wwPDB X-ray Structure Validation Summary Report (i)

Apr 8, 2025 – 04:10 PM JST

PDB ID	:	9U98 / pdb_00009u98
Title	:	Glycoside hydrolase family 1 beta-glucosidase (E318G mutant) from Streptomyces griseus (sophorose complex)
Authors	:	Kumakura, H.; Motouchi, S.; Nakai, H.; Nakajima, M.
Deposited on	:	2025-03-27
Resolution	:	2.13 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 (1)) were used in the production of this report:

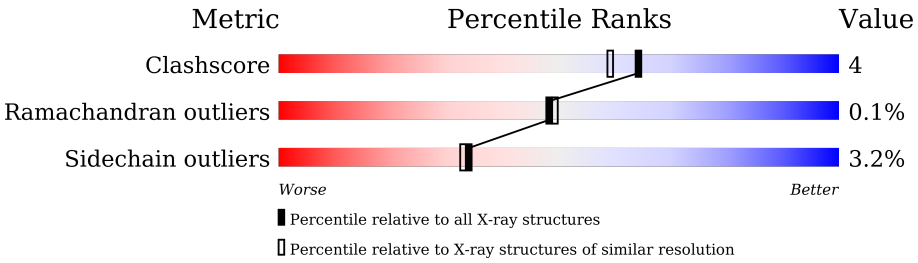
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.13 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))
Clashscore	180529	3585 (2.16-2.12)
Ramachandran outliers	177936	3554 (2.16-2.12)
Sidechain outliers	177891	3553 (2.16-2.12)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	414	87% 8% • •
1	B	414	86% 7% • 5%
1	C	414	86% 9% • •
1	D	414	74% 12% • 12%
2	E	2	50% 50%
2	H	2	50% 50%
3	F	2	50% 50%
3	G	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	I	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12837 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 Putative beta-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3114	1968	548	590	8			
1	B	395	Total	C	N	O	S	0	0	0
			3067	1939	538	582	8			
1	C	400	Total	C	N	O	S	0	0	0
			3110	1967	545	590	8			
1	D	364	Total	C	N	O	S	0	0	0
			2854	1807	502	537	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	GLY	GLU	engineered mutation	UNP B1W1N0
A	407	LEU	-	expression tag	UNP B1W1N0
A	408	GLU	-	expression tag	UNP B1W1N0
A	409	HIS	-	expression tag	UNP B1W1N0
A	410	HIS	-	expression tag	UNP B1W1N0
A	411	HIS	-	expression tag	UNP B1W1N0
A	412	HIS	-	expression tag	UNP B1W1N0
A	413	HIS	-	expression tag	UNP B1W1N0
A	414	HIS	-	expression tag	UNP B1W1N0
B	318	GLY	GLU	engineered mutation	UNP B1W1N0
B	407	LEU	-	expression tag	UNP B1W1N0
B	408	GLU	-	expression tag	UNP B1W1N0
B	409	HIS	-	expression tag	UNP B1W1N0
B	410	HIS	-	expression tag	UNP B1W1N0
B	411	HIS	-	expression tag	UNP B1W1N0
B	412	HIS	-	expression tag	UNP B1W1N0
B	413	HIS	-	expression tag	UNP B1W1N0
B	414	HIS	-	expression tag	UNP B1W1N0
C	318	GLY	GLU	engineered mutation	UNP B1W1N0
C	407	LEU	-	expression tag	UNP B1W1N0
C	408	GLU	-	expression tag	UNP B1W1N0

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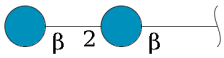
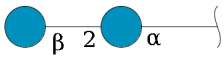
Chain	Residue	Modelled	Actual	Comment	Reference
C	409	HIS	-	expression tag	UNP B1W1N0
C	410	HIS	-	expression tag	UNP B1W1N0
C	411	HIS	-	expression tag	UNP B1W1N0
C	412	HIS	-	expression tag	UNP B1W1N0
C	413	HIS	-	expression tag	UNP B1W1N0
C	414	HIS	-	expression tag	UNP B1W1N0
D	318	GLY	GLU	engineered mutation	UNP B1W1N0
D	407	LEU	-	expression tag	UNP B1W1N0
D	408	GLU	-	expression tag	UNP B1W1N0
D	409	HIS	-	expression tag	UNP B1W1N0
D	410	HIS	-	expression tag	UNP B1W1N0
D	411	HIS	-	expression tag	UNP B1W1N0
D	412	HIS	-	expression tag	UNP B1W1N0
D	413	HIS	-	expression tag	UNP B1W1N0
D	414	HIS	-	expression tag	UNP B1W1N0

- Molecule 2 is an oligosaccharide called beta-D-glucopyranose-(1-2)-beta-D-glucopyranose.



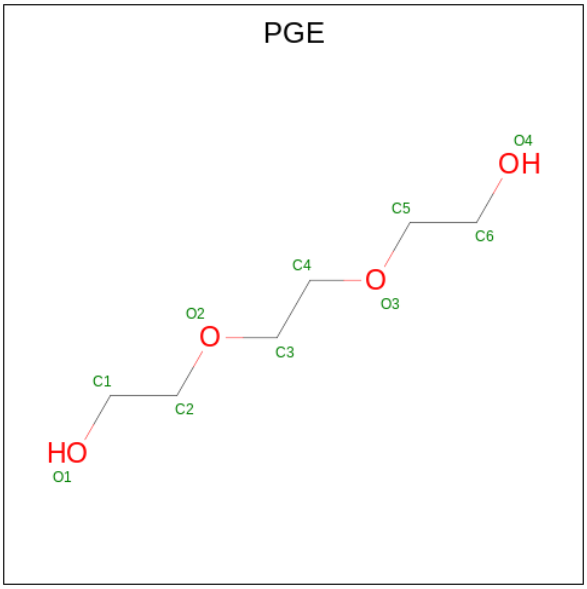
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is an oligosaccharide called beta-D-glucopyranose-(1-2)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	F	2	Total	C	O	0	0	0
			23	12	11			
3	G	2	Total	C	O	0	0	0
			23	12	11			
3	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).

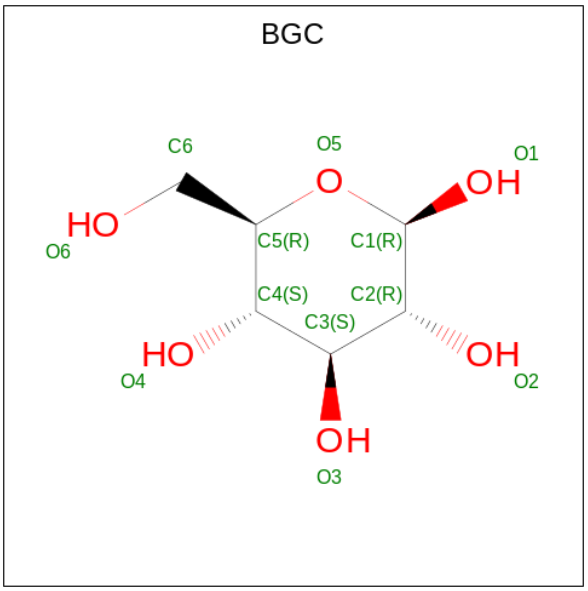


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0
4	C	1	Total C O 10 6 4	0	0

- 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	2	Total Cl 2 2	0	0
5	B	2	Total Cl 2 2	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total C O 12 6 6	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	168	Total O 168 168	0	0
7	B	138	Total O 138 138	0	0
7	C	145	Total O 145 145	0	0
7	D	79	Total O 79 79	0	0

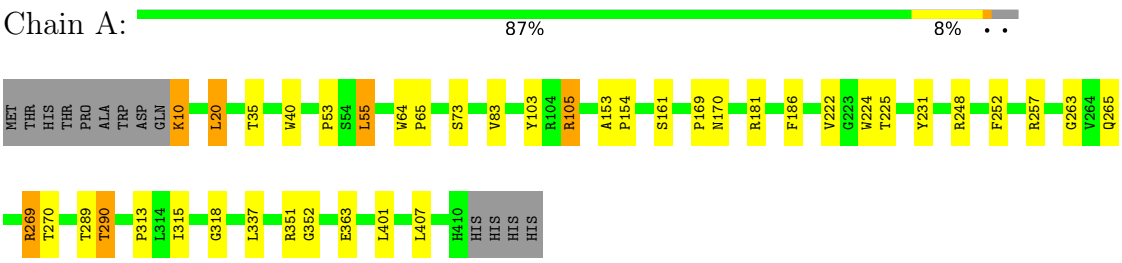
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

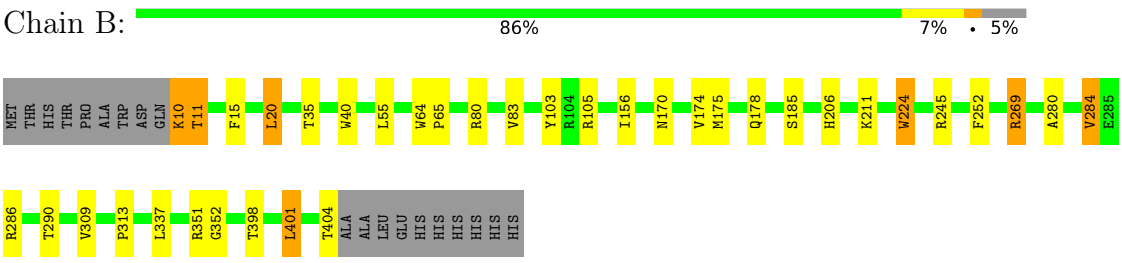
- Molecule 1: Putative beta-glucosidase

Chain A:



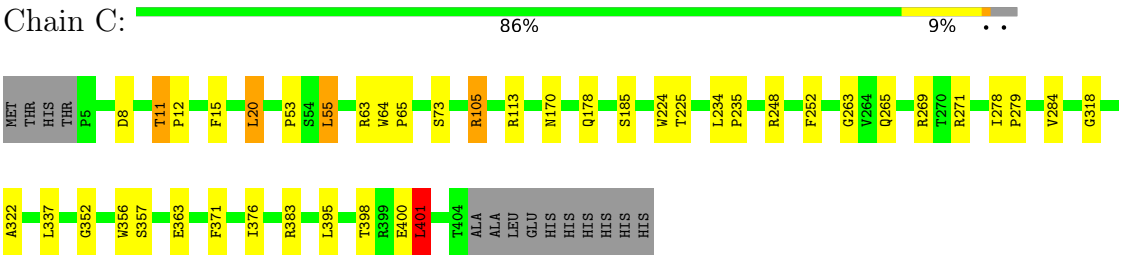
- Molecule 1: Putative beta-glucosidase

Chain B:



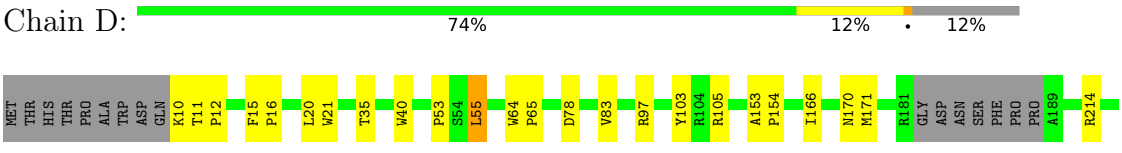
- Molecule 1: Putative beta-glucosidase

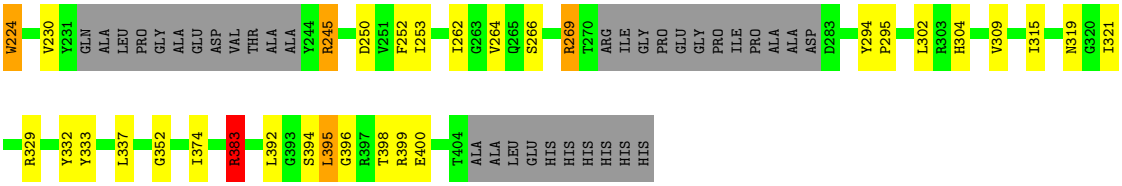
Chain C:



- Molecule 1: Putative beta-glucosidase

Chain D:





- Molecule 2: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose

Chain E:

- Molecule 2: beta-D-glucopyranose-(1-2)-beta-D-glucopyranose

Chain H:

- Molecule 3: beta-D-glucopyranose-(1-2)-alpha-D-glucopyranose

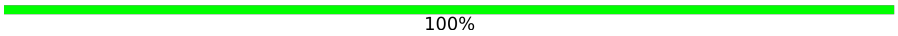
Chain F:

- Molecule 3: beta-D-glucopyranose-(1-2)-alpha-D-glucopyranose

Chain G:

- Molecule 3: beta-D-glucopyranose-(1-2)-alpha-D-glucopyranose

Chain I:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.79Å 100.18Å 96.05Å 90.00° 102.87° 90.00°	Depositor
Resolution (Å)	46.82 – 2.13	Depositor
% Data completeness (in resolution range)	98.5 (46.82-2.13)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.181 , 0.228	Depositor
Wilson B-factor (Å^2)	25.6	Xtriage
Anisotropy	0.024	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
Total number of atoms	12837	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: PGE, GLC, BGC, 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	0.49	0/3205	0.86	2/4386 (0.0%)
1	B	0.50	0/3156	0.88	2/4319 (0.0%)
1	C	0.52	0/3202	0.89	3/4383 (0.1%)
1	D	0.49	0/2933	0.88	0/4005
All	All	0.50	0/12496	0.88	7/17093 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	248	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	C	20	LEU	CB-CG-CD1	5.87	120.98	111.00
1	B	80	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	401	LEU	CB-CG-CD1	5.38	120.14	111.00
1	A	257	ARG	NE-CZ-NH2	5.32	122.96	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	269	ARG	Sidechain
1	B	245	ARG	Sidechain
1	B	269	ARG	Sidechain
1	C	105	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3114	0	2945	20	0
1	B	3067	0	2904	17	0
1	C	3110	0	2939	23	0
1	D	2854	0	2703	31	0
2	E	23	0	21	1	0
2	H	23	0	21	0	0
3	F	23	0	21	0	0
3	G	23	0	21	0	0
3	I	23	0	21	0	0
4	A	10	0	14	2	0
4	B	10	0	14	0	0
4	C	10	0	14	0	0
5	A	2	0	0	0	0
5	B	2	0	0	2	0
5	C	1	0	0	1	0
6	D	12	0	12	0	0
7	A	168	0	0	1	0
7	B	138	0	0	2	0
7	C	145	0	0	1	0
7	D	79	0	0	2	0
All	All	12837	0	11650	91	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.

The worst 5 of 91 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:D:250:ASP:OD1	1:D:304:HIS:NE2	2.25	0.69
1:D:20:LEU:HB2	1:D:352:GLY:HA3	1.81	0.63
1:A:20:LEU:HB2	1:A:352:GLY:HA3	1.82	0.62
1:C:363:GLU:OE1	5:C:502:CL:CL	2.58	0.59
1:D:230:VAL:HG12	1:D:230:VAL:O	2.03	0.58

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	399/414 (96%)	384 (96%)	15 (4%)	0	100	100
1	B	393/414 (95%)	382 (97%)	11 (3%)	0	100	100
1	C	398/414 (96%)	388 (98%)	10 (2%)	0	100	100
1	D	356/414 (86%)	335 (94%)	19 (5%)	2 (1%)	22	16
All	All	1546/1656 (93%)	1489 (96%)	55 (4%)	2 (0%)	48	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	395	LEU
1	D	16	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	310/322 (96%)	299 (96%)	11 (4%)	31	29
1	B	306/322 (95%)	295 (96%)	11 (4%)	30	28
1	C	310/322 (96%)	301 (97%)	9 (3%)	37	36
1	D	285/322 (88%)	277 (97%)	8 (3%)	38	38
All	All	1211/1288 (94%)	1172 (97%)	39 (3%)	34	33

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	284	VAL
1	D	269	ARG
1	C	337	LEU
1	D	171	MET
1	D	383	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	9	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)

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

5.5 Carbohydrates (i)

10 monosaccharides 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	$\#\|Z\|>2$
2	BGC	E	1	2	12,12,12	0.30	0	17,17,17	0.48	0
2	BGC	E	2	2	11,11,12	0.64	0	15,15,17	1.57	3 (20%)
3	GLC	F	1	3	12,12,12	0.21	0	17,17,17	0.30	0
3	BGC	F	2	3	11,11,12	0.33	0	15,15,17	0.76	1 (6%)
3	GLC	G	1	3	12,12,12	0.26	0	17,17,17	0.39	0
3	BGC	G	2	3	11,11,12	0.46	0	15,15,17	1.45	2 (13%)
2	BGC	H	1	2	12,12,12	0.28	0	17,17,17	0.51	0
2	BGC	H	2	2	11,11,12	0.57	0	15,15,17	1.91	3 (20%)
3	GLC	I	1	3	12,12,12	0.16	0	17,17,17	0.29	0
3	BGC	I	2	3	11,11,12	0.34	0	15,15,17	0.64	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
2	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
3	GLC	F	1	3	-	0/2/22/22	0/1/1/1
3	BGC	F	2	3	-	0/2/19/22	0/1/1/1
3	GLC	G	1	3	-	0/2/22/22	0/1/1/1
3	BGC	G	2	3	-	0/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	BGC	H	2	2	-	0/2/19/22	0/1/1/1
3	GLC	I	1	3	-	0/2/22/22	0/1/1/1
3	BGC	I	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	2	BGC	O5-C1-C2	4.96	118.43	110.77
3	G	2	BGC	C1-C2-C3	4.12	114.73	109.67
2	E	2	BGC	O5-C1-C2	4.02	116.97	110.77
2	H	2	BGC	C1-O5-C5	3.85	117.40	112.19
2	H	2	BGC	C1-C2-C3	3.38	113.82	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	BGC	C4-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6

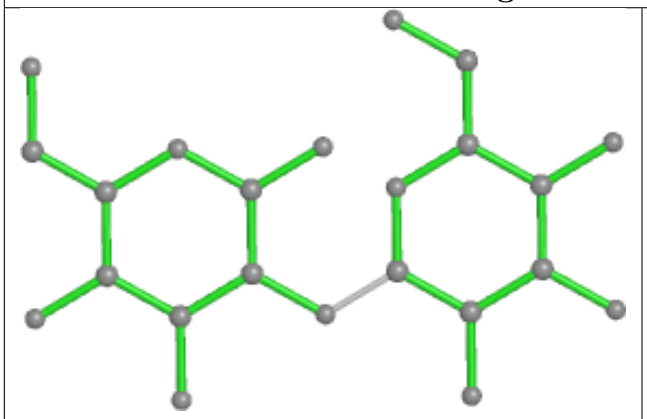
There are no ring outliers.

1 monomer is involved in 1 short contact:

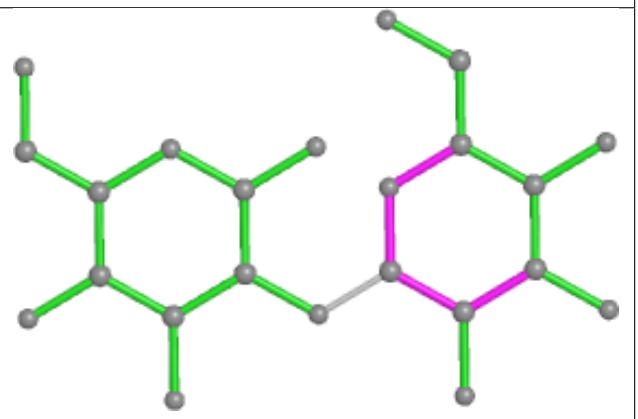
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	BGC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

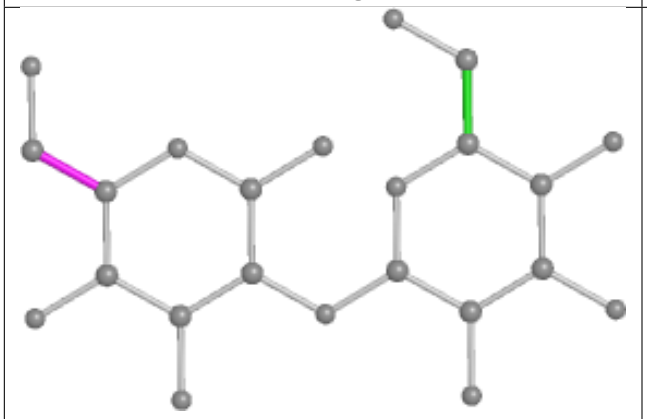
Oligosaccharide Chain E



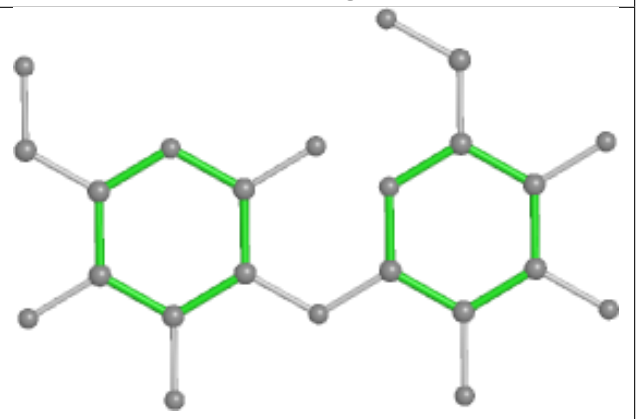
Bond lengths



Bond angles

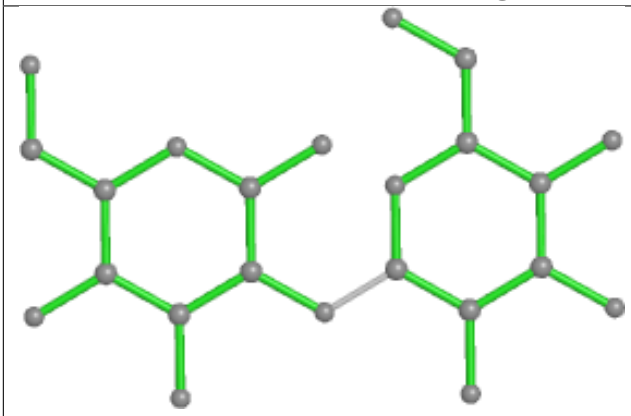


Torsions

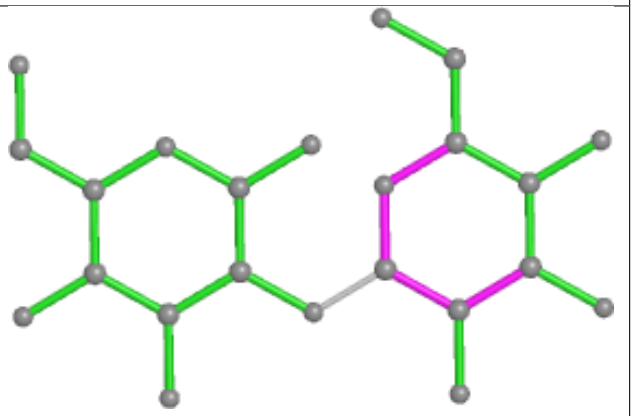


Rings

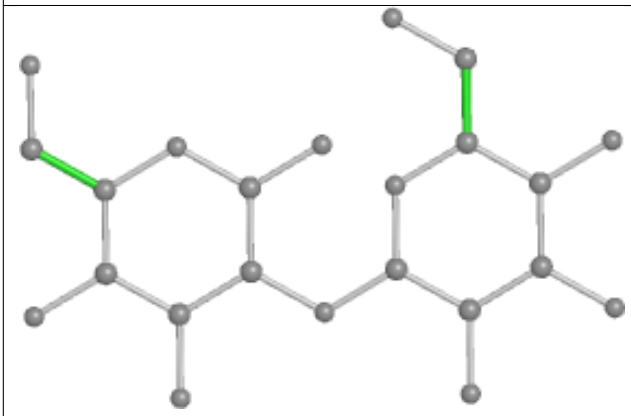
Oligosaccharide Chain H



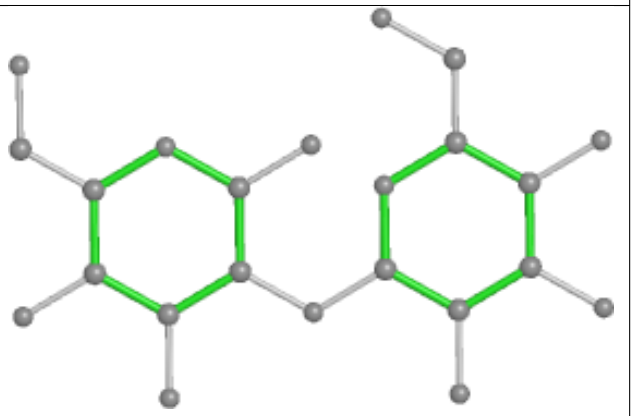
Bond lengths



Bond angles

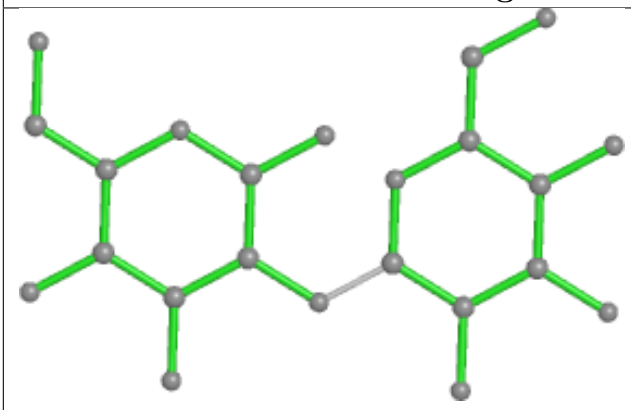


Torsions

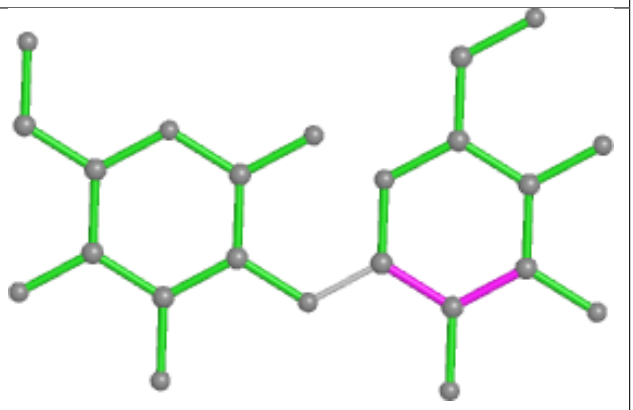


Rings

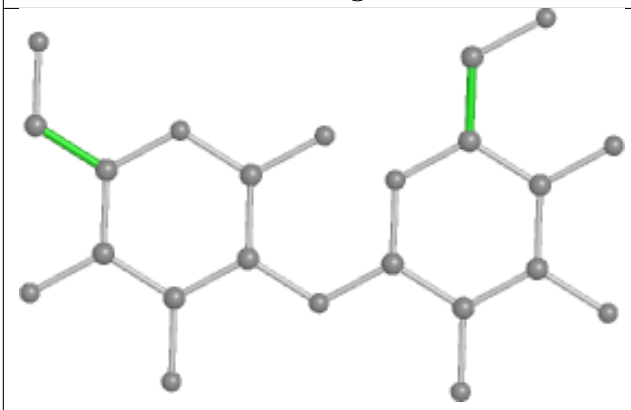
Oligosaccharide Chain F



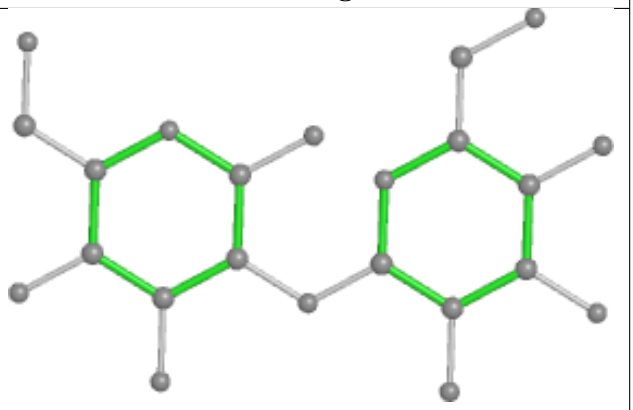
Bond lengths



Bond angles

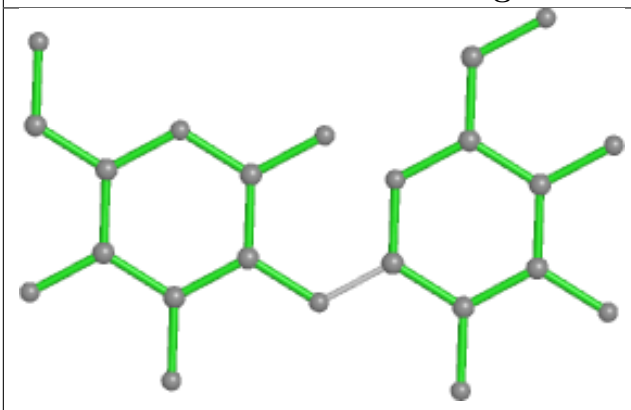


Torsions

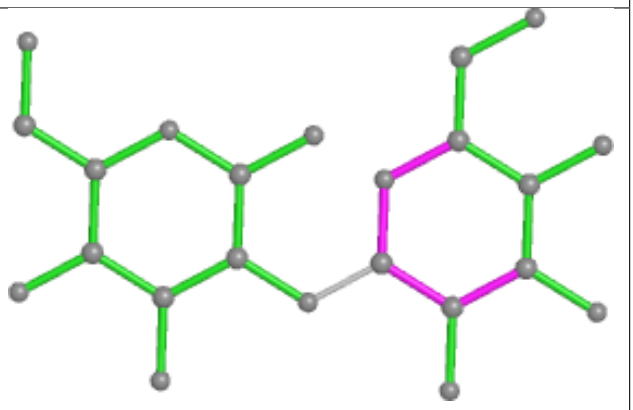


Rings

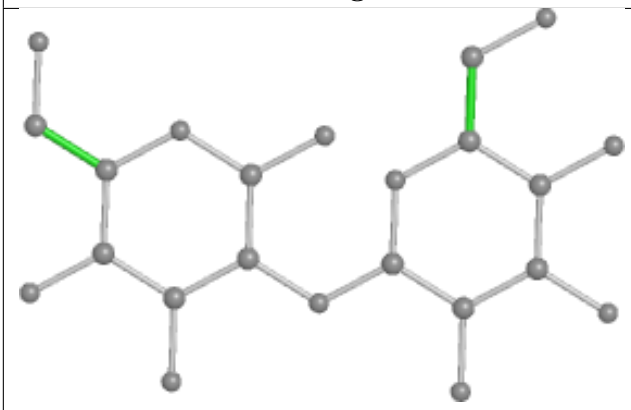
Oligosaccharide Chain G



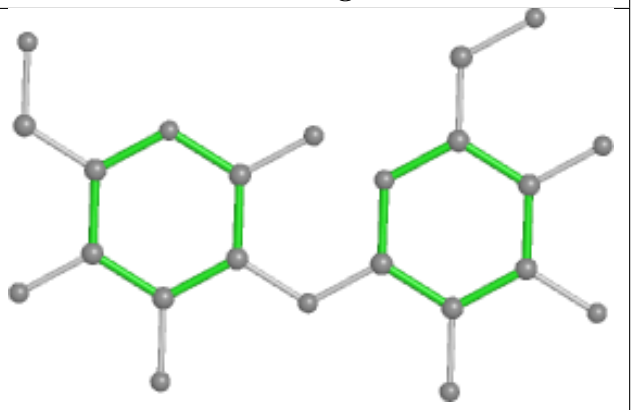
Bond lengths



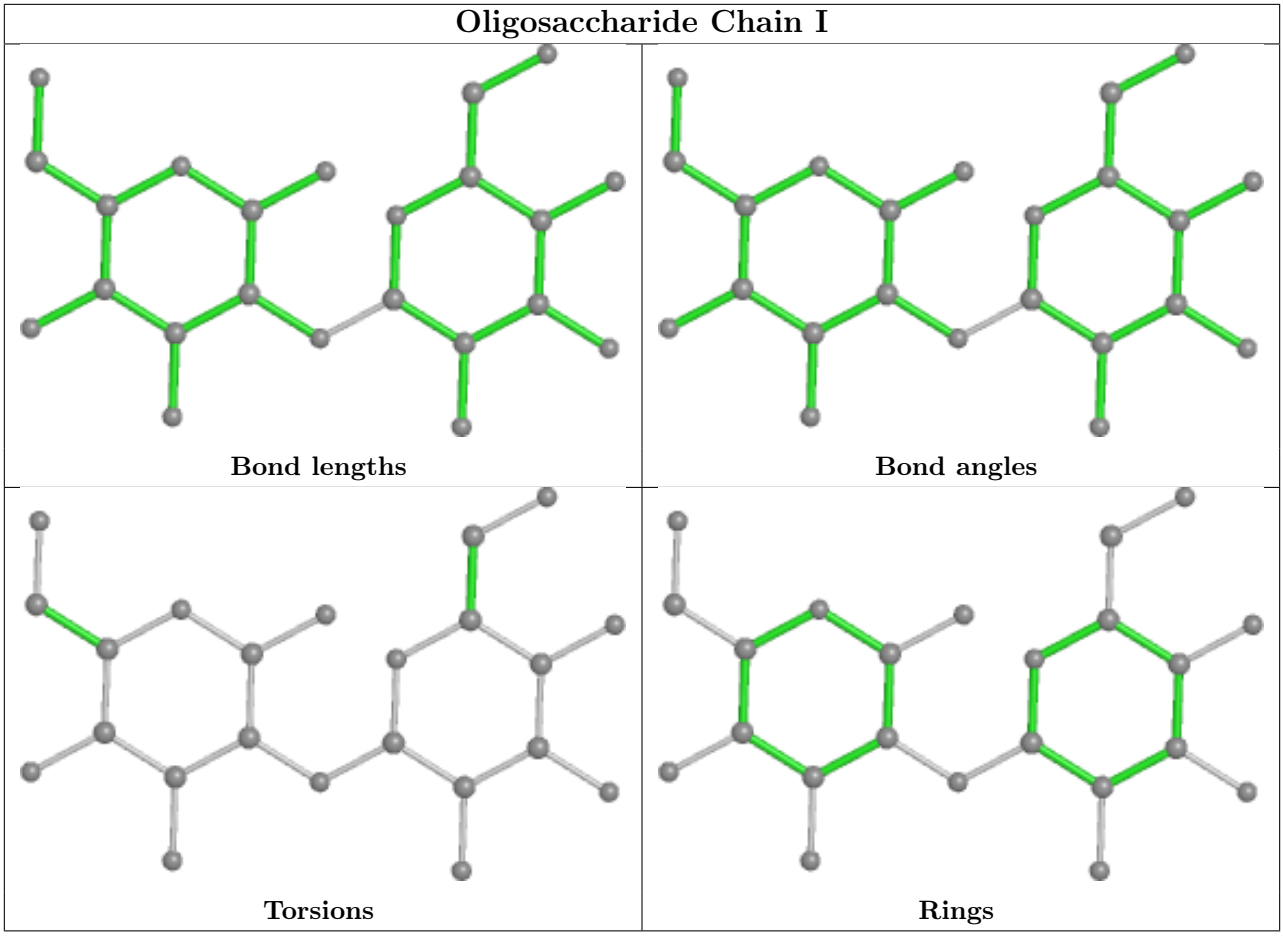
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
6	BGC	D	501	-	12,12,12	0.45	0	17,17,17	1.62	3 (17%)
4	PGE	C	501	-	9,9,9	0.30	0	8,8,8	0.38	0
4	PGE	B	501	-	9,9,9	0.34	0	8,8,8	0.30	0
4	PGE	A	501	-	9,9,9	0.34	0	8,8,8	0.31	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
6	BGC	D	501	-	-	0/2/22/22	0/1/1/1
4	PGE	C	501	-	-	4/7/7/7	-
4	PGE	B	501	-	-	6/7/7/7	-
4	PGE	A	501	-	-	4/7/7/7	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	501	BGC	C1-O5-C5	4.31	121.80	113.66
6	D	501	BGC	O5-C1-C2	2.52	114.77	110.28
6	D	501	BGC	C1-C2-C3	2.20	114.87	110.31

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	PGE	C4-C3-O2-C2
4	A	501	PGE	O2-C3-C4-O3
4	A	501	PGE	O1-C1-C2-O2
4	B	501	PGE	O3-C5-C6-O4
4	A	501	PGE	O3-C5-C6-O4

There are no ring outliers.

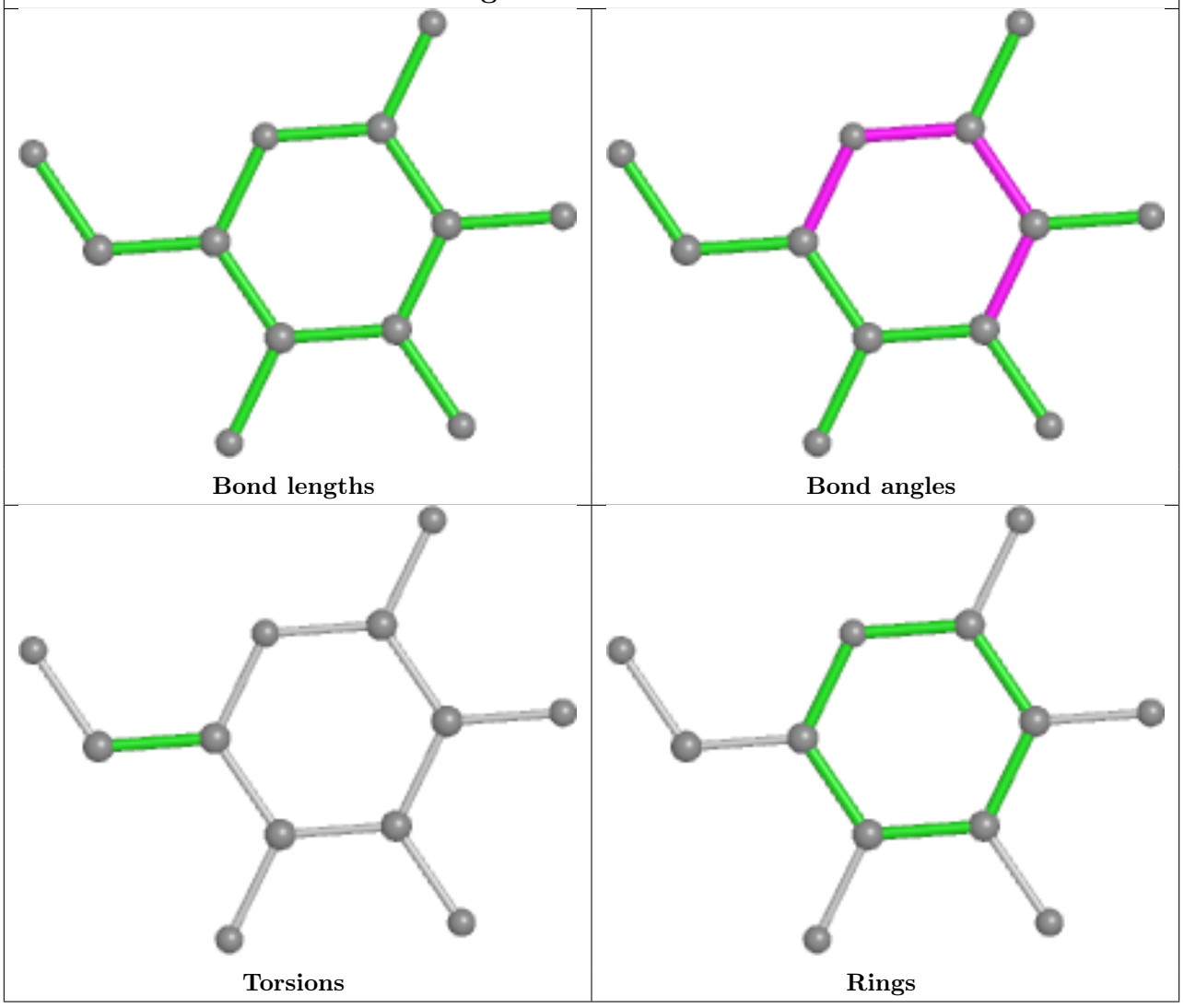
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	PGE	2	0

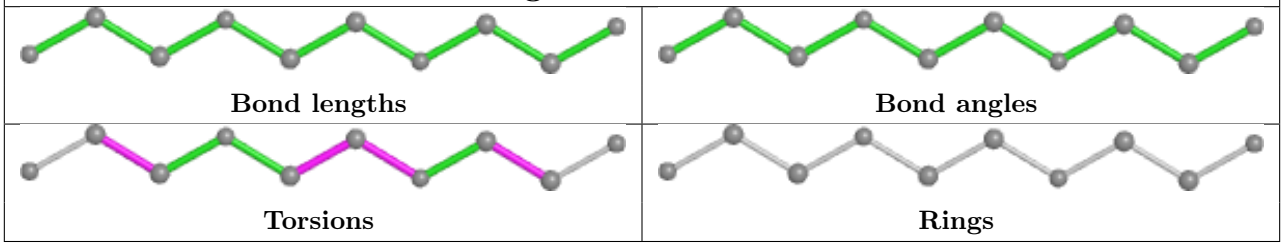
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

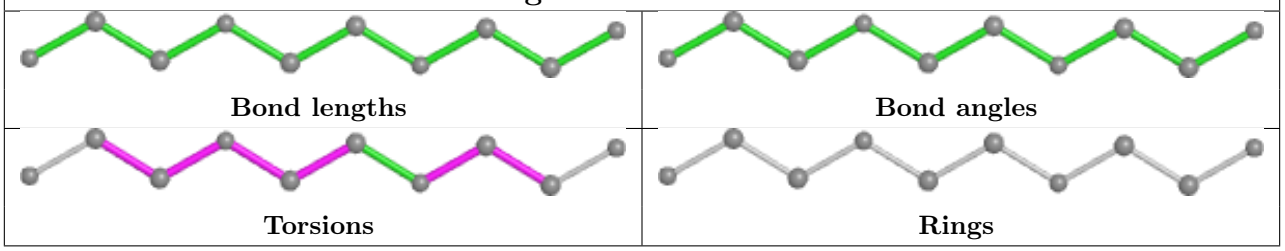
Ligand BGC D 501

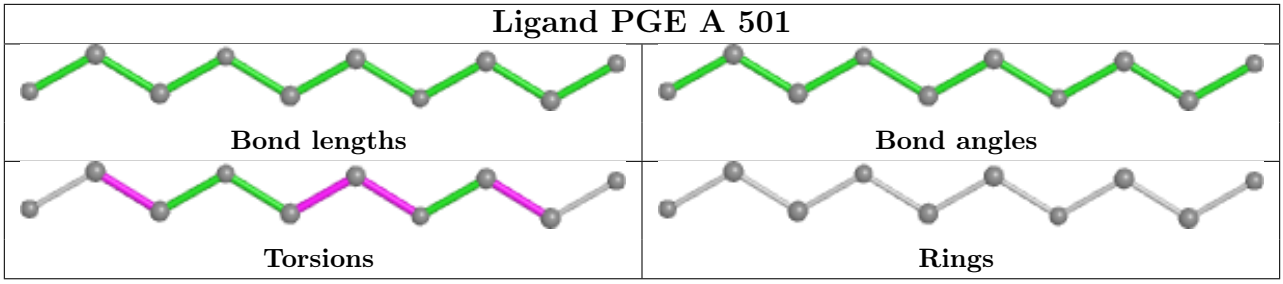


Ligand PGE C 501



Ligand PGE B 501





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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

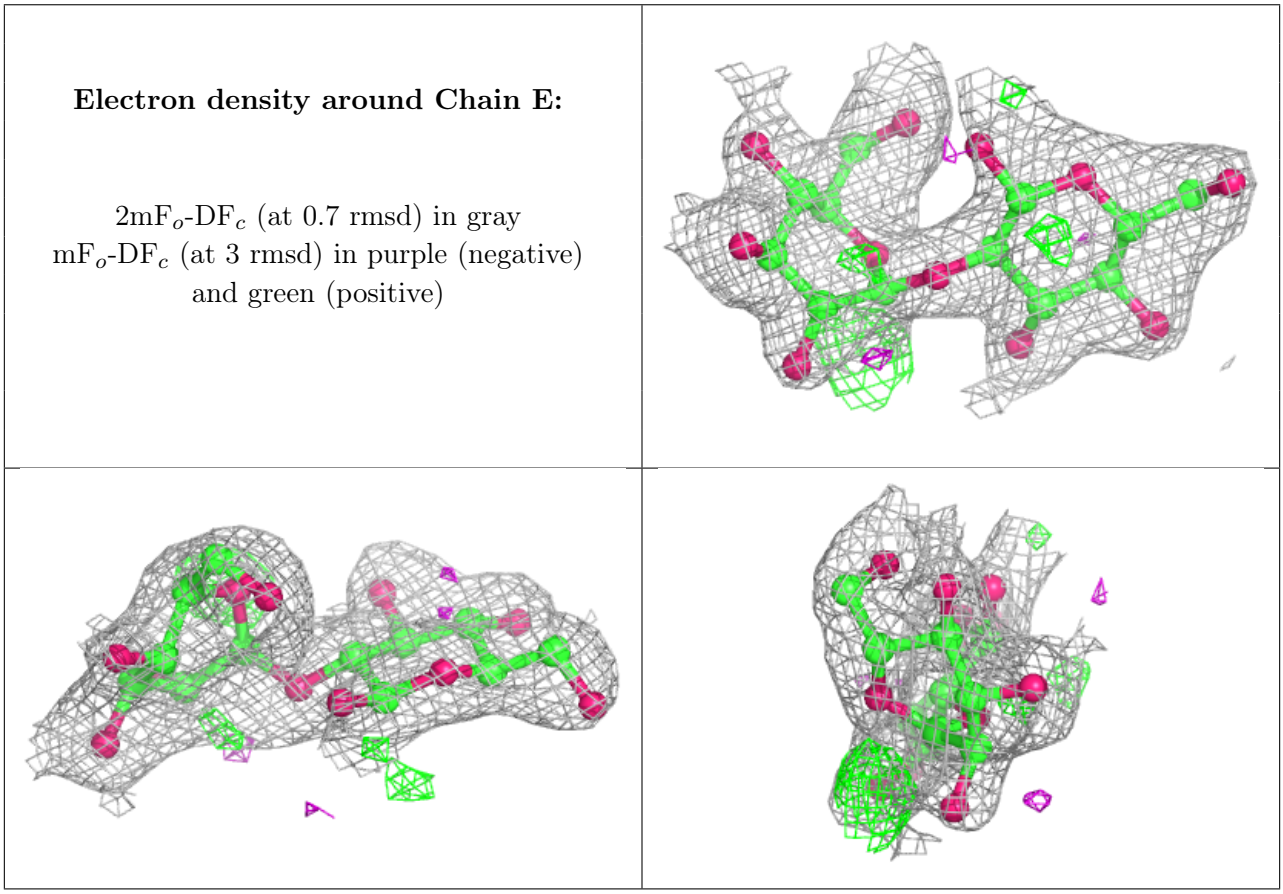
6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

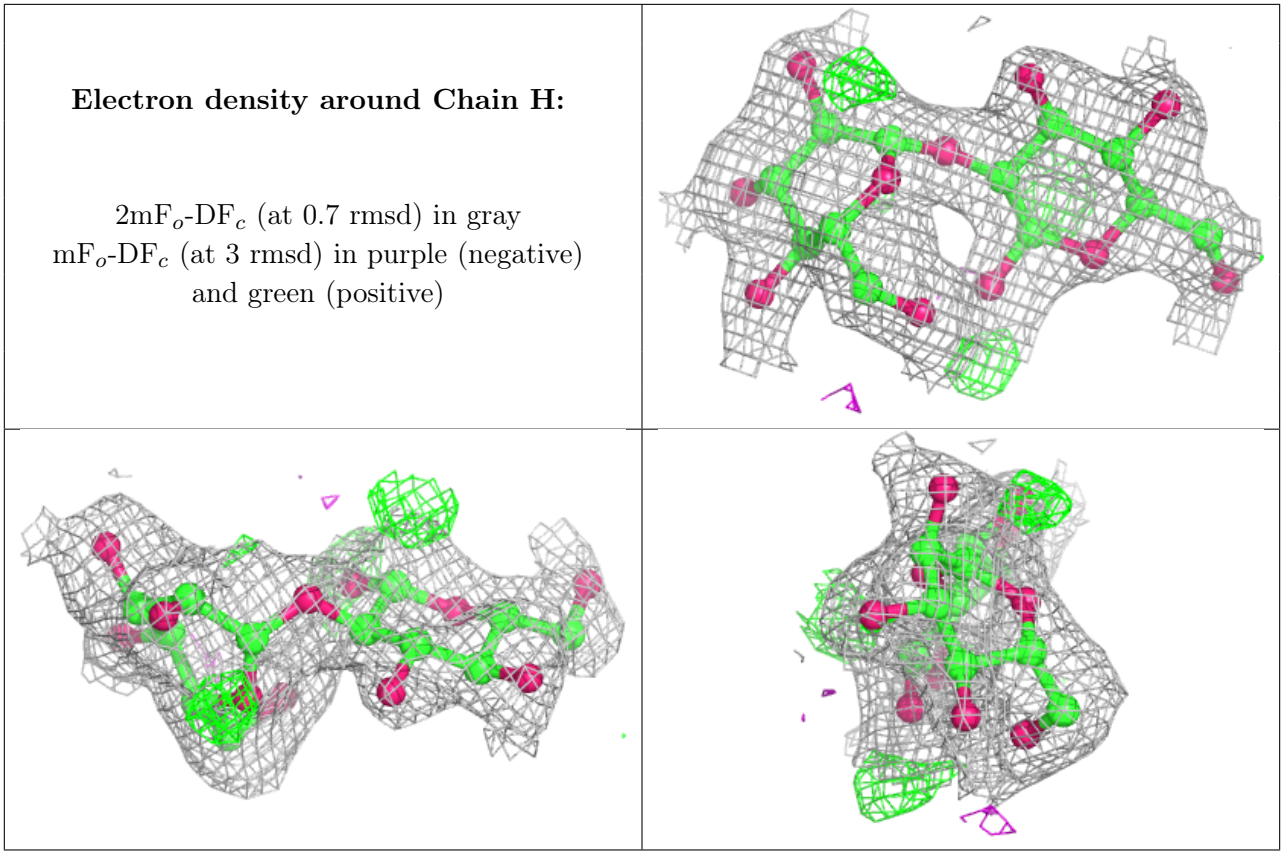
Electron density around Chain E:

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



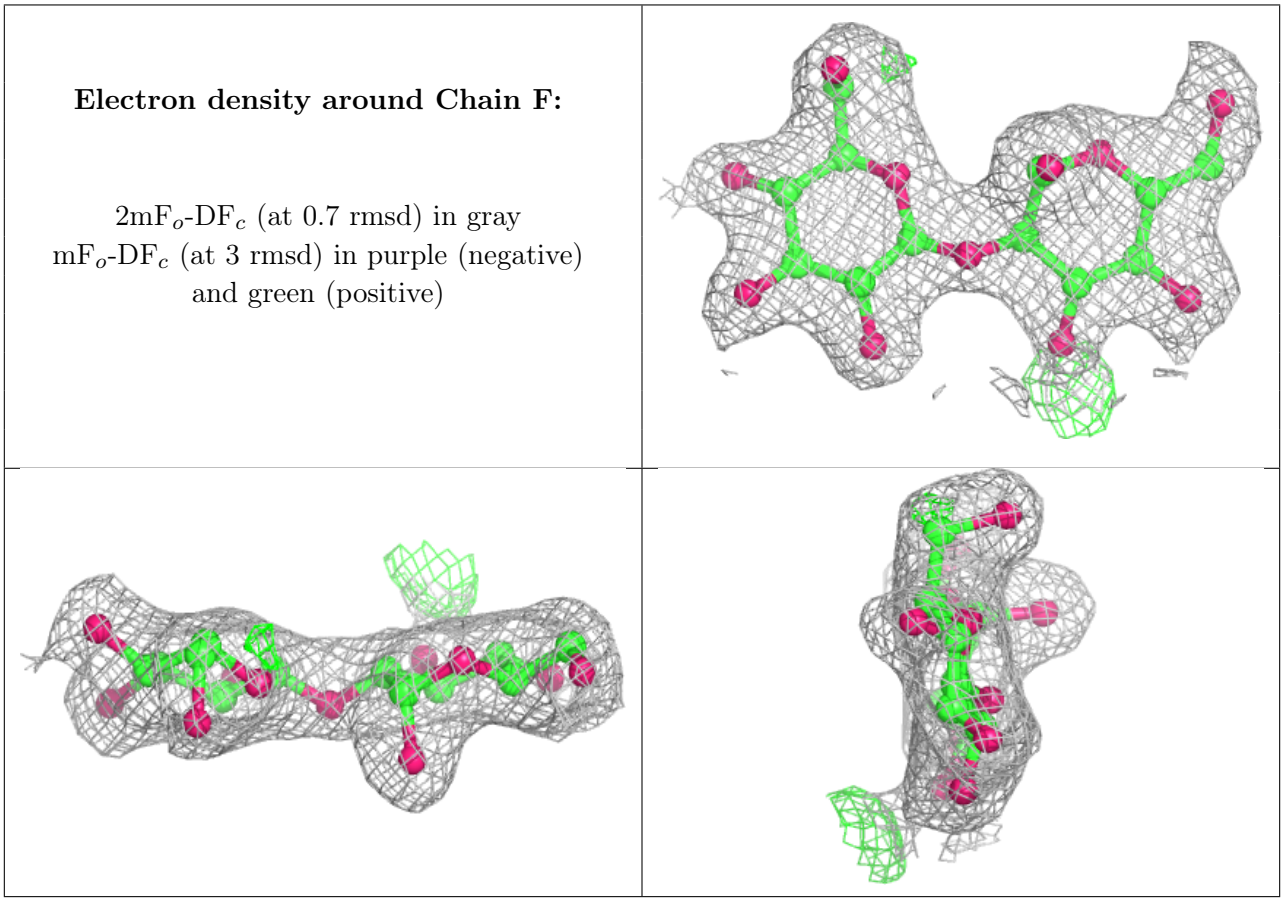
Electron density around Chain H:

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



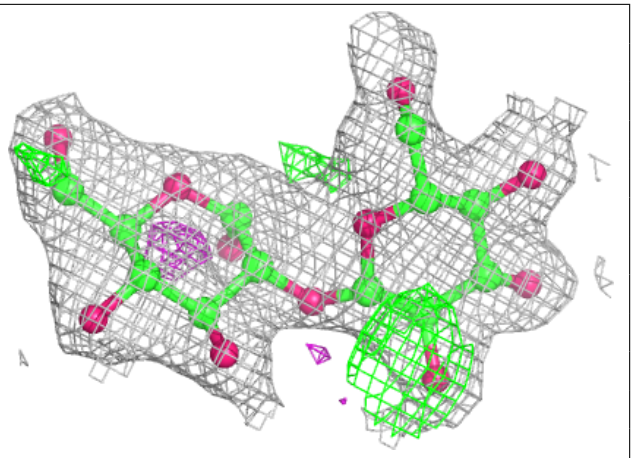
Electron density around Chain F:

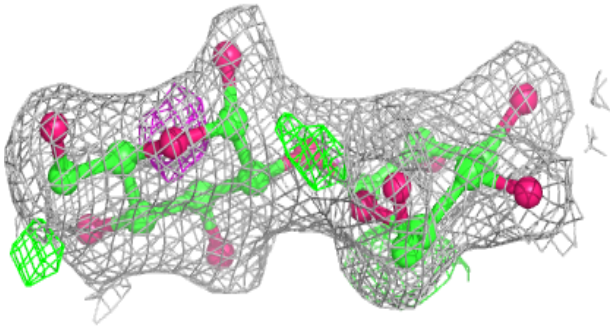
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

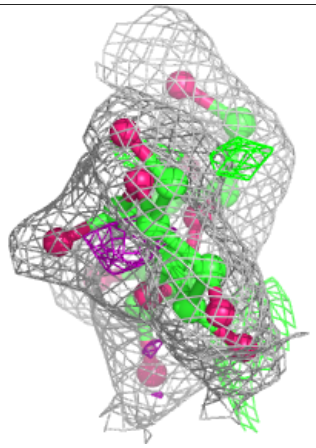


Electron density around Chain G:

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

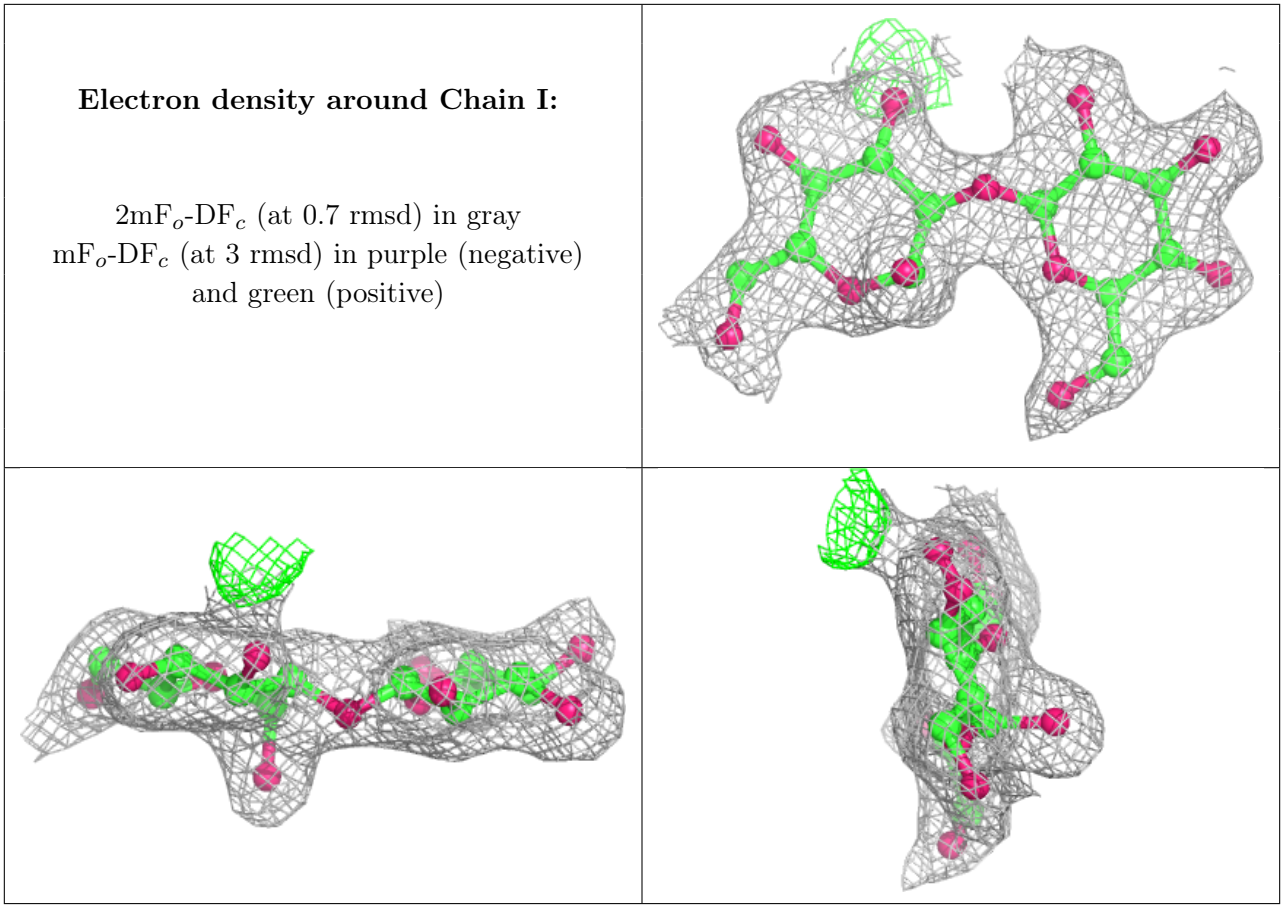






Electron density around Chain I:

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



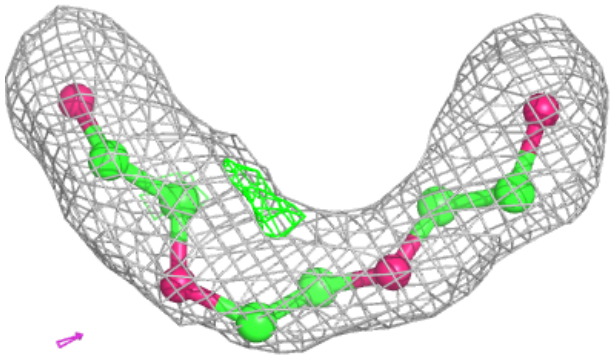
6.4 Ligands

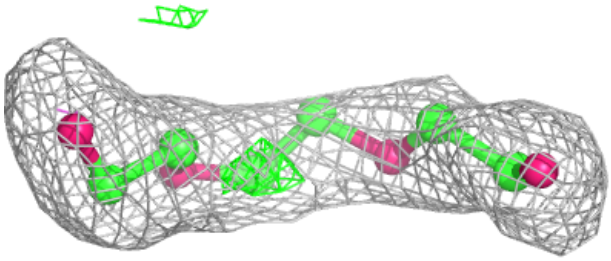
EDS failed to run properly - this section is therefore empty.

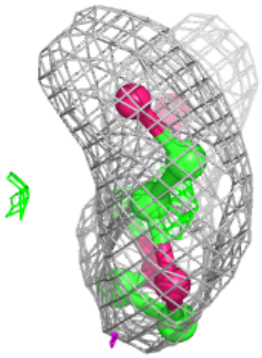
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGE A 501:

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

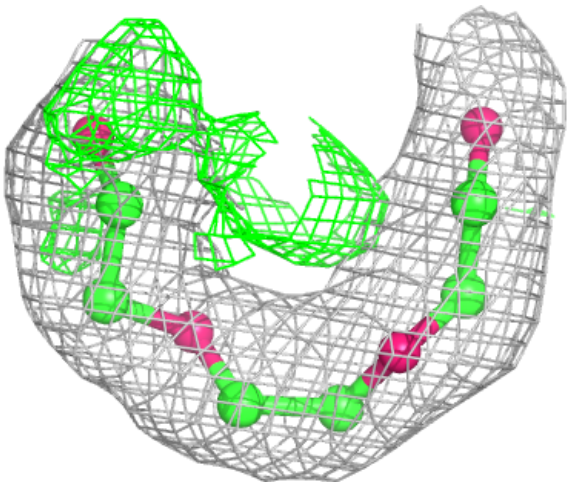


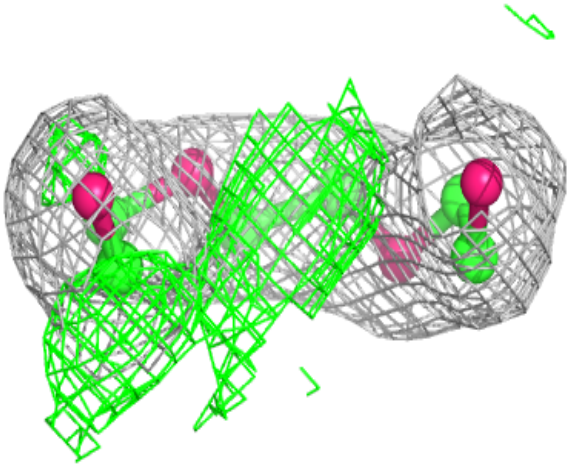


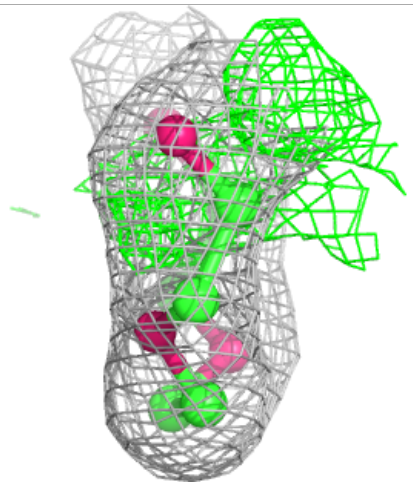


Electron density around PGE B 501:

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

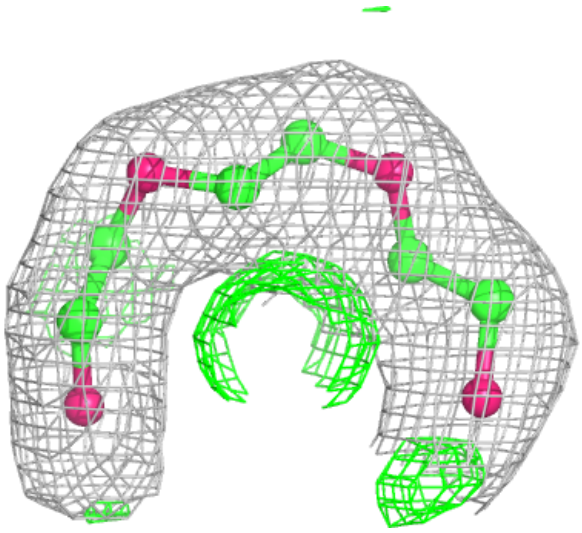


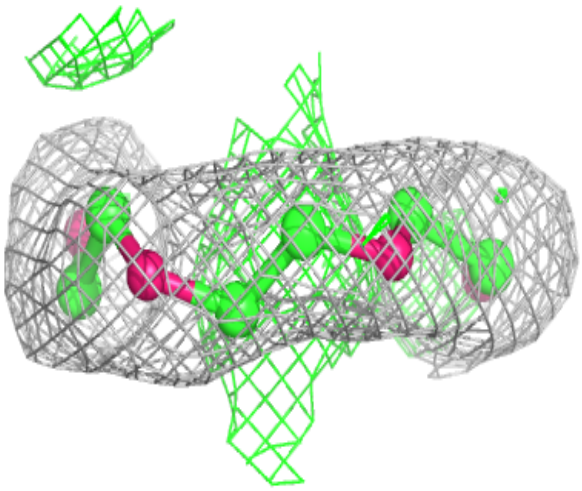


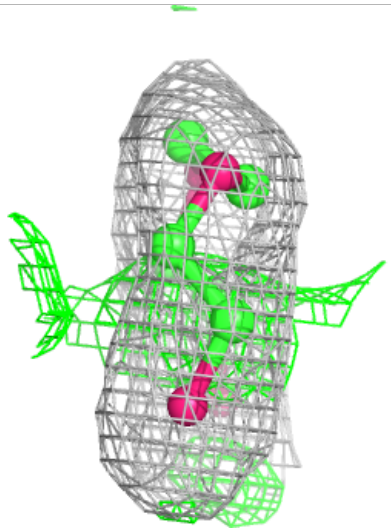


Electron density around PGE C 501:

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

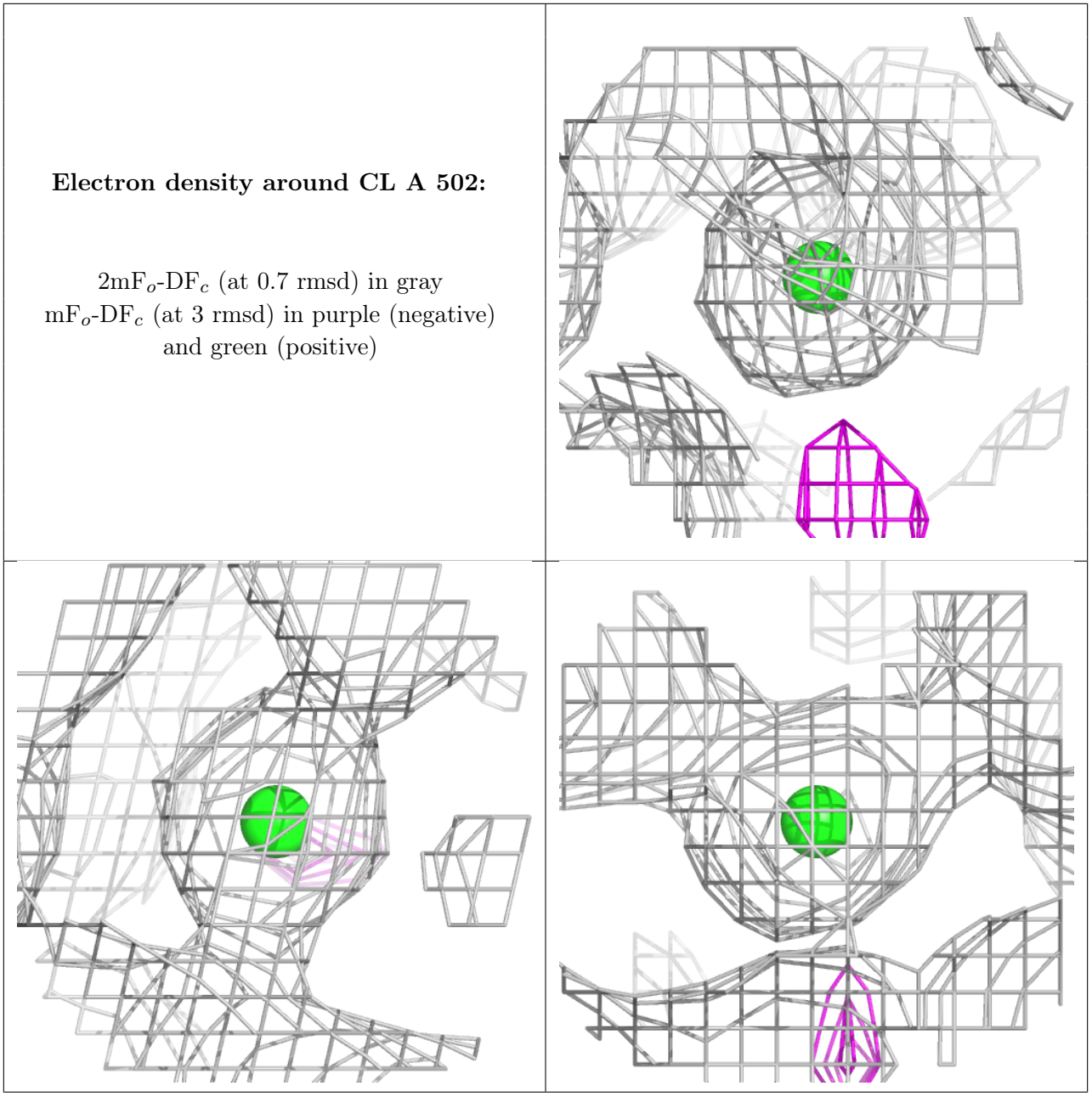






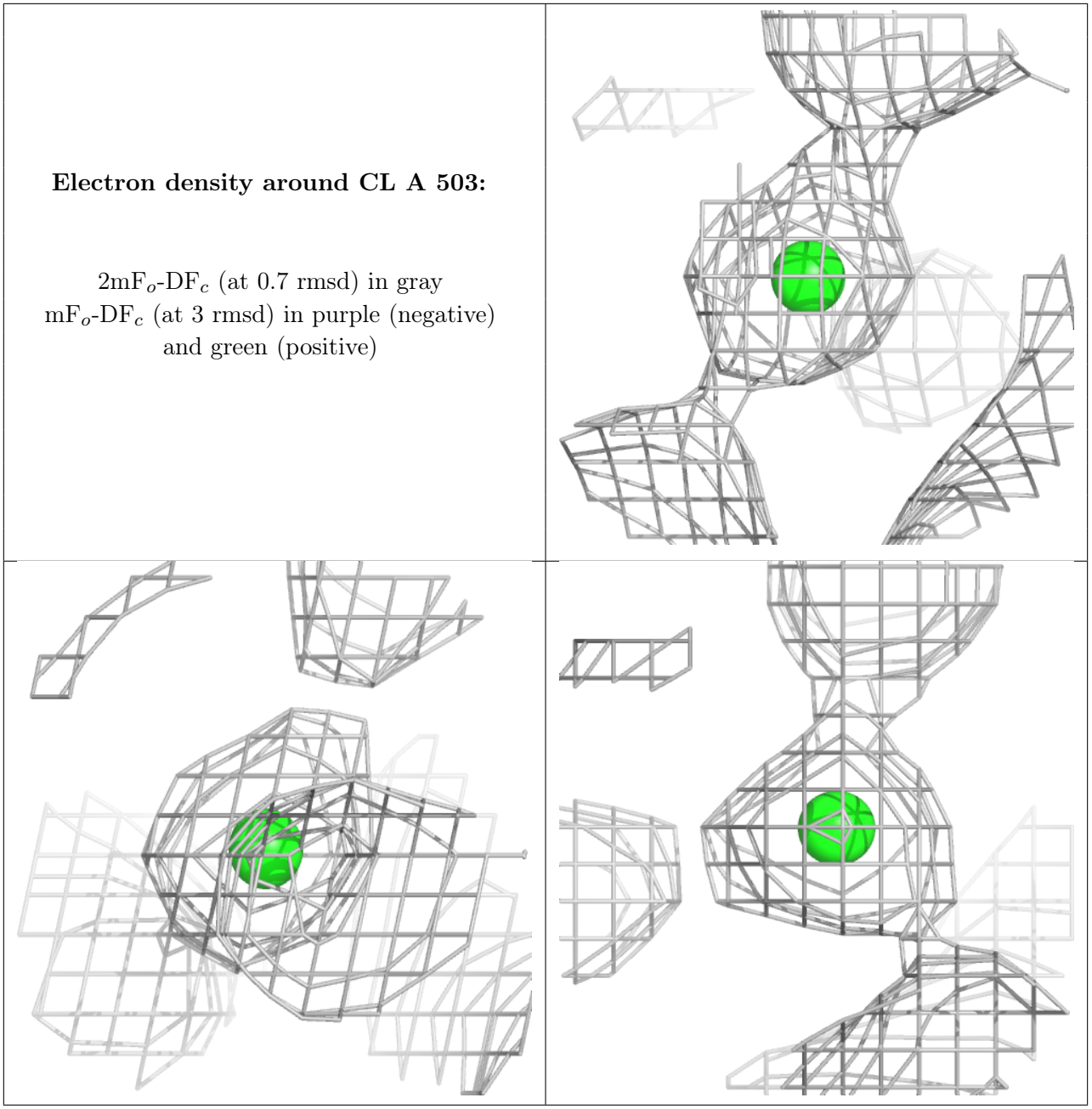
Electron density around CL A 502:

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



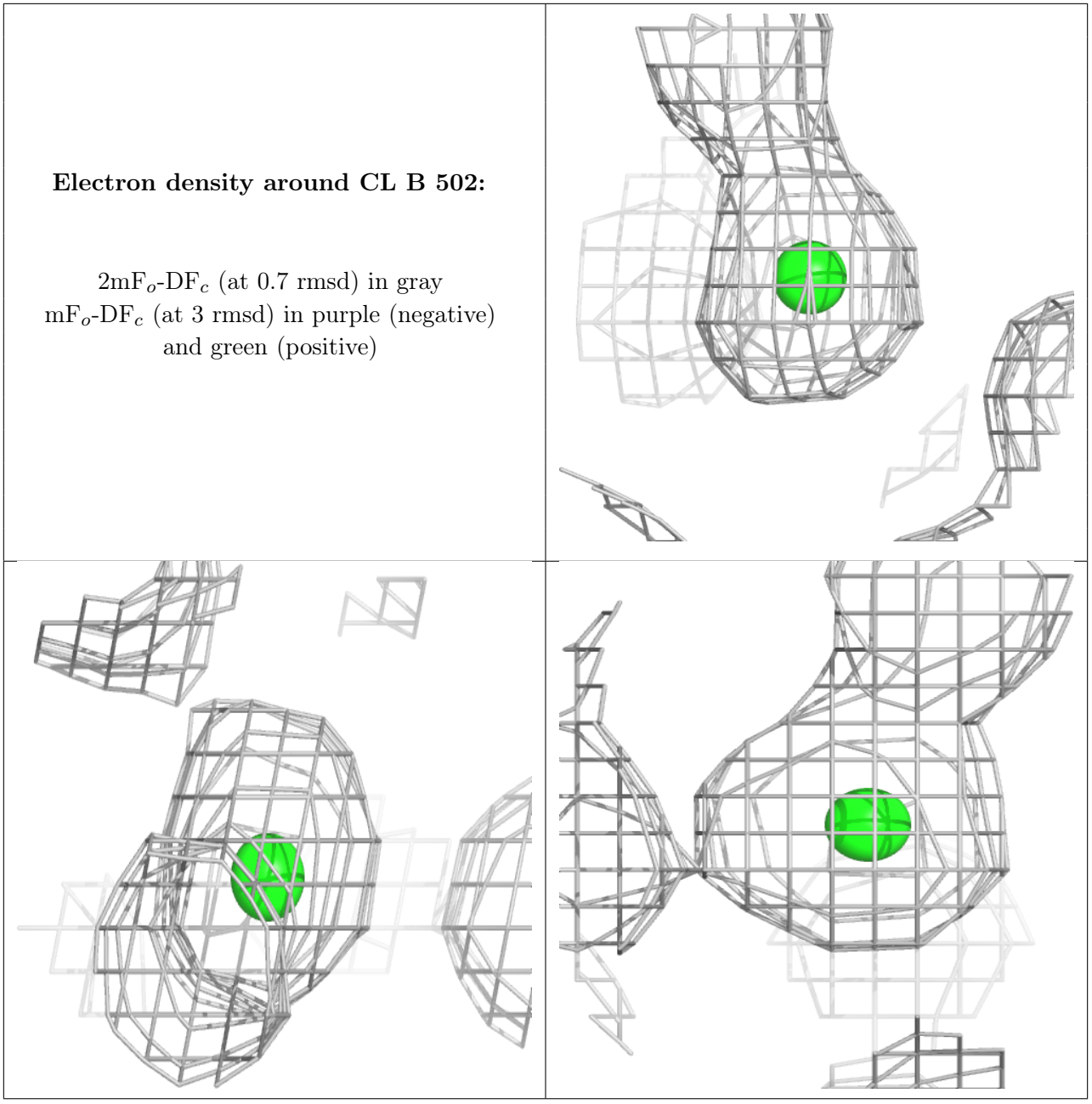
Electron density around CL A 503:

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



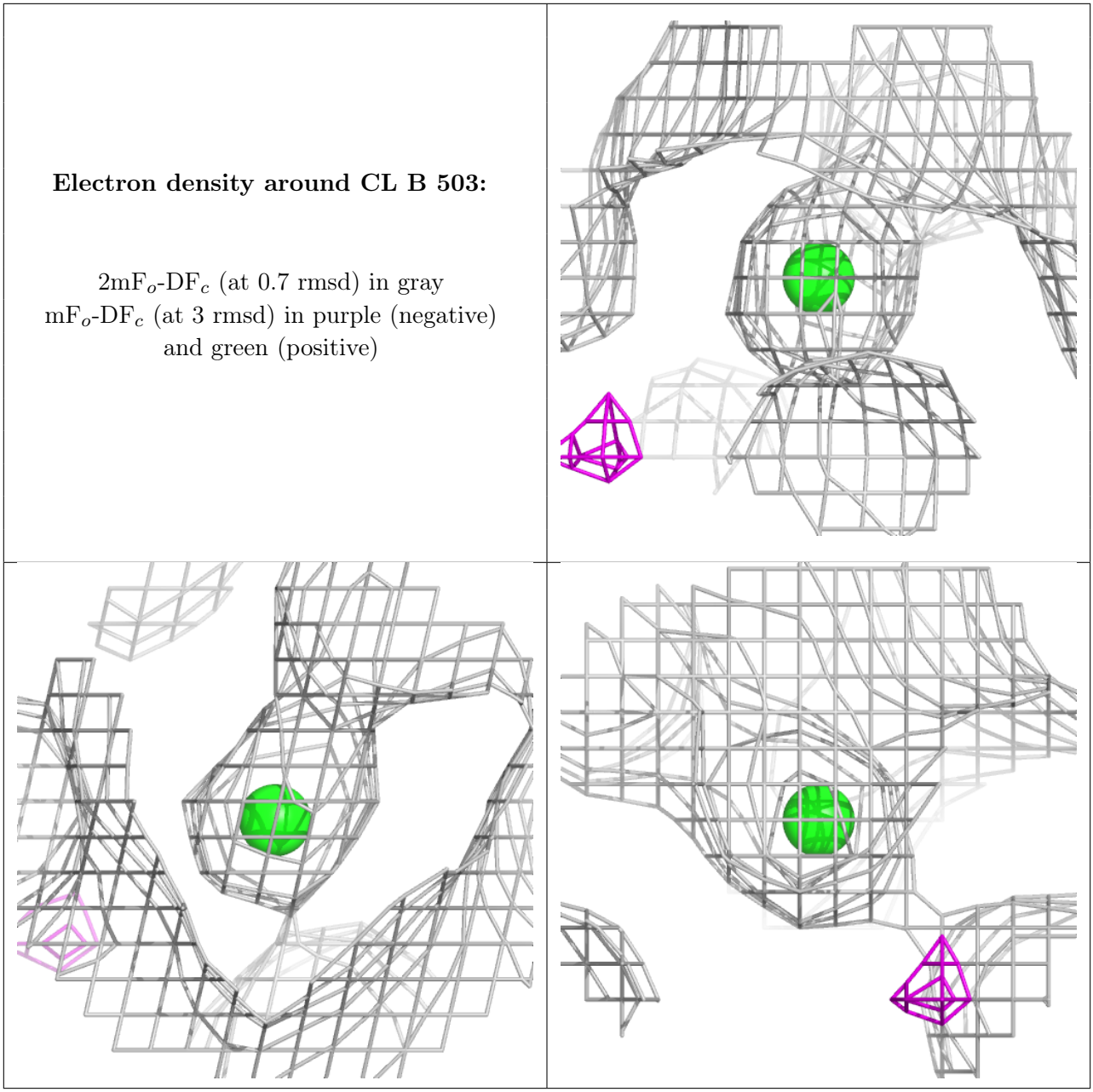
Electron density around CL B 502:

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



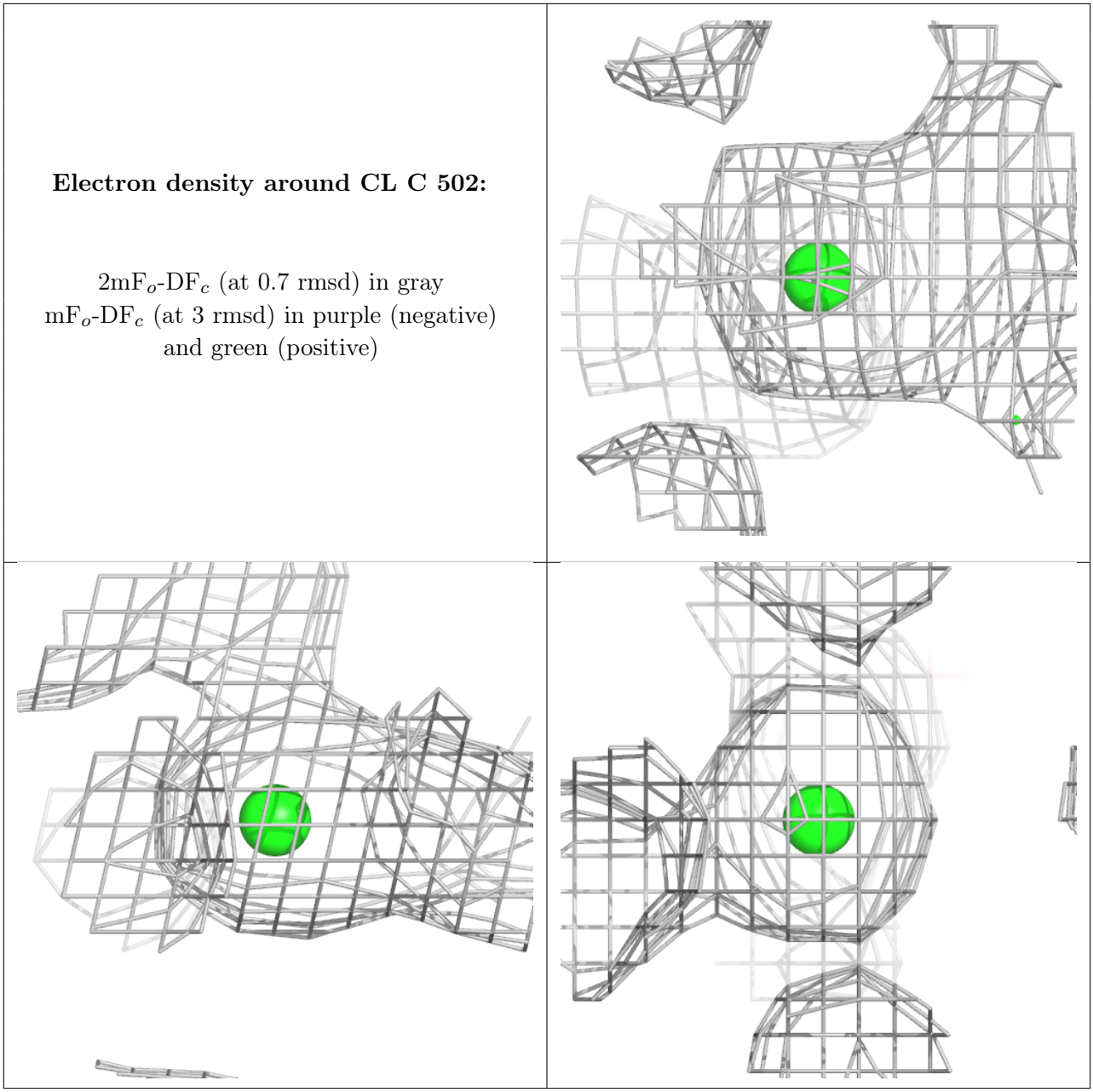
Electron density around CL B 503:

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



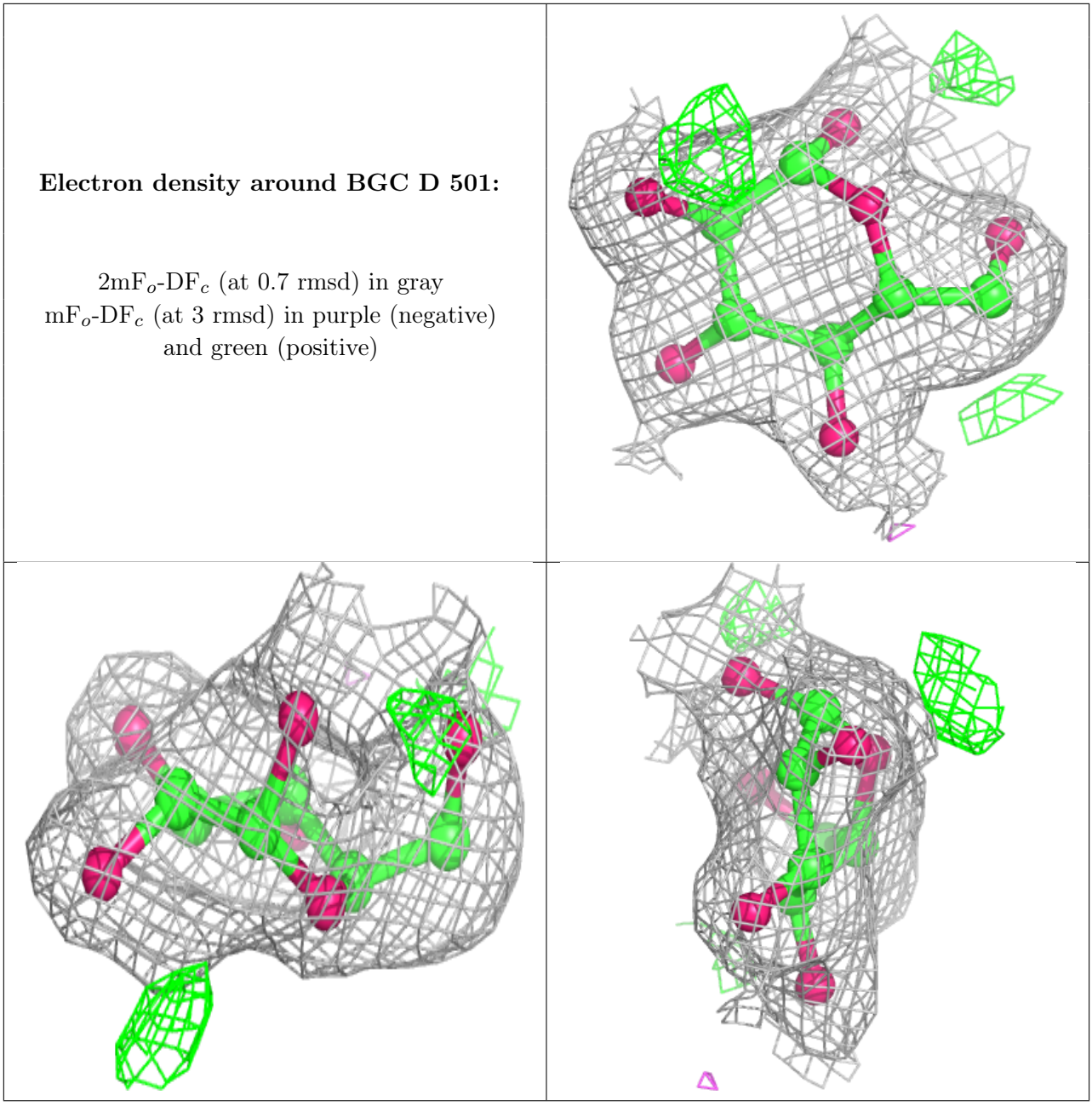
Electron density around CL C 502:

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



Electron density around BGC D 501:

$2mF_o$-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 (i)

EDS failed to run properly - this section is therefore empty.