wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2023 – 10:39 AM EDT

PDB ID	:	7UQC
Title	:	phospho-GlialCAM peptide AA370-389 with Fab MS39p2w174
Authors	:	Lanz, T.V.; Robinson, W.H.; Fernandez, D.
Deposited on	:	2022-04-19
Resolution	:	2.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

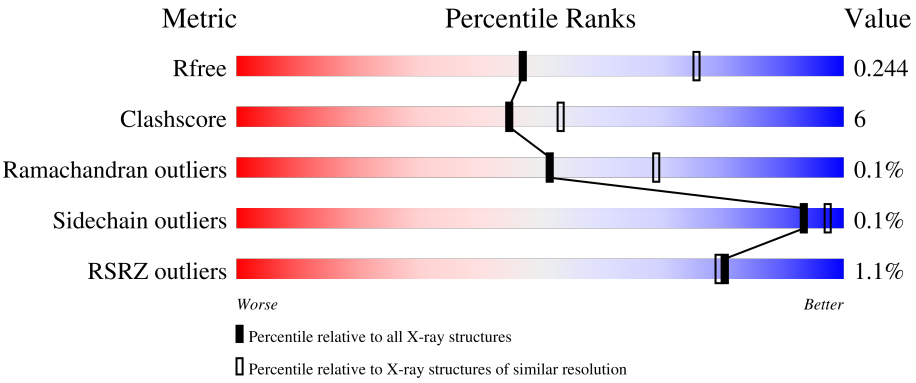
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	219	78% 21%
1	D	219	79% 20%
1	G	219	85% 13%
1	I	219	84% 16%
2	B	219	91% 9%

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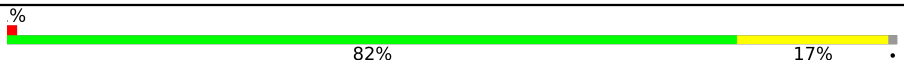
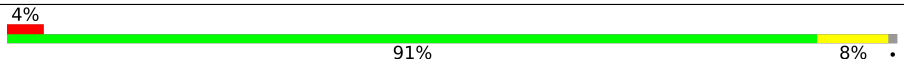
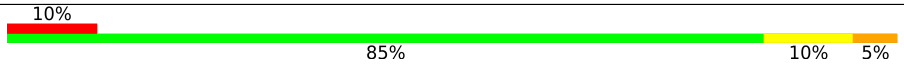
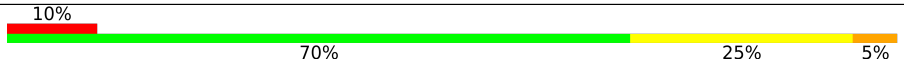
Mol	Chain	Length	Quality of chain
2	E	219	
2	H	219	
2	J	219	
3	C	20	
3	F	20	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13969 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 Fab MS39p2w174 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1701	1064	293	338	6			
1	G	218	Total	C	N	O	S	0	0	0
			1695	1061	292	337	5			
1	I	219	Total	C	N	O	S	0	0	0
			1701	1064	293	338	6			
1	D	218	Total	C	N	O	S	0	0	0
			1691	1059	292	335	5			

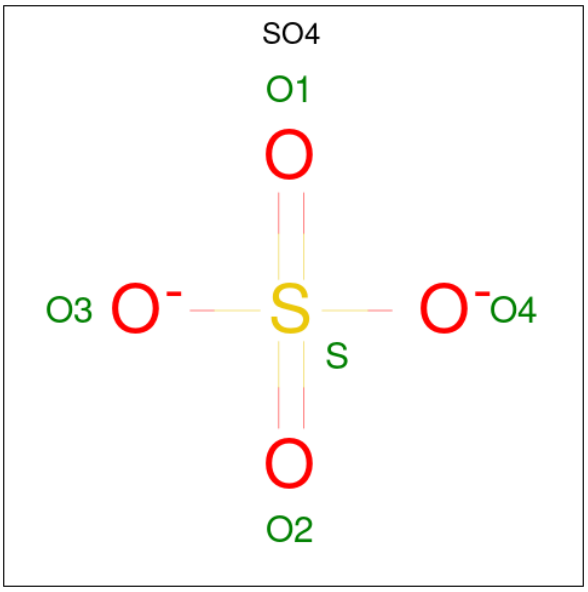
- Molecule 2 is a protein called Fab MS39p2w174 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1639	1033	276	325	5			
2	H	218	Total	C	N	O	S	0	0	0
			1639	1033	276	325	5			
2	J	217	Total	C	N	O	S	0	0	0
			1627	1026	274	322	5			
2	E	217	Total	C	N	O	S	0	0	0
			1633	1030	275	323	5			

- Molecule 3 is a protein called Hepatocyte cell adhesion molecule.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	20	Total	C	N	O	P	0	0	0
			152	83	34	33	2			
3	F	20	Total	C	N	O	P	0	0	0
			152	83	34	33	2			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	G	2	Total Cl 2 2	0	0
5	H	2	Total Cl 2 2	0	0
5	I	2	Total Cl 2 2	0	0
5	J	2	Total Cl 2 2	0	0
5	E	2	Total Cl 2 2	0	0
5	F	1	Total Cl 1 1	0	0

- Molecule 6 is water.

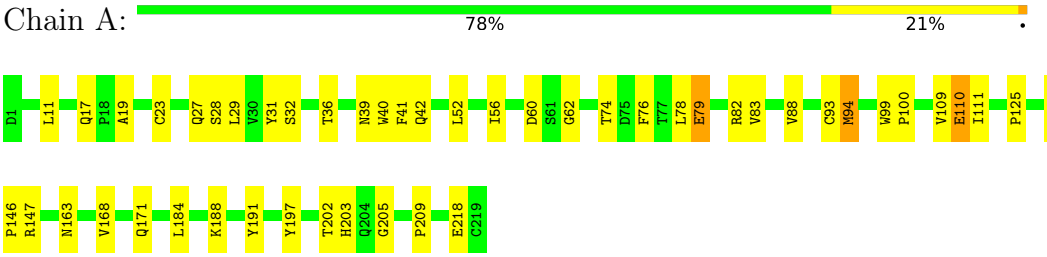
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	38	Total O 38 38	0	0
6	B	30	Total O 30 30	0	0
6	C	6	Total O 6 6	0	0
6	G	61	Total O 61 61	0	0
6	H	41	Total O 41 41	0	0
6	I	37	Total O 37 37	0	0
6	J	26	Total O 26 26	0	0
6	D	46	Total O 46 46	0	0
6	E	24	Total O 24 24	0	0
6	F	8	Total O 8 8	0	0

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.

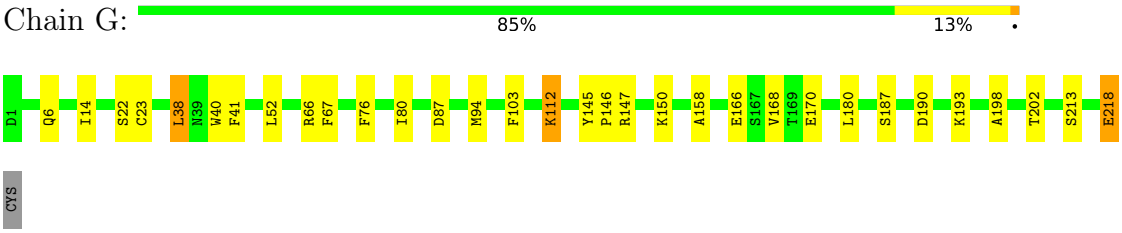
• Molecule 1: Fab MS39p2w174 Light Chain

Chain A:



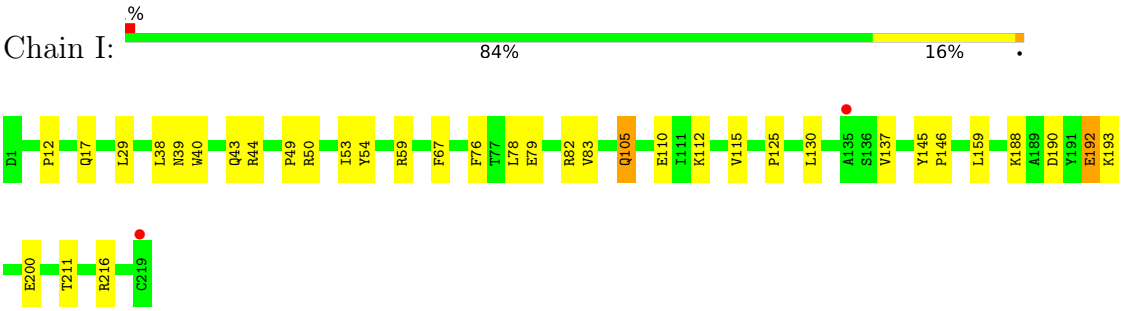
• Molecule 1: Fab MS39p2w174 Light Chain

Chain G:



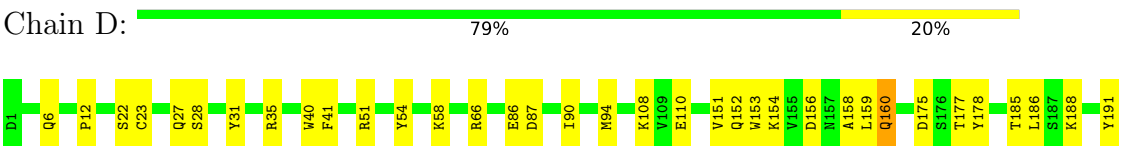
• Molecule 1: Fab MS39p2w174 Light Chain

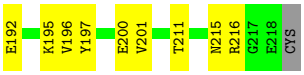
Chain I:



• Molecule 1: Fab MS39p2w174 Light Chain

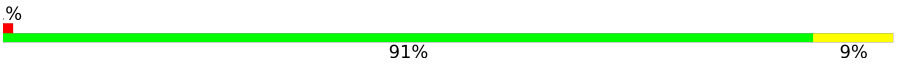
Chain D:

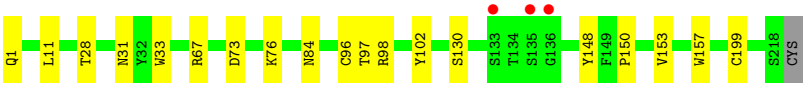




• Molecule 2: Fab MS39p2w174 Heavy Chain

Chain B:



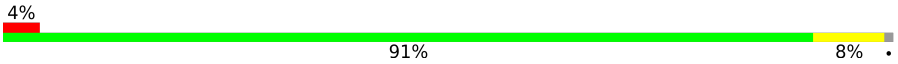


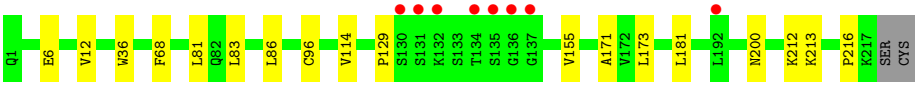
• Molecule 2: Fab MS39p2w174 Heavy Chain

Chain H:

• Molecule 2: Fab MS39p2w174 Heavy Chain

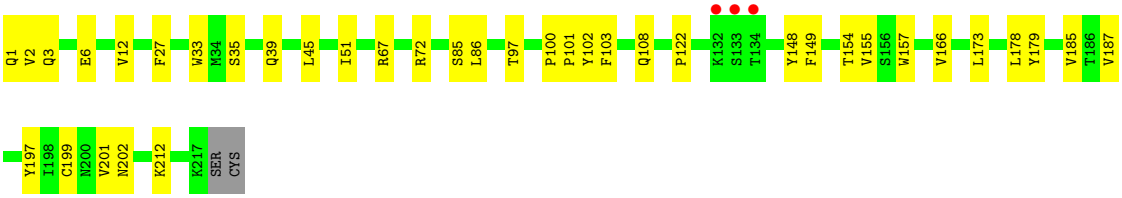
Chain J:





• Molecule 2: Fab MS39p2w174 Heavy Chain

Chain E:

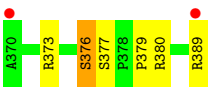


• Molecule 3: Hepatocyte cell adhesion molecule

Chain C:

• Molecule 3: Hepatocyte cell adhesion molecule

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	195.03Å 99.51Å 136.41Å 90.00° 112.81° 90.00°	Depositor
Resolution (Å)	44.11 – 2.65 44.11 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.8 (44.11-2.65) 96.0 (44.11-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.65Å)	Xtriage
Refinement program	REFMAC 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.176 , 0.237 0.187 , 0.244	Depositor DCC
R_{free} test set	3503 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.2	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	0.94	EDS
Total number of atoms	13969	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: SO4, SEP, CL

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	0.59	2/1738 (0.1%)	0.77	4/2357 (0.2%)
1	D	0.53	0/1728	0.70	0/2344
1	G	0.58	2/1732 (0.1%)	0.76	5/2349 (0.2%)
1	I	0.57	2/1738 (0.1%)	0.78	3/2357 (0.1%)
2	B	0.49	1/1680 (0.1%)	0.67	0/2289
2	E	0.50	0/1674	0.70	0/2281
2	H	0.51	0/1680	0.67	1/2289 (0.0%)
2	J	0.50	0/1668	0.68	1/2274 (0.0%)
3	C	0.41	0/135	0.62	0/180
3	F	0.43	0/135	0.63	0/180
All	All	0.53	7/13908 (0.1%)	0.72	14/18900 (0.1%)

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	2
1	D	0	1
1	I	0	1
All	All	0	4

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	218	GLU	CD-OE2	9.23	1.35	1.25
1	I	50	ARG	NE-CZ	-7.94	1.22	1.33
1	A	110	GLU	CD-OE2	7.87	1.34	1.25
2	B	96	CYS	CB-SG	-6.08	1.72	1.82
1	A	79	GLU	CD-OE2	5.20	1.31	1.25

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	G	38	LEU	CA-CB-CG	-6.75	99.77	115.30
2	H	65	LYS	CD-CE-NZ	-6.66	96.38	111.70
1	I	50	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	60	ASP	N-CA-CB	6.25	121.84	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLU	Sidechain
1	A	62	GLY	Peptide
1	D	160	GLN	Peptide
1	I	105	GLN	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	1701	0	1662	29	0
1	D	1691	0	1653	33	0
1	G	1695	0	1657	23	0
1	I	1701	0	1662	22	0
2	B	1639	0	1596	10	0
2	E	1633	0	1591	29	0
2	H	1639	0	1596	20	0
2	J	1627	0	1575	11	0
3	C	152	0	138	2	0
3	F	152	0	138	5	0
4	A	5	0	0	0	0
4	I	5	0	0	0	0
5	B	1	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	2	0	0	0	0
5	J	2	0	0	0	0
6	A	38	0	0	0	0
6	B	30	0	0	0	0
6	C	6	0	0	0	0
6	D	46	0	0	0	0
6	E	24	0	0	1	0
6	F	8	0	0	1	0
6	G	61	0	0	0	0
6	H	41	0	0	0	0
6	I	37	0	0	0	0
6	J	26	0	0	0	0
All	All	13969	0	13268	175	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 6.

The worst 5 of 175 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)
2:E:35:SER:HB2	2:E:100:PRO:HG3	1.62	0.81
1:A:27:GLN:HE21	1:A:28:SER:H	1.27	0.80
1:D:156:ASP:HA	1:D:196:VAL:HB	1.65	0.78
2:H:204:LYS:HG3	2:H:205:PRO:HD3	1.68	0.76
2:E:1:GLN:N	2:E:1:GLN:OE1	2.19	0.75

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	217/219 (99%)	209 (96%)	7 (3%)	1 (0%)	29 43
1	D	216/219 (99%)	205 (95%)	11 (5%)	0	100 100
1	G	216/219 (99%)	208 (96%)	8 (4%)	0	100 100
1	I	217/219 (99%)	209 (96%)	8 (4%)	0	100 100
2	B	216/219 (99%)	203 (94%)	12 (6%)	1 (0%)	29 43
2	E	215/219 (98%)	209 (97%)	6 (3%)	0	100 100
2	H	216/219 (99%)	210 (97%)	6 (3%)	0	100 100
2	J	215/219 (98%)	204 (95%)	11 (5%)	0	100 100
3	C	16/20 (80%)	16 (100%)	0	0	100 100
3	F	16/20 (80%)	15 (94%)	1 (6%)	0	100 100
All	All	1760/1792 (98%)	1688 (96%)	70 (4%)	2 (0%)	51 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLU
2	B	130	SER

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	195/195 (100%)	194 (100%)	1 (0%)	88 94
1	D	193/195 (99%)	193 (100%)	0	100 100
1	G	194/195 (100%)	194 (100%)	0	100 100
1	I	195/195 (100%)	194 (100%)	1 (0%)	88 94
2	B	187/188 (100%)	187 (100%)	0	100 100
2	E	186/188 (99%)	186 (100%)	0	100 100
2	H	187/188 (100%)	187 (100%)	0	100 100
2	J	184/188 (98%)	184 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	14/14 (100%)	14 (100%)	0	100	100
3	F	14/14 (100%)	14 (100%)	0	100	100
All	All	1549/1560 (99%)	1547 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	I	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	HIS
2	B	31	ASN
1	I	143	ASN
1	A	39	ASN
1	A	27	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	SEP	C	376	3	8,9,10	1.65	2 (25%)	8,12,14	1.35	1 (12%)
3	SEP	F	377	3	8,9,10	1.51	1 (12%)	8,12,14	1.42	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SEP	C	377	3	8,9,10	1.40	1 (12%)	8,12,14	2.20	3 (37%)
3	SEP	F	376	3	8,9,10	1.61	3 (37%)	8,12,14	1.41	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	C	376	3	-	0/5/8/10	-
3	SEP	F	377	3	-	0/5/8/10	-
3	SEP	C	377	3	-	0/5/8/10	-
3	SEP	F	376	3	-	0/5/8/10	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	377	SEP	P-O1P	3.39	1.61	1.50
3	C	376	SEP	P-O1P	3.38	1.61	1.50
3	C	377	SEP	P-O1P	3.01	1.60	1.50
3	F	376	SEP	P-O1P	2.91	1.59	1.50
3	F	376	SEP	P-O3P	2.48	1.64	1.54

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	377	SEP	OG-CB-CA	4.23	112.26	108.14
3	C	377	SEP	O3P-P-OG	3.28	115.46	106.73
3	F	377	SEP	P-OG-CB	-2.72	110.81	118.30
3	C	376	SEP	P-OG-CB	-2.62	111.09	118.30
3	F	376	SEP	O3P-P-OG	2.46	113.27	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	376	SEP	1	0
3	F	376	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	SO4	A	301	-	4,4,4	0.26	0	6,6,6	0.28	0
4	SO4	I	301	-	4,4,4	0.16	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

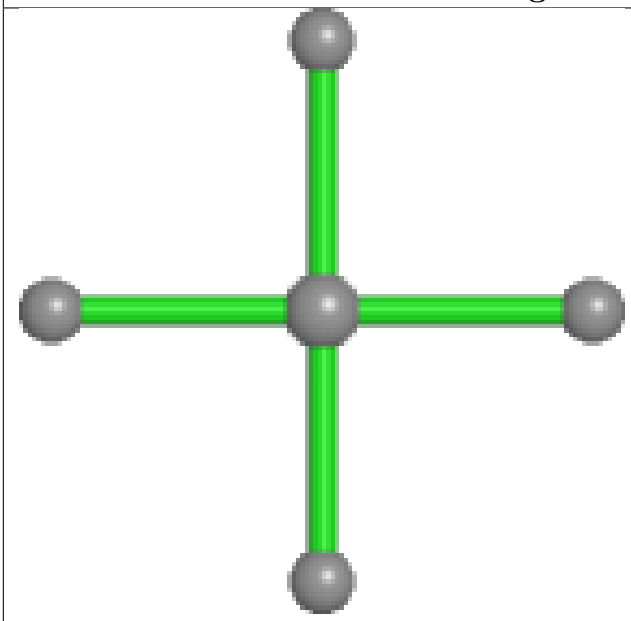
There are no torsion outliers.

There are no ring outliers.

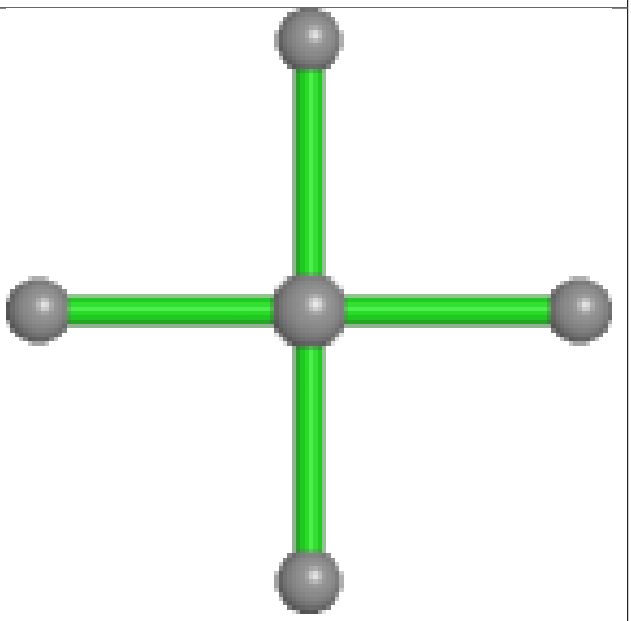
No monomer is involved in short contacts.

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.

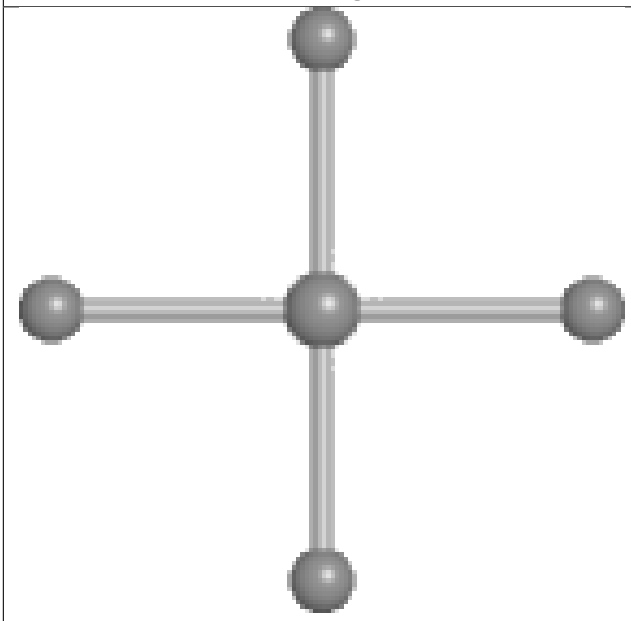
Ligand SO4 A 301



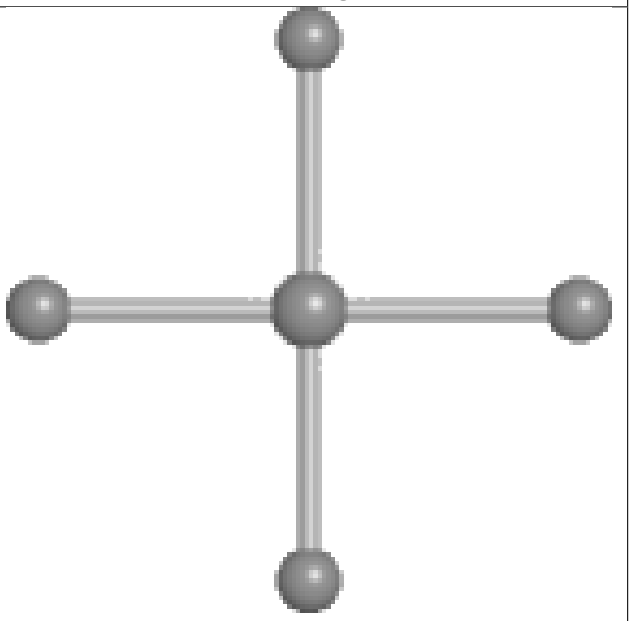
Bond lengths



Bond angles

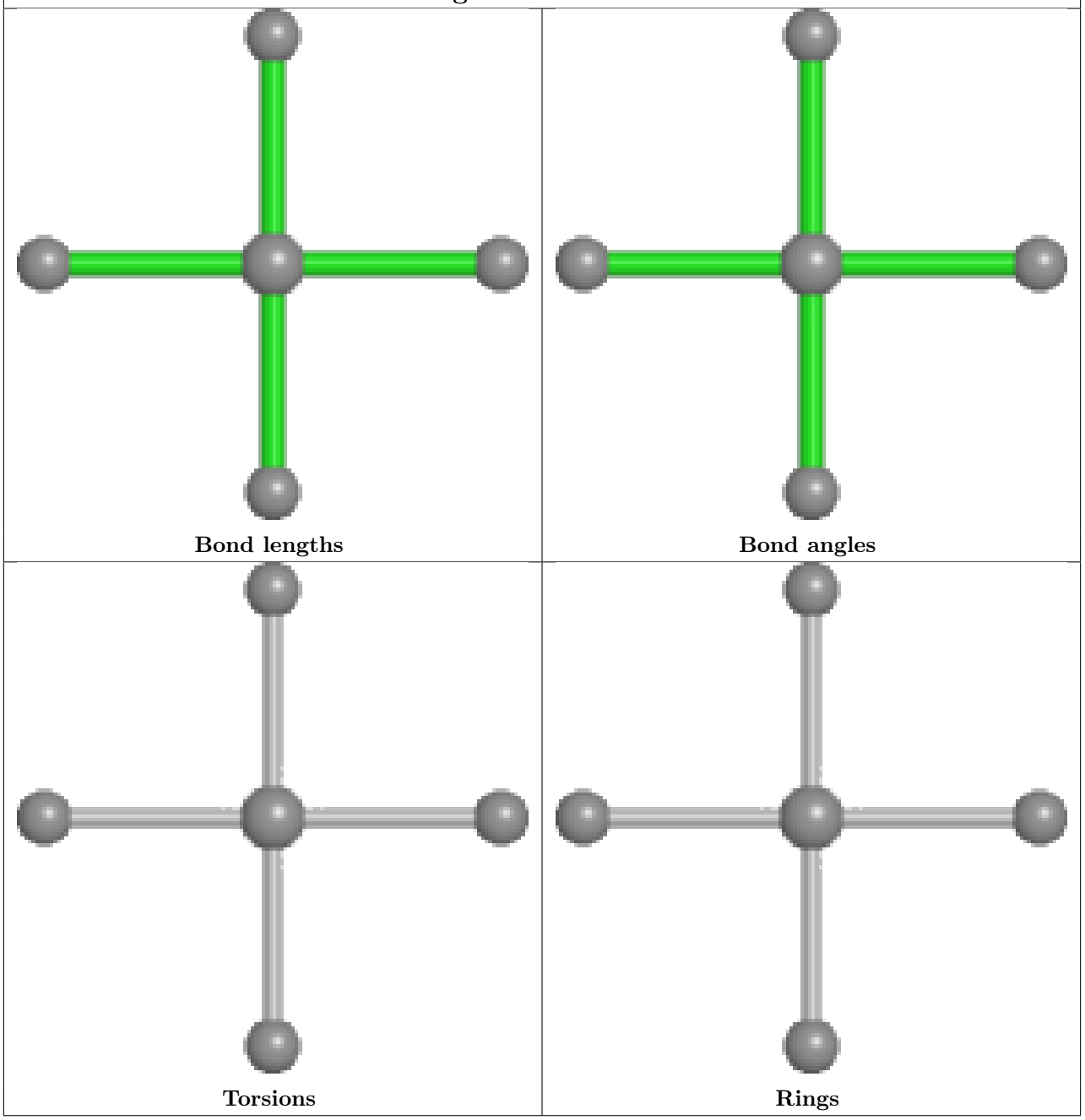


Torsions



Rings

Ligand SO4 I 301



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	219/219 (100%)	-0.28	0 100 100	27, 49, 67, 89	0
1	D	218/219 (99%)	-0.20	0 100 100	29, 48, 85, 99	0
1	G	218/219 (99%)	-0.28	0 100 100	28, 42, 62, 78	0
1	I	219/219 (100%)	-0.05	2 (0%) 84 83	30, 54, 76, 112	0
2	B	218/219 (99%)	-0.14	3 (1%) 75 73	29, 48, 77, 132	0
2	E	217/219 (99%)	-0.15	3 (1%) 75 73	29, 47, 79, 113	0
2	H	218/219 (99%)	-0.35	0 100 100	31, 43, 58, 75	0
2	J	217/219 (99%)	-0.00	8 (3%) 41 38	34, 51, 99, 138	0
3	C	18/20 (90%)	0.23	2 (11%) 5 3	30, 40, 81, 92	0
3	F	18/20 (90%)	0.25	2 (11%) 5 3	31, 38, 75, 86	0
All	All	1780/1792 (99%)	-0.17	20 (1%) 80 79	27, 48, 78, 138	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	135	SER	6.7
2	B	136	GLY	5.6
2	J	136	GLY	4.9
3	F	370	ALA	4.6
1	I	219	CYS	4.0

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

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	SEP	C	376	10/11	0.97	0.16	38,41,48,52	0
3	SEP	F	376	10/11	0.98	0.16	38,42,46,48	0
3	SEP	C	377	10/11	0.99	0.15	27,33,38,41	0
3	SEP	F	377	10/11	0.99	0.19	29,33,36,38	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

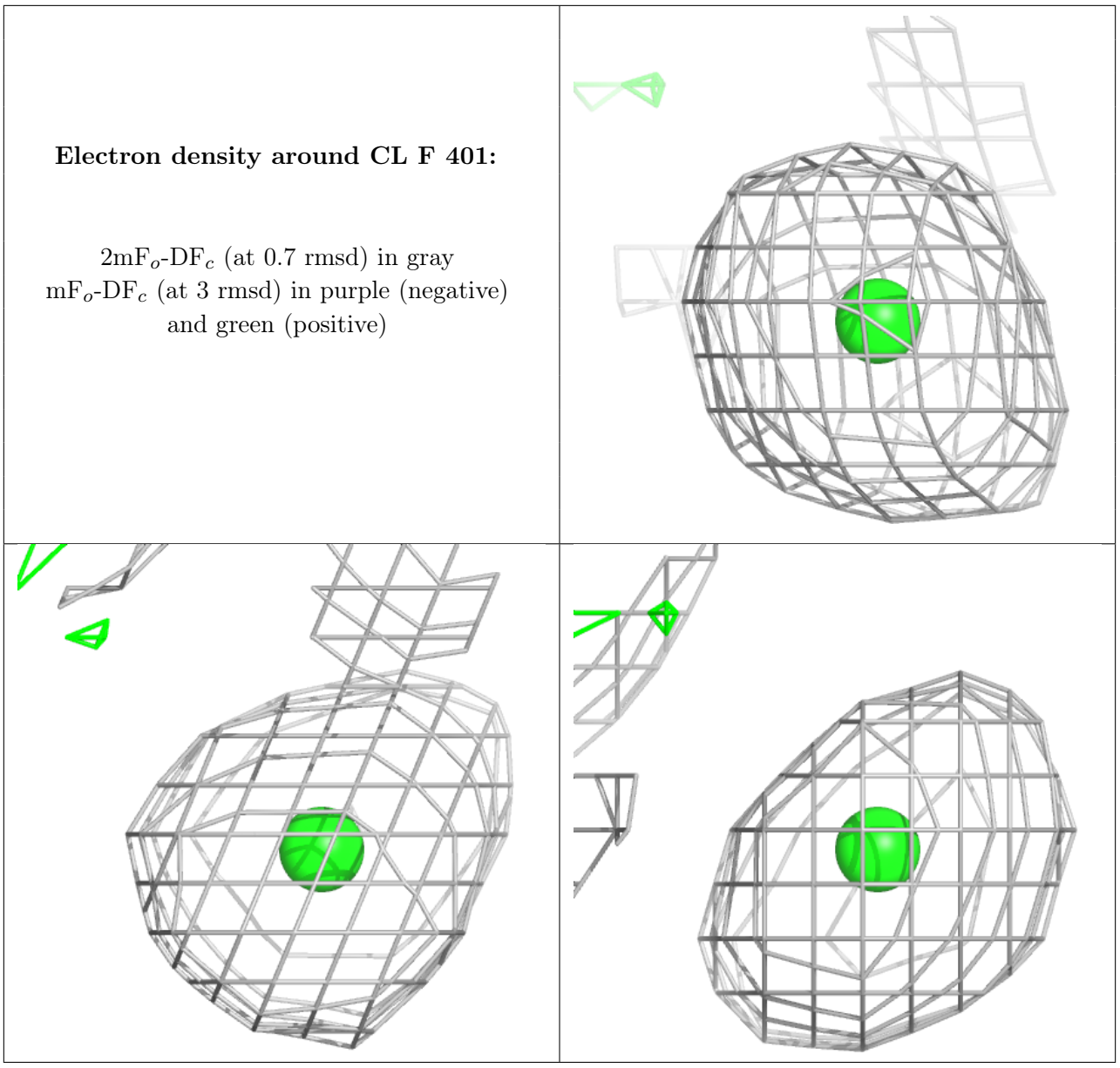
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	F	401	1/1	0.85	0.13	69,69,69,69	0
5	CL	I	302	1/1	0.92	0.07	64,64,64,64	0
5	CL	J	301	1/1	0.94	0.13	60,60,60,60	0
5	CL	H	301	1/1	0.95	0.07	48,48,48,48	0
5	CL	J	302	1/1	0.96	0.08	60,60,60,60	0
5	CL	E	301	1/1	0.97	0.12	45,45,45,45	0
5	CL	B	301	1/1	0.97	0.06	44,44,44,44	0
5	CL	G	302	1/1	0.98	0.09	41,41,41,41	0
5	CL	I	303	1/1	0.98	0.08	34,34,34,34	0
5	CL	E	302	1/1	0.98	0.03	58,58,58,58	0
5	CL	G	301	1/1	0.98	0.36	73,73,73,73	0
4	SO4	I	301	5/5	0.99	0.17	30,32,36,38	0
5	CL	H	302	1/1	0.99	0.28	76,76,76,76	1
4	SO4	A	301	5/5	0.99	0.17	28,32,36,39	0

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

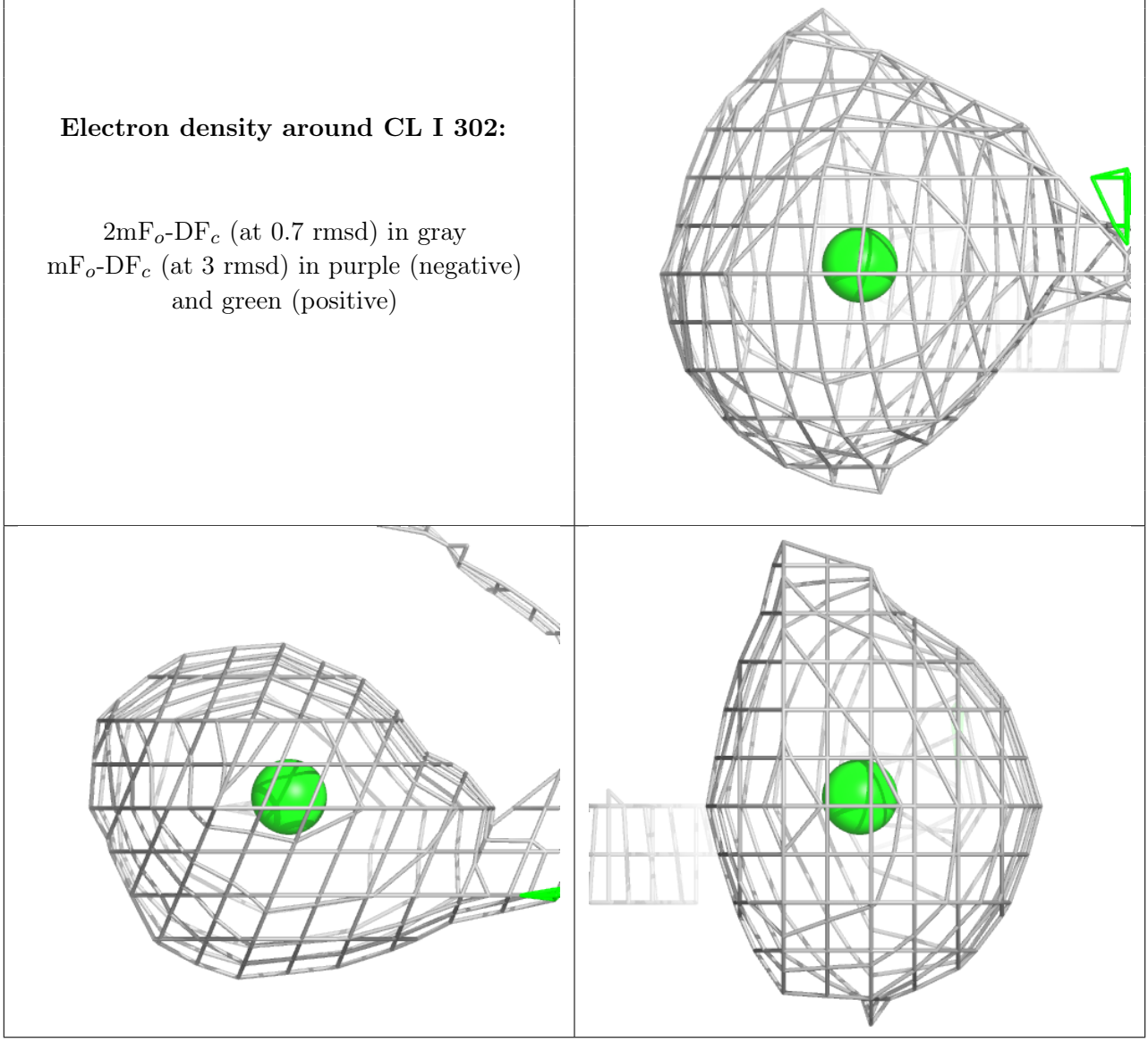
Electron density around CL F 401:

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



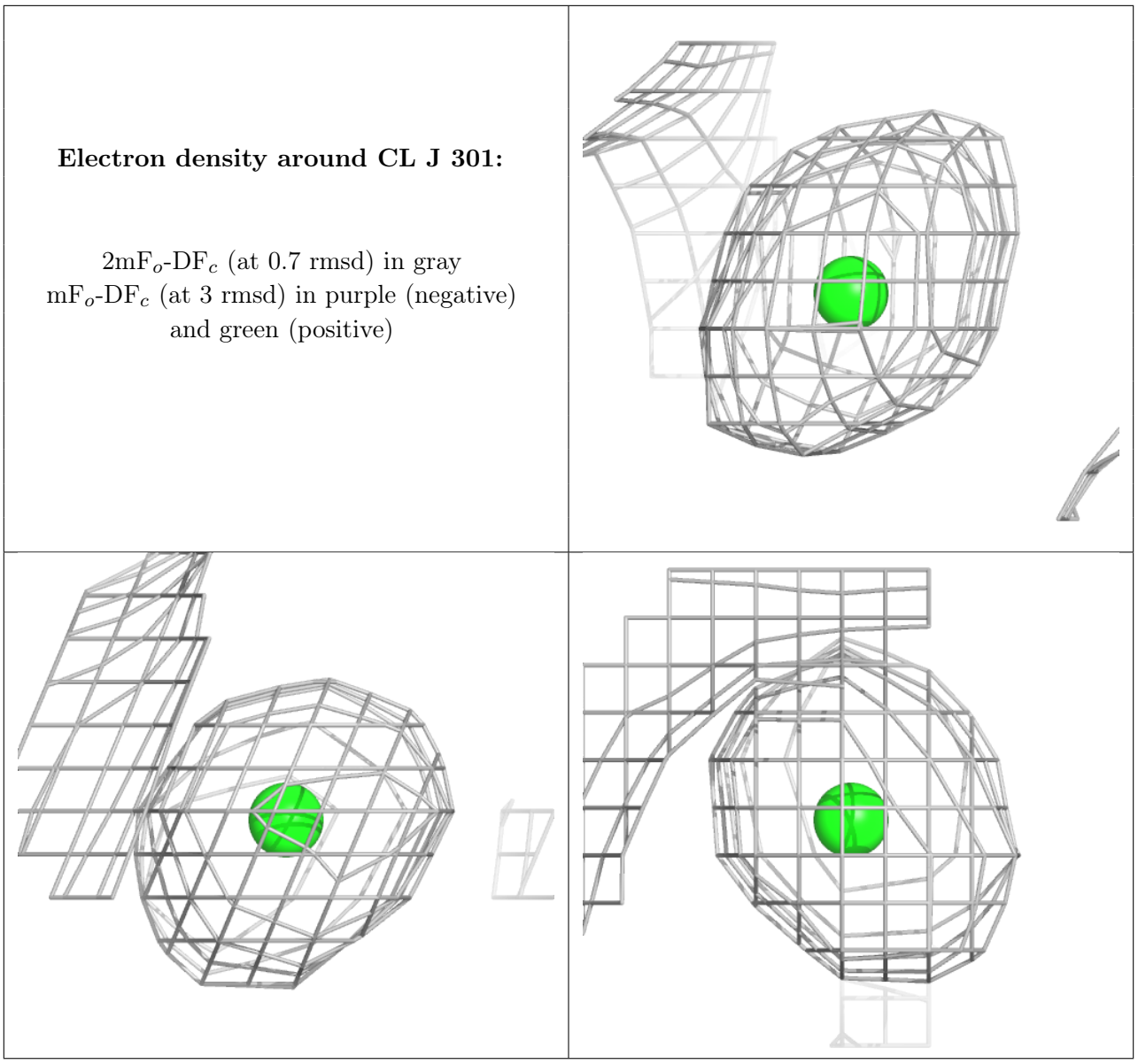
Electron density around CL I 302:

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



Electron density around CL J 301:

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



Electron density around CL H 301:

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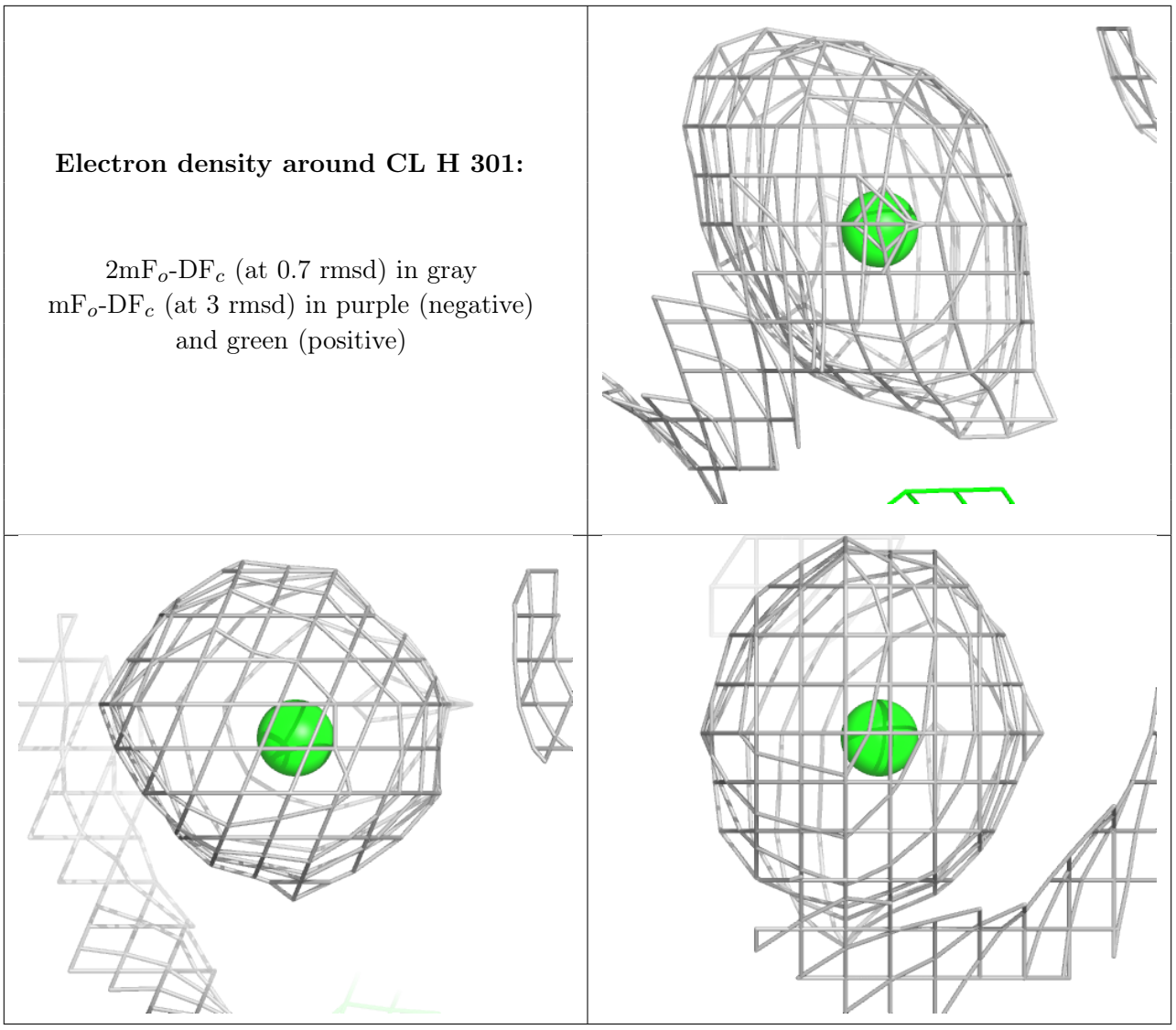
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CL J 302:

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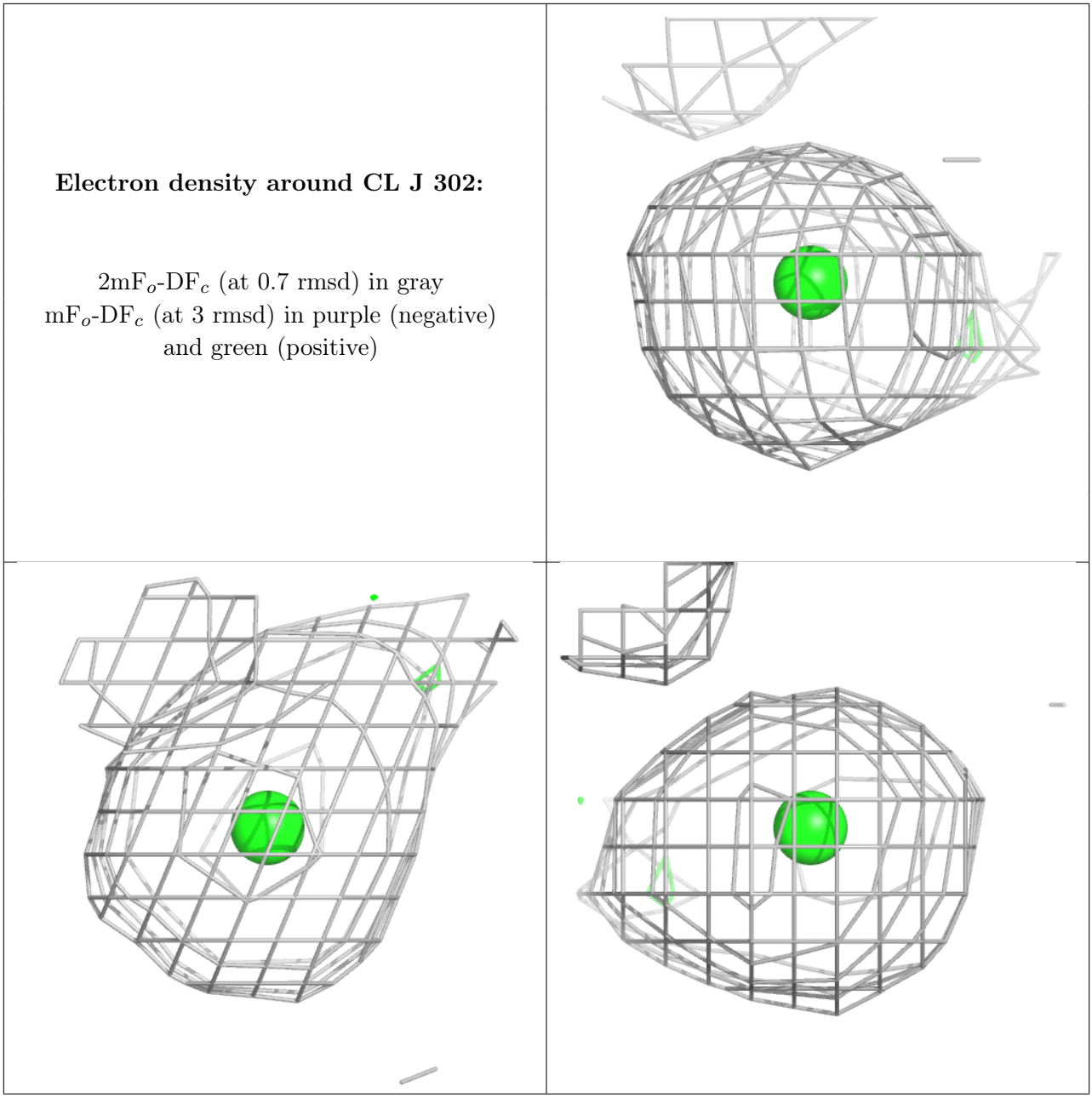
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CL E 301:

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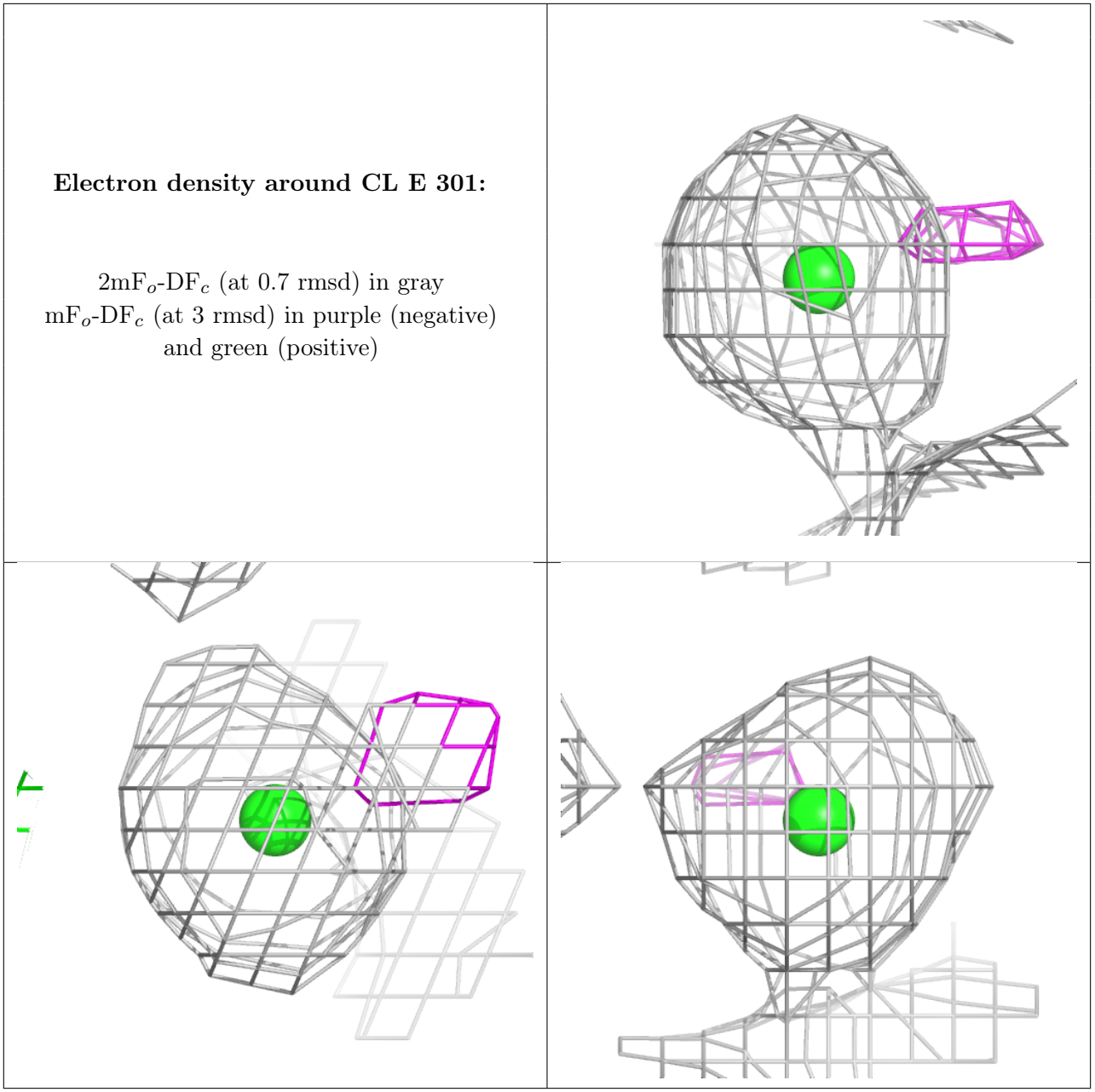
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CL B 301:

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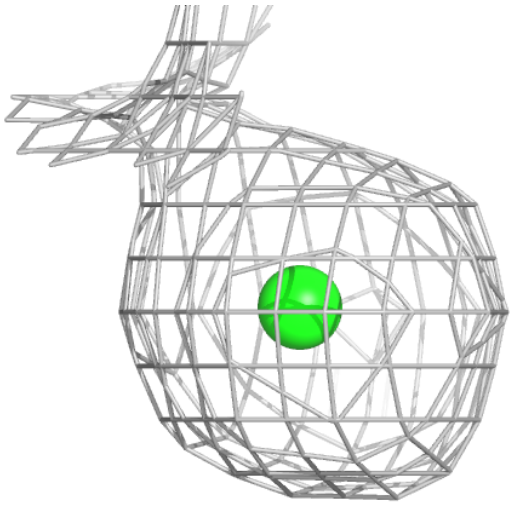
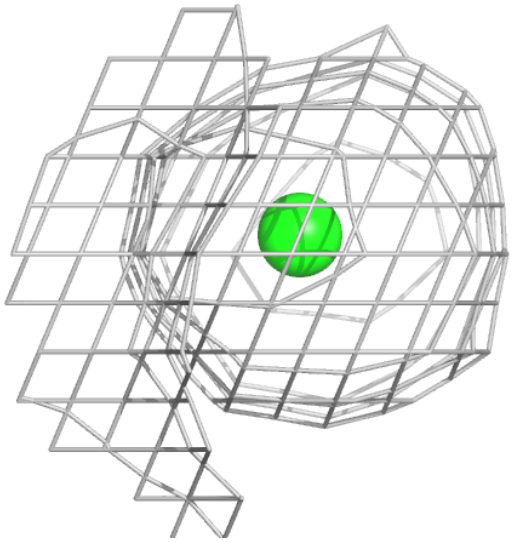
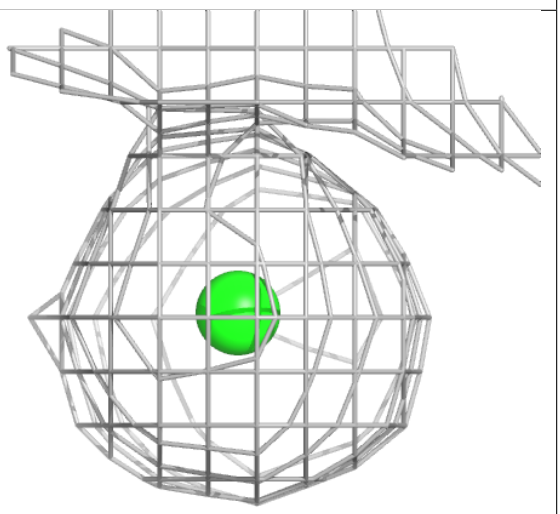
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around CL G 302:

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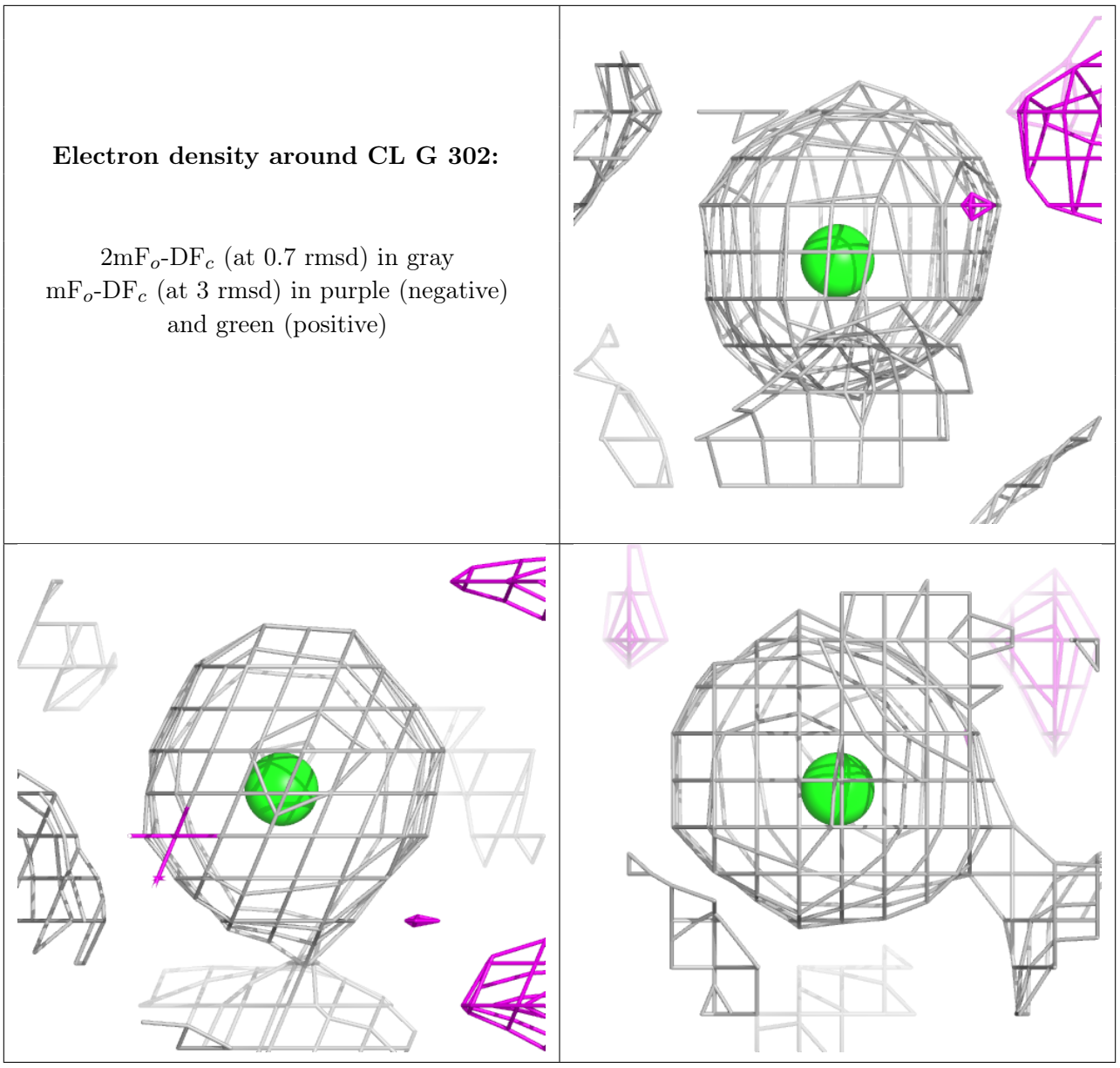
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CL I 303:

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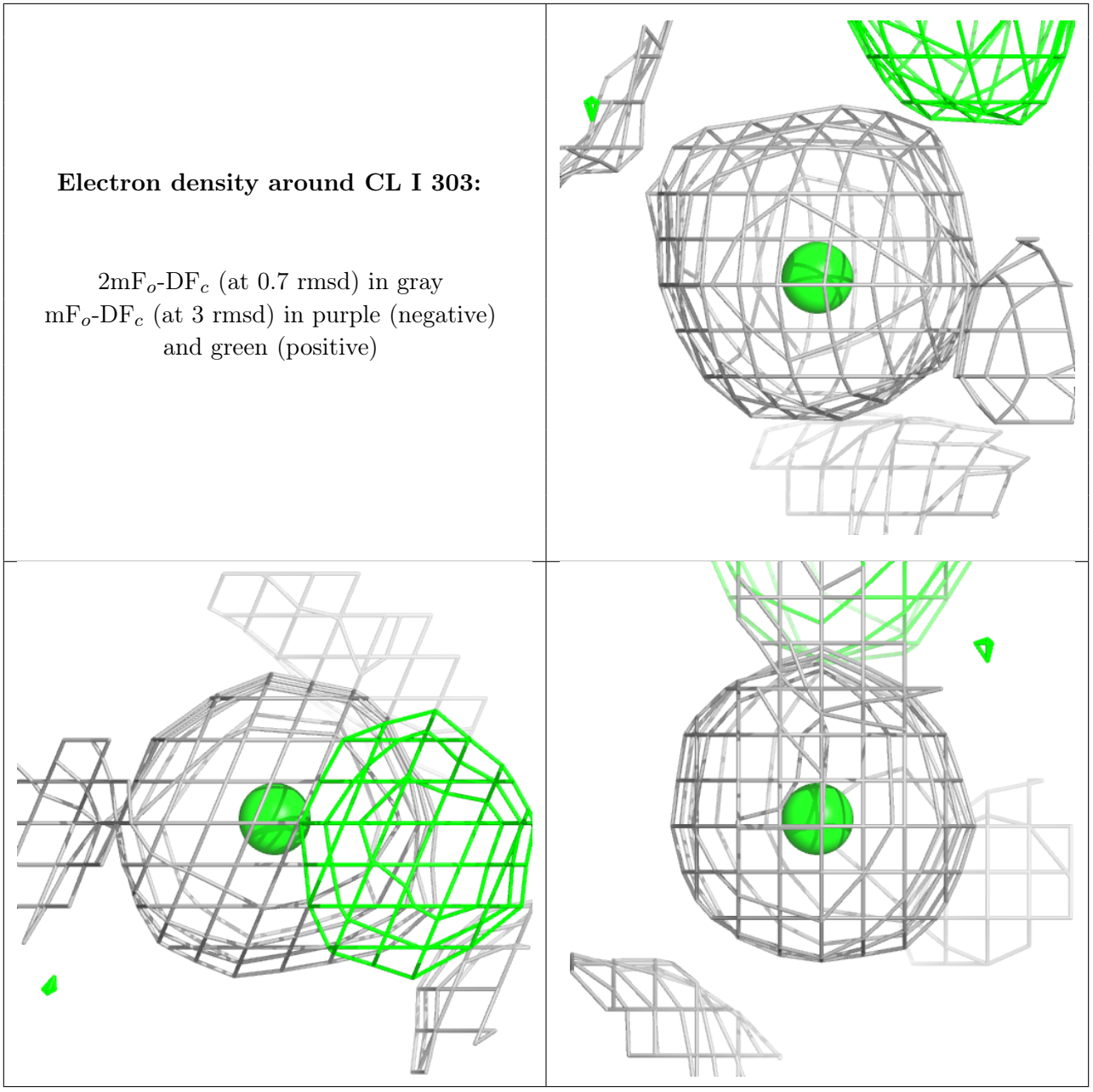
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CL E 302:

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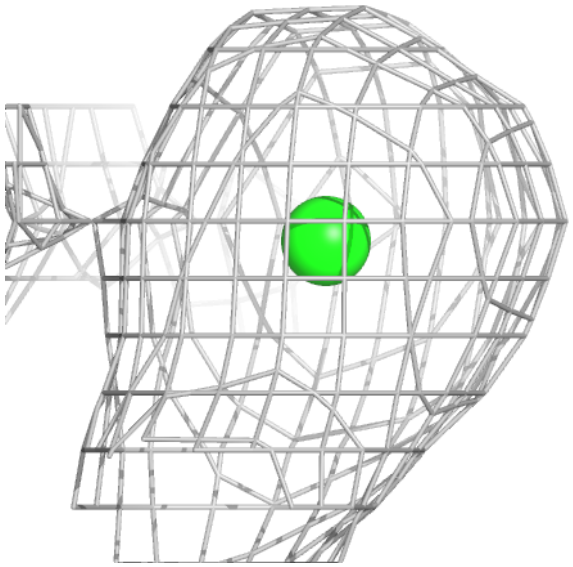
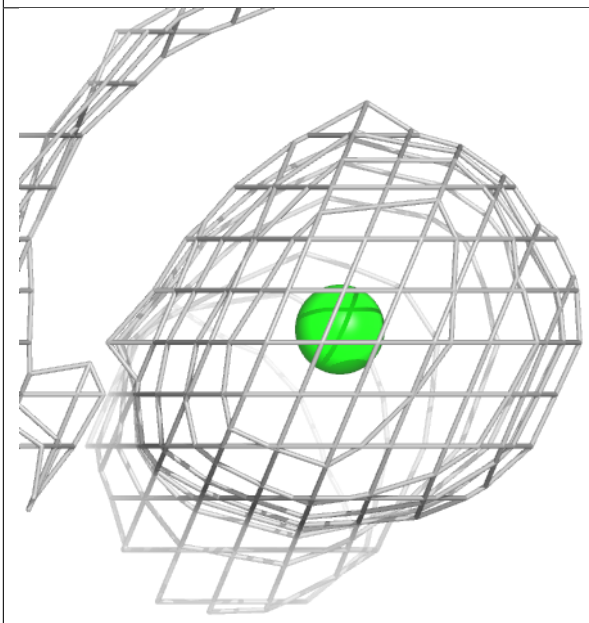
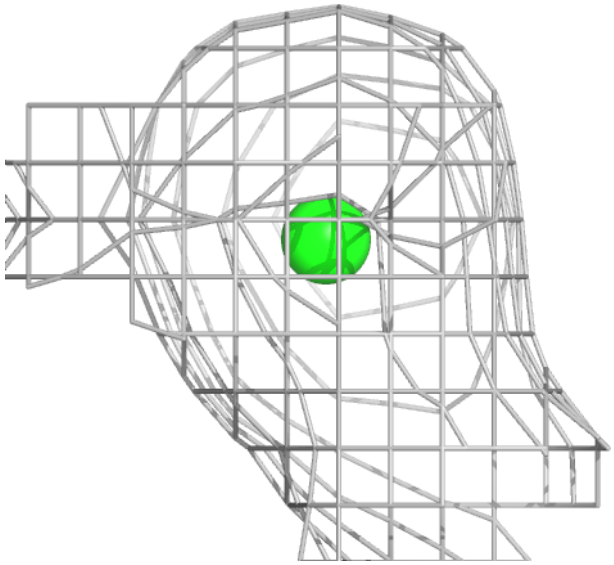
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around CL G 301:

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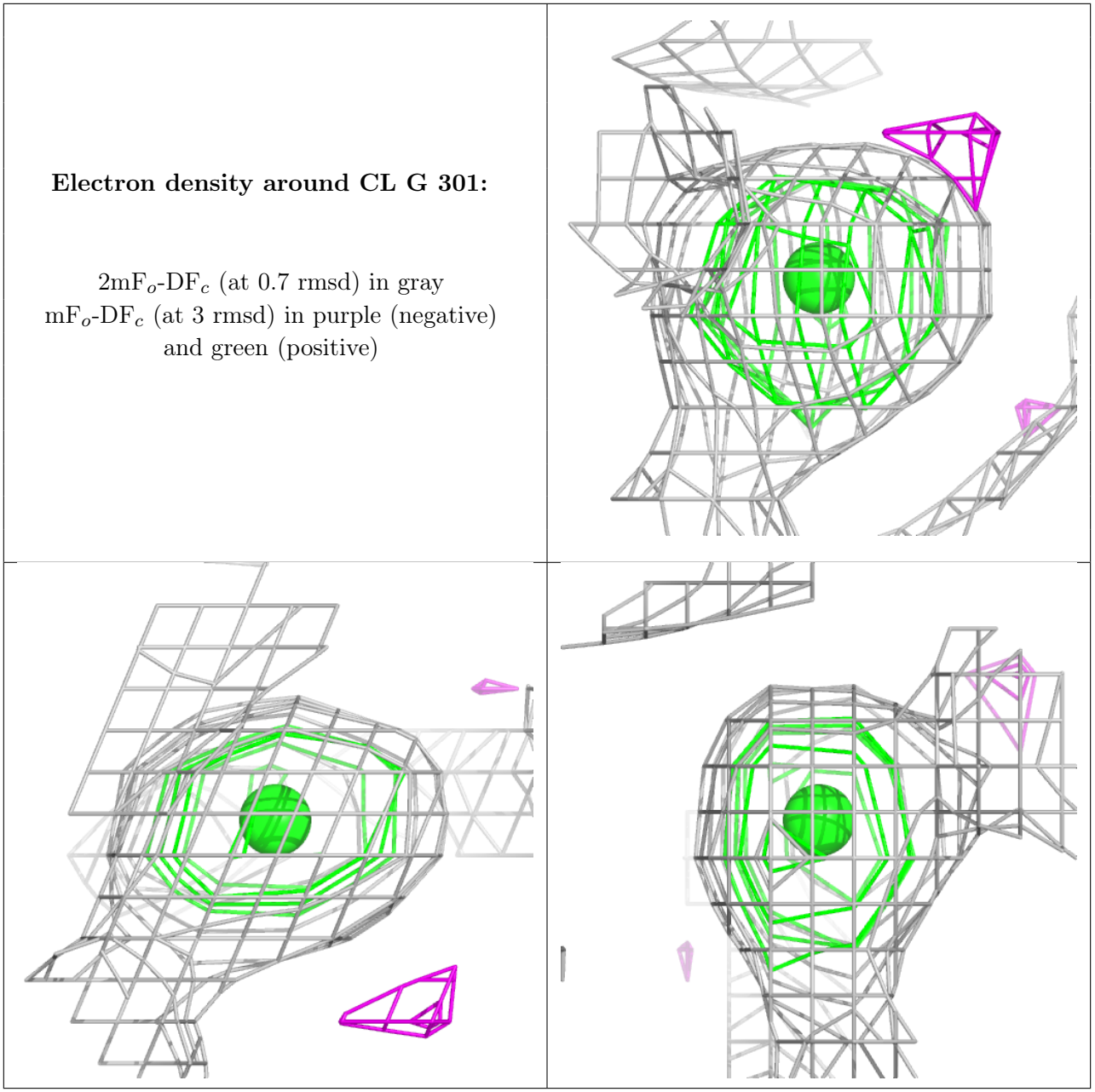
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SO4 I 301:

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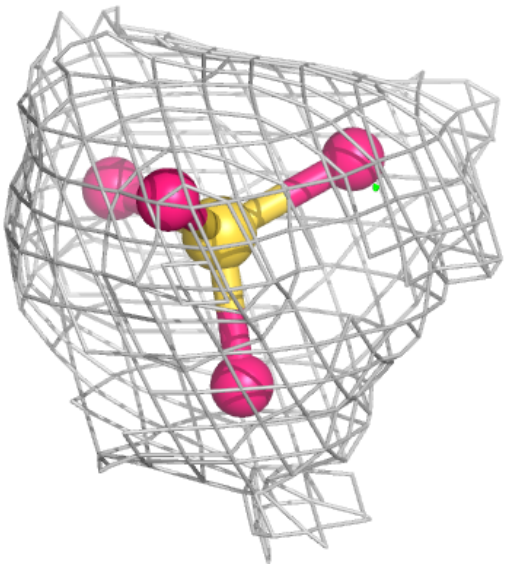
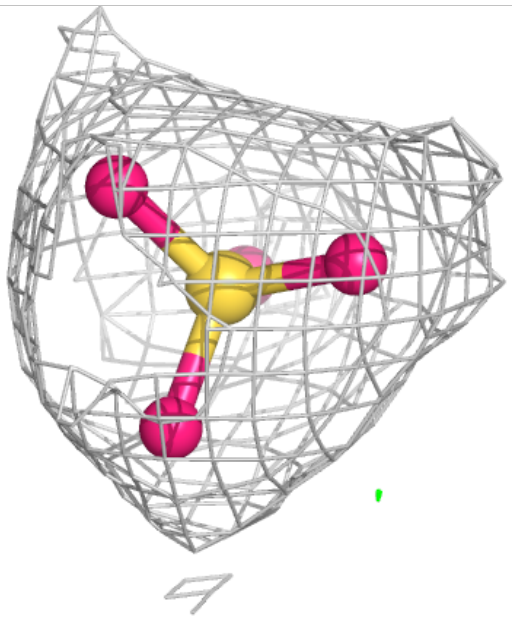
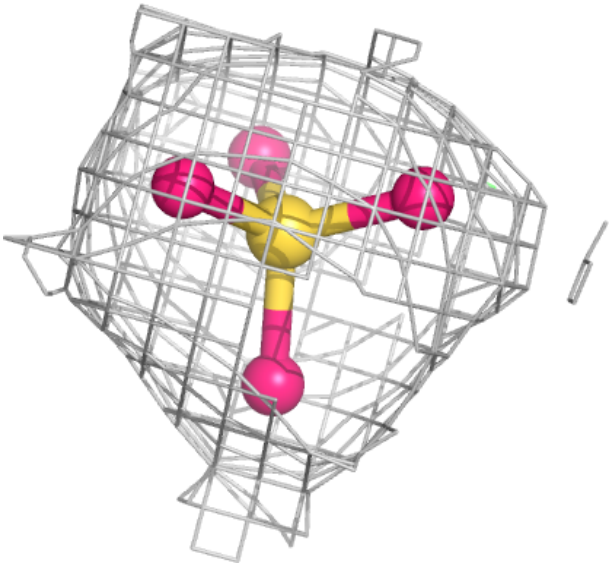
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

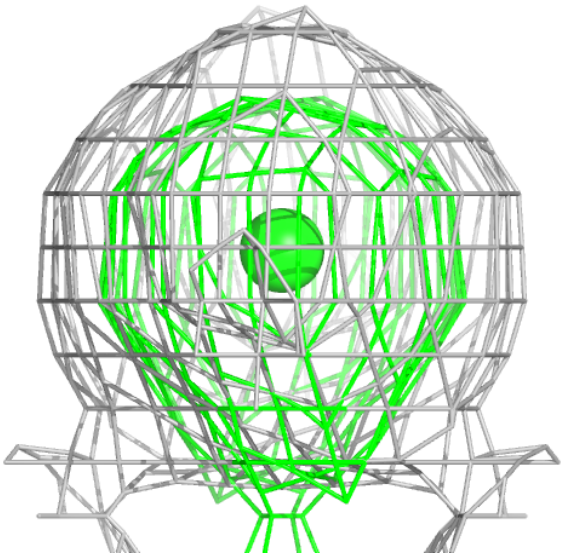


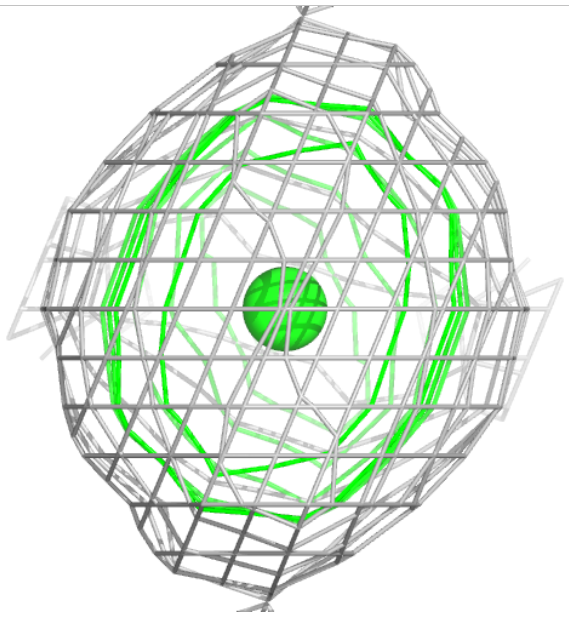


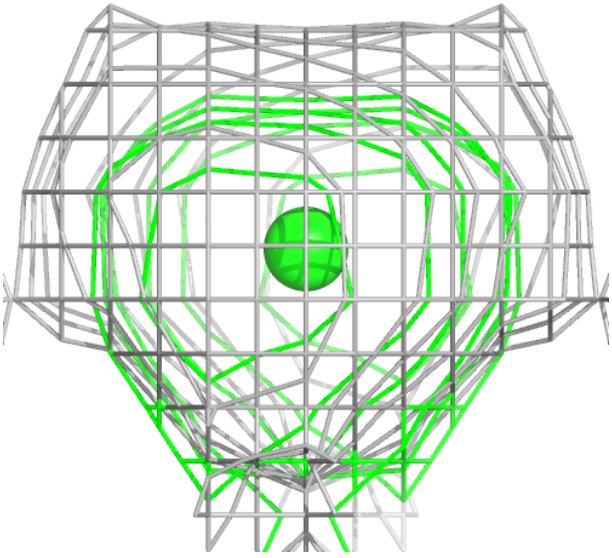


Electron density around CL H 302:

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

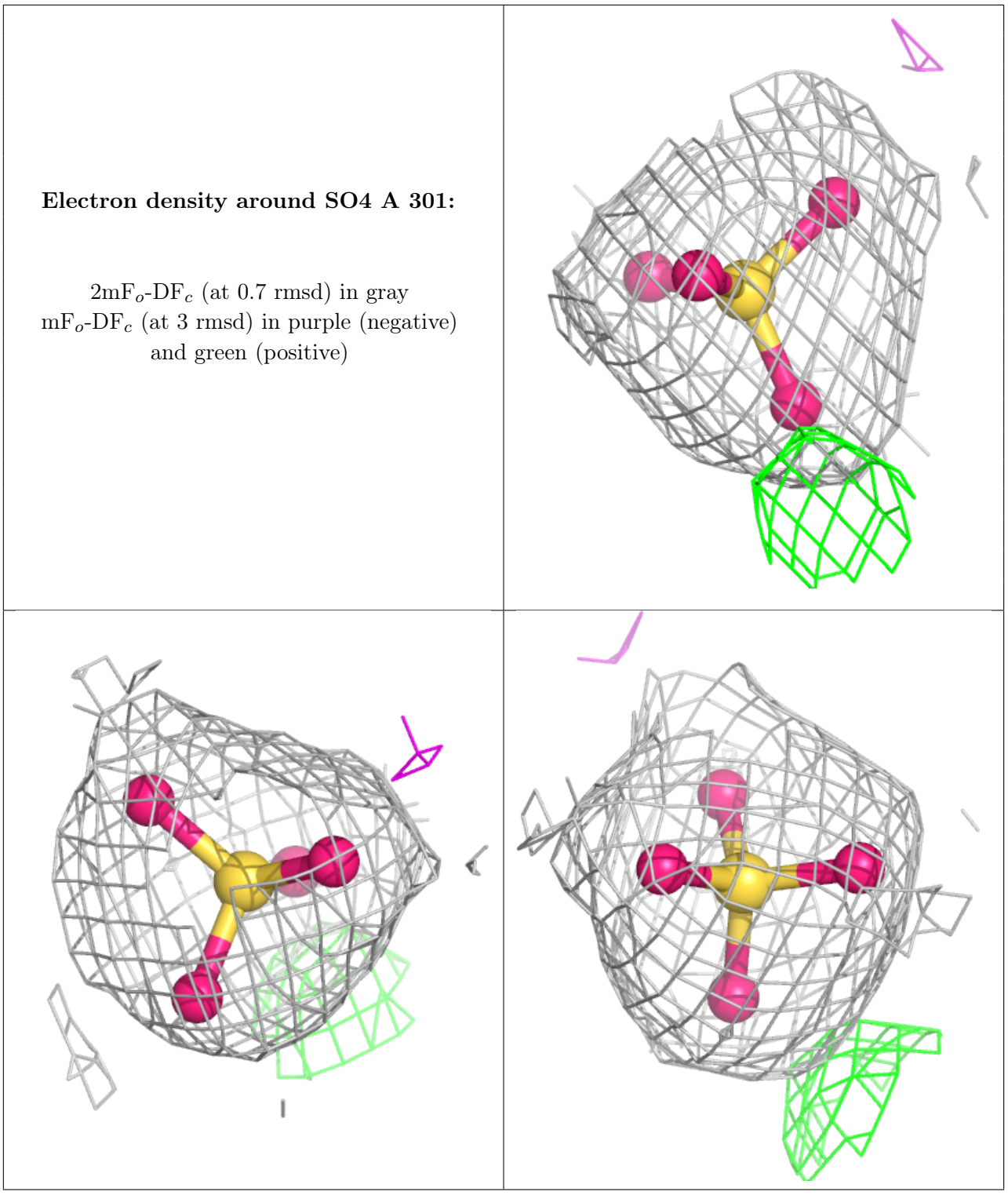






Electron density around SO4 A 301:

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



6.5 Other polymers

There are no such residues in this entry.