Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2025 – 06:33 PM JST

PDB ID	:	9V59 / pdb_00009v59
Title	:	Crystal structure of calcium indicator WHaloCaMP1a labeled with BD566-HTL substrate
Authors	:	Zhang, K.; Chen, Z.X.
Deposited on	:	2025-05-25
Resolution	:	2.17 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:

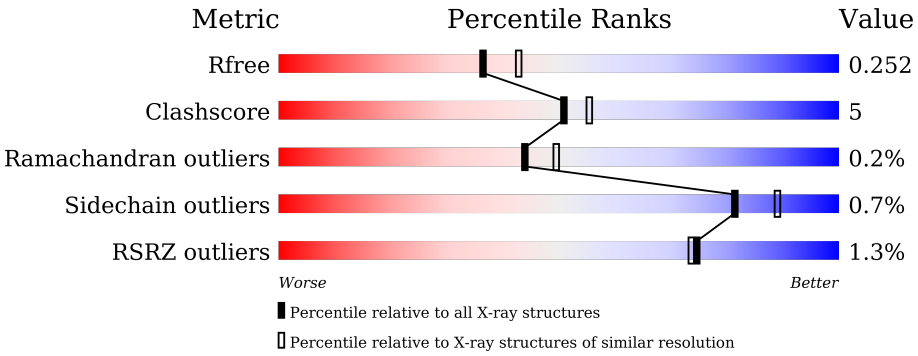
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

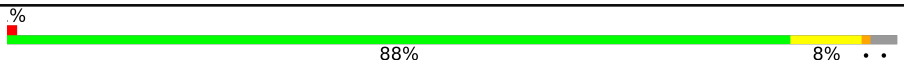
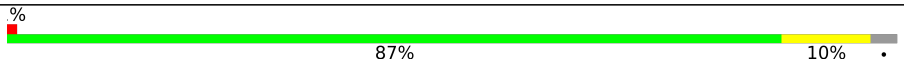
The reported resolution of this entry is 2.17 Å.

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}	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (2.20-2.16)

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	474	
1	B	474	

2 Entry composition

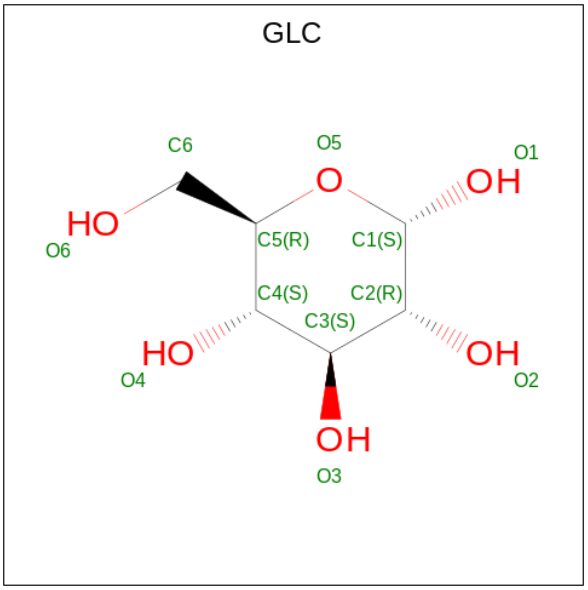
There are 6 unique types of molecules in this entry. The entry contains 7736 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 WHaloCaMP1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	1	0
			3595	2298	608	671	18			
1	B	462	Total	C	N	O	S	0	1	0
			3595	2298	608	671	18			

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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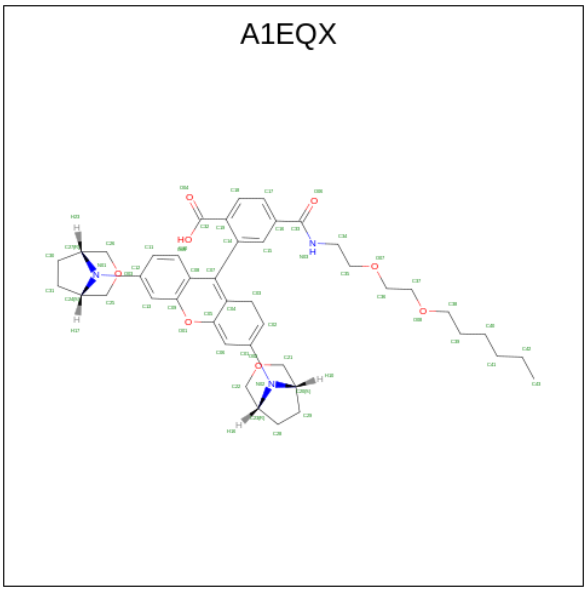
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Ca 4 4	0	0
3	B	4	Total Ca 4 4	0	0

- Molecule 4 is 2-[3,6-bis[(1R,5S)-3-oxa-8-azabicyclo[3.2.1]octan-8-yl]-1H-xanthen-9-yl]-4-[2-(2-hexoxyethoxy)ethylcarbamoyl]benzoic acid (CCD ID: A1EQX) (formula: $C_{43}H_{53}N_3O_8$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 54 43 3 8	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			54	43	3	8		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

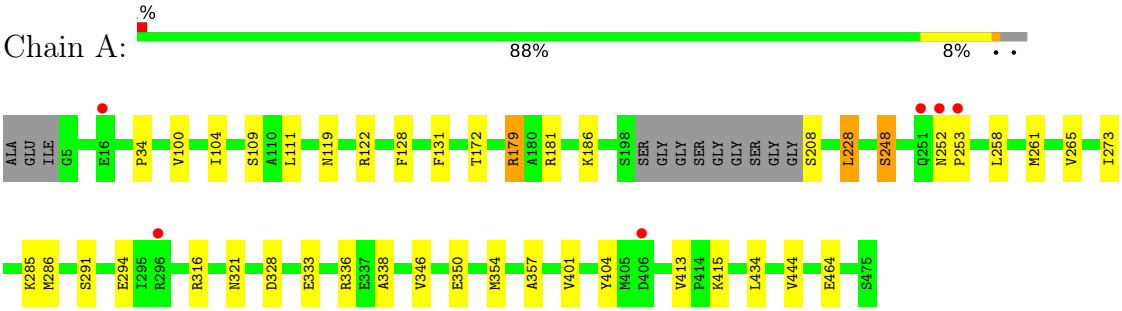
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	197	Total	O	0	0
			197	197		
6	B	195	Total	O	0	0
			195	195		

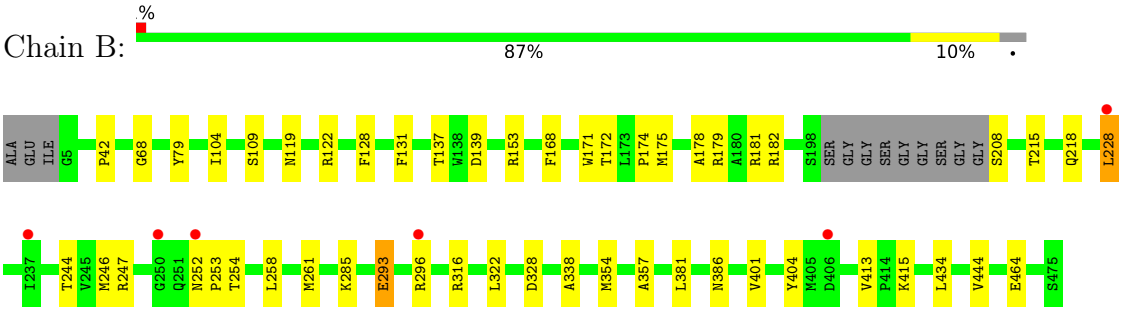
3 Residue-property plots (i)

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: WHaloCaMP1a



• Molecule 1: WHaloCaMP1a



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.94Å 94.18Å 76.04Å 90.00° 101.34° 90.00°	Depositor
Resolution (Å)	32.80 – 2.17 32.80 – 2.17	Depositor EDS
% Data completeness (in resolution range)	93.0 (32.80-2.17) 92.9 (32.80-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.16_3549: ???	Depositor
R, R_{free}	0.205 , 0.255 0.204 , 0.252	Depositor DCC
R_{free} test set	43010 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	1.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 95.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2908e-09. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GLC, CL, A1EQX

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	0.36	0/3693	0.57	1/5032 (0.0%)
1	B	0.37	0/3693	0.56	0/5032
All	All	0.37	0/7386	0.57	1/10064 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	ASN	CB-CA-C	6.92	119.35	109.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3595	0	3401	25	0
1	B	3595	0	3401	36	0
2	A	20	0	15	2	0
2	B	16	0	12	4	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	54	0	0	6	0
4	B	54	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	197	0	0	1	0
6	B	195	0	0	2	0
All	All	7736	0	6829	72	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 5.

All (72) 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)
4:A:608:A1EQX:C21	4:A:608:A1EQX:O02	1.80	1.28
4:B:706:A1EQX:O02	4:B:706:A1EQX:C22	1.81	1.28
4:B:706:A1EQX:O02	4:B:706:A1EQX:C21	1.80	1.27
4:A:608:A1EQX:C25	4:A:608:A1EQX:O03	1.83	1.27
4:A:608:A1EQX:O02	4:A:608:A1EQX:C22	1.82	1.26
4:A:608:A1EQX:O03	4:A:608:A1EQX:C26	1.82	1.26
4:B:706:A1EQX:C26	4:B:706:A1EQX:O03	1.81	1.25
4:B:706:A1EQX:O03	4:B:706:A1EQX:C25	1.83	1.24
1:B:137:THR:HG22	1:B:139:ASP:H	1.26	0.99
1:B:338:ALA:HA	1:B:354:MET:HE3	1.64	0.80
1:A:338:ALA:HA	1:A:354:MET:HE3	1.68	0.73
1:B:228:LEU:HD11	1:B:322:LEU:O	1.90	0.70
1:A:286:MET:HE3	1:A:291:SER:HA	1.76	0.67
1:A:444:VAL:HG21	1:A:464:GLU:HG2	1.79	0.64
1:B:413:VAL:O	1:B:415:LYS:NZ	2.33	0.62
1:A:179:ARG:HD3	1:A:333:GLU:OE1	2.00	0.61
1:B:444:VAL:HG21	1:B:464:GLU:HG2	1.82	0.60
1:B:338:ALA:HA	1:B:354:MET:CE	2.33	0.59
1:B:316[B]:ARG:NH2	1:B:328:ASP:OD1	2.36	0.58
1:B:247:ARG:HA	1:B:252:ASN:OD1	2.04	0.58
1:B:228:LEU:HD21	1:B:322:LEU:O	2.04	0.57
1:A:181:ARG:HD3	1:A:357:ALA:O	2.05	0.56
1:B:181:ARG:HD3	1:B:357:ALA:O	2.05	0.55
1:B:244:THR:HA	2:B:709:GLC:H62	1.89	0.55
1:B:104:ILE:HB	1:B:109:SER:HA	1.88	0.54
1:A:104:ILE:HB	1:A:109:SER:HA	1.88	0.54
1:B:137:THR:HG22	1:B:139:ASP:N	2.08	0.54
1:B:258:LEU:HA	1:B:261:MET:HE3	1.91	0.52
1:A:413:VAL:O	1:A:415:LYS:NZ	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:PHE:HE1	1:A:415:LYS:HB3	1.76	0.49
1:A:316[B]:ARG:NH2	1:A:328:ASP:OD1	2.39	0.49
1:B:293:GLU:HG2	1:B:296:ARG:NH1	2.28	0.49
1:B:254:THR:O	1:B:258:LEU:HG	2.13	0.48
1:B:293:GLU:HG2	1:B:296:ARG:HH12	1.77	0.48
1:A:286:MET:HE1	1:A:294:GLU:CD	2.38	0.48
1:B:208:SER:HA	1:B:285:LYS:O	2.13	0.48
1:A:186:LYS:HE2	1:A:228:LEU:HD22	1.95	0.48
1:B:215:THR:OG1	1:B:218:GLN:HG3	2.14	0.48
1:B:252:ASN:HB3	6:B:852:HOH:O	2.13	0.47
1:A:131:PHE:HZ	1:A:434:LEU:HD13	1.80	0.47
1:B:246:MET:HE3	1:B:261:MET:HE1	1.97	0.47
1:B:178:ALA:O	2:B:710:GLC:H62	2.15	0.47
1:B:172:THR:HG23	4:B:706:A1EQX:C34	2.46	0.46
1:B:182:ARG:HG3	2:B:710:GLC:H61	1.97	0.46
1:B:131:PHE:HZ	1:B:434:LEU:HD13	1.80	0.45
1:B:119:ASN:HB3	1:B:122:ARG:HD3	1.97	0.45
1:A:172:THR:HG23	4:A:608:A1EQX:C34	2.46	0.45
1:A:34:PRO:HG2	1:A:100:VAL:HG12	1.98	0.44
4:A:608:A1EQX:C21	4:A:608:A1EQX:C22	2.95	0.44
1:A:401:VAL:HG13	1:A:404:TYR:CZ	2.53	0.44
1:B:153:ARG:HA	1:B:386:ASN:OD1	2.17	0.44
1:B:401:VAL:HG13	1:B:404:TYR:CZ	2.53	0.44
1:A:265:VAL:HG21	1:A:273:ILE:HD13	1.99	0.44
1:A:286:MET:HE3	1:A:291:SER:CA	2.47	0.43
1:A:248:SER:HB2	1:A:321:ASN:O	2.19	0.43
1:A:346:VAL:HA	1:A:350:GLU:OE1	2.18	0.43
1:A:119:ASN:HB3	1:A:122:ARG:HD3	1.99	0.43
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.89	0.42
1:B:171:TRP:O	1:B:174:PRO:HD2	2.19	0.42
1:B:179:ARG:HG2	6:B:812:HOH:O	2.19	0.42
1:A:336:ARG:NE	2:A:602:GLC:O6	2.53	0.42
1:B:42:PRO:HB3	1:B:381:LEU:HD22	2.02	0.42
4:B:706:A1EQX:C22	4:B:706:A1EQX:C21	2.97	0.42
1:B:42:PRO:HG3	1:B:168:PHE:CD1	2.55	0.41
1:B:175:MET:HA	2:B:710:GLC:C5	2.50	0.41
1:B:128:PHE:HE1	1:B:415:LYS:HB3	1.84	0.41
1:B:68:GLY:HA3	1:B:79:TYR:CE1	2.56	0.41
1:A:258:LEU:HA	1:A:261:MET:HE3	2.02	0.41
1:B:171:TRP:C	1:B:174:PRO:HD2	2.46	0.40
1:A:208:SER:HA	1:A:285:LYS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HA	1:A:228:LEU:HD12	1.80	0.40
2:A:601:GLC:H61	6:A:754:HOH:O	2.21	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	459/474 (97%)	443 (96%)	15 (3%)	1 (0%)	44 49
1	B	459/474 (97%)	444 (97%)	14 (3%)	1 (0%)	44 49
All	All	918/948 (97%)	887 (97%)	29 (3%)	2 (0%)	44 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	PRO
1	B	253	PRO

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	369/399 (92%)	366 (99%)	3 (1%)	79 87
1	B	369/399 (92%)	367 (100%)	2 (0%)	86 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	738/798 (92%)	733 (99%)	5 (1%)	81 89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	ARG
1	A	228	LEU
1	A	248	SER
1	B	228	LEU
1	B	293	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	374	ASN
1	B	345	GLN
1	B	367	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 10 are monoatomic - leaving 11 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	A1EQX	A	608	-	60,61,61	7.22	44 (73%)	70,86,86	1.95	17 (24%)
2	GLC	B	709	-	3,3,12	0.47	0	2,2,17	0.43	0
2	GLC	B	710	-	3,3,12	0.55	0	2,2,17	0.22	0
4	A1EQX	B	706	-	60,61,61	7.21	46 (76%)	70,86,86	2.02	19 (27%)
2	GLC	B	701	-	3,3,12	0.54	0	2,2,17	0.07	0
2	GLC	A	602	-	3,3,12	0.49	0	2,2,17	0.43	0
2	GLC	A	610	-	3,3,12	0.50	0	2,2,17	0.61	0
2	GLC	A	601	-	3,3,12	0.55	0	2,2,17	0.12	0
2	GLC	A	611	-	3,3,12	0.40	0	2,2,17	0.46	0
2	GLC	B	708	-	3,3,12	0.44	0	2,2,17	0.65	0
2	GLC	A	603	-	3,3,12	0.44	0	2,2,17	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A1EQX	A	608	-	-	9/33/96/96	0/10/8/8
2	GLC	B	709	-	-	1/1/1/22	-
2	GLC	B	710	-	-	1/1/1/22	-
4	A1EQX	B	706	-	-	9/33/96/96	0/10/8/8
2	GLC	B	701	-	-	0/1/1/22	-
2	GLC	A	602	-	-	1/1/1/22	-
2	GLC	A	610	-	-	0/1/1/22	-
2	GLC	A	601	-	-	0/1/1/22	-
2	GLC	A	611	-	-	0/1/1/22	-
2	GLC	B	708	-	-	1/1/1/22	-
2	GLC	A	603	-	-	1/1/1/22	-

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	706	A1EQX	O03-C25	21.10	1.83	1.42
4	A	608	A1EQX	O03-C25	20.86	1.83	1.42
4	A	608	A1EQX	O03-C26	20.31	1.82	1.42
4	A	608	A1EQX	O02-C22	20.16	1.82	1.42
4	B	706	A1EQX	O02-C22	20.09	1.81	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	706	A1EQX	O03-C26	19.99	1.81	1.42
4	B	706	A1EQX	O02-C21	19.50	1.80	1.42
4	A	608	A1EQX	O02-C21	19.29	1.80	1.42
4	A	608	A1EQX	C18-C19	15.17	1.64	1.39
4	B	706	A1EQX	C18-C19	15.00	1.63	1.39
4	A	608	A1EQX	C15-C14	12.72	1.59	1.39
4	B	706	A1EQX	C17-C16	12.68	1.61	1.39
4	A	608	A1EQX	C17-C16	12.54	1.60	1.39
4	B	706	A1EQX	C15-C14	12.38	1.59	1.39
4	A	608	A1EQX	C07-C04	12.17	1.46	1.35
4	B	706	A1EQX	C07-C04	11.88	1.46	1.35
4	A	608	A1EQX	C14-C07	11.53	1.65	1.49
4	B	706	A1EQX	C14-C07	11.41	1.64	1.49
4	B	706	A1EQX	C33-N03	8.82	1.53	1.33
4	A	608	A1EQX	C33-N03	8.56	1.52	1.33
4	B	706	A1EQX	C01-N02	7.84	1.59	1.36
4	A	608	A1EQX	C01-N02	7.80	1.59	1.36
4	B	706	A1EQX	O01-C05	6.18	1.48	1.37
4	A	608	A1EQX	O01-C05	6.08	1.48	1.37
4	B	706	A1EQX	C12-N01	5.99	1.53	1.40
4	A	608	A1EQX	O01-C09	5.95	1.47	1.38
4	A	608	A1EQX	C12-N01	5.83	1.53	1.40
4	A	608	A1EQX	C16-C33	5.70	1.62	1.50
4	B	706	A1EQX	C16-C33	5.41	1.61	1.50
4	B	706	A1EQX	O01-C09	5.40	1.46	1.38
4	B	706	A1EQX	C19-C32	5.39	1.61	1.49
4	A	608	A1EQX	C19-C32	5.23	1.60	1.49
4	B	706	A1EQX	C10-C11	4.87	1.47	1.38
4	B	706	A1EQX	C27-N01	-4.85	1.42	1.47
4	A	608	A1EQX	C34-N03	4.83	1.57	1.46
4	A	608	A1EQX	C27-N01	-4.79	1.42	1.47
4	B	706	A1EQX	C34-N03	4.72	1.57	1.46
4	A	608	A1EQX	C10-C11	4.68	1.47	1.38
4	B	706	A1EQX	C13-C09	4.52	1.47	1.38
4	B	706	A1EQX	C34-C35	4.47	1.66	1.50
4	A	608	A1EQX	C34-C35	4.46	1.66	1.50
4	A	608	A1EQX	C02-C01	4.43	1.49	1.35
4	B	706	A1EQX	C21-C20	4.41	1.59	1.51
4	A	608	A1EQX	C21-C20	4.38	1.59	1.51
4	B	706	A1EQX	C02-C01	4.36	1.49	1.35
4	A	608	A1EQX	C10-C08	4.34	1.46	1.39
4	B	706	A1EQX	C10-C08	4.19	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	A1EQX	C13-C09	4.15	1.46	1.38
4	B	706	A1EQX	C06-C05	3.87	1.47	1.36
4	B	706	A1EQX	C31-C30	-3.82	1.43	1.54
4	A	608	A1EQX	C22-C23	3.82	1.58	1.51
4	A	608	A1EQX	C06-C05	3.77	1.46	1.36
4	A	608	A1EQX	C31-C30	-3.73	1.43	1.54
4	B	706	A1EQX	C29-C28	-3.72	1.43	1.54
4	B	706	A1EQX	C22-C23	3.66	1.58	1.51
4	A	608	A1EQX	C29-C28	-3.65	1.44	1.54
4	B	706	A1EQX	C03-C04	-3.59	1.43	1.50
4	A	608	A1EQX	C03-C04	-3.57	1.43	1.50
4	B	706	A1EQX	C25-C24	3.48	1.58	1.51
4	B	706	A1EQX	C39-C38	3.39	1.65	1.51
4	A	608	A1EQX	C25-C24	3.39	1.57	1.51
4	A	608	A1EQX	O04-C32	3.39	1.32	1.22
4	B	706	A1EQX	O04-C32	3.34	1.32	1.22
4	A	608	A1EQX	C39-C38	3.30	1.65	1.51
4	B	706	A1EQX	C11-C12	3.24	1.45	1.39
4	A	608	A1EQX	C11-C12	3.22	1.45	1.39
4	A	608	A1EQX	C26-C27	3.14	1.57	1.51
4	B	706	A1EQX	C13-C12	3.14	1.45	1.39
4	A	608	A1EQX	C13-C12	3.10	1.45	1.39
4	B	706	A1EQX	C30-C27	2.96	1.61	1.53
4	A	608	A1EQX	C30-C27	2.89	1.60	1.53
4	B	706	A1EQX	C06-C01	2.84	1.47	1.40
4	B	706	A1EQX	C26-C27	2.78	1.56	1.51
4	A	608	A1EQX	C06-C01	2.77	1.47	1.40
4	B	706	A1EQX	C08-C09	2.64	1.45	1.40
4	B	706	A1EQX	C37-C36	2.54	1.62	1.49
4	A	608	A1EQX	C20-N02	-2.53	1.44	1.47
4	B	706	A1EQX	O08-C37	2.46	1.52	1.42
4	B	706	A1EQX	C20-N02	-2.46	1.44	1.47
4	A	608	A1EQX	C37-C36	2.36	1.61	1.49
4	A	608	A1EQX	C29-C20	2.34	1.59	1.53
4	B	706	A1EQX	C29-C20	2.32	1.59	1.53
4	A	608	A1EQX	C08-C09	2.24	1.44	1.40
4	A	608	A1EQX	O08-C37	2.23	1.51	1.42
4	B	706	A1EQX	C41-C40	2.21	1.64	1.51
4	B	706	A1EQX	O07-C36	2.17	1.51	1.42
4	B	706	A1EQX	C43-C42	2.17	1.67	1.49
4	B	706	A1EQX	C31-C24	2.08	1.58	1.53
4	A	608	A1EQX	C31-C24	2.06	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	608	A1EQX	C41-C40	2.05	1.63	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	706	A1EQX	C30-C27-N01	6.47	106.42	102.11
4	A	608	A1EQX	C30-C27-N01	6.24	106.27	102.11
4	B	706	A1EQX	C29-C20-N02	5.02	107.32	101.70
4	B	706	A1EQX	C12-N01-C27	4.54	126.18	121.18
4	A	608	A1EQX	C34-N03-C33	-4.41	112.03	122.08
4	A	608	A1EQX	C31-C24-N01	4.35	105.01	102.11
4	A	608	A1EQX	C29-C20-N02	4.33	106.56	101.70
4	B	706	A1EQX	C14-C07-C08	4.32	124.98	119.94
4	B	706	A1EQX	C29-C20-C21	-3.82	108.12	111.64
4	B	706	A1EQX	C31-C24-N01	3.67	104.55	102.11
4	A	608	A1EQX	C12-N01-C24	3.65	125.20	121.18
4	B	706	A1EQX	C34-N03-C33	-3.62	113.82	122.08
4	B	706	A1EQX	O01-C05-C04	3.62	122.98	119.12
4	A	608	A1EQX	C14-C07-C08	3.57	124.11	119.94
4	A	608	A1EQX	O02-C21-C20	-3.50	106.28	110.99
4	A	608	A1EQX	O01-C05-C04	3.43	122.78	119.12
4	A	608	A1EQX	C12-N01-C27	3.34	124.86	121.18
4	A	608	A1EQX	C02-C03-C04	3.30	120.58	112.29
4	B	706	A1EQX	O03-C26-C27	-3.30	106.56	110.99
4	B	706	A1EQX	C02-C03-C04	3.21	120.36	112.29
4	B	706	A1EQX	C28-C23-N02	3.04	105.11	101.70
4	A	608	A1EQX	C15-C14-C07	-2.98	113.92	119.21
4	B	706	A1EQX	C12-N01-C24	2.92	124.40	121.18
4	B	706	A1EQX	C30-C27-C26	-2.76	109.09	111.64
4	B	706	A1EQX	O02-C21-C20	-2.57	107.53	110.99
4	B	706	A1EQX	C15-C14-C07	-2.57	114.66	119.21
4	A	608	A1EQX	C28-C23-N02	2.53	104.53	101.70
4	A	608	A1EQX	O03-C26-C27	-2.46	107.68	110.99
4	B	706	A1EQX	C41-C40-C39	-2.34	102.56	114.42
4	A	608	A1EQX	O02-C22-C23	-2.29	107.91	110.99
4	B	706	A1EQX	C15-C16-C33	-2.27	112.91	120.44
4	A	608	A1EQX	C15-C16-C33	-2.26	112.94	120.44
4	B	706	A1EQX	C17-C16-C15	2.24	121.89	119.24
4	B	706	A1EQX	C28-C23-C22	-2.15	109.65	111.64
4	A	608	A1EQX	C41-C40-C39	-2.03	104.12	114.42
4	A	608	A1EQX	C17-C16-C15	2.01	121.61	119.24

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	608	A1EQX	C02-C01-N02-C20
4	A	608	A1EQX	C14-C07-C08-C10
4	A	608	A1EQX	C04-C07-C08-C10
4	B	706	A1EQX	C02-C01-N02-C20
4	B	706	A1EQX	C14-C07-C08-C10
4	B	706	A1EQX	C04-C07-C08-C10
4	B	706	A1EQX	C36-C37-O08-C38
4	A	608	A1EQX	C36-C37-O08-C38
4	B	706	A1EQX	O07-C36-C37-O08
4	A	608	A1EQX	O07-C36-C37-O08
4	B	706	A1EQX	C37-C36-O07-C35
2	B	710	GLC	O5-C5-C6-O6
4	A	608	A1EQX	C37-C36-O07-C35
4	A	608	A1EQX	C40-C41-C42-C43
2	A	603	GLC	O5-C5-C6-O6
4	A	608	A1EQX	C34-C35-O07-C36
4	B	706	A1EQX	C34-C35-O07-C36
4	B	706	A1EQX	O08-C38-C39-C40
2	B	709	GLC	O5-C5-C6-O6
2	B	708	GLC	O5-C5-C6-O6
4	B	706	A1EQX	C15-C16-C33-N03
4	A	608	A1EQX	C15-C16-C33-N03
2	A	602	GLC	O5-C5-C6-O6

There are no ring outliers.

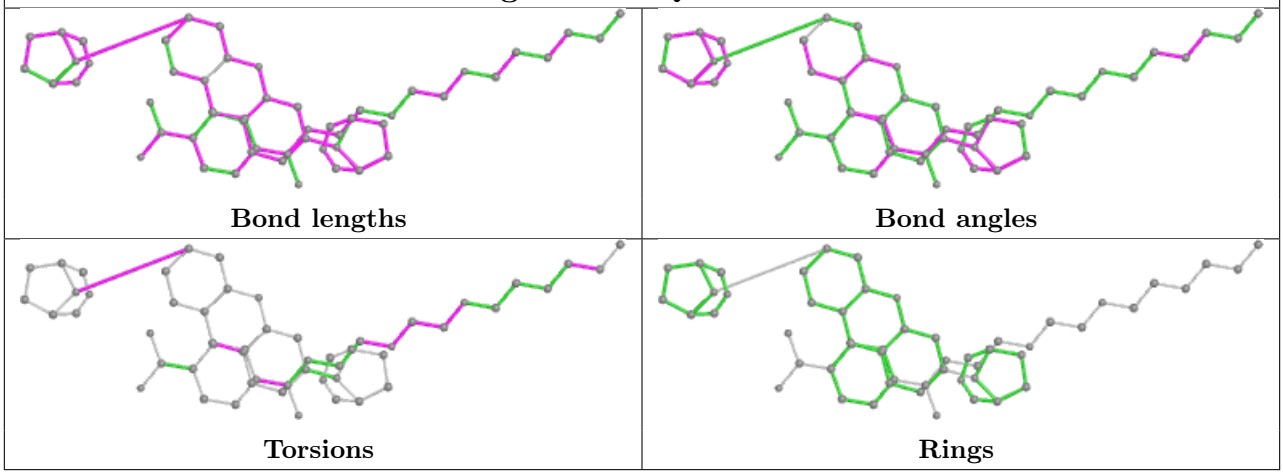
6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	608	A1EQX	6	0
2	B	709	GLC	1	0
2	B	710	GLC	3	0
4	B	706	A1EQX	6	0
2	A	602	GLC	1	0
2	A	601	GLC	1	0

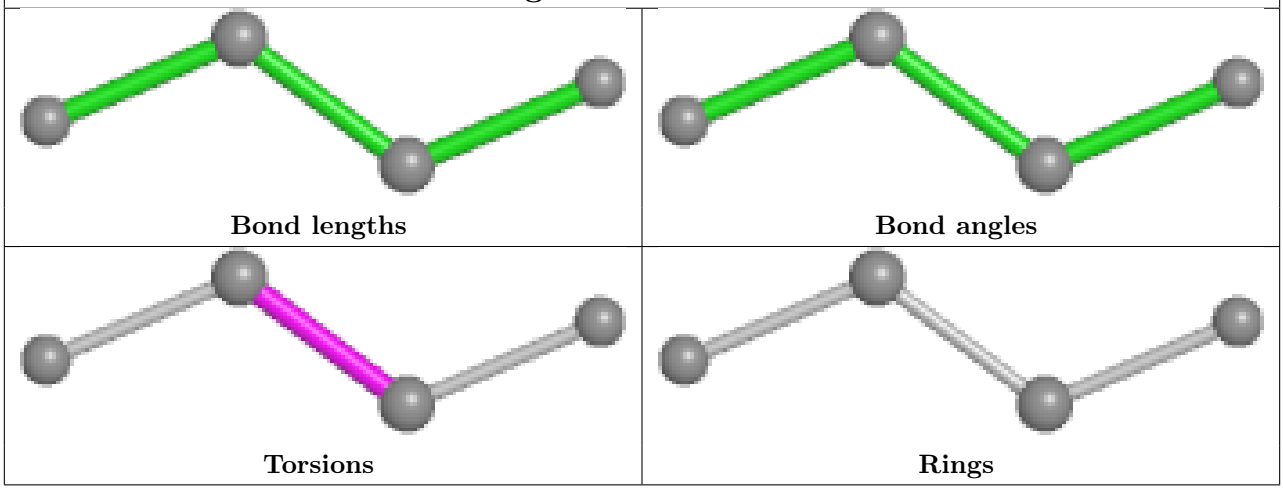
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1EQX A 608



Ligand GLC B 709



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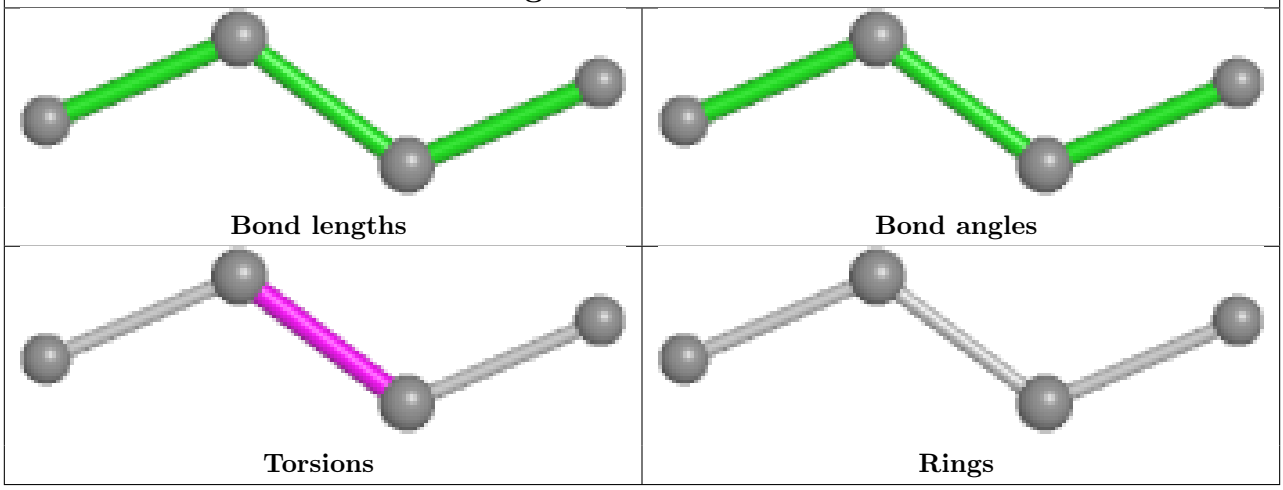
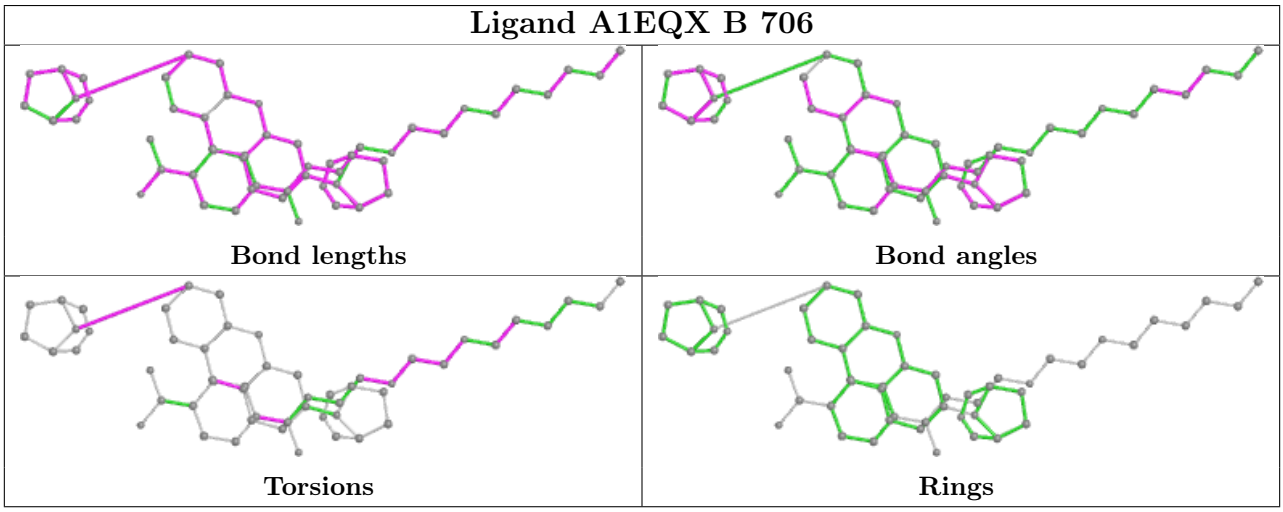


Ligand A1EQX B 706



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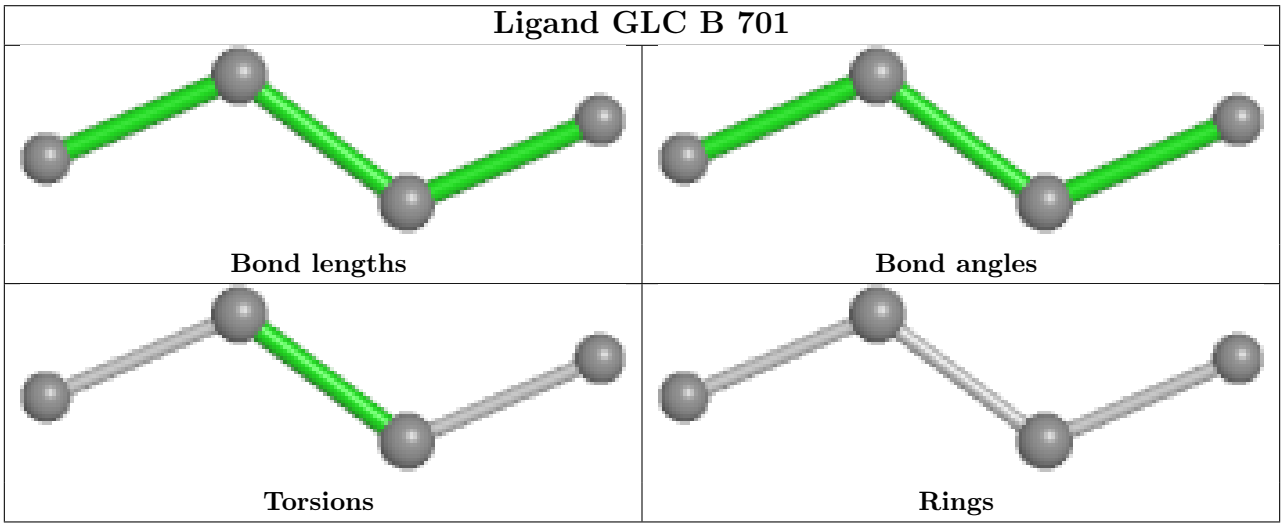
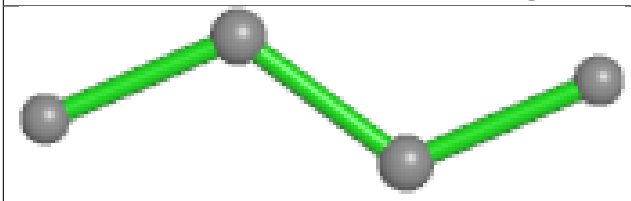
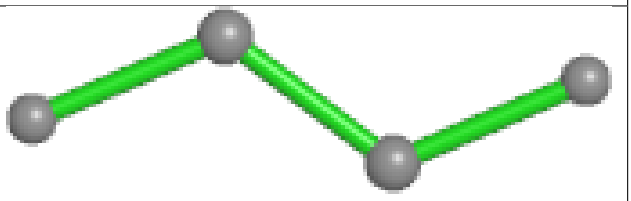


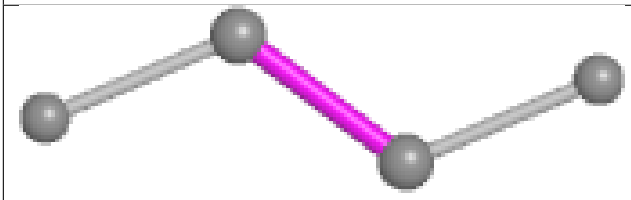
Ligand GLC A 602



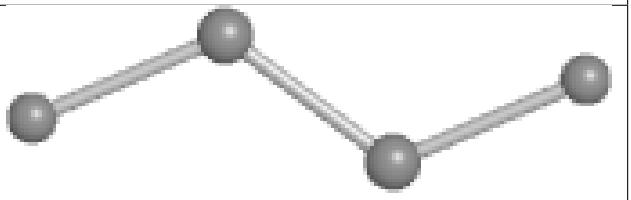
Bond lengths



Bond angles

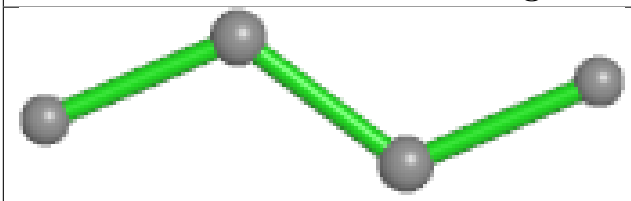


Torsions

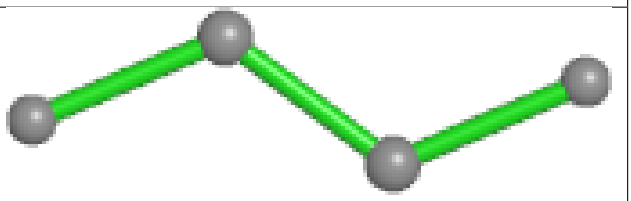


Rings

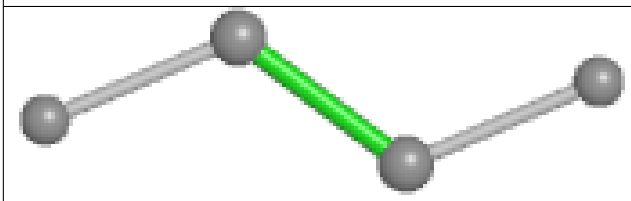
Ligand GLC A 610



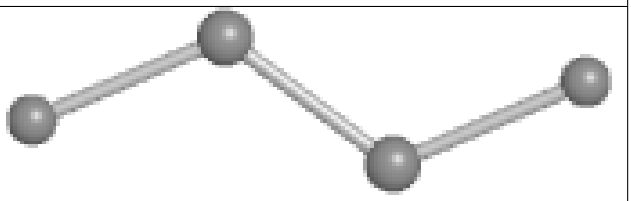
Bond lengths



Bond angles

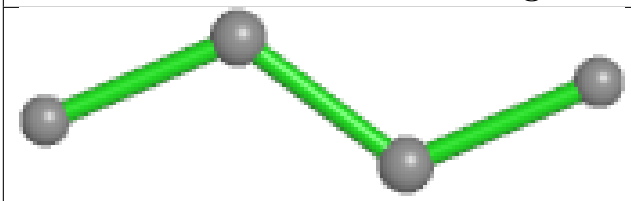


Torsions

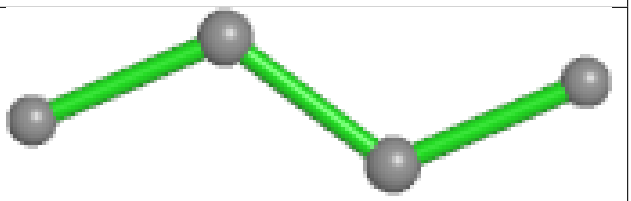


Rings

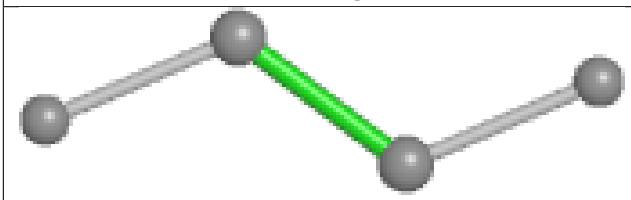
Ligand GLC A 601



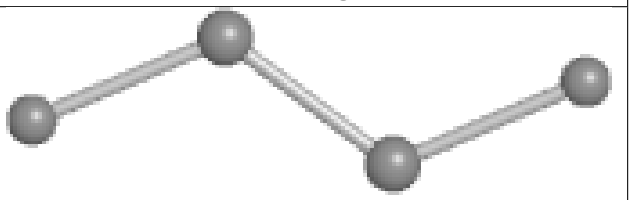
Bond lengths



Bond angles

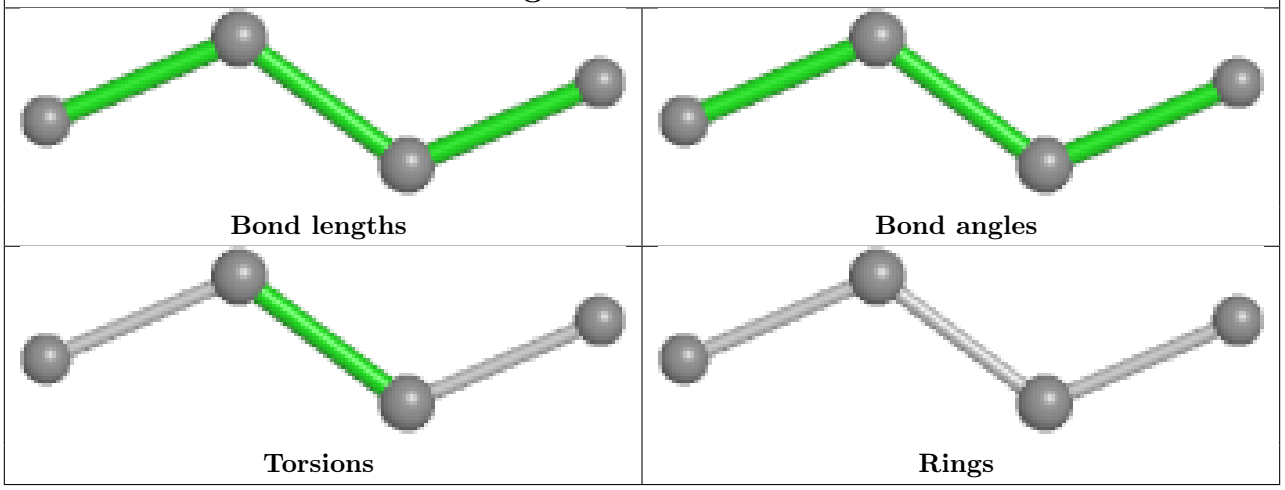


Torsions

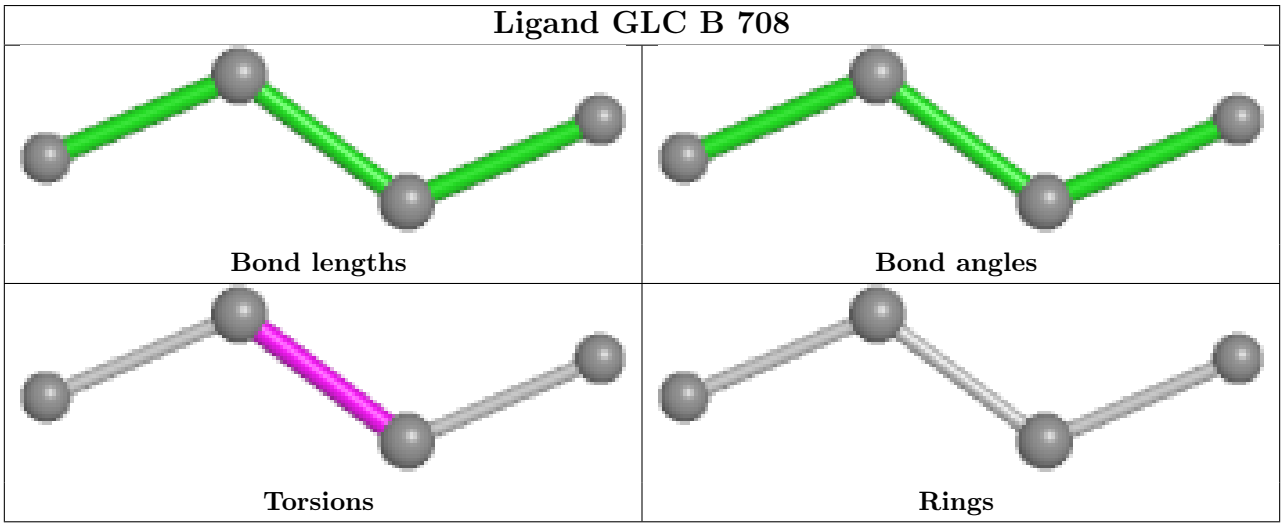


Rings

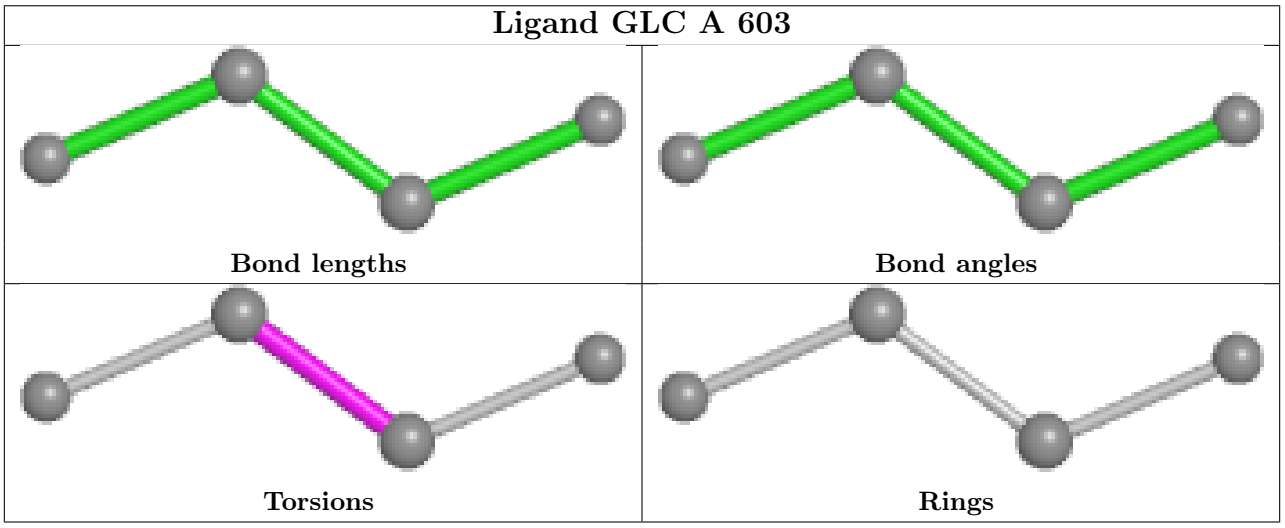
Ligand GLC A 611



Ligand GLC B 708



Ligand GLC A 603



5.7 Other polymers

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	462/474 (97%)	-0.05	6 (1%)	74	73	9, 21, 33, 48	2 (0%)
1	B	462/474 (97%)	-0.13	6 (1%)	74	73	9, 20, 36, 48	1 (0%)
All	All	924/948 (97%)	-0.09	12 (1%)	74	73	9, 21, 34, 48	3 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	ASP	3.7
1	B	228	LEU	3.5
1	A	252	ASN	3.2
1	A	251	GLN	3.0
1	A	296	ARG	2.9
1	A	16	GLU	2.6
1	B	296	ARG	2.5
1	A	406	ASP	2.4
1	B	252	ASN	2.3
1	B	237	ILE	2.3
1	A	253	PRO	2.1
1	B	250	GLY	2.0

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)

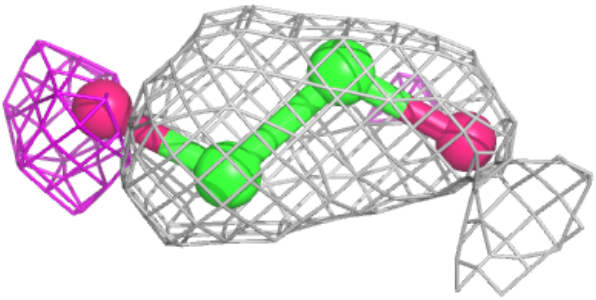
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

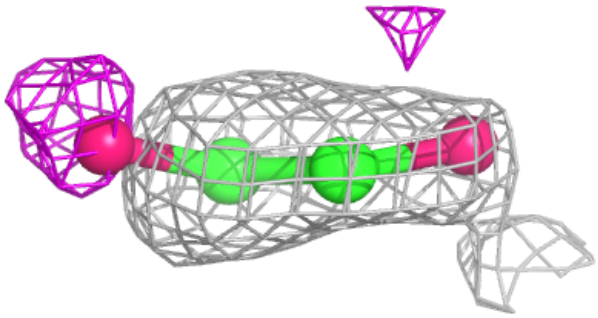
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	A	602	4/12	0.74	0.20	29,29,32,40	0
2	GLC	A	610	4/12	0.76	0.13	22,23,29,29	0
2	GLC	A	603	4/12	0.79	0.18	28,30,33,37	0
2	GLC	A	601	4/12	0.83	0.19	32,34,36,39	0
2	GLC	B	701	4/12	0.83	0.18	34,35,36,38	0
2	GLC	B	710	4/12	0.83	0.17	33,34,35,41	0
2	GLC	B	708	4/12	0.84	0.11	18,20,23,33	0
2	GLC	A	611	4/12	0.88	0.12	28,28,32,35	0
3	CA	A	605	1/1	0.88	0.07	33,33,33,33	0
4	A1EQX	A	608	54/54	0.89	0.10	10,18,30,34	0
4	A1EQX	B	706	54/54	0.89	0.11	14,22,35,38	0
2	GLC	B	709	4/12	0.93	0.11	34,35,35,40	0
3	CA	B	702	1/1	0.95	0.06	39,39,39,39	0
3	CA	B	703	1/1	0.95	0.04	35,35,35,35	0
3	CA	A	607	1/1	0.96	0.06	28,28,28,28	0
3	CA	B	704	1/1	0.96	0.04	27,27,27,27	0
3	CA	A	604	1/1	0.97	0.04	30,30,30,30	0
3	CA	B	705	1/1	0.97	0.05	18,18,18,18	0
3	CA	A	606	1/1	0.98	0.03	32,32,32,32	0
5	CL	A	609	1/1	0.99	0.02	9,9,9,9	0
5	CL	B	707	1/1	0.99	0.09	15,15,15,15	0

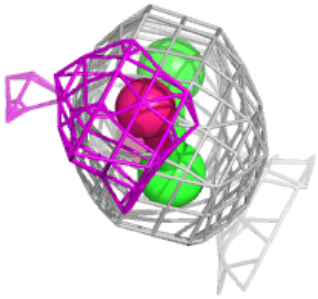
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GLC 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)

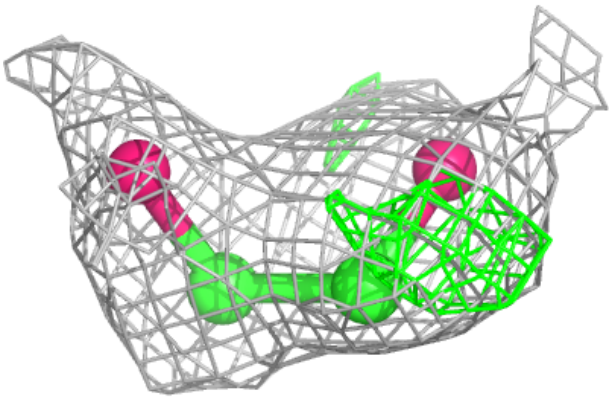


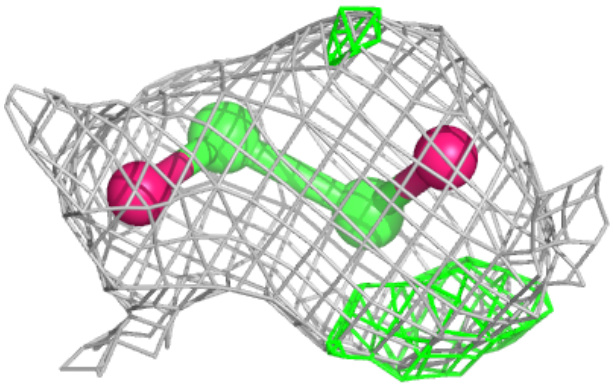


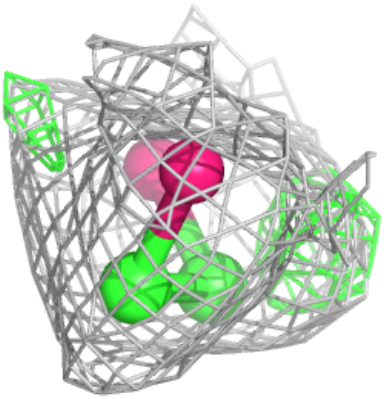


Electron density around GLC A 610:

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

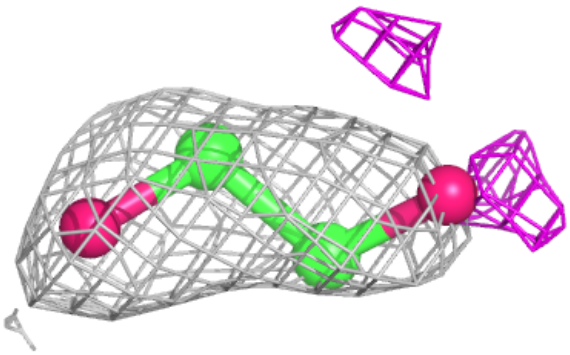


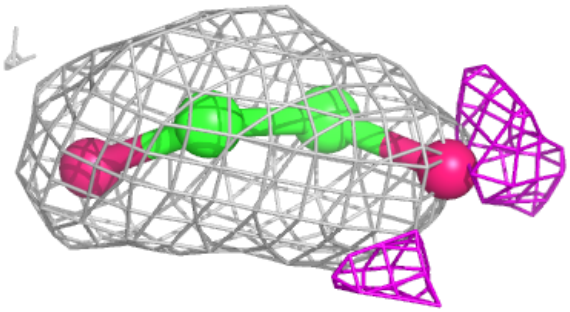


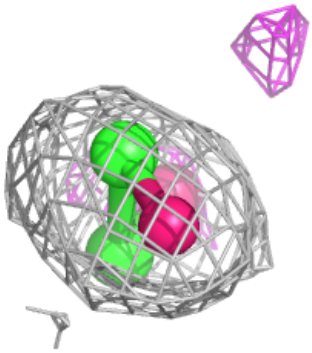


Electron density around GLC A 603:

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

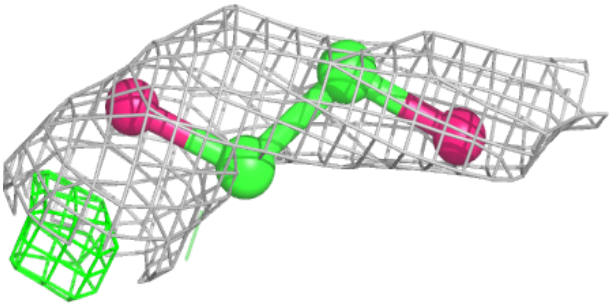


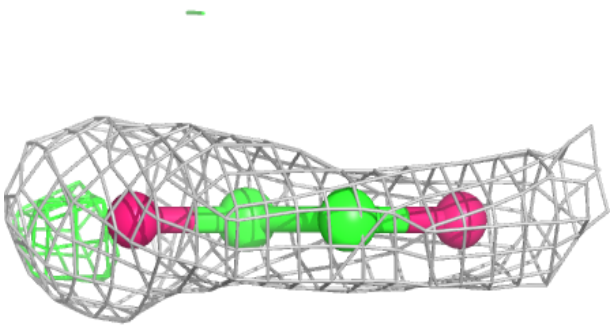


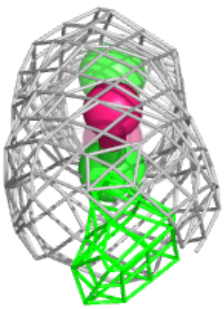


Electron density around GLC A 601:

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

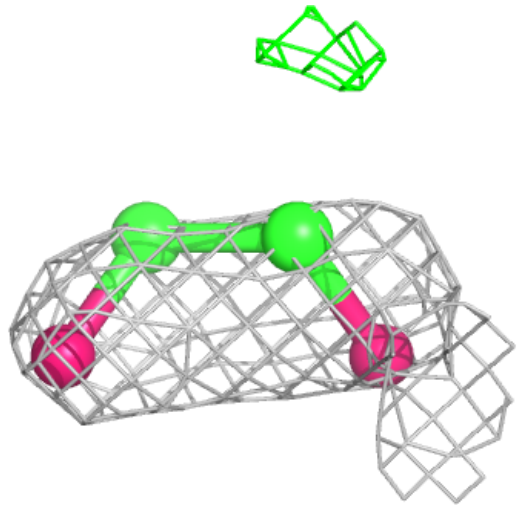


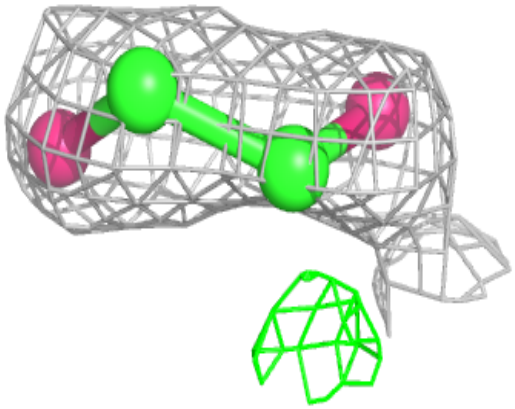


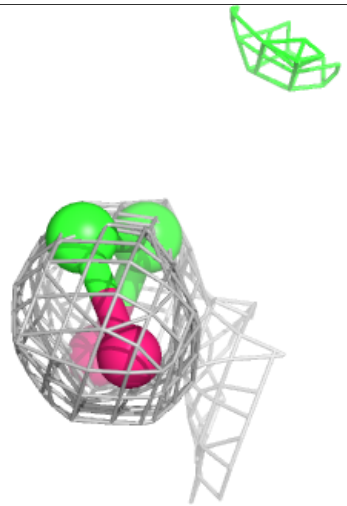


Electron density around GLC B 701:

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

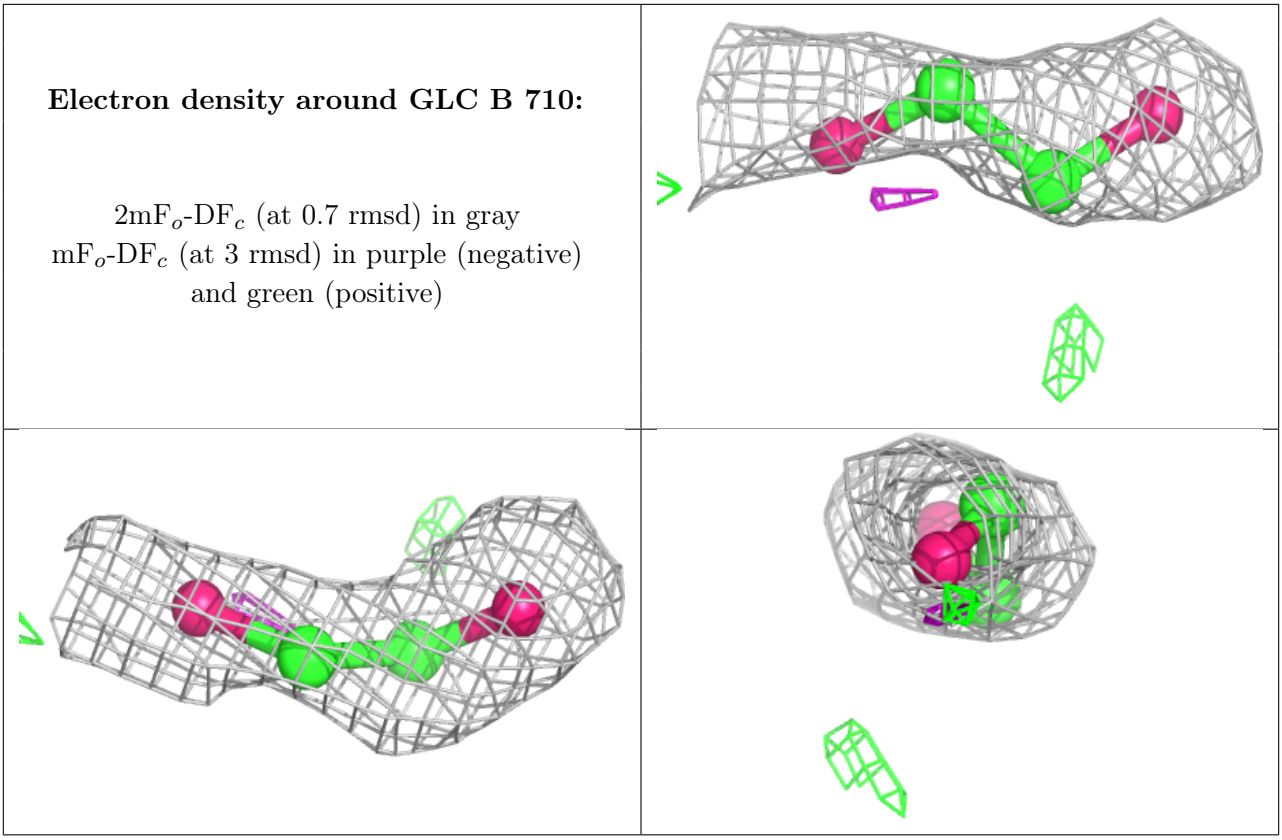






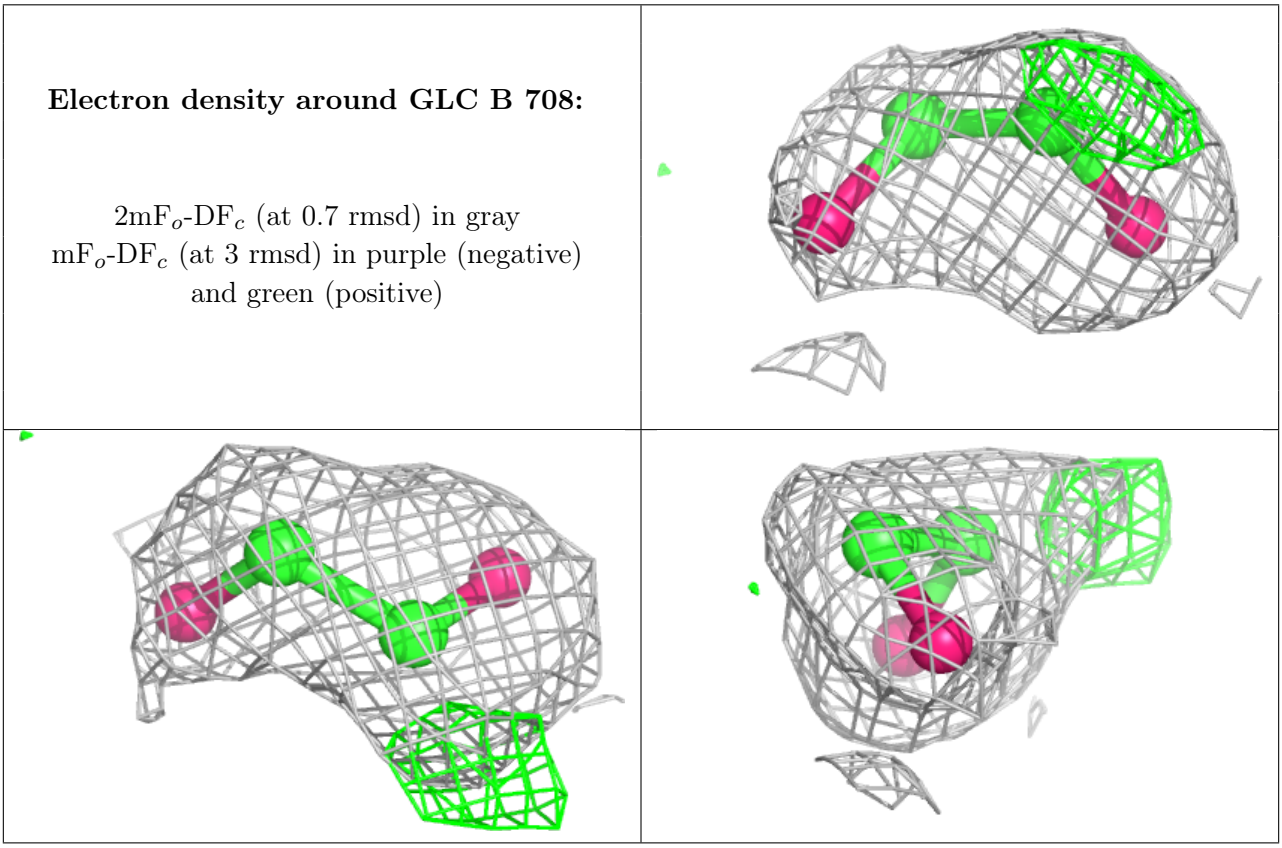
Electron density around GLC B 710:

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



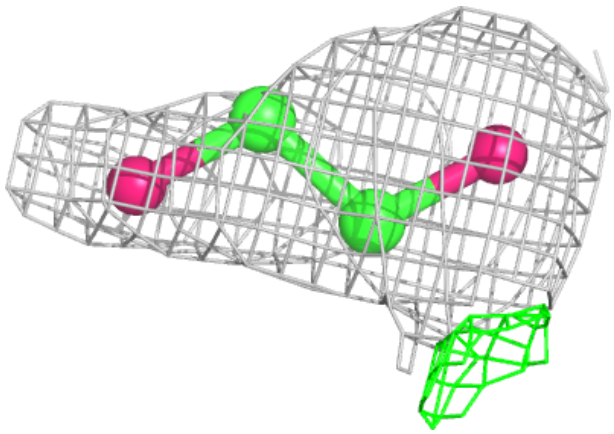
Electron density around GLC B 708:

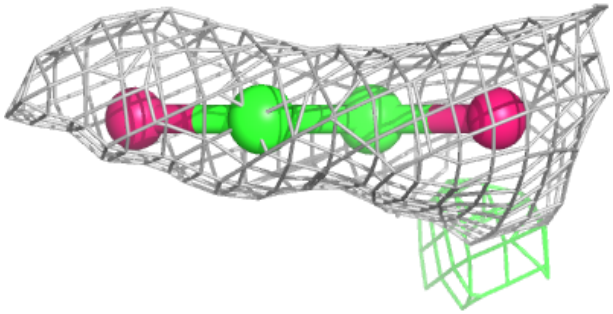
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

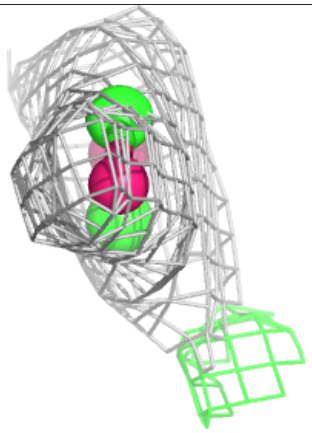


Electron density around GLC A 611:

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

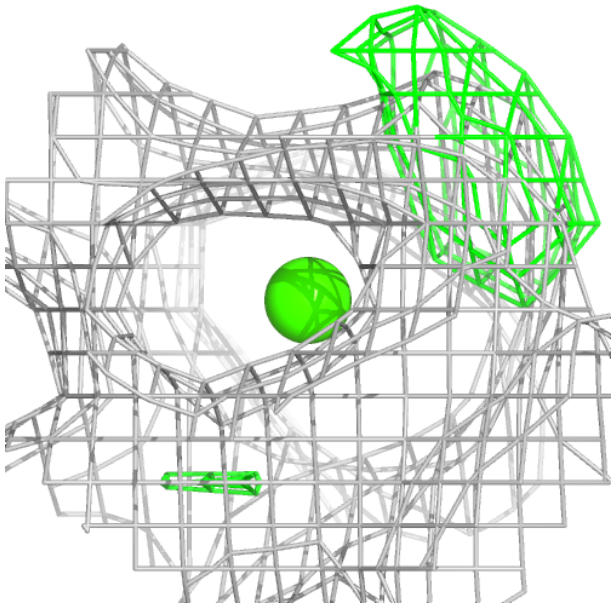


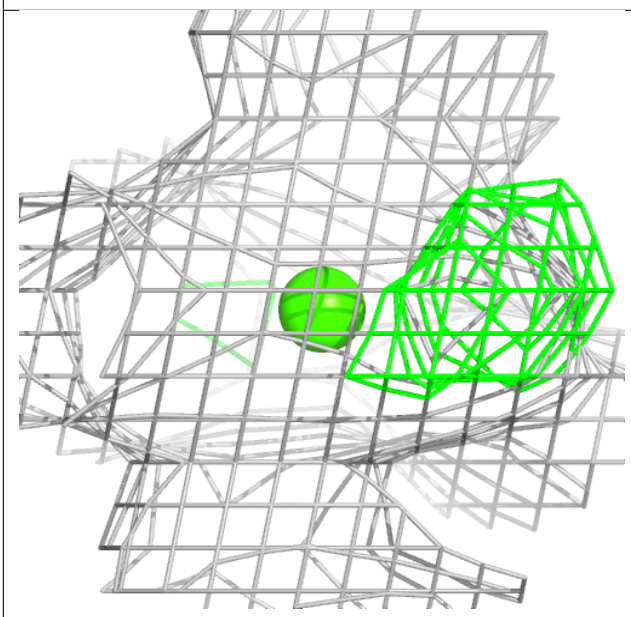


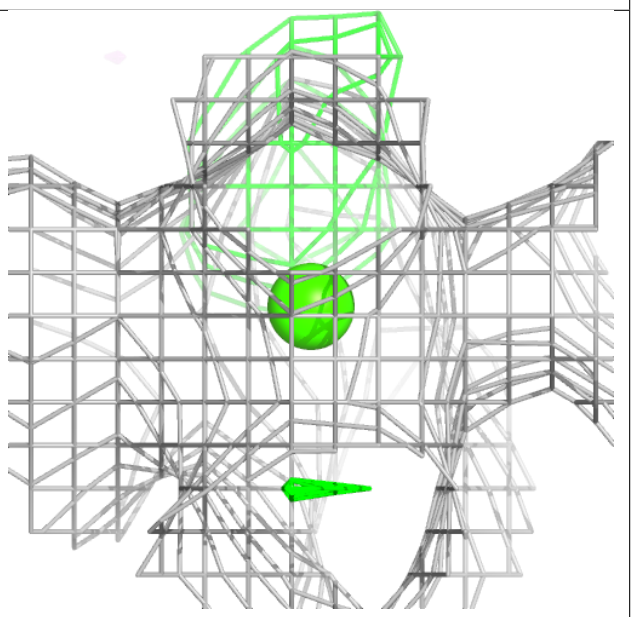


Electron density around CA A 605:

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

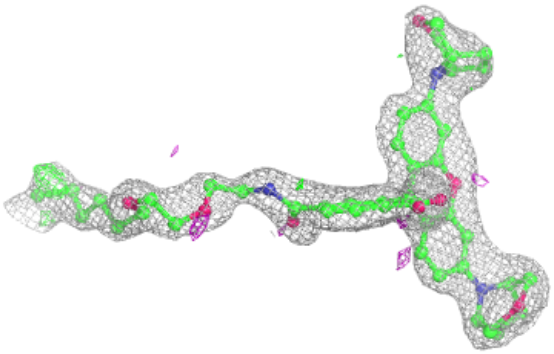


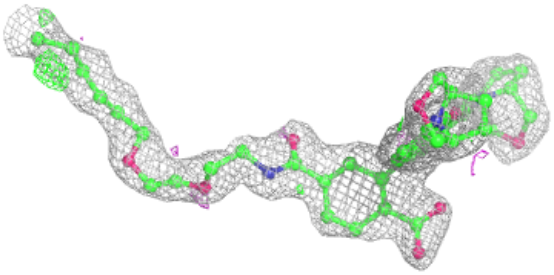


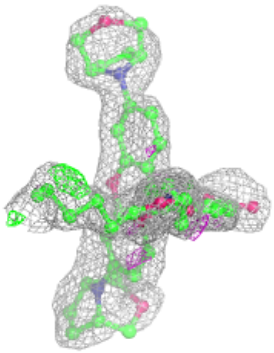


Electron density around A1EQX A 608:

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

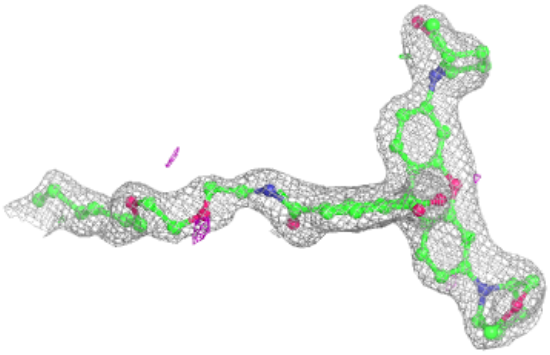


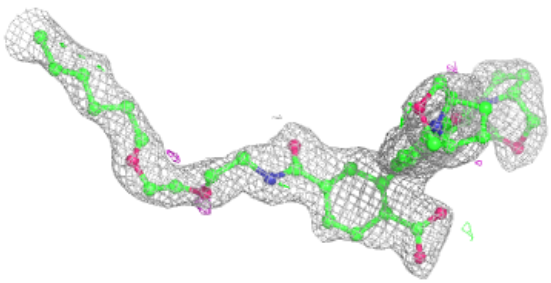


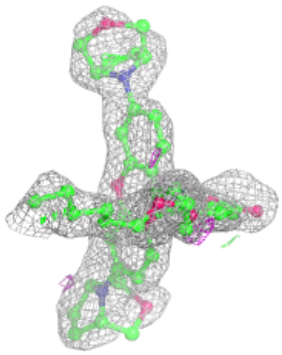


Electron density around A1EQX B 706:

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

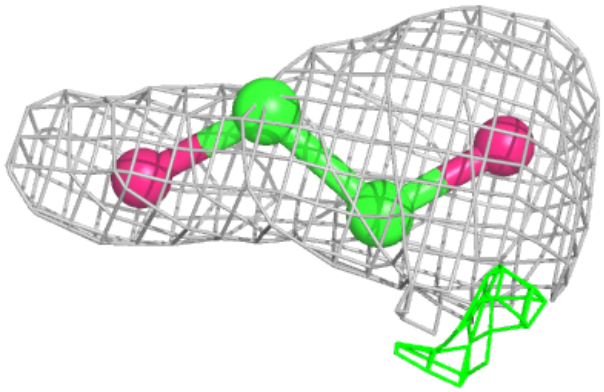


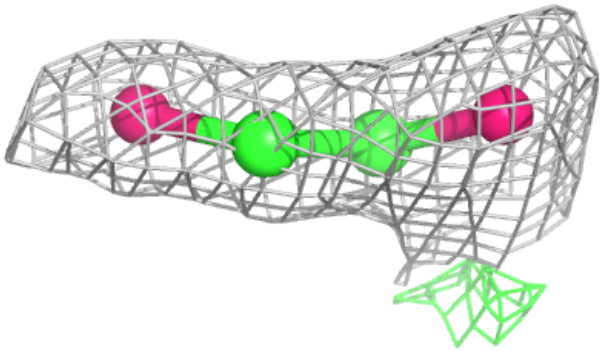


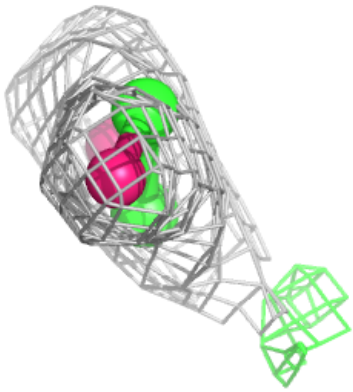


Electron density around GLC B 709:

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

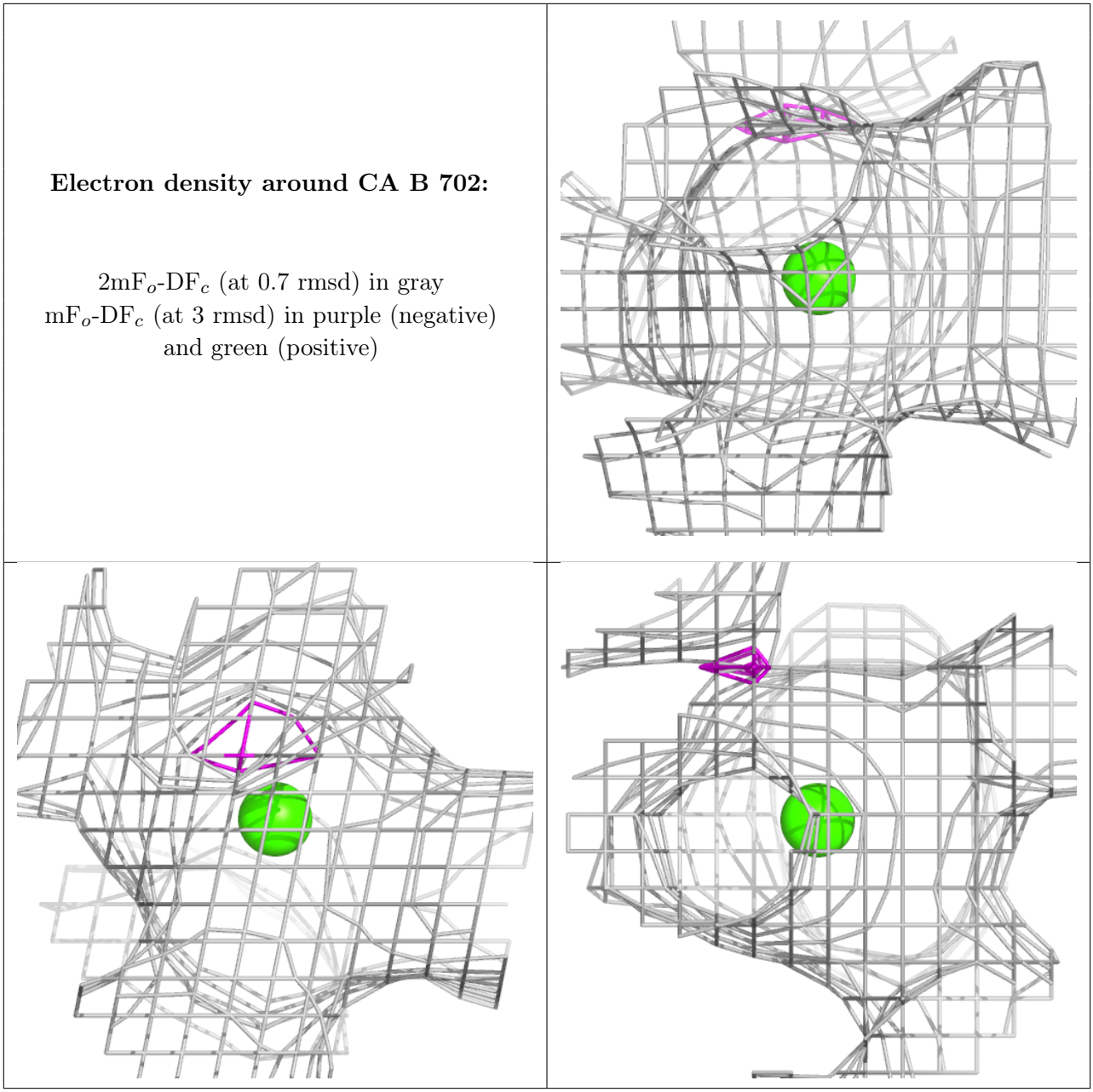






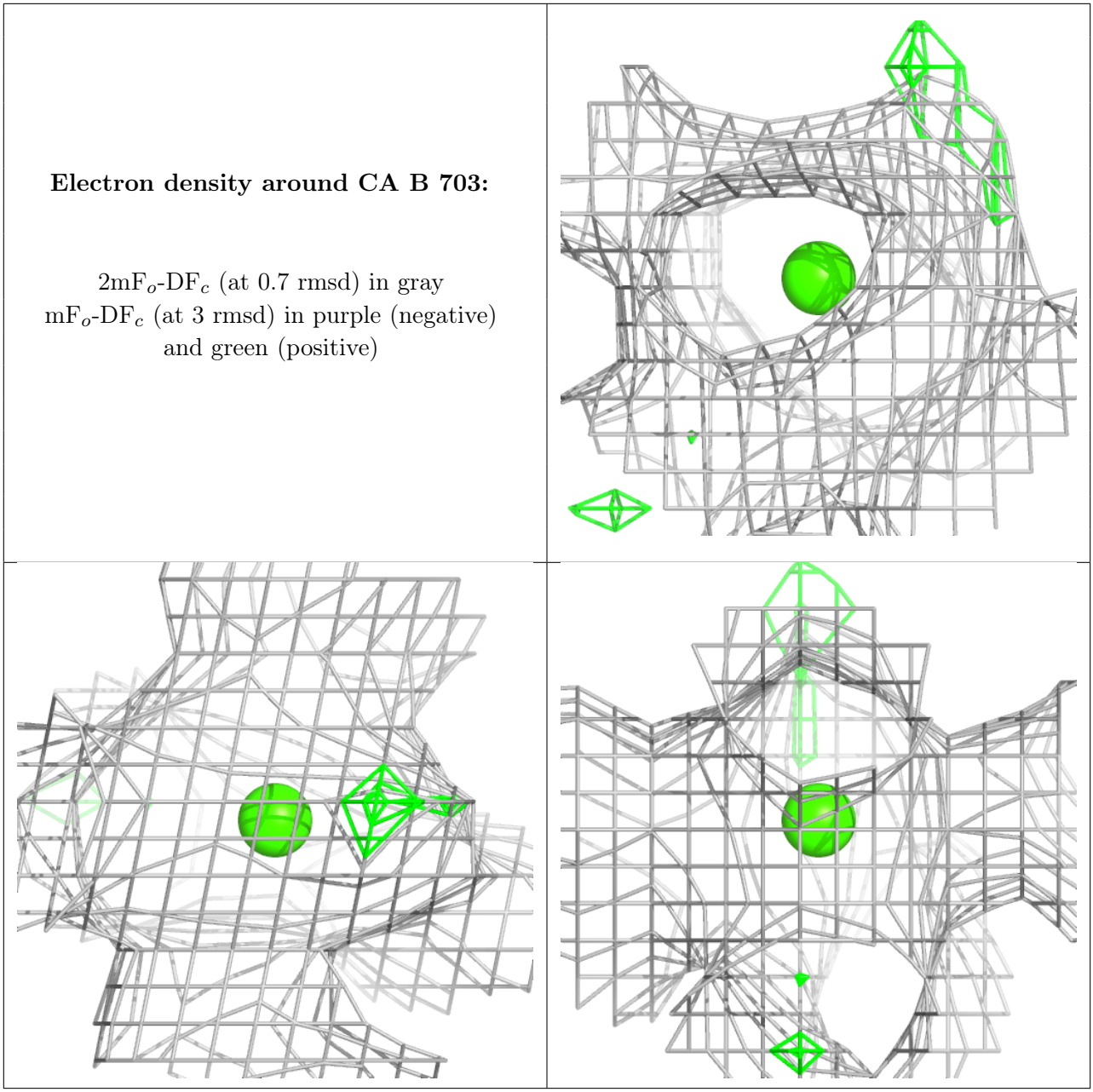
Electron density around CA B 702:

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



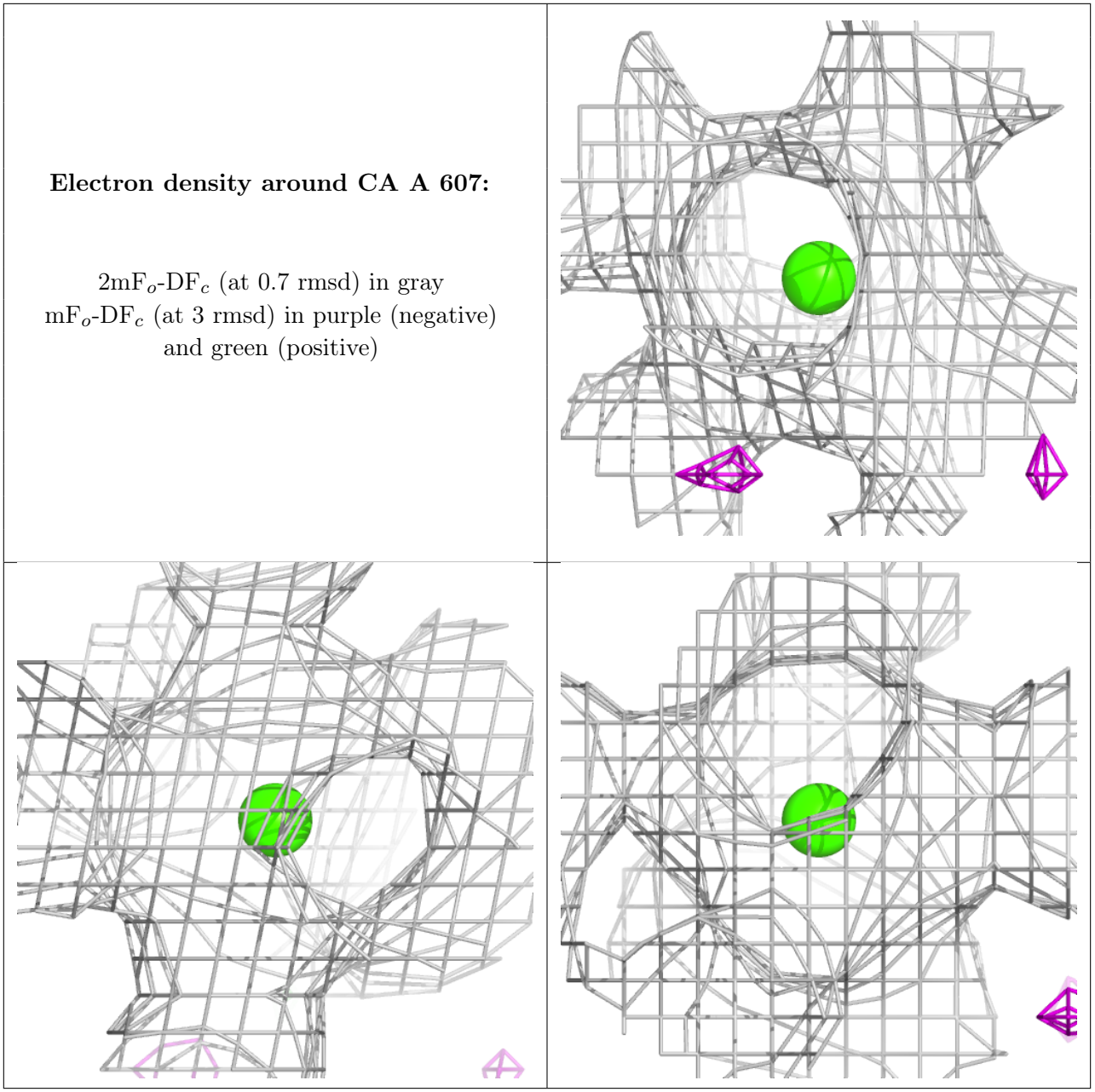
Electron density around CA B 703:

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



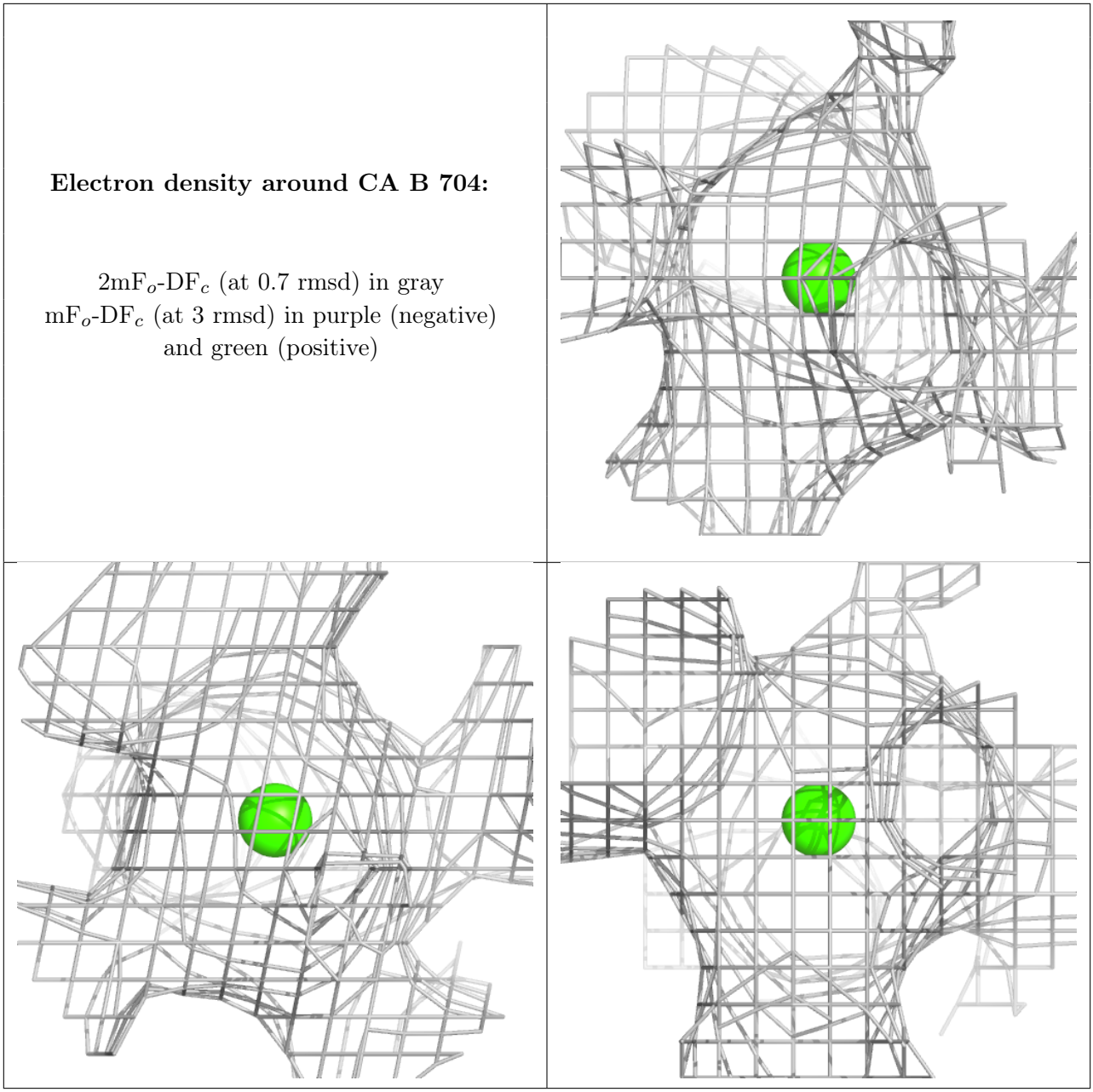
Electron density around CA A 607:

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



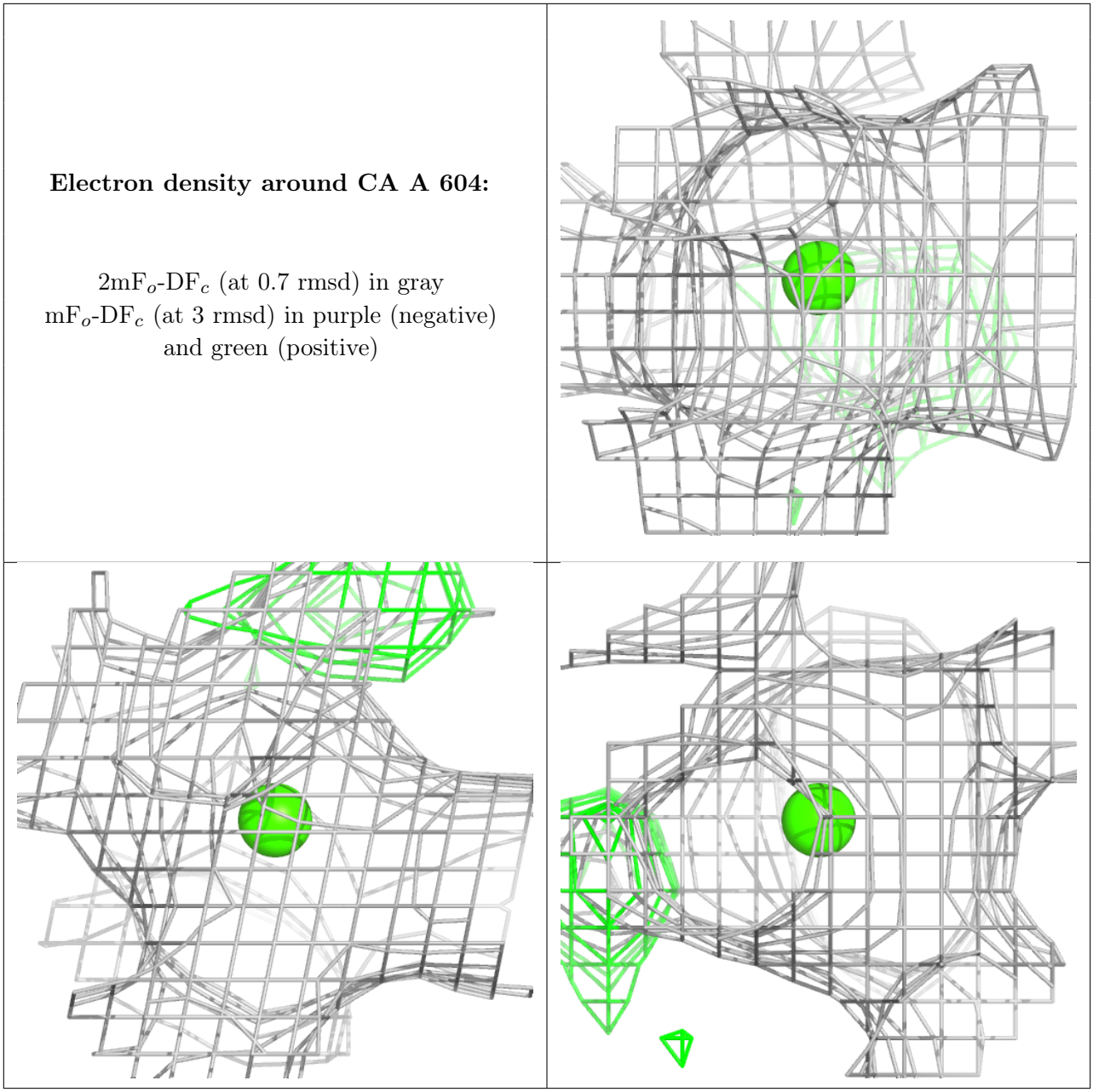
Electron density around CA B 704:

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



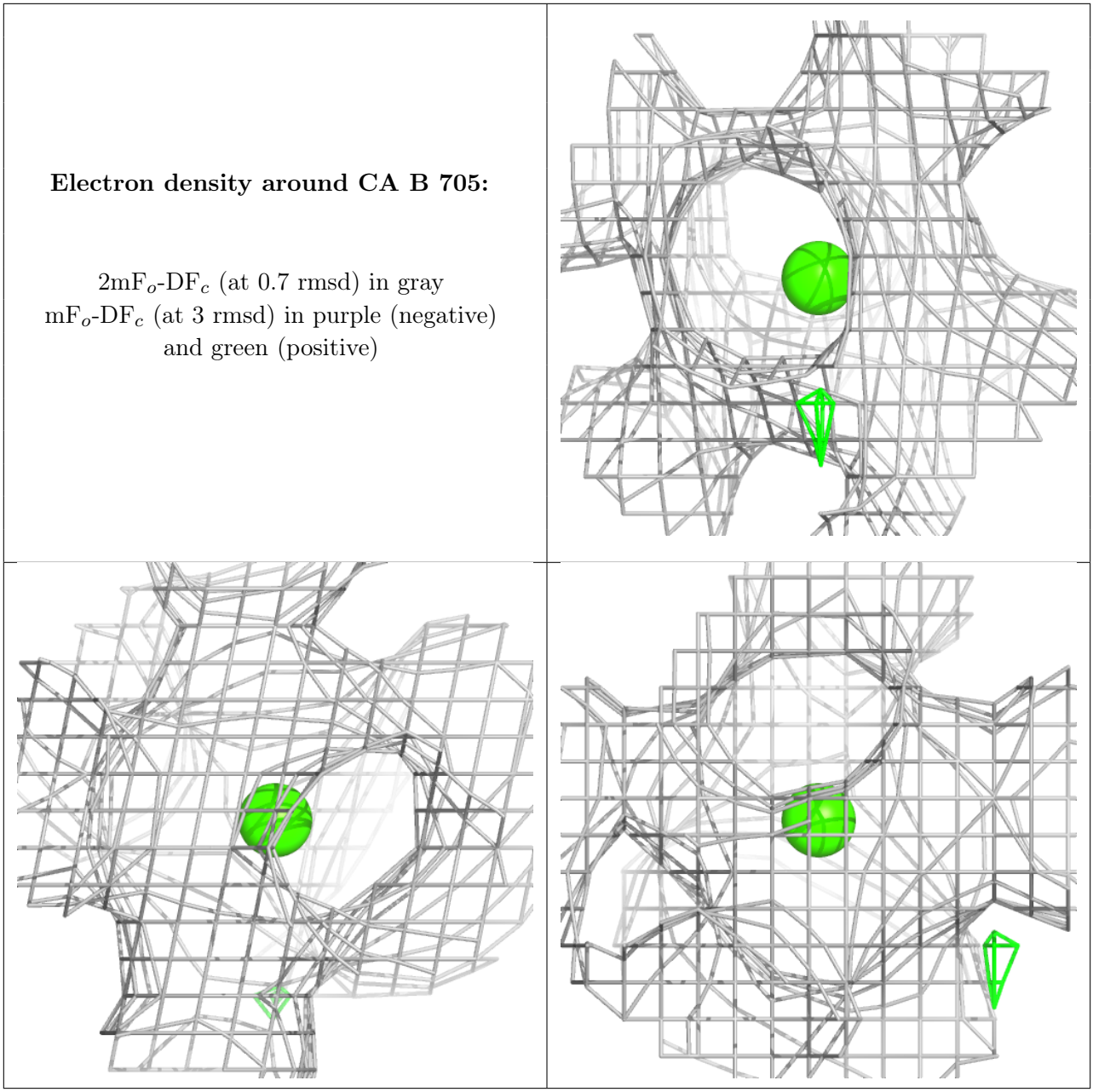
Electron density around CA A 604:

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



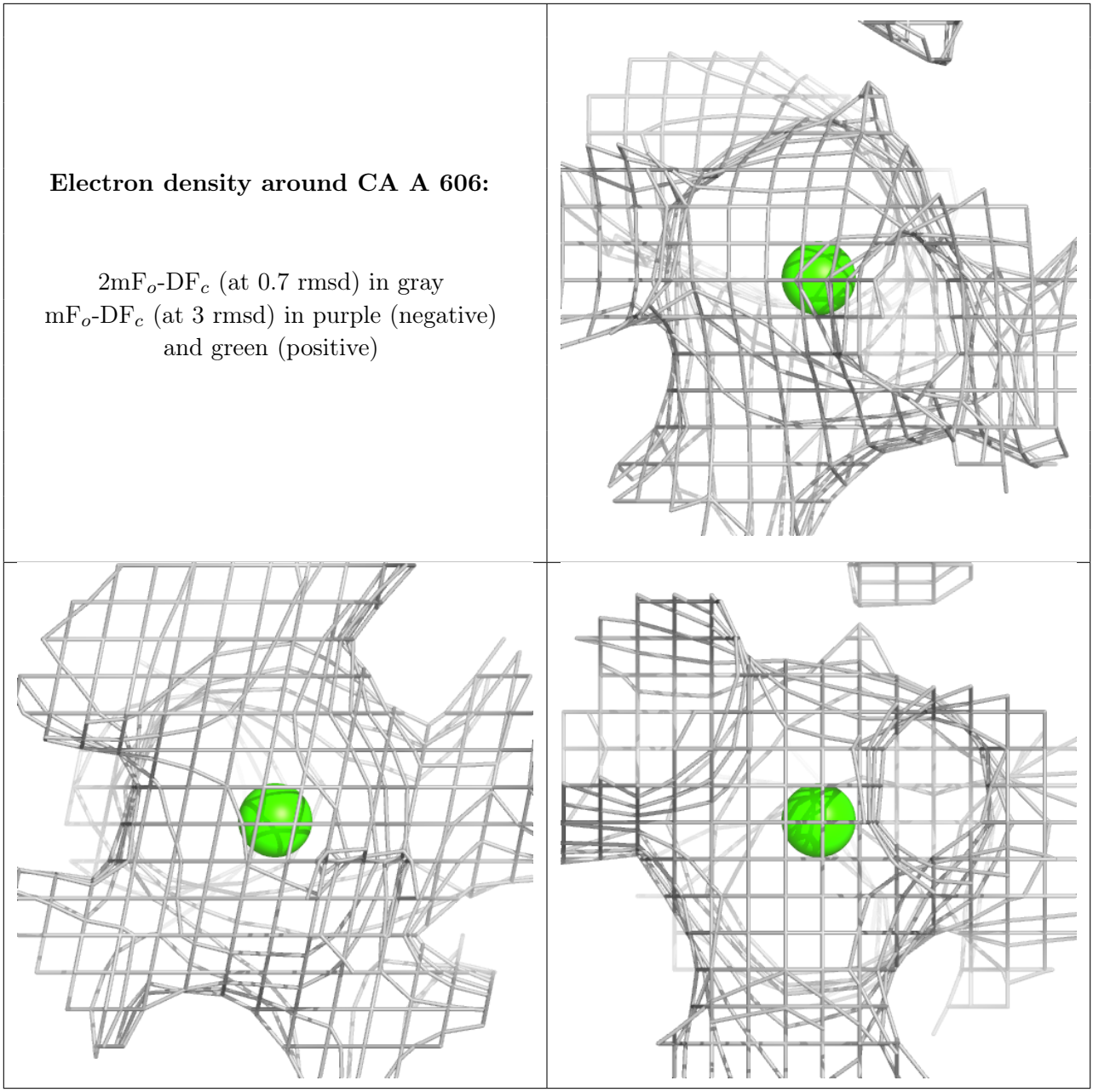
Electron density around CA B 705:

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



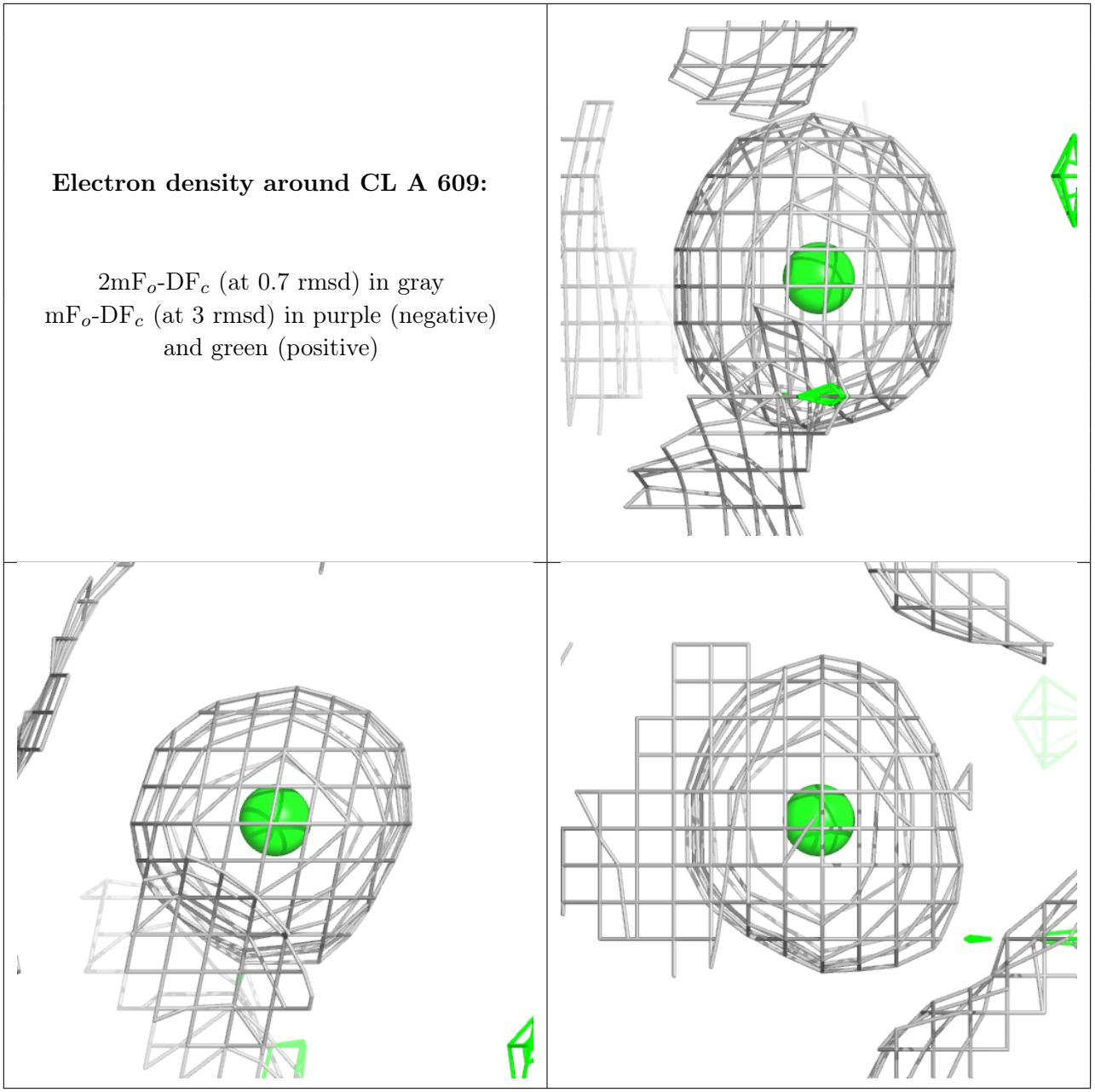
Electron density around CA A 606:

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



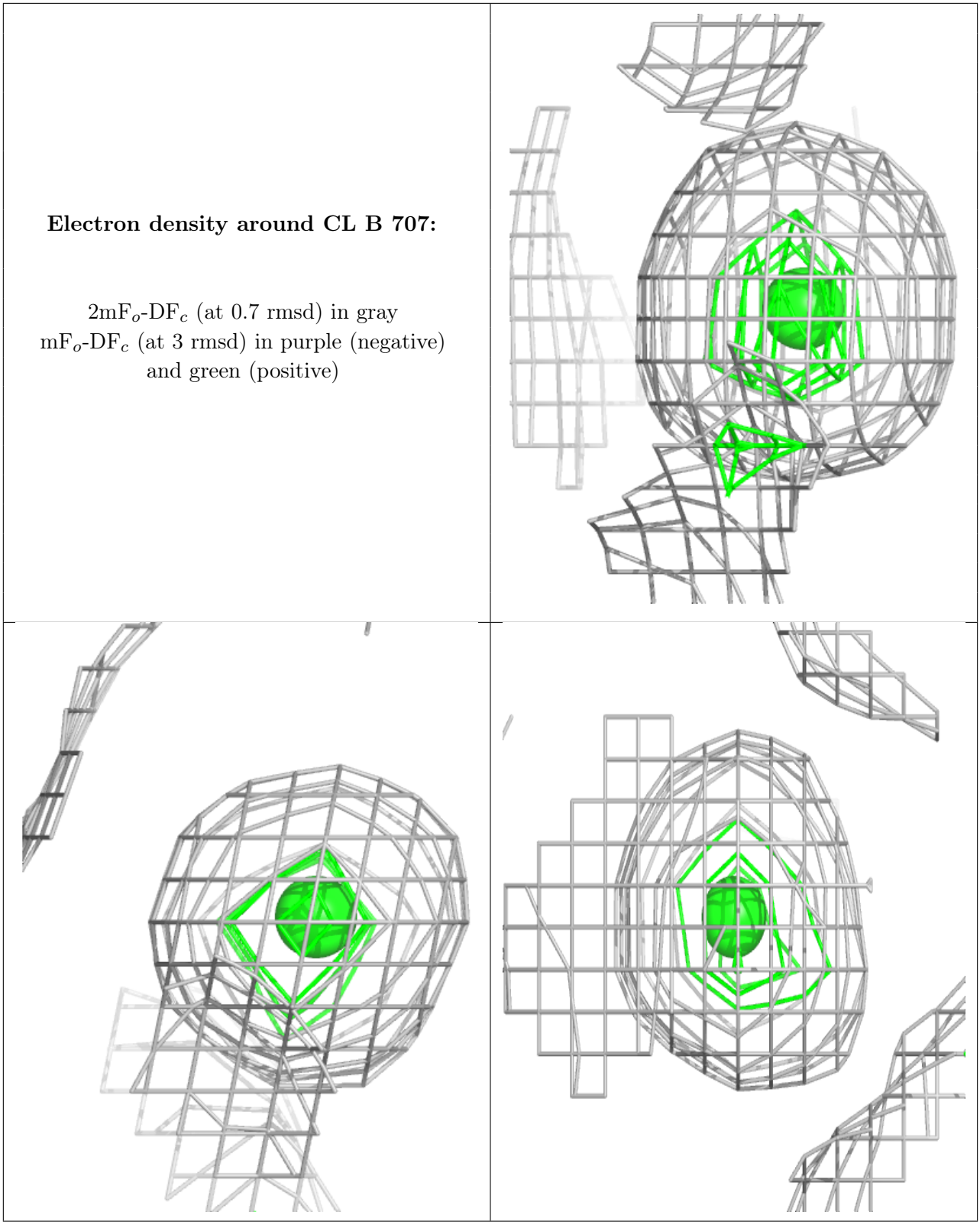
Electron density around CL A 609:

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



Electron density around CL B 707:

$2mF_o$-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.