Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2025 – 02:43 PM JST

PDB ID	:	8XVP
Title	:	Crystal structure of inulosucrase from Lactobacillus reuteri 121
Authors	:	Ni, D.; Hou, X.; Cheng, M.; Xu, W.; Rao, Y.; Mu, W.
Deposited on	:	2024-01-15
Resolution	:	1.98 Å(reported)

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

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

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

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

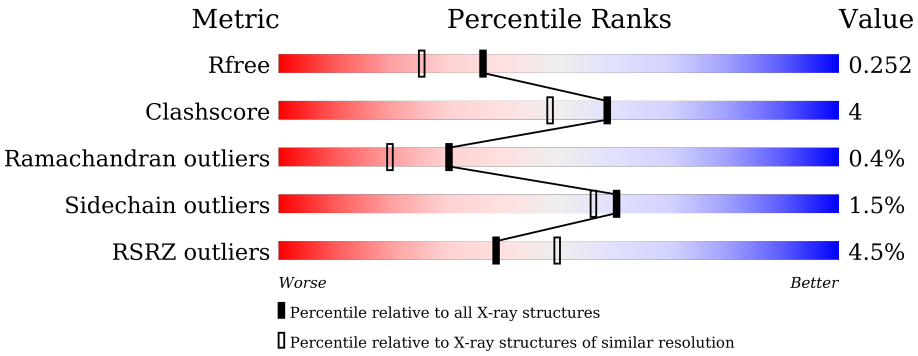
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

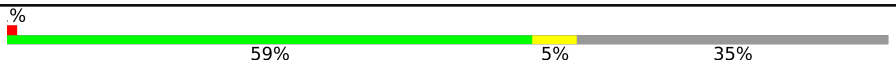
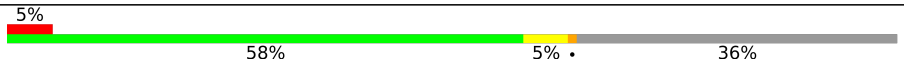
The reported resolution of this entry is 1.98 Å.

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	1356 (1.98-1.98)
Clashscore	180529	1437 (1.98-1.98)
Ramachandran outliers	177936	1426 (1.98-1.98)
Sidechain outliers	177891	1426 (1.98-1.98)
RSRZ outliers	164620	1356 (1.98-1.98)

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	798	
1	B	798	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8450 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.

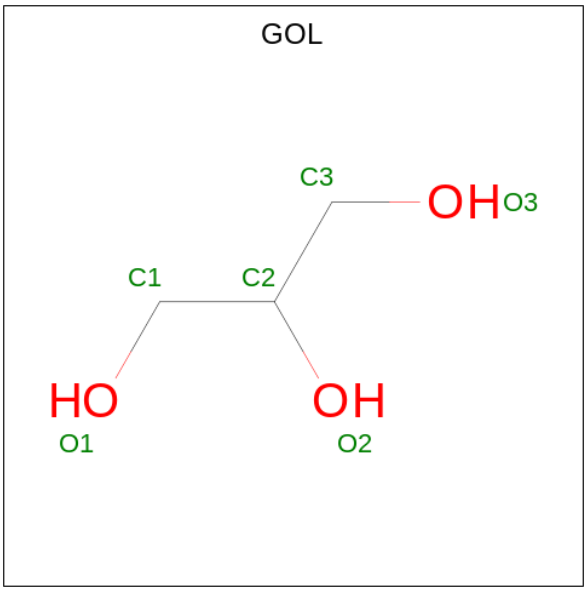
- Molecule 1 is a protein called Inulosucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	517	Total	C	N	O	S	0	0	0
			4050	2540	683	814	13			
1	B	507	Total	C	N	O	S	0	1	0
			3982	2496	669	804	13			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

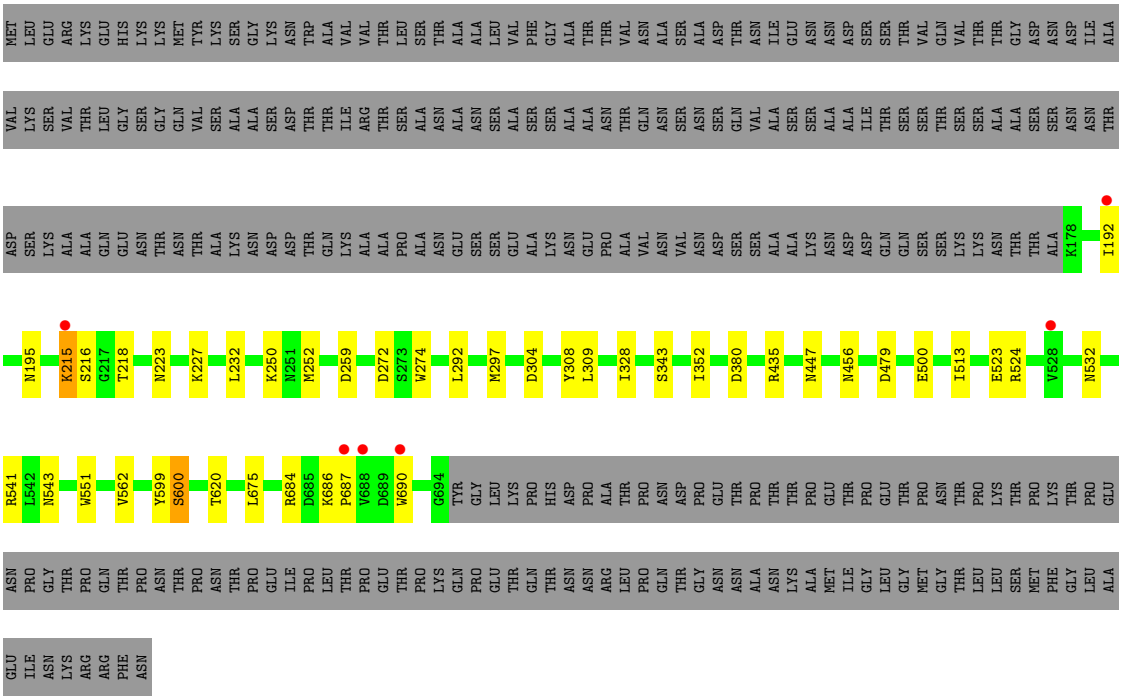
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	212	Total O 212 212	0	0
4	B	188	Total O 188 188	0	0

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.

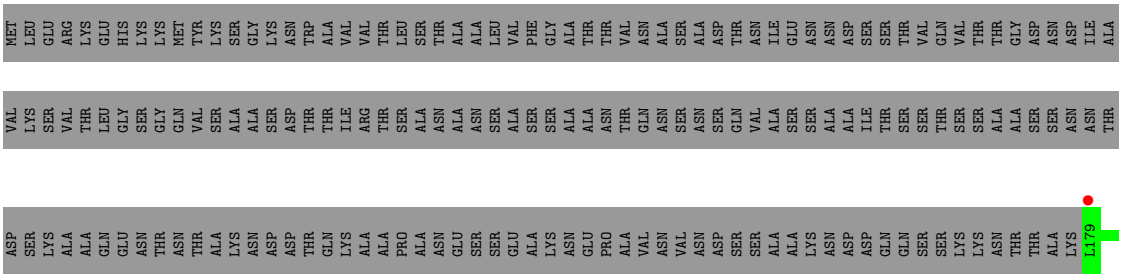
• Molecule 1: Inulosucrase

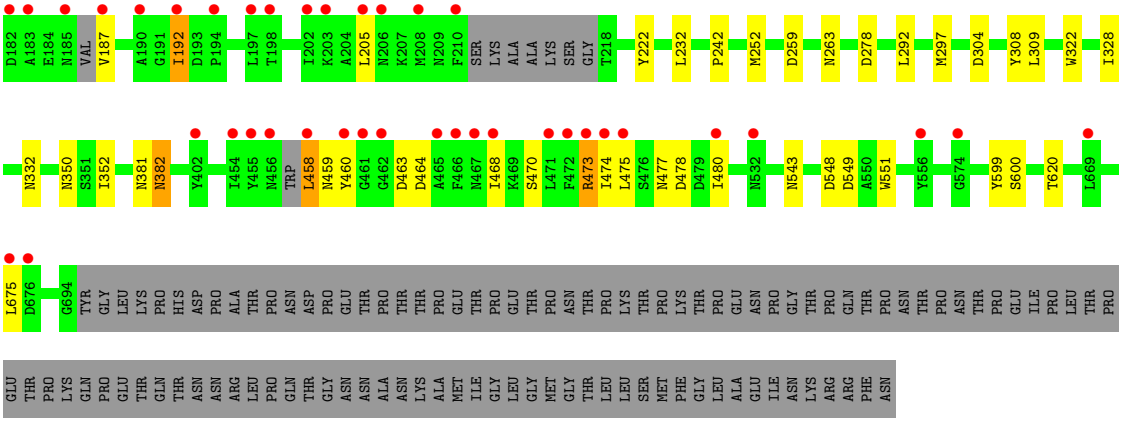
Chain A:



• Molecule 1: Inulosucrase

Chain B:




D182 A183 E184 N185 VAL V187 A190 G191 I192 D193 P194 L197 T198 I202 K203 A204 L205 N206 K207 M208 N209 F210 SER LYS ALA ALA LYS SER GLY T218 Y222 L232 P242 M252 D259 N263 D278 L292 M297 D304 Y308 L309 W322 I328
N332 N350 S351 I352 N381 N382 Y402 I454 Y455 N456 TRP L458 N459 Y460 G461 G462 D463 D464 A465 F466 N467 I468 K469 S470 L471 F472 R473 I474 L475 S476 N477 D478 D479 I480 N532 N543 D548 D549 A550 W551 Y556 G574 Y599 S600 T620 L669
L675 D676 G694 TYR GLY LEU LYS PRO HIS ASP PRO ALA THR PRO ASN ASP PRO GLU THR PRO THR THR PRO GLU THR PRO GLU THR PRO ASN THR PRO LYS THR PRO LYS THR PRO GLU ASN PRO GLY THR PRO GLN THR PRO ASN THR PRO ASN THR PRO GLU ILE PRO LEU THR PRO
GLU THR PRO LYS GLN PRO GLU THR GLN THR ASN ASN ARG LEU PRO GLN THR GLY ASN ASN ALA ASN LYS ALA MET ILE GLY LEU GLY MET GLY THR LEU LEU SER MET PHE GLY LEU ALA GLU ILE ASN LYS ARG ARG PHE ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.91Å 98.69Å 139.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.42 – 1.98 49.42 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.42-1.98) 99.9 (49.42-1.98)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.245 0.209 , 0.252	Depositor DCC
R_{free} test set	3350 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 33.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8450	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: CA, GOL

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	0.60	1/4139 (0.0%)	0.70	0/5640
1	B	0.57	0/4069	0.72	0/5542
All	All	0.59	1/8208 (0.0%)	0.71	0/11182

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ASP	C-N	-5.84	1.20	1.34

There are no bond angle outliers.

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	4050	0	3857	28	0
1	B	3982	0	3779	38	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	6	0	8	3	0
3	B	6	0	8	1	0
4	A	212	0	0	5	0
4	B	188	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8450	0	7652	67	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:SER:HB2	4:B:1033:HOH:O	1.49	1.07
1:B:458:LEU:HD12	1:B:459:ASN:N	1.73	1.02
3:B:804:GOL:H2	4:B:932:HOH:O	1.67	0.95
1:B:473:ARG:HD3	1:B:549:ASP:OD2	1.68	0.91
3:A:804:GOL:H12	4:A:905:HOH:O	1.78	0.83
1:B:460:TYR:HD2	4:B:1033:HOH:O	1.65	0.80
1:B:473:ARG:HA	1:B:473:ARG:HE	1.48	0.79
1:B:473:ARG:HH22	1:B:477:ASN:HB2	1.49	0.77
1:B:473:ARG:HE	1:B:473:ARG:CA	1.98	0.76
1:B:458:LEU:HD12	1:B:459:ASN:H	1.50	0.75
1:A:524:ARG:HD3	1:A:600:SER:OG	1.89	0.73
1:A:456:ASN:HB3	4:A:1095:HOH:O	1.89	0.71
1:A:532:ASN:HB3	4:A:1083:HOH:O	1.90	0.71
1:B:474:ILE:HG22	1:B:475:LEU:HD23	1.76	0.67
1:B:187:VAL:HG13	1:B:192:ILE:HG22	1.76	0.67
1:B:473:ARG:NH2	1:B:477:ASN:HB2	2.10	0.66
1:A:252:MET:SD	4:A:1040:HOH:O	2.56	0.60
1:B:263:ASN:ND2	1:B:332:ASN:OD1	2.27	0.58
1:B:381:ASN:HB2	4:B:916:HOH:O	2.04	0.57
1:A:272:ASP:OD2	3:A:804:GOL:H2	2.06	0.55
1:B:458:LEU:HD12	1:B:458:LEU:C	2.19	0.54
1:B:464:ASP:O	1:B:468:ILE:HG12	2.08	0.54
1:B:278:ASP:HB3	4:B:969:HOH:O	2.09	0.53
1:A:541:ARG:HG2	1:A:562:VAL:HG12	1.92	0.51
1:B:292:LEU:HD13	1:B:352:ILE:HD11	1.93	0.51
1:A:292:LEU:HD13	1:A:352:ILE:HD11	1.92	0.51
1:B:460:TYR:CD2	4:B:1033:HOH:O	2.47	0.50
1:B:473:ARG:CA	1:B:473:ARG:NE	2.70	0.50
1:A:309:LEU:HB2	1:A:328:ILE:HD11	1.93	0.50
1:A:435:ARG:NH2	1:A:500:GLU:HG2	2.28	0.49
1:B:543:ASN:HA	1:B:551:TRP:CG	2.49	0.48
1:A:523:GLU:OE2	3:A:804:GOL:H12	2.14	0.47
1:A:686:LYS:HG3	1:A:687:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:MET:HB2	1:B:308:TYR:CE1	2.50	0.47
1:B:473:ARG:HA	1:B:473:ARG:NE	2.25	0.47
1:A:543:ASN:HA	1:A:551:TRP:CG	2.50	0.47
1:B:222:TYR:CE2	1:B:470:SER:HB3	2.50	0.46
1:A:435:ARG:CZ	1:A:500:GLU:HG2	2.46	0.46
1:A:218:THR:O	1:A:513:ILE:HA	2.15	0.46
1:B:458:LEU:C	1:B:458:LEU:CD1	2.85	0.45
1:A:297:MET:HB2	1:A:308:TYR:CE1	2.51	0.45
1:A:223:ASN:OD1	1:A:227:LYS:HE3	2.17	0.45
1:B:381:ASN:O	1:B:382:ASN:CB	2.64	0.45
1:A:684:ARG:HG3	4:A:1006:HOH:O	2.17	0.44
1:B:309:LEU:HB2	1:B:328:ILE:HD11	1.99	0.44
1:A:690:TRP:HD1	1:B:549:ASP:OD1	2.00	0.44
1:B:474:ILE:HA	1:B:480:ILE:HG21	2.00	0.44
1:B:259:ASP:OD1	1:B:304:ASP:OD2	2.36	0.44
1:A:599:TYR:CG	1:A:600:SER:N	2.87	0.43
1:A:274:TRP:CD1	1:A:343:SER:HA	2.54	0.42
1:B:232:LEU:HD23	1:B:232:LEU:C	2.39	0.42
1:B:599:TYR:CG	1:B:600:SER:N	2.87	0.42
1:A:259:ASP:OD1	1:A:304:ASP:OD2	2.37	0.42
1:A:686:LYS:CG	1:A:687:PRO:HD2	2.49	0.42
1:B:548:ASP:HA	1:B:551:TRP:NE1	2.34	0.42
1:B:252:MET:HE2	1:B:322:TRP:HB2	2.01	0.42
1:B:470:SER:CB	4:B:1033:HOH:O	2.30	0.41
1:A:309:LEU:HB2	1:A:328:ILE:CD1	2.51	0.41
1:B:292:LEU:CD1	1:B:352:ILE:HD11	2.50	0.41
1:A:232:LEU:C	1:A:232:LEU:HD23	2.40	0.41
1:A:524:ARG:CD	1:A:600:SER:OG	2.66	0.41
1:B:309:LEU:HB2	1:B:328:ILE:CD1	2.51	0.41
1:B:205:LEU:HD21	1:B:468:ILE:HD12	2.03	0.41
1:B:475:LEU:HD23	1:B:475:LEU:HA	1.64	0.41
1:A:192:ILE:HD12	1:A:192:ILE:HA	1.99	0.41
1:A:215:LYS:NZ	1:A:447:ASN:HD22	2.19	0.41
1:A:195:ASN:N	1:A:195:ASN:HD22	2.19	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	515/798 (64%)	498 (97%)	15 (3%)	2 (0%)	30	20
1	B	500/798 (63%)	482 (96%)	16 (3%)	2 (0%)	30	20
All	All	1015/1596 (64%)	980 (97%)	31 (3%)	4 (0%)	30	20

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	382	ASN
1	A	216	SER
1	A	620	THR
1	B	620	THR

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	436/671 (65%)	431 (99%)	5 (1%)	70	68
1	B	430/671 (64%)	422 (98%)	8 (2%)	52	46
All	All	866/1342 (64%)	853 (98%)	13 (2%)	60	56

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	LYS
1	A	250	LYS

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Mol	Chain	Res	Type
1	A	380	ASP
1	A	600	SER
1	A	675	LEU
1	B	192	ILE
1	B	242	PRO
1	B	350	ASN
1	B	458	LEU
1	B	463	ASP
1	B	473	ARG
1	B	478	ASP
1	B	675	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	195	ASN
1	A	219	GLN
1	A	288	ASN
1	A	301	ASN
1	B	288	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
3	GOL	B	804	-	5,5,5	0.42	0	5,5,5	0.52	0
3	GOL	A	804	-	5,5,5	0.28	0	5,5,5	0.86	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
3	GOL	B	804	-	-	2/4/4/4	-
3	GOL	A	804	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	GOL	C1-C2-C3-O3
3	B	804	GOL	O1-C1-C2-C3
3	A	804	GOL	O2-C2-C3-O3
3	B	804	GOL	O1-C1-C2-O2

There are no ring outliers.

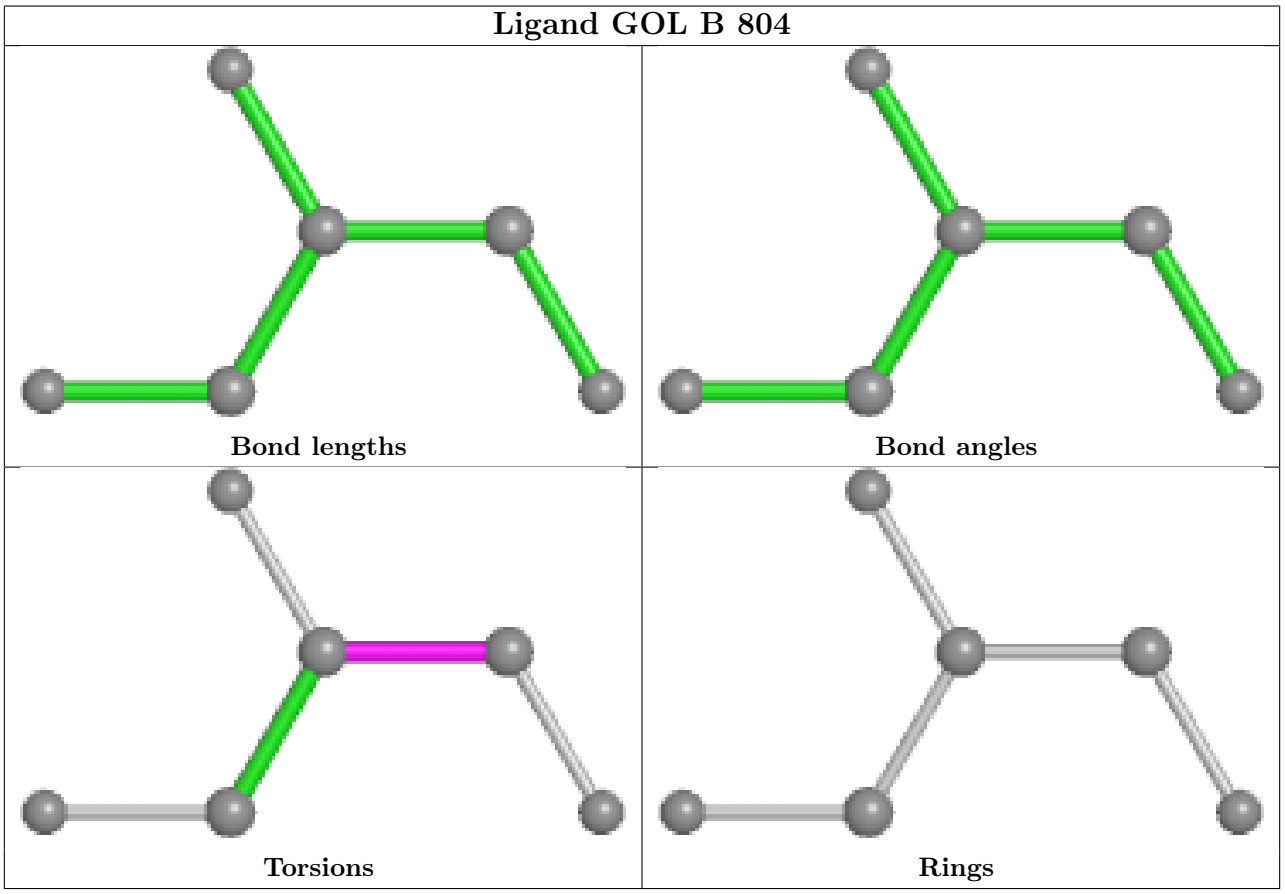
2 monomers are involved in 4 short contacts:

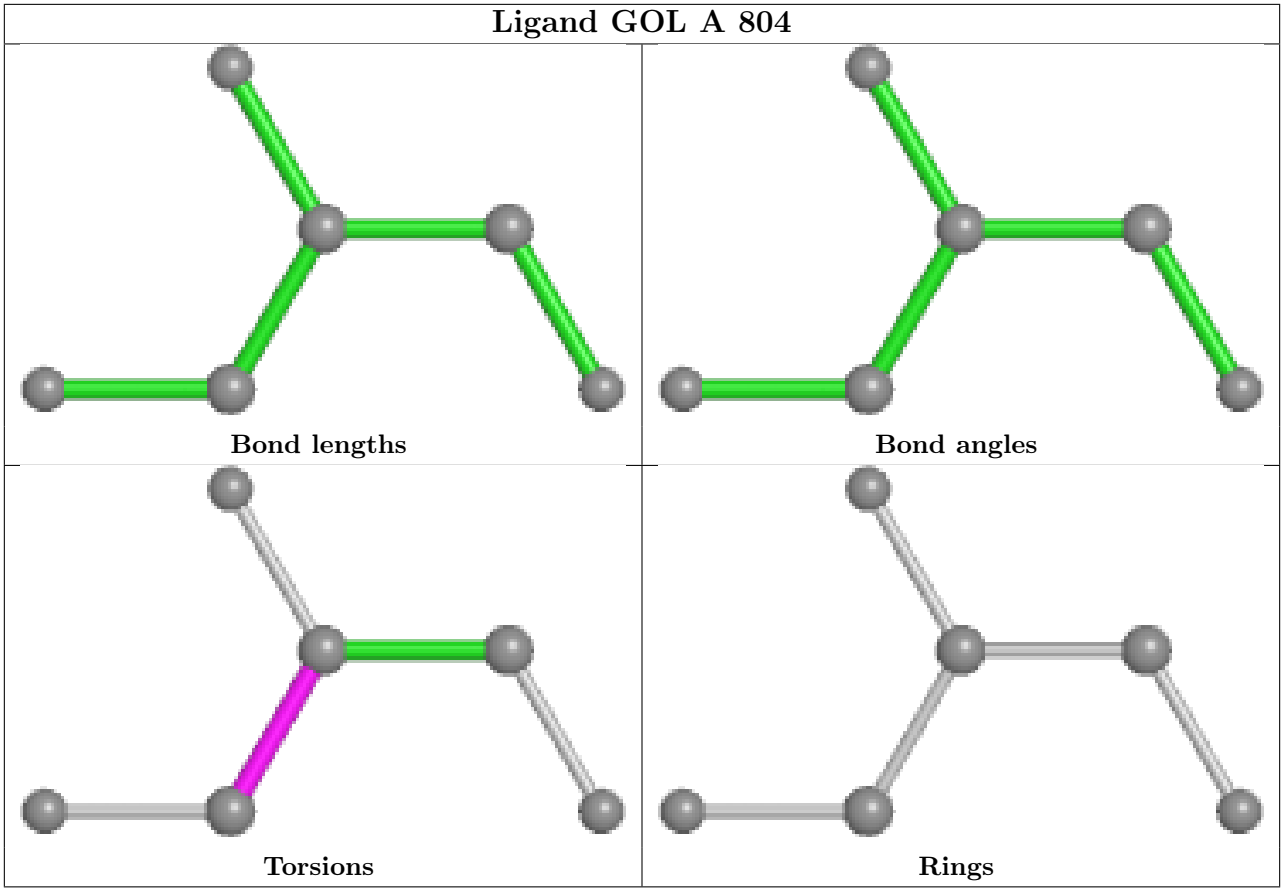
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	804	GOL	1	0
3	A	804	GOL	3	0

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 GOL B 804





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	517/798 (64%)	0.10	6 (1%)	76	83	21, 32, 54, 70	0
1	B	507/798 (63%)	0.42	40 (7%)	20	29	22, 35, 68, 86	1 (0%)
All	All	1024/1596 (64%)	0.26	46 (4%)	39	50	21, 33, 62, 86	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	458	LEU	5.8
1	B	210	PHE	5.2
1	A	192	ILE	4.6
1	B	474	ILE	4.3
1	B	179	LEU	4.2
1	B	456	ASN	4.1
1	B	455	TYR	3.5
1	B	471	LEU	3.4
1	B	556	TYR	3.3
1	B	192	ILE	3.3
1	B	472	PHE	3.2
1	A	688	VAL	3.1
1	B	675	LEU	3.1
1	B	187	VAL	3.1
1	B	462	GLY	3.1
1	B	475	LEU	3.1
1	B	468	ILE	3.0
1	B	473	ARG	2.9
1	B	202	ILE	2.9
1	B	190	ALA	2.8
1	A	215	LYS	2.8
1	B	461	GLY	2.7
1	B	194	PRO	2.7
1	B	205	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	203	LYS	2.6
1	A	687	PRO	2.6
1	B	466	PHE	2.6
1	B	669	LEU	2.5
1	B	183	ALA	2.5
1	B	480	ILE	2.4
1	A	528	VAL	2.4
1	B	465	ALA	2.4
1	B	206	ASN	2.4
1	B	676	ASP	2.3
1	B	185	ASN	2.2
1	B	460	TYR	2.2
1	B	454	ILE	2.2
1	B	208	MET	2.2
1	B	197	LEU	2.2
1	B	574	GLY	2.1
1	B	402	TYR	2.1
1	B	198	THR	2.1
1	B	532	ASN	2.1
1	B	182	ASP	2.0
1	A	690	TRP	2.0
1	B	467	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	GOL	A	804	6/6	0.90	0.10	29,32,35,35	0

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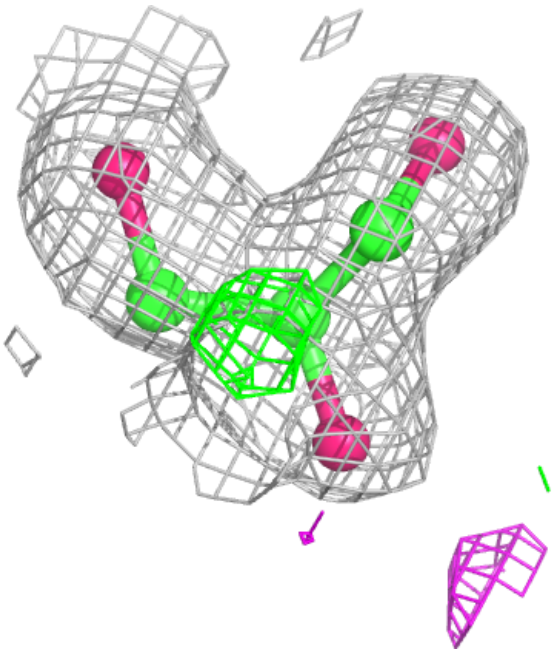
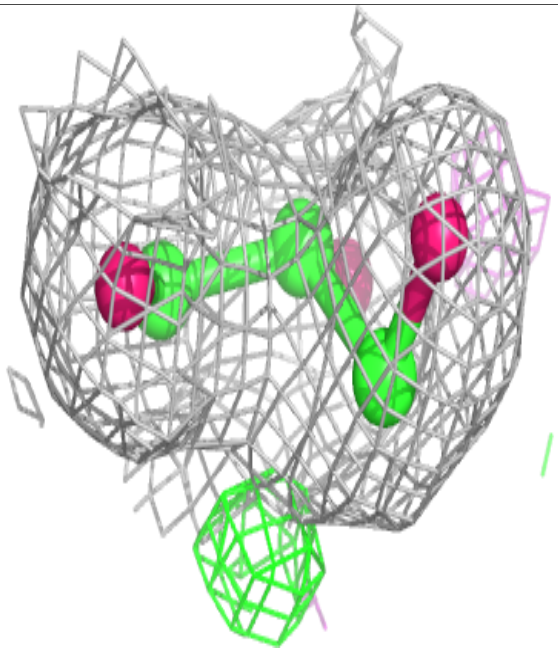
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	804	6/6	0.93	0.08	32,35,35,38	0
2	CA	A	803	1/1	0.98	0.03	30,30,30,30	0
2	CA	B	803	1/1	0.98	0.04	35,35,35,35	0
2	CA	B	802	1/1	0.99	0.03	37,37,37,37	0
2	CA	A	802	1/1	0.99	0.03	29,29,29,29	0
2	CA	A	801	1/1	0.99	0.03	24,24,24,24	0
2	CA	B	801	1/1	0.99	0.03	29,29,29,29	0

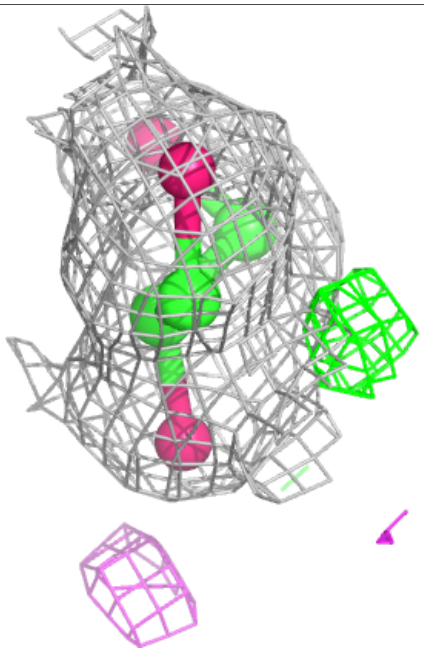
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GOL A 804:

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

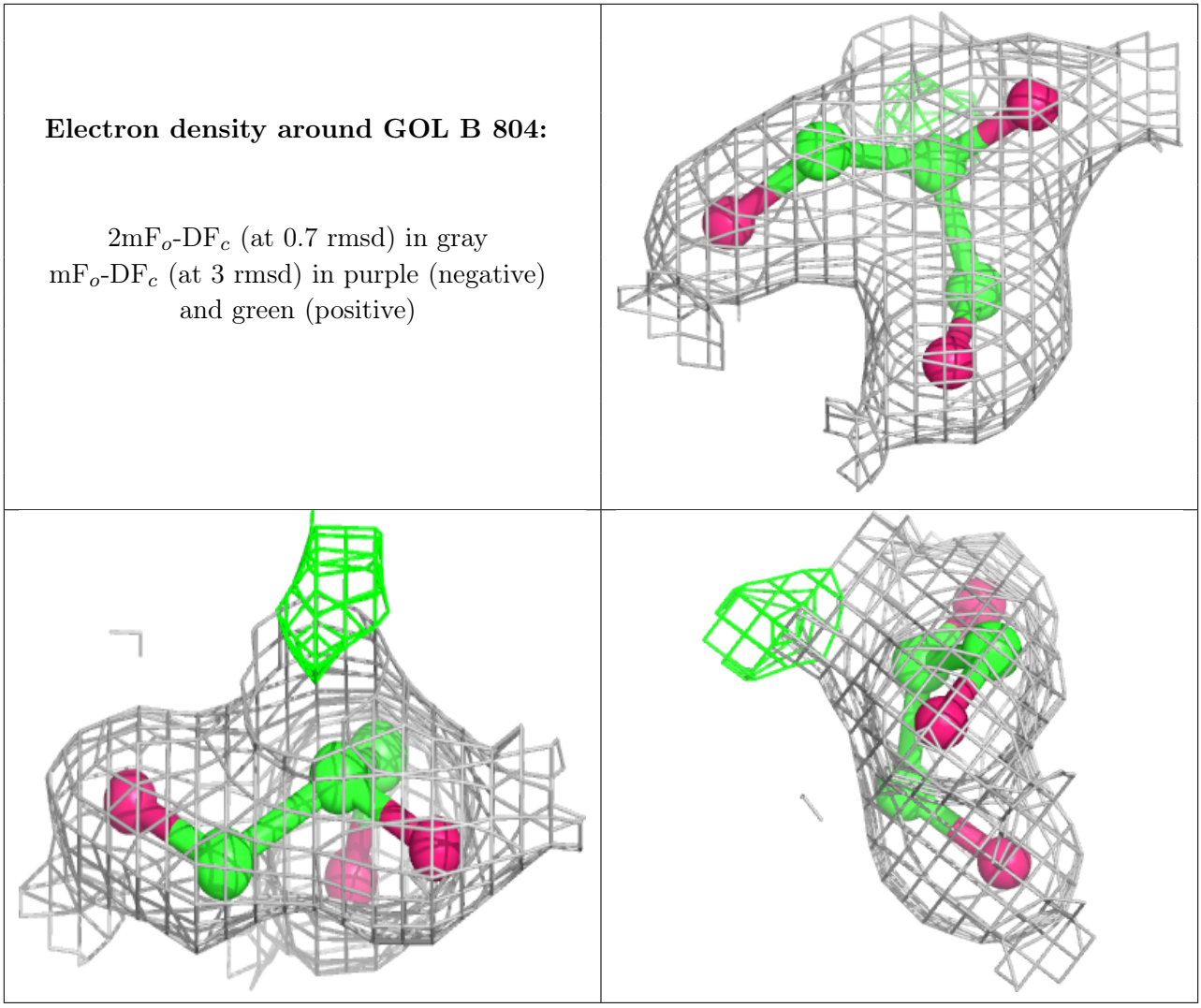






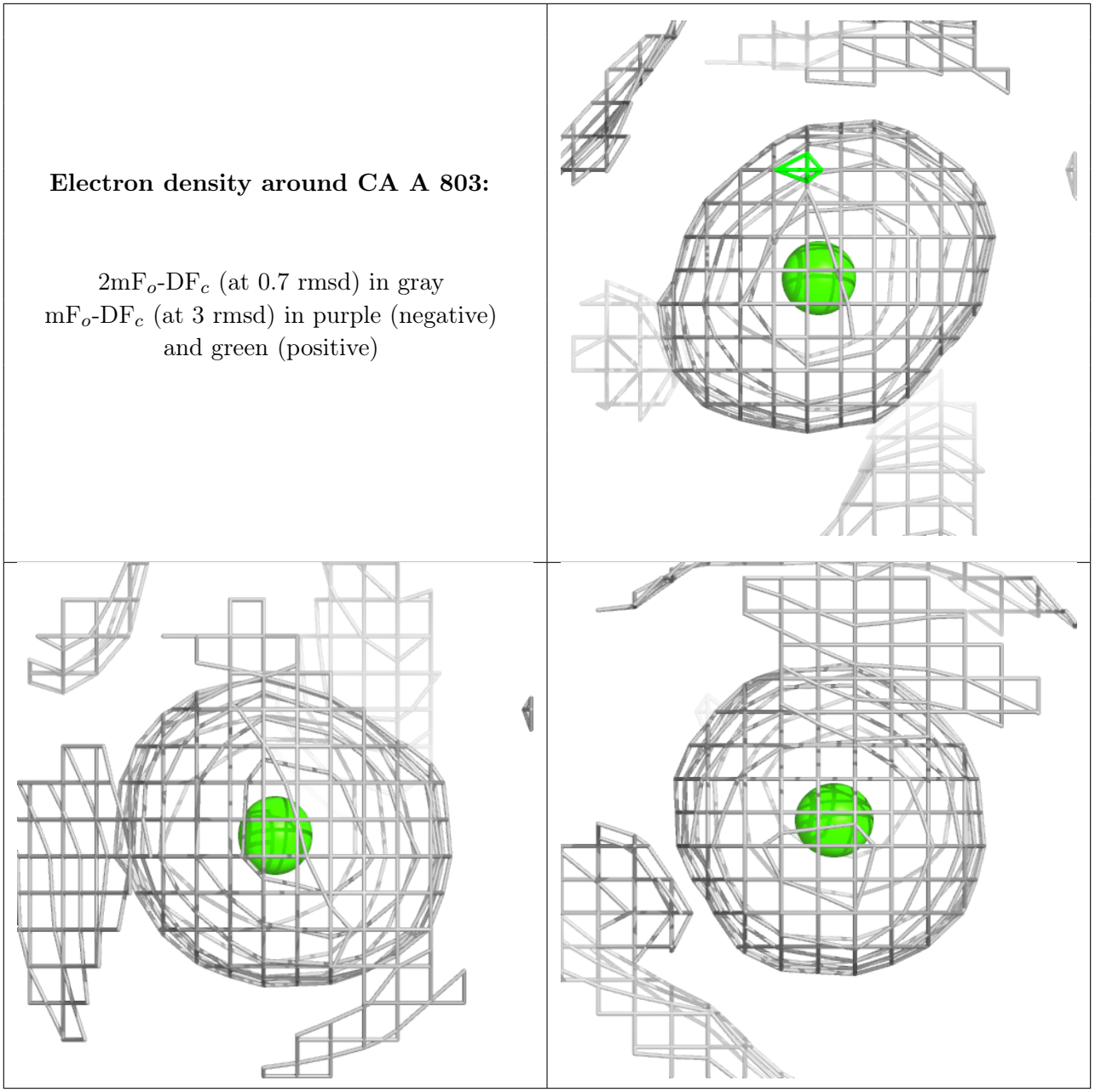
Electron density around GOL B 804:

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



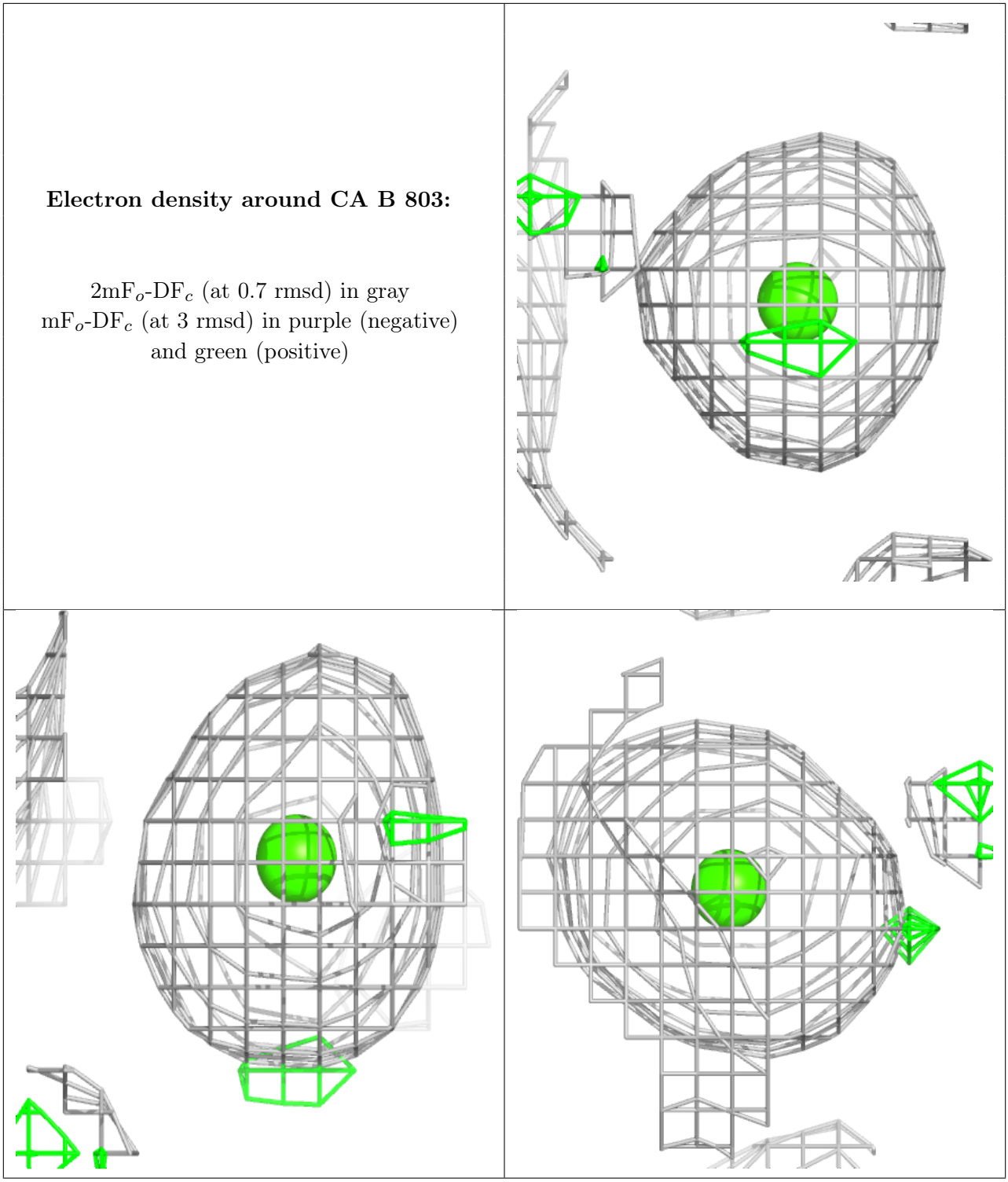
Electron density around CA A 803:

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



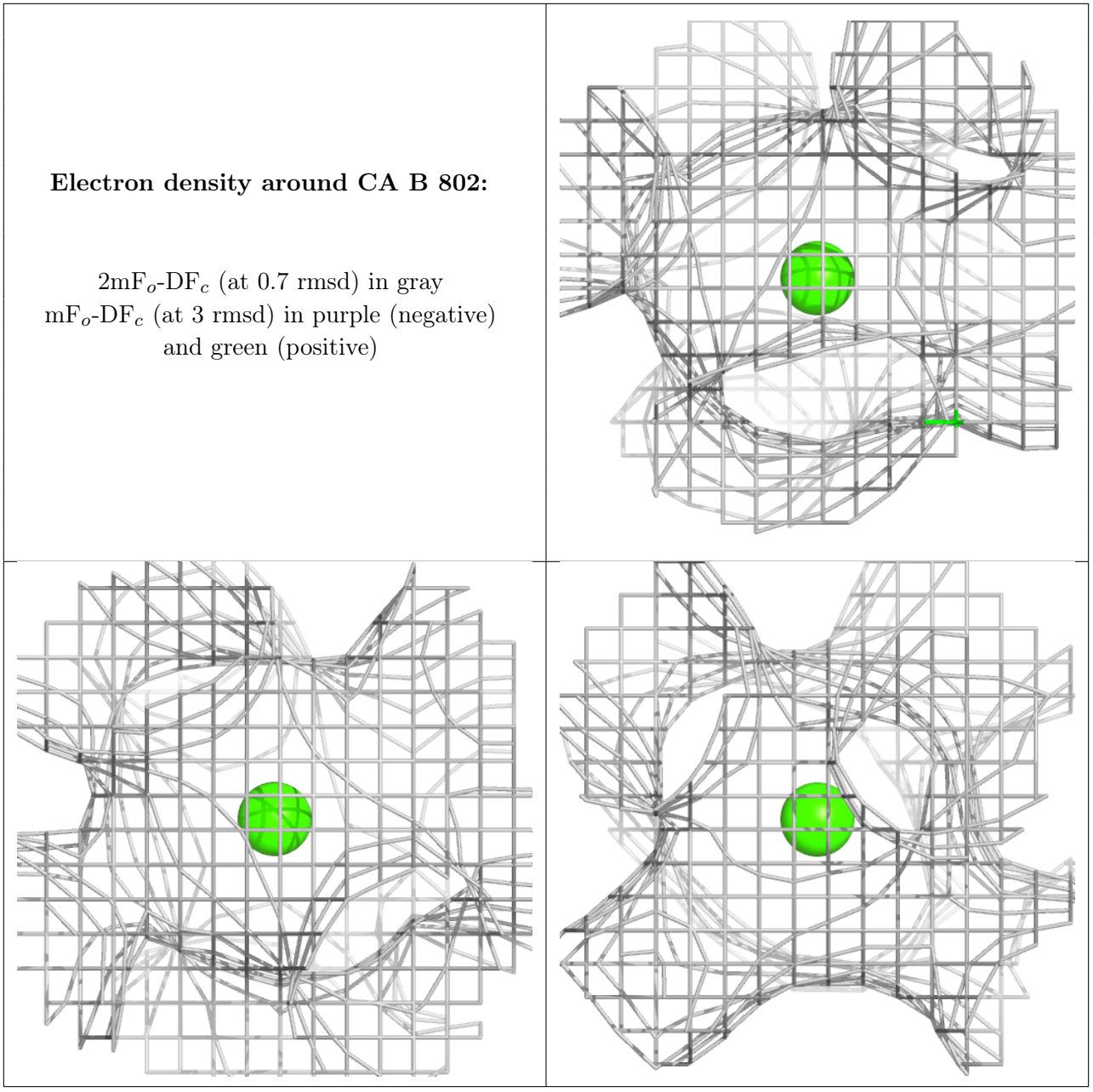
Electron density around CA B 803:

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



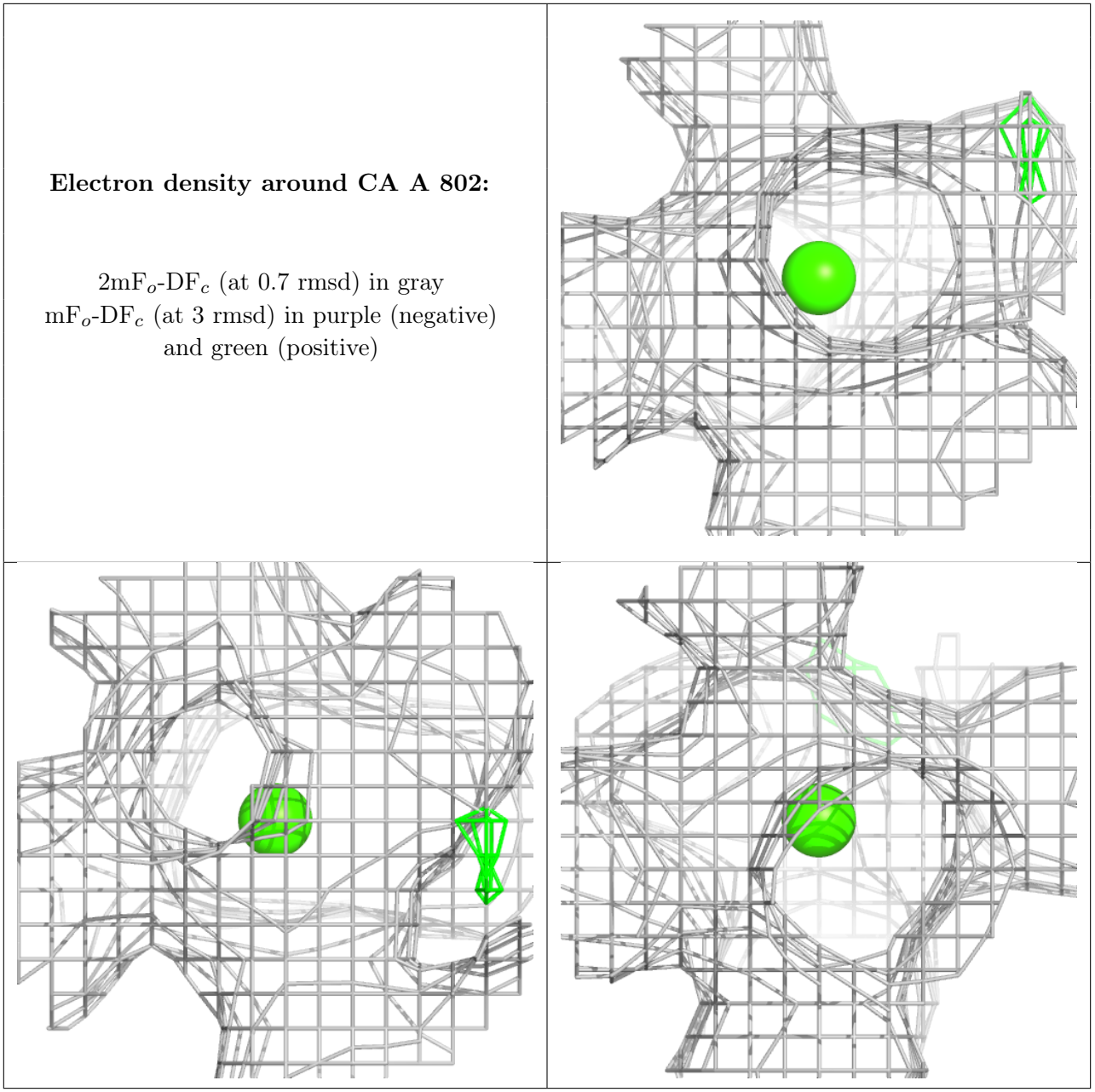
Electron density around CA B 802:

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



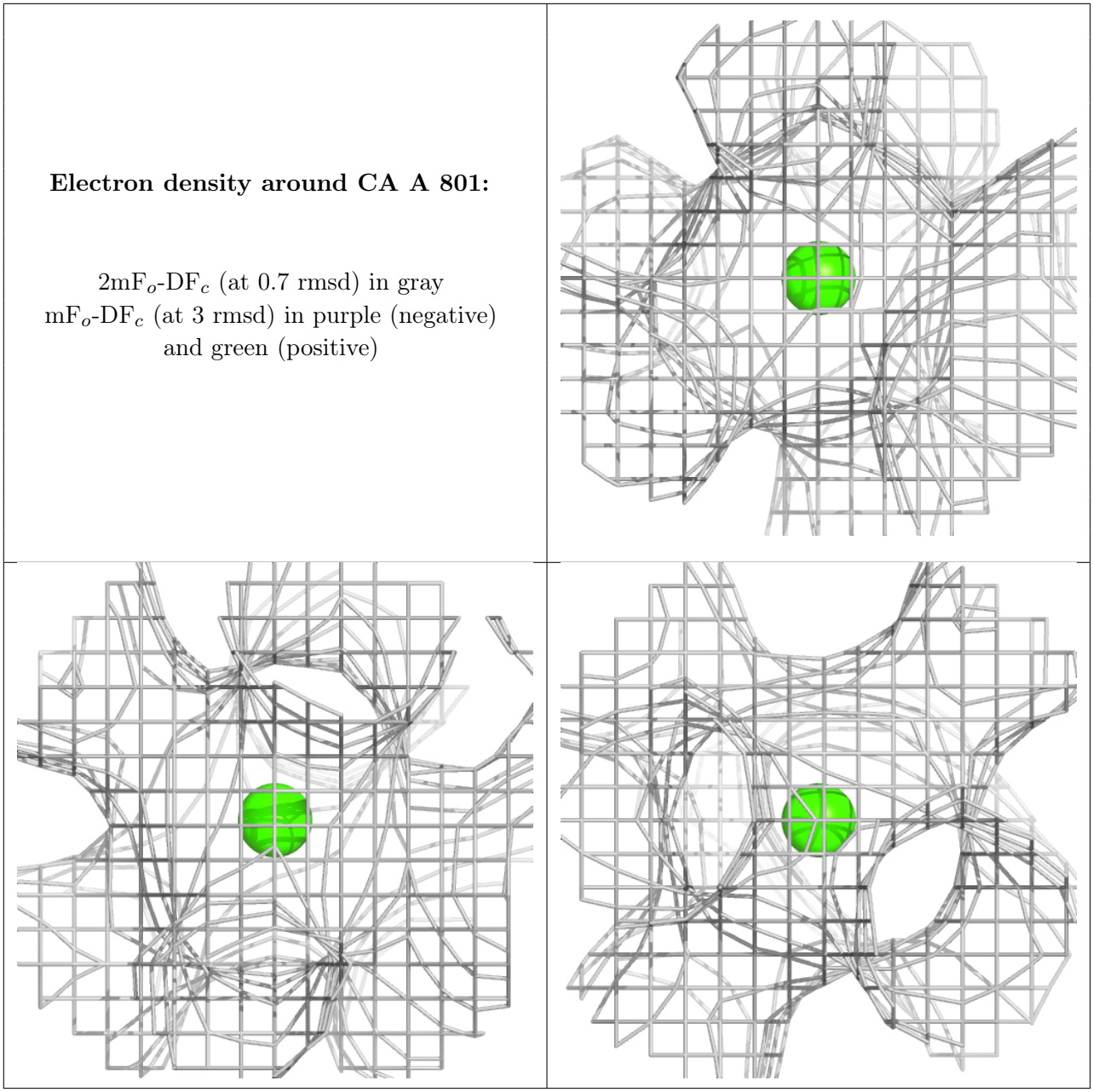
Electron density around CA A 802:

$2mF_o$-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 801:

$2mF_o$-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 801:

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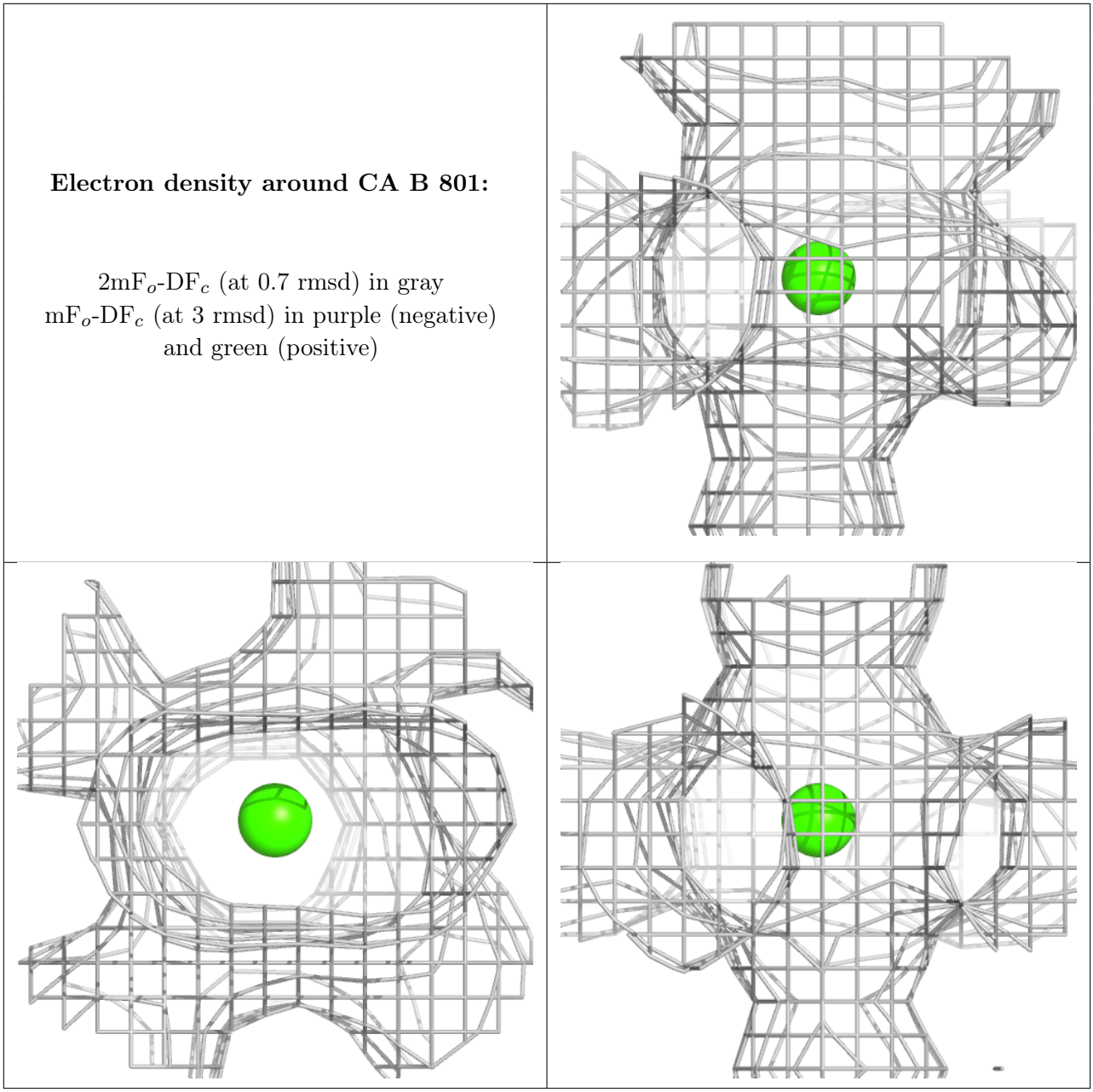
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.