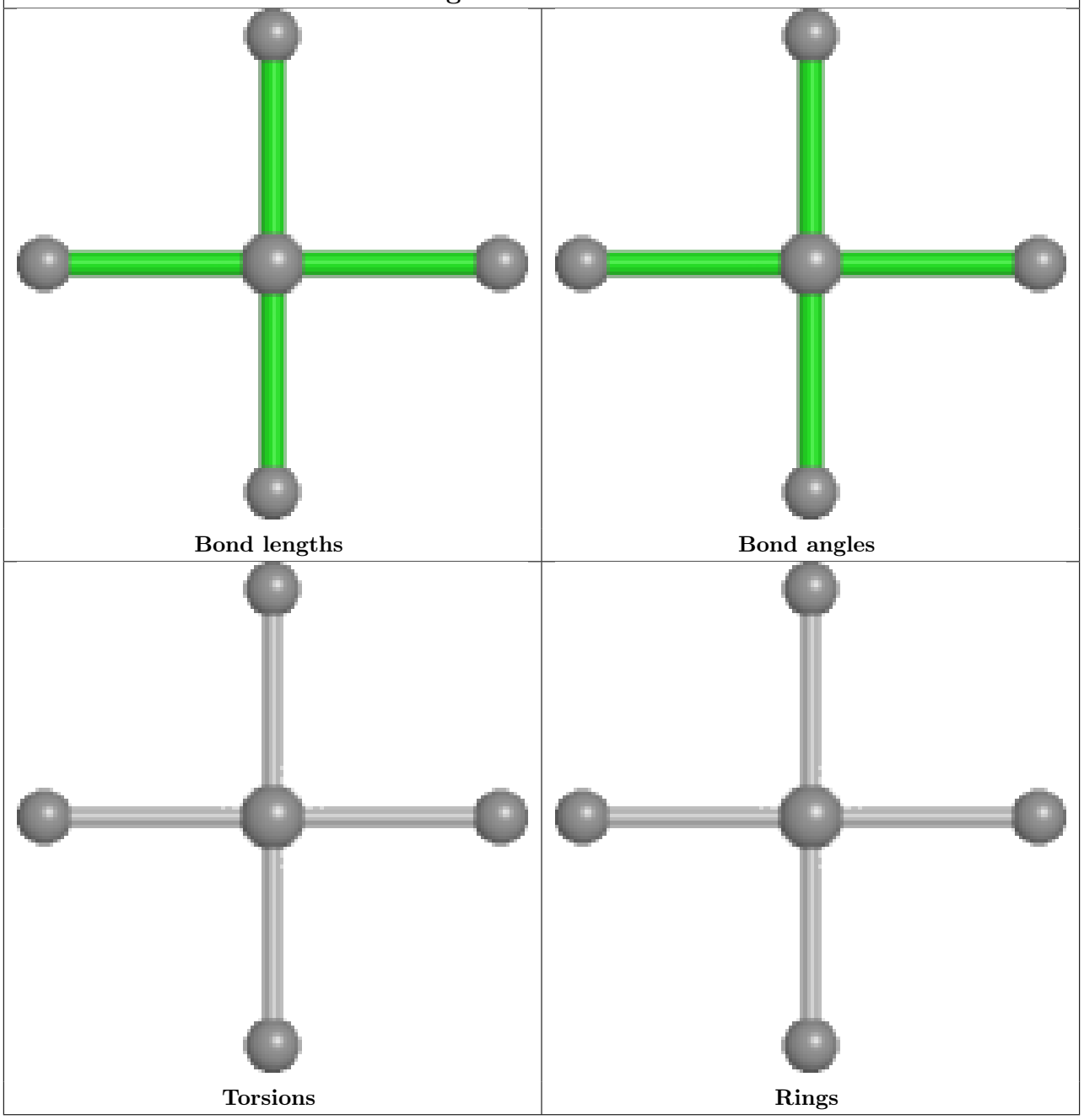


Torsions



Rings

Ligand SO4 K 604



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	470/470 (100%)	-0.43	2 (0%)	92	90	15, 22, 35, 64	0
1	B	467/470 (99%)	-0.46	1 (0%)	95	93	15, 20, 34, 66	0
1	J	467/470 (99%)	-0.45	1 (0%)	95	93	15, 21, 35, 65	0
1	K	467/470 (99%)	-0.46	3 (0%)	89	87	16, 22, 33, 60	0
All	All	1871/1880 (99%)	-0.45	7 (0%)	92	90	15, 21, 35, 66	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	MET	3.7
1	J	430	GLY	2.8
1	K	429	ARG	2.5
1	B	430	GLY	2.2
1	K	428	TRP	2.2
1	K	165	GLY	2.1
1	A	429	ARG	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

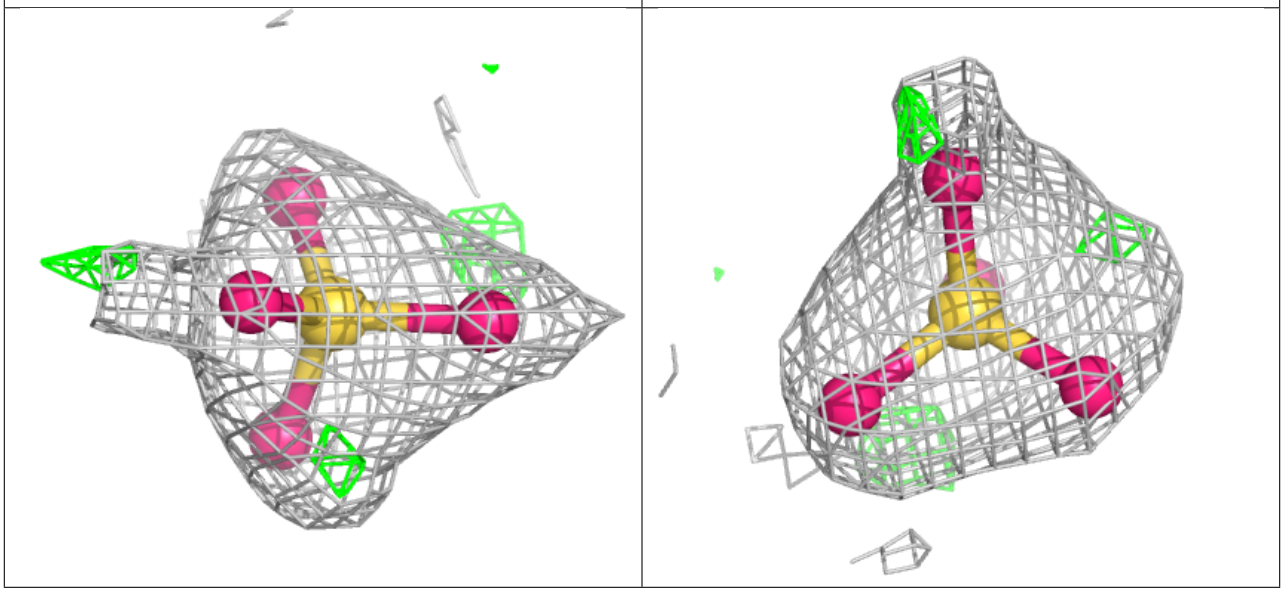
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	K	604	5/5	0.95	0.17	26,28,32,33	5
3	SO4	A	603	5/5	0.96	0.20	19,20,22,22	5
3	SO4	A	604	5/5	0.97	0.20	25,25,27,28	5
2	CU	B	602	1/1	1.00	0.11	22,22,22,22	1
2	CU	J	601	1/1	1.00	0.11	20,20,20,20	1
2	CU	J	602	1/1	1.00	0.11	23,23,23,23	1
2	CU	K	601	1/1	1.00	0.11	20,20,20,20	1
2	CU	K	602	1/1	1.00	0.12	21,21,21,21	1
2	CU	K	603	1/1	1.00	0.09	29,29,29,29	1
2	CU	A	601	1/1	1.00	0.10	20,20,20,20	1
2	CU	A	602	1/1	1.00	0.10	22,22,22,22	1
2	CU	B	601	1/1	1.00	0.10	17,17,17,17	1

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.

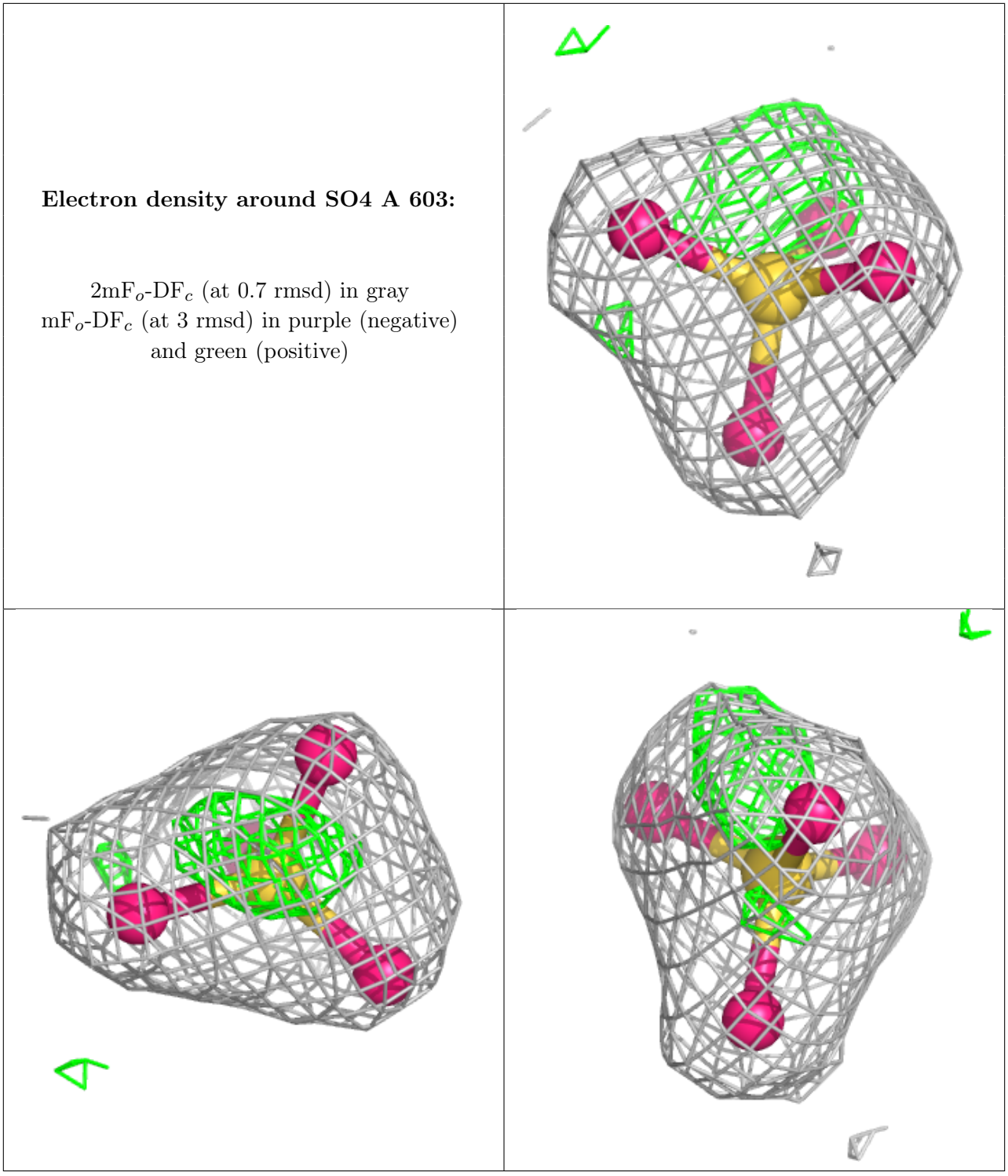
Electron density around SO4 K 604:

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



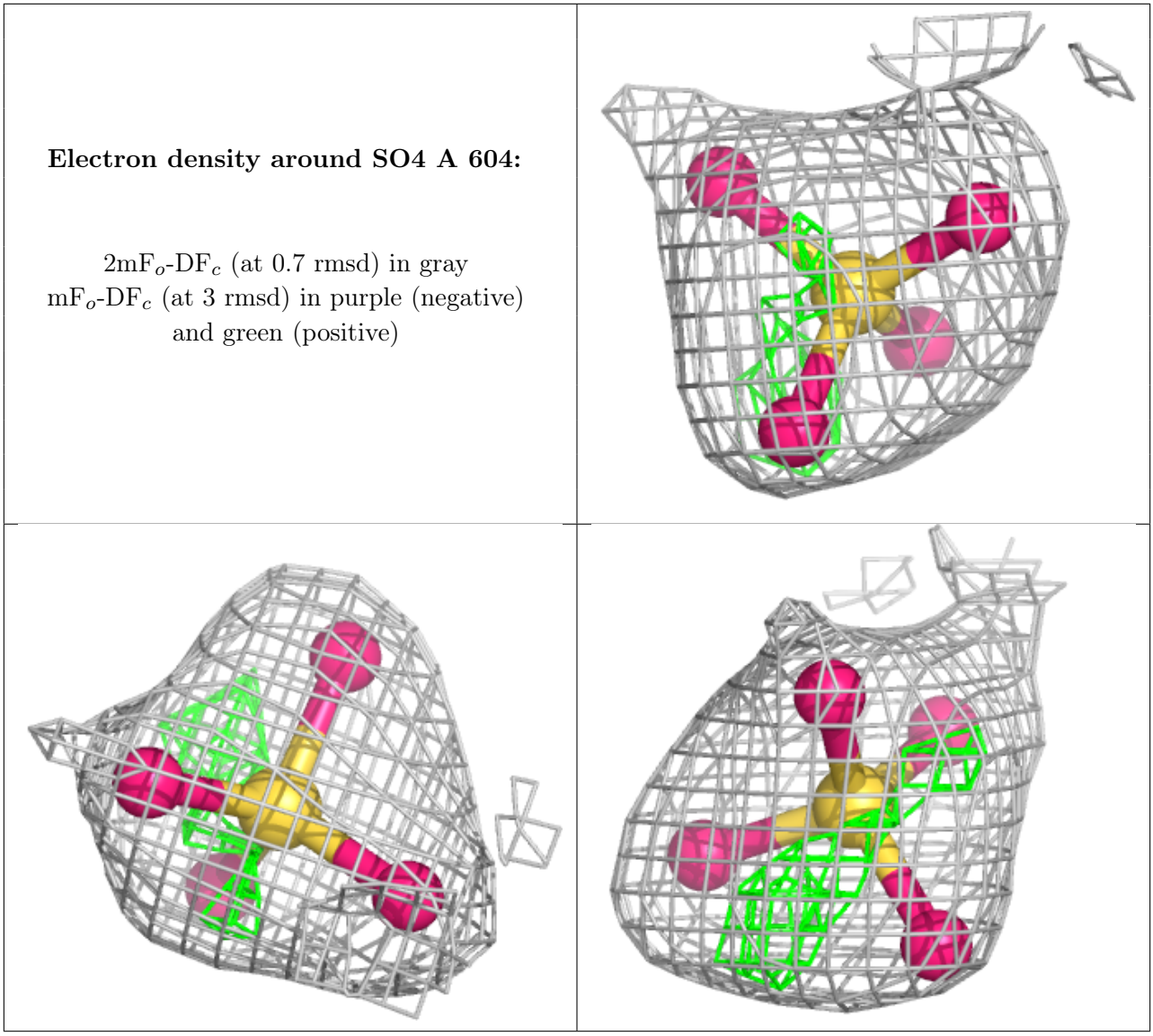
Electron density around SO4 A 603:

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



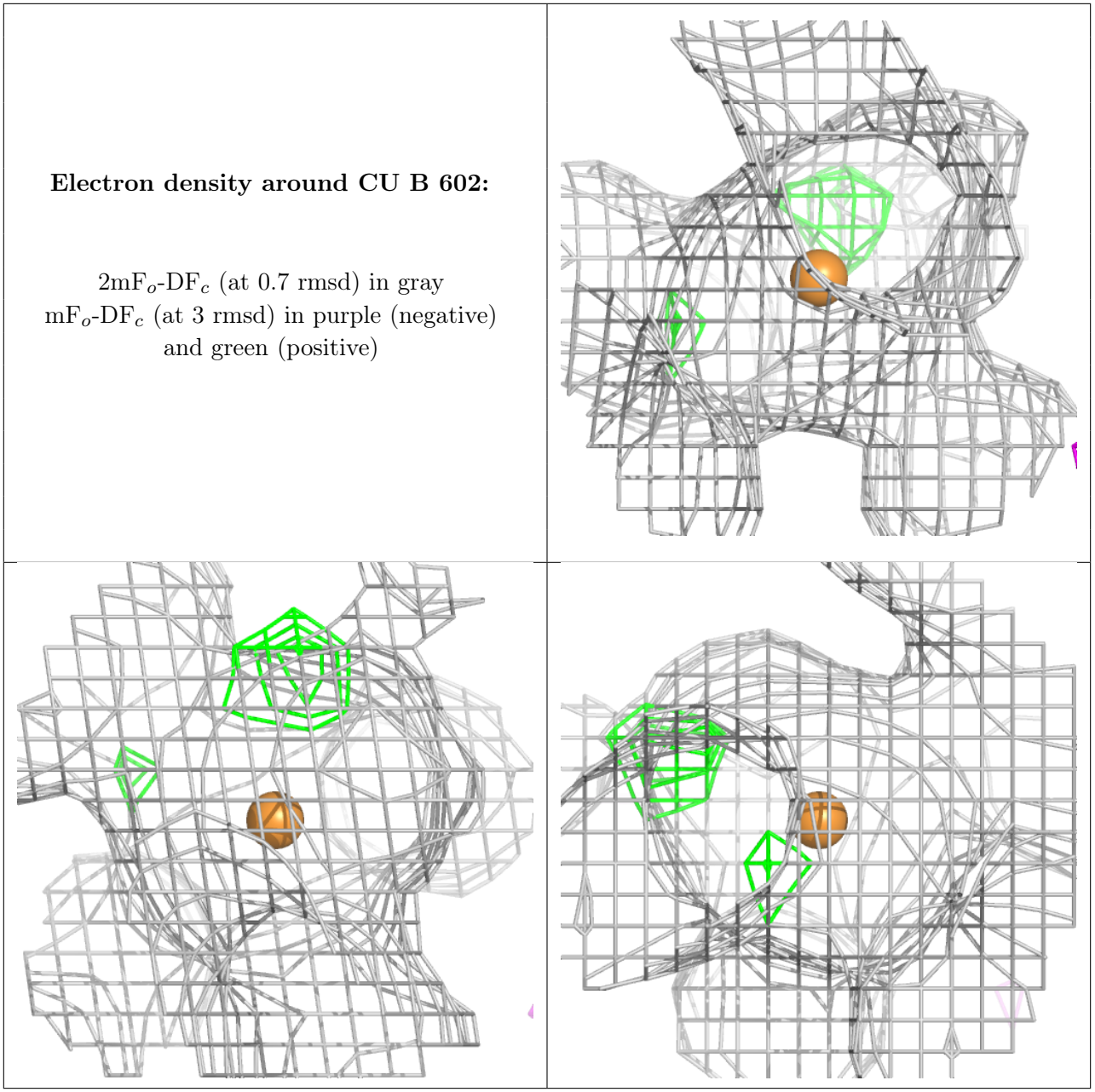
Electron density around SO4 A 604:

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



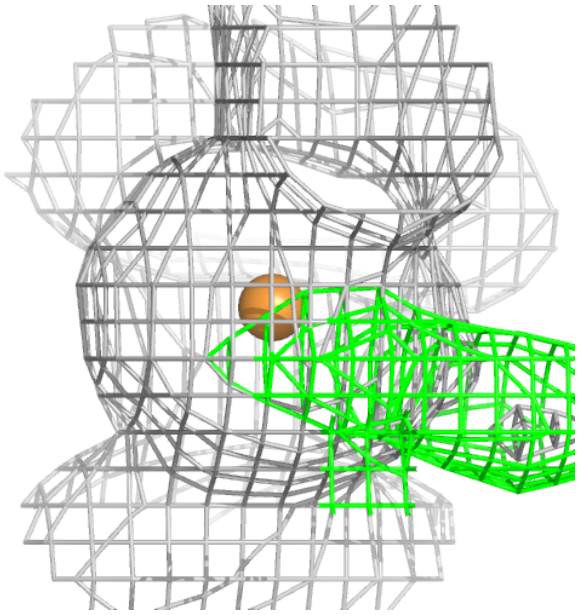
Electron density around CU B 602:

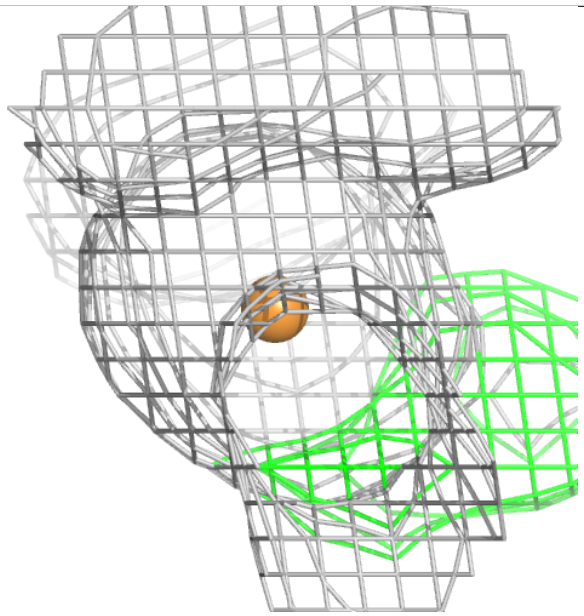
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

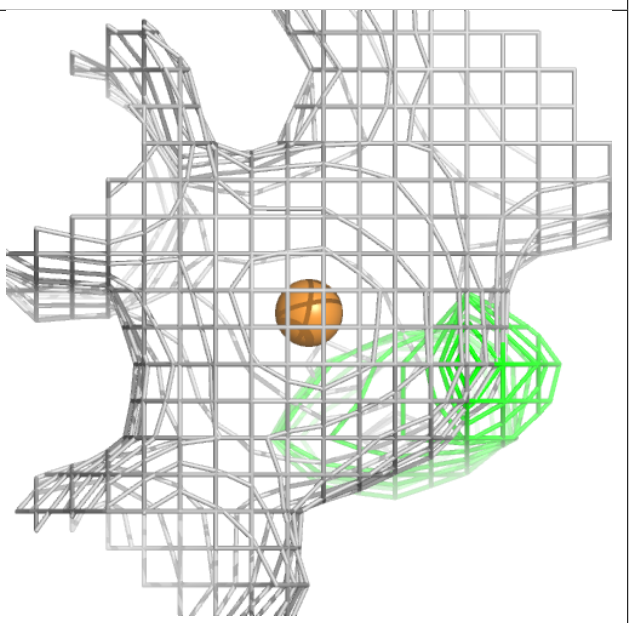


Electron density around CU J 601:

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

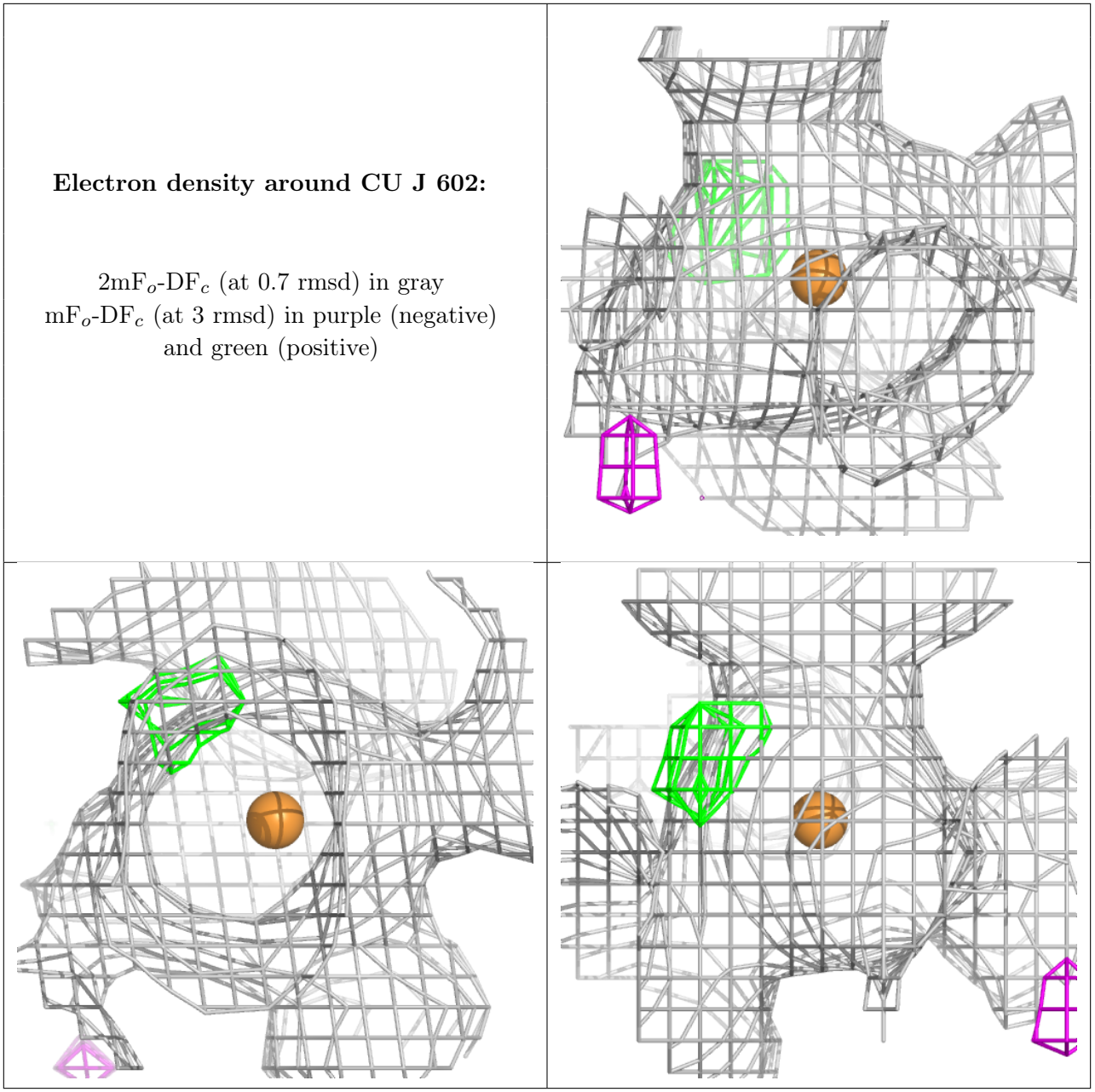






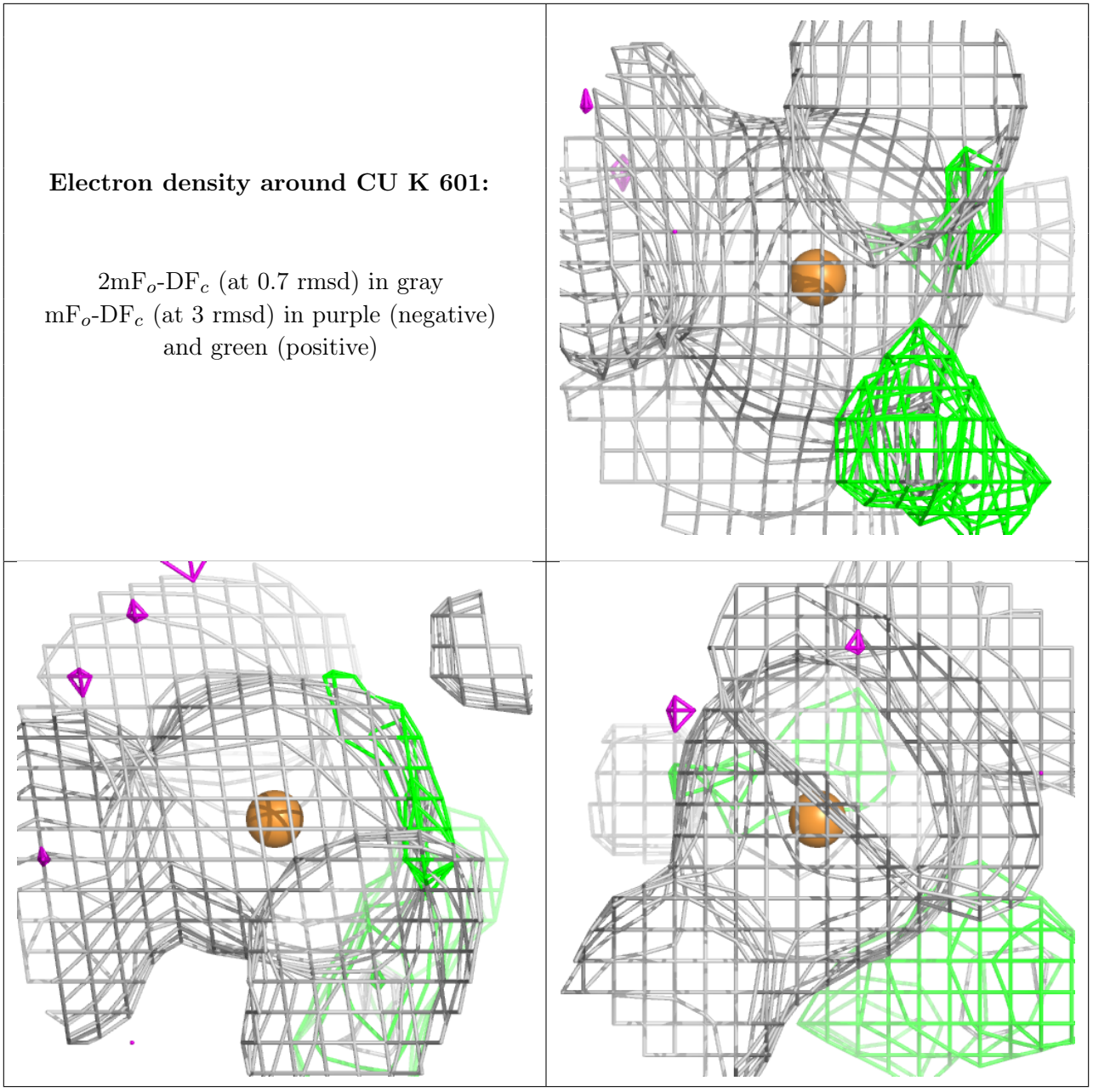
Electron density around CU J 602:

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



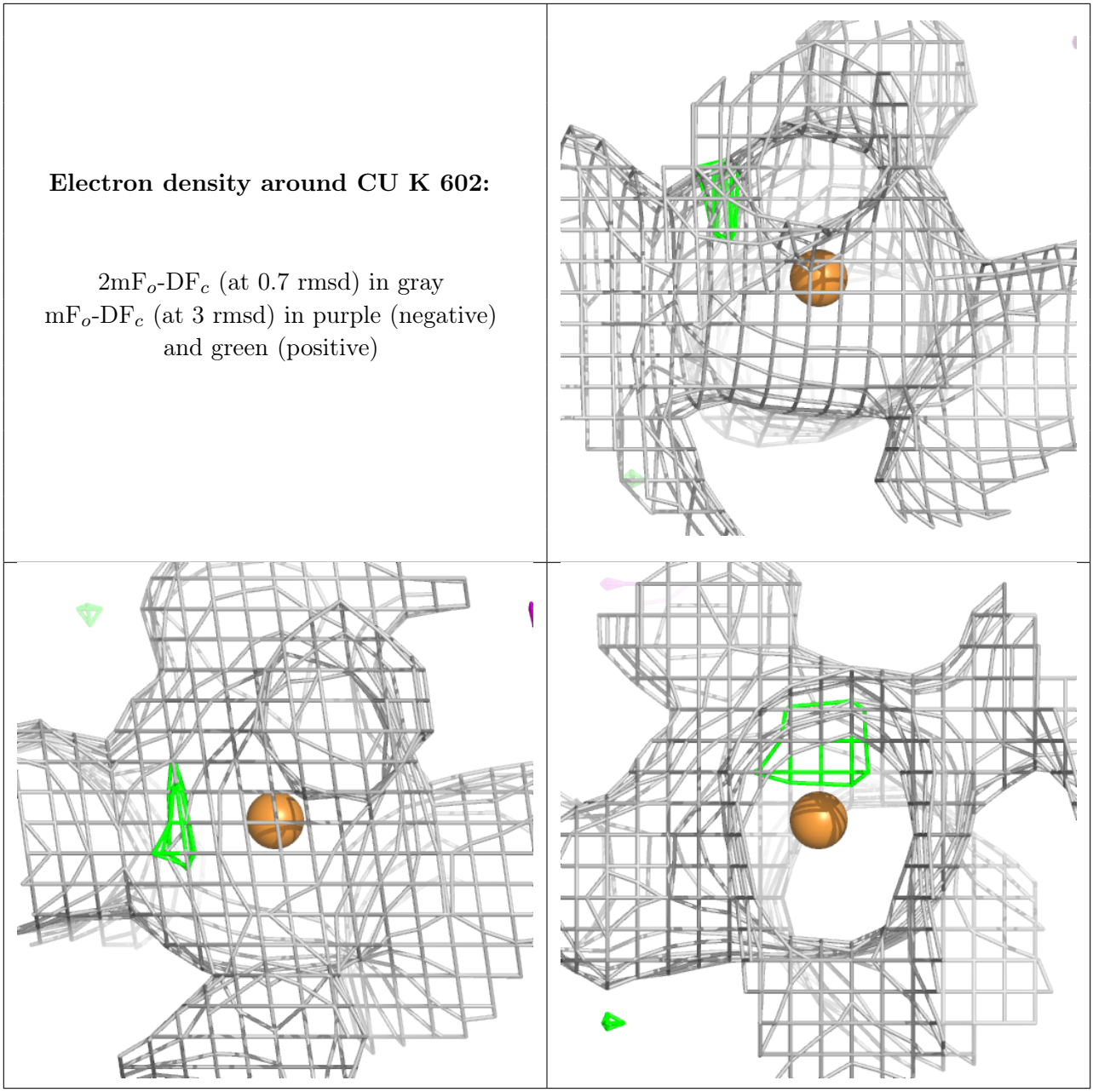
Electron density around CU K 601:

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



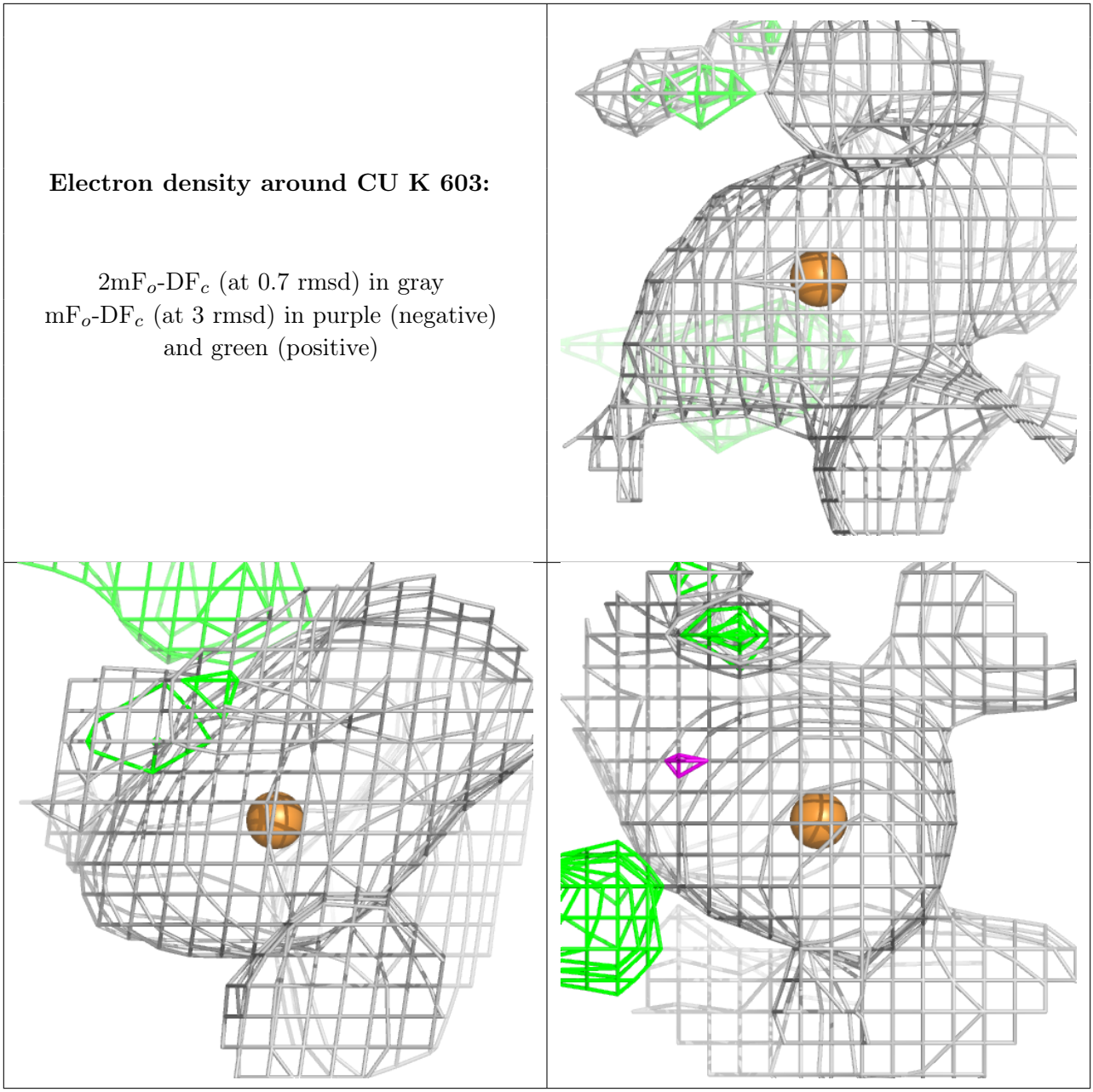
Electron density around CU K 602:

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



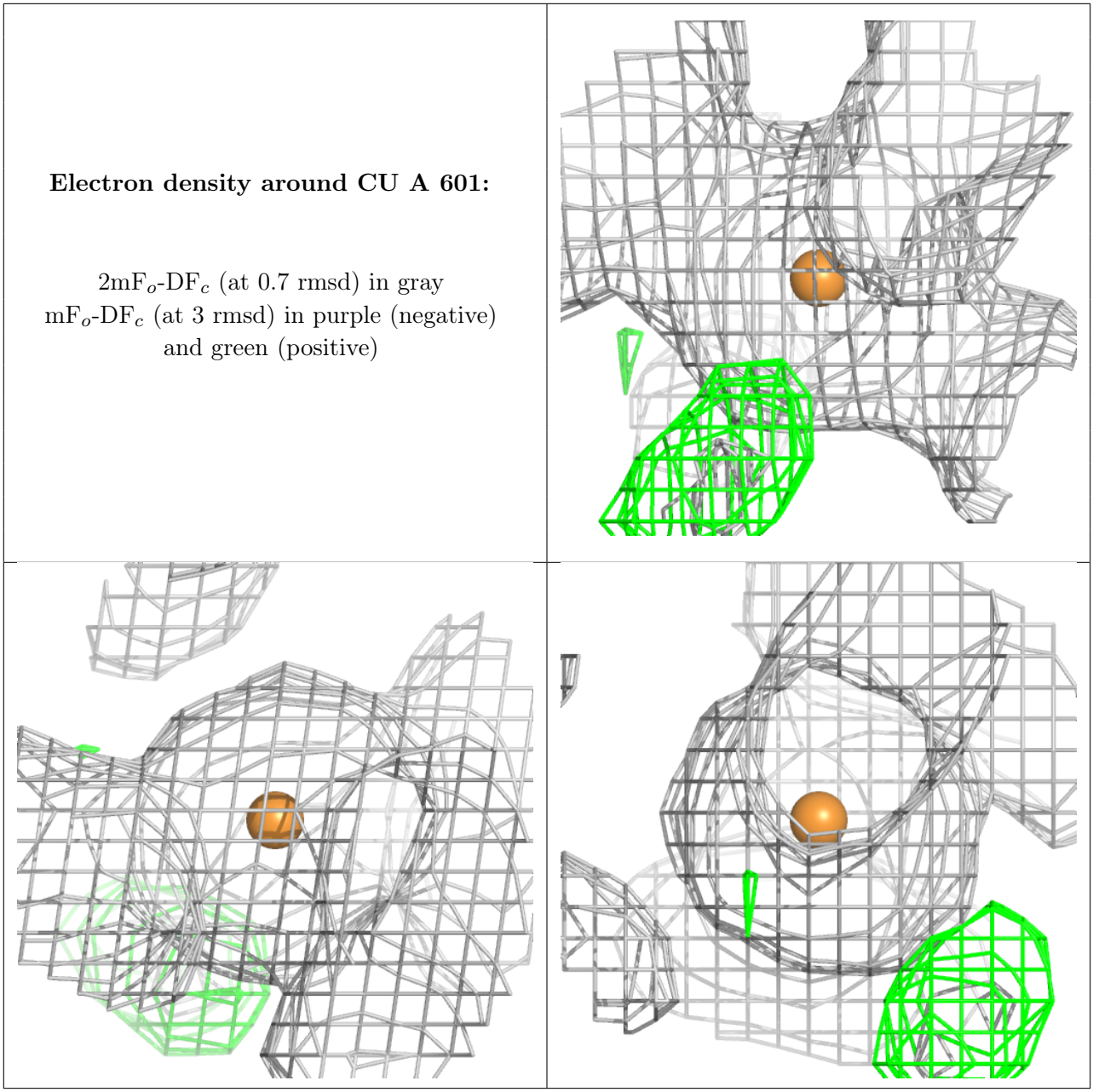
Electron density around CU K 603:

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



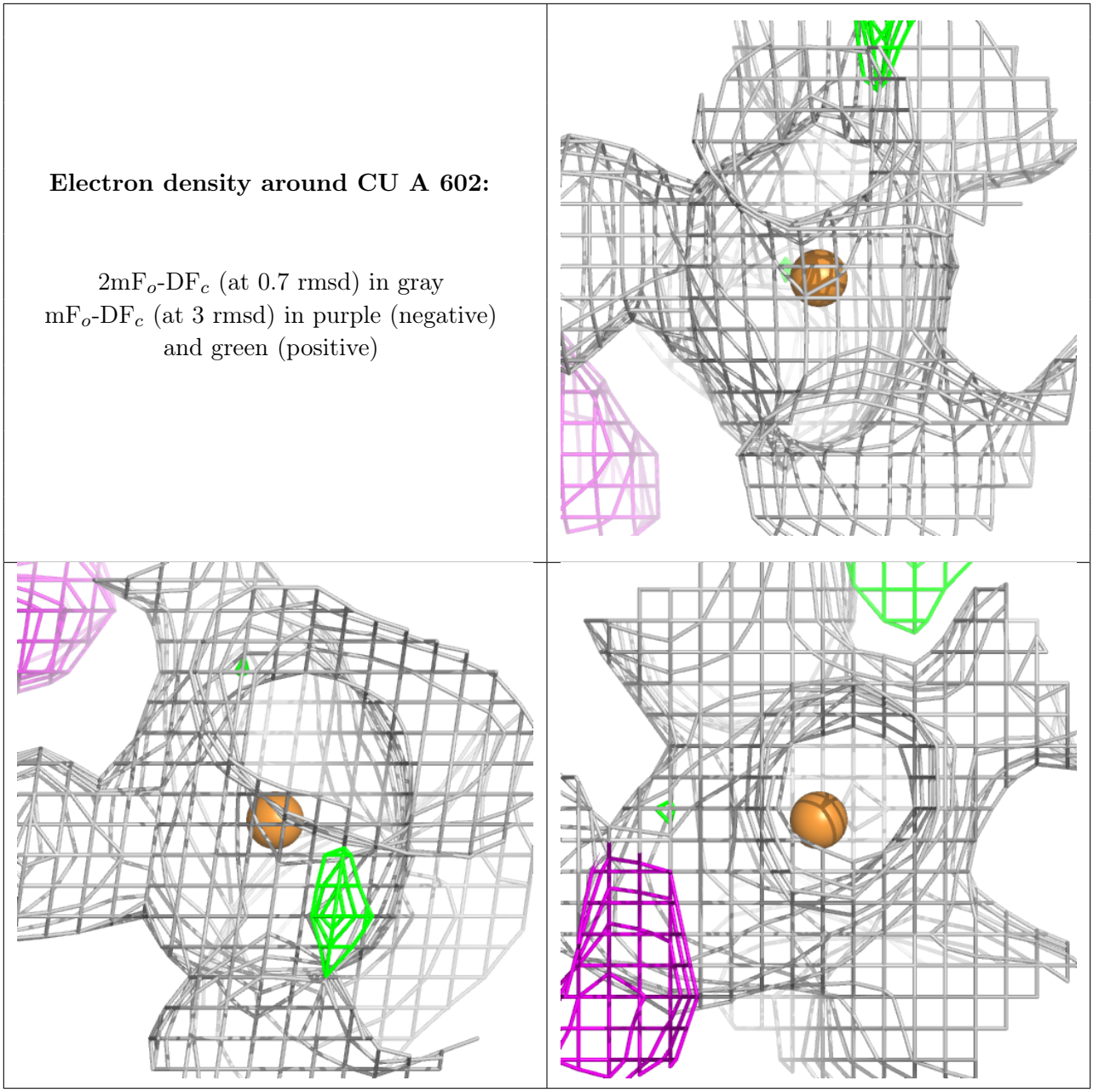
Electron density around CU A 601:

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



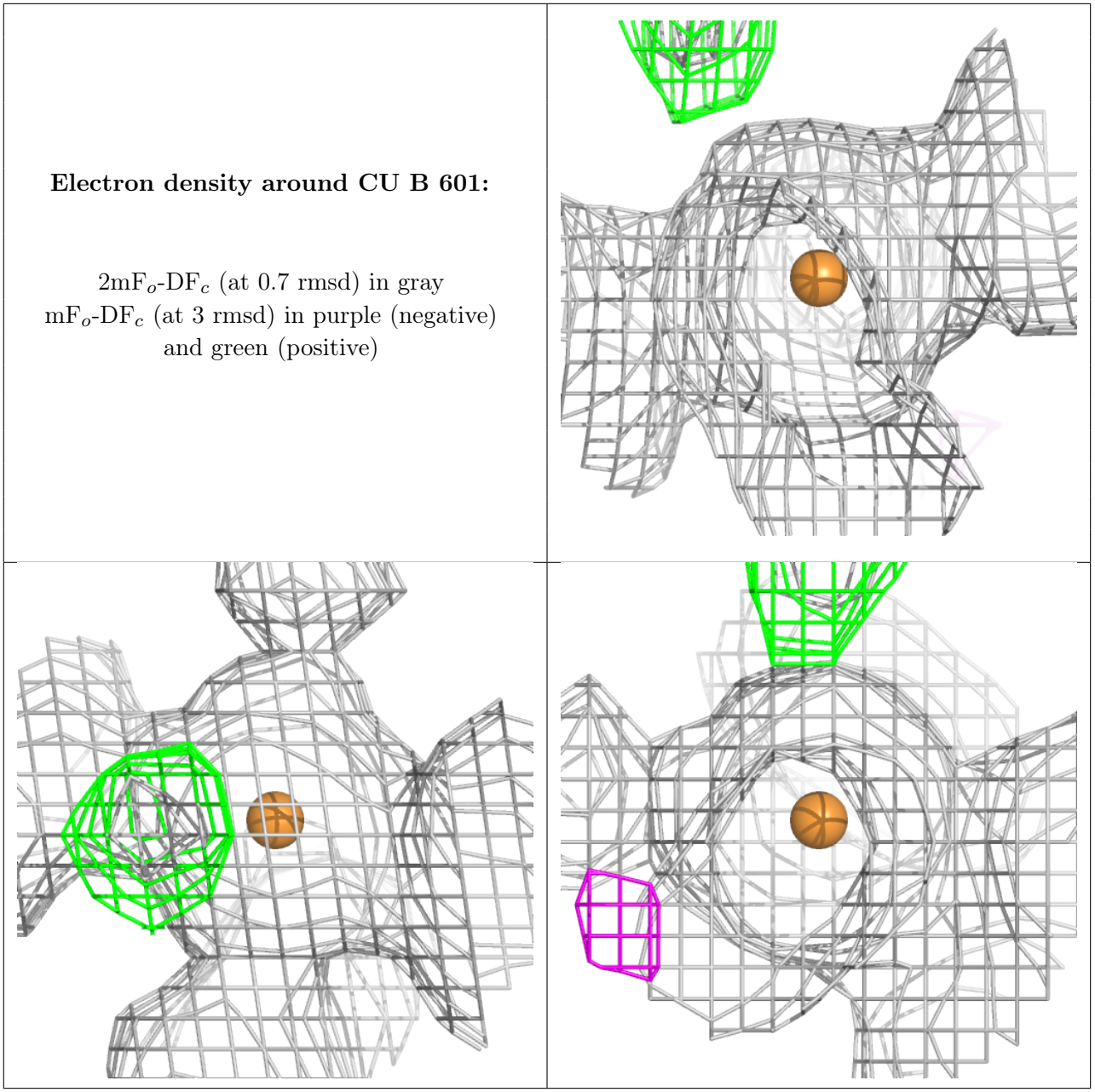
Electron density around CU A 602:

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



Electron density around CU B 601:

$2mF_o$-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.