Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 01:23 pm GMT

PDB ID	:	7QZR
Title	:	Structure of native leukocyte myeloperoxidase in complex with the Staphylococcal Peroxidase Inhibitor SPIN from Staphylococcus aureus
Authors	:	Pfanzagl, V.; Brito, J.A.
Deposited on	:	2022-01-31
Resolution	:	2.18 Å(reported)

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

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

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

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

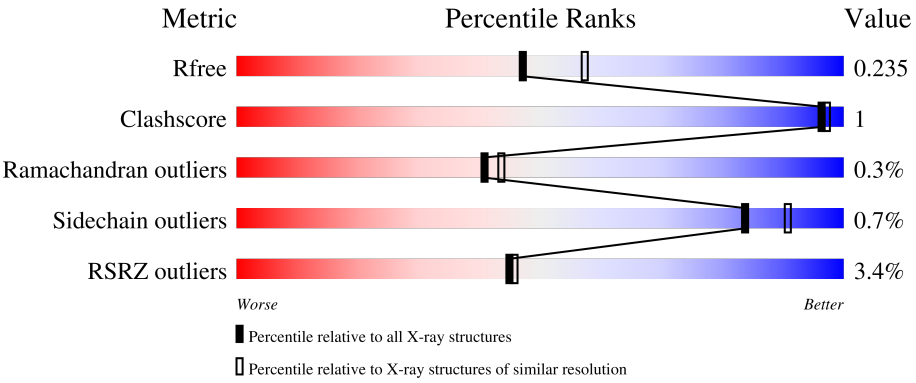
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.18 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (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	114	2% 89% · 8%
1	C	114	4% 88% · 8%
2	B	467	2% 97% ·
3	D	467	2% 95% ·
4	E	102	7% 69% 31%

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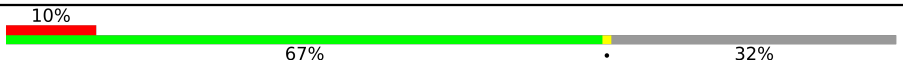
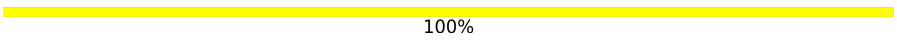
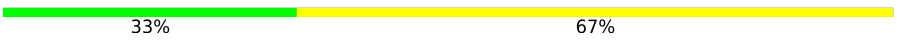
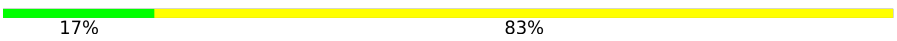
Mol	Chain	Length	Quality of chain
4	F	102	
5	G	2	
5	H	2	
5	J	2	
5	K	2	
6	I	6	
6	L	6	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21609 atoms, of which 10440 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 Myeloperoxidase light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	105	Total	C	H	N	O	S	800	0	0
			1642	532	800	149	156	5			
1	C	105	Total	C	H	N	O	S	800	0	0
			1642	532	800	149	156	5			

- Molecule 2 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	466	Total	C	H	N	O	S	3731	0	0
			7461	2351	3728	687	668	27			

- Molecule 3 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	465	Total	C	H	N	O	S	3724	0	0
			7451	2348	3723	686	667	27			

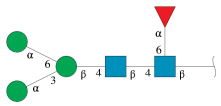
- Molecule 4 is a protein called Exported protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	70	Total	C	H	N	O	546	0	0
			1112	357	546	95	114			
4	F	69	Total	C	H	N	O	531	0	0
			1091	352	531	95	113			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

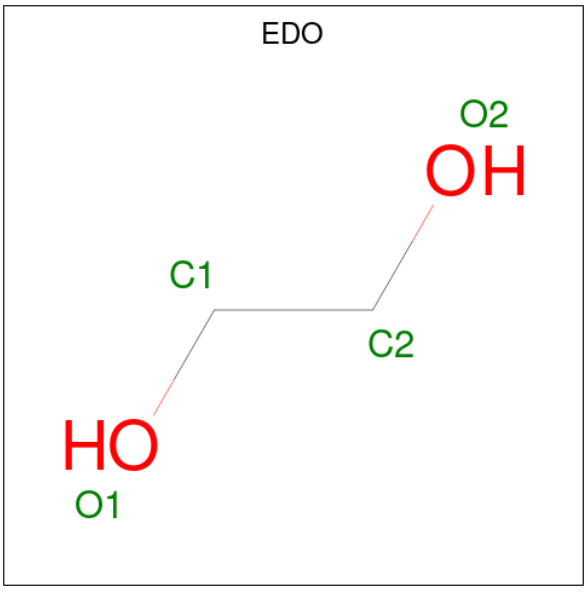
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			
5	H	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			
5	J	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			
5	K	2	Total	C	H	N	O	25	0	0
			53	16	25	2	10			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



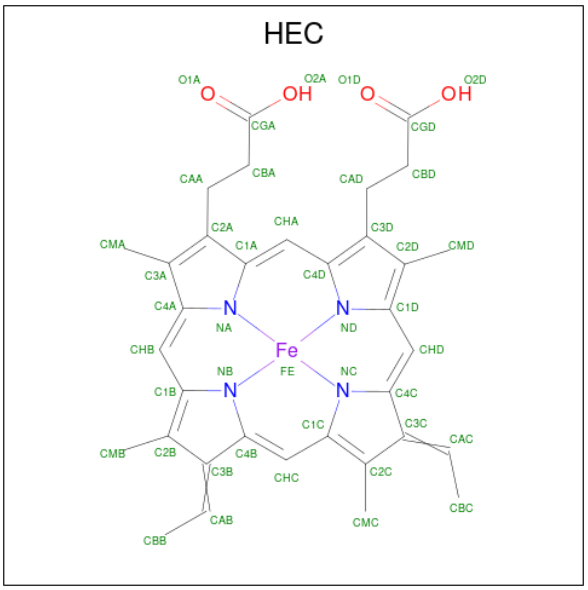
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	6	Total	C	H	N	O	61	0	0
			132	40	61	2	29			
6	L	6	Total	C	H	N	O	61	0	0
			132	40	61	2	29			

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 10 2 6 2	6	0
7	B	1	Total C H O 10 2 6 2	6	0
7	B	1	Total C H O 10 2 6 2	6	0
7	B	1	Total C H O 10 2 6 2	6	0

- Molecule 8 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C Fe H N O 71 34 1 28 4 4	28	0
8	C	1	Total C Fe H N O 71 34 1 28 4 4	28	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

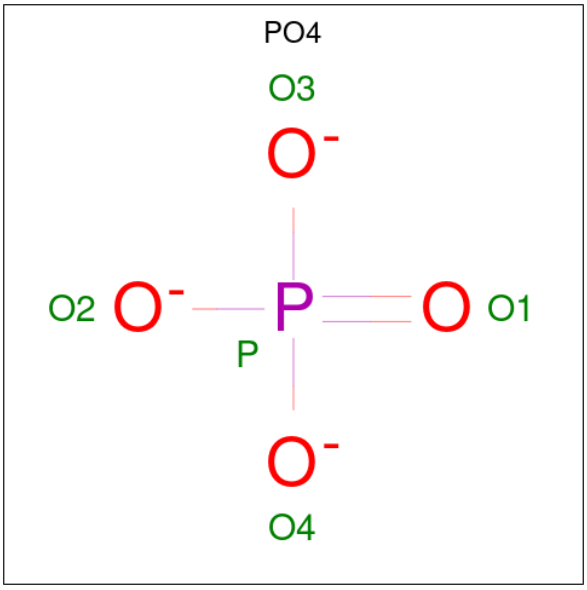
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0
9	C	1	Total Cl 1 1	0	0

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand

of Interest" by depositor).

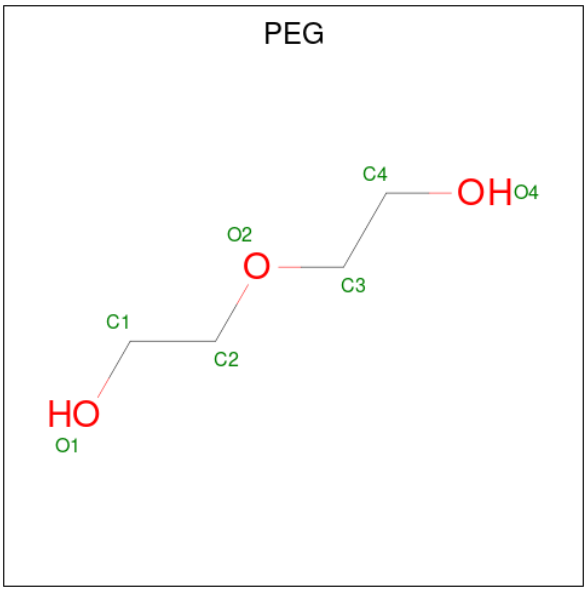
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Ca 1 1	0	0
10	D	1	Total Ca 1 1	0	0

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total O P 5 4 1	0	0

- Molecule 12 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total C H O 17 4 10 3	10	0

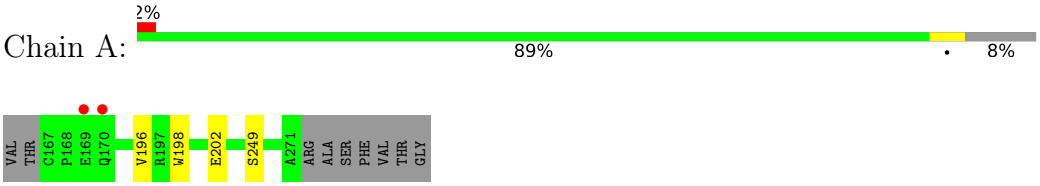
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	56	Total O 56 56	0	0
13	B	211	Total O 211 211	0	0
13	C	51	Total O 51 51	0	0
13	D	181	Total O 181 181	0	0
13	E	16	Total O 16 16	0	0
13	F	11	Total O 11 11	0	0

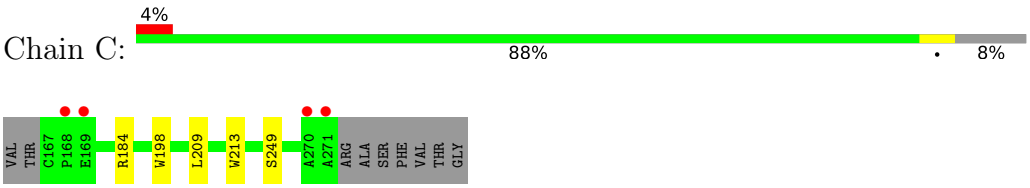
3 Residue-property plots (i)

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.

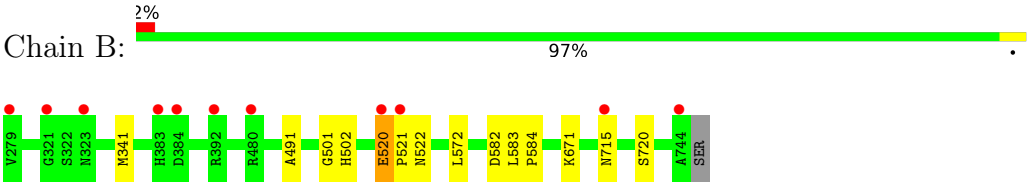
• Molecule 1: Myeloperoxidase light chain



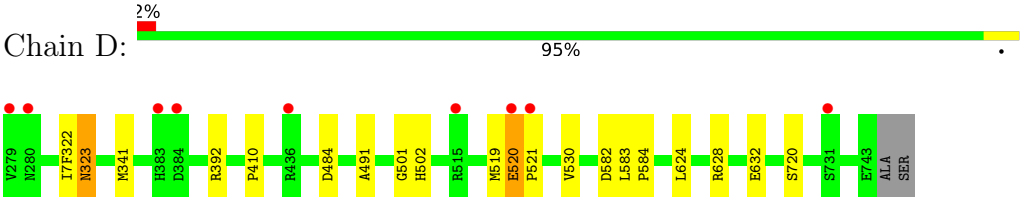
• Molecule 1: Myeloperoxidase light chain



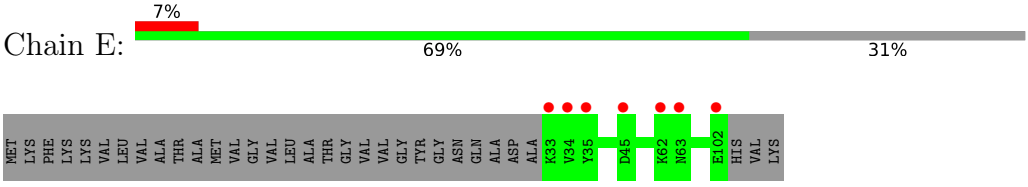
• Molecule 2: Myeloperoxidase heavy chain



• Molecule 3: Myeloperoxidase heavy chain

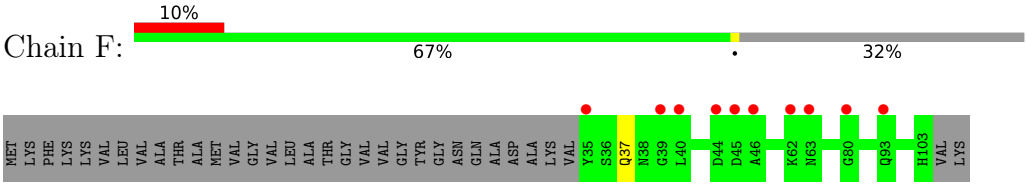


• Molecule 4: Exported protein



• Molecule 4: Exported protein

Chain F:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

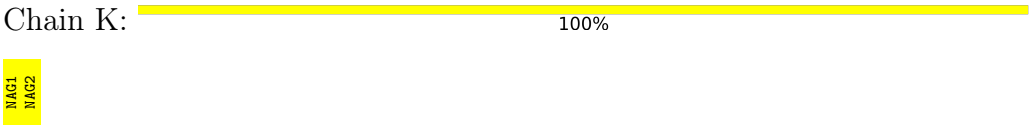
Chain H:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:


NAG1
NAG2
BMA3
MAN4
MAN5
FUC6

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.08Å 112.08Å 249.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 2.18 19.81 – 2.18	Depositor EDS
% Data completeness (in resolution range)	82.4 (19.81-2.18) 82.4 (19.81-2.18)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.19Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.204 , 0.244 0.196 , 0.235	Depositor DCC
R_{free} test set	3513 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21609	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: PEG, 2CO, HEC, I7F, NAG, CSO, CA, CL, EDO, BMA, MAN, FUC, PO4

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	0.44	0/867	0.66	0/1181
1	C	0.42	0/867	0.65	0/1181
2	B	0.44	0/3810	0.58	0/5168
3	D	0.44	0/3798	0.59	1/5150 (0.0%)
4	E	0.37	0/575	0.49	0/773
4	F	0.36	0/570	0.48	0/767
All	All	0.43	0/10487	0.59	1/14220 (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})
3	D	323	ASN	N-CA-CB	6.88	122.99	110.60

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	842	800	800	5	0
1	C	842	800	800	4	0
2	B	3733	3728	3724	8	0
3	D	3728	3723	3715	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	566	546	546	0	0
4	F	560	531	531	0	0
5	G	28	25	25	0	0
5	H	28	25	25	0	0
5	J	28	25	25	0	0
5	K	28	25	25	0	0
6	I	71	61	61	0	0
6	L	71	61	61	0	0
7	A	4	6	6	0	0
7	B	12	18	18	3	0
8	A	43	28	28	1	0
8	C	43	28	29	2	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
11	B	5	0	0	0	0
12	B	7	10	10	0	0
13	A	56	0	0	0	0
13	B	211	0	0	0	0
13	C	51	0	0	0	0
13	D	181	0	0	0	0
13	E	16	0	0	0	0
13	F	11	0	0	0	0
All	All	11169	10440	10429	21	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 1.

All (21) 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)
8:A:302:HEC:HBC2	2:B:501:GLY:HA3	1.71	0.71
1:A:196:VAL:HG11	7:B:802:EDO:H12	1.84	0.60
8:C:301:HEC:HBC2	3:D:501:GLY:HA3	1.82	0.60
2:B:671:LYS:HD3	7:B:802:EDO:O1	2.04	0.58
3:D:502:HIS:CE1	3:D:583:LEU:HD21	2.42	0.55
1:C:249:SER:HB3	3:D:720:SER:O	2.09	0.52
3:D:520:GLU:HB3	3:D:521:PRO:CD	2.45	0.47
1:A:202:GLU:OE2	1:C:184:ARG:NH1	2.47	0.47
1:C:209:LEU:HD22	1:C:213:TRP:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:301:HEC:HMC1	8:C:301:HEC:HBC3	1.98	0.44
1:A:249:SER:HB3	2:B:720:SER:O	2.17	0.44
1:A:198:TRP:CE2	2:B:491:ALA:HB2	2.53	0.44
2:B:582:ASP:OD1	2:B:584:PRO:HD2	2.17	0.44
3:D:582:ASP:OD1	3:D:584:PRO:HD2	2.17	0.44
1:A:196:VAL:HG11	7:B:802:EDO:C1	2.48	0.43
2:B:502:HIS:CE1	2:B:583:LEU:HD21	2.54	0.43
1:C:198:TRP:CE2	3:D:491:ALA:HB2	2.55	0.42
2:B:572:LEU:HD22	2:B:583:LEU:HB2	2.03	0.40
2:B:520:GLU:CB	2:B:521:PRO:HD3	2.51	0.40
3:D:410:PRO:HD3	3:D:530:VAL:O	2.21	0.40
3:D:624:LEU:O	3:D:628:ARG:HG3	2.22	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	103/114 (90%)	101 (98%)	2 (2%)	0	100	100
1	C	103/114 (90%)	102 (99%)	1 (1%)	0	100	100
2	B	463/467 (99%)	448 (97%)	13 (3%)	2 (0%)	34	35
3	D	461/467 (99%)	445 (96%)	14 (3%)	2 (0%)	34	35
4	E	68/102 (67%)	67 (98%)	1 (2%)	0	100	100
4	F	67/102 (66%)	66 (98%)	1 (2%)	0	100	100
All	All	1265/1366 (93%)	1229 (97%)	32 (2%)	4 (0%)	41	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	520	GLU

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Mol	Chain	Res	Type
2	B	715	ASN
3	D	323	ASN
3	D	520	GLU

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	90/97 (93%)	90 (100%)	0	100 100
1	C	90/97 (93%)	90 (100%)	0	100 100
2	B	410/411 (100%)	408 (100%)	2 (0%)	88 94
3	D	409/410 (100%)	404 (99%)	5 (1%)	71 81
4	E	62/85 (73%)	62 (100%)	0	100 100
4	F	61/85 (72%)	60 (98%)	1 (2%)	62 74
All	All	1122/1185 (95%)	1114 (99%)	8 (1%)	84 91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	341	MET
2	B	522	ASN
3	D	341	MET
3	D	392	ARG
3	D	484	ASP
3	D	519	MET
3	D	632	GLU
4	F	37	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	66	GLN
4	E	82	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	I7F	D	322	3	4,6,7	1.52	1 (25%)	0,6,8	-	-
2	2CO	B	316	2	3,7,8	0.53	0	1,7,9	0.00	0
3	CSO	D	316	3	3,6,7	0.78	0	0,6,8	-	-

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	I7F	D	322	3	-	0/0/5/7	-
2	2CO	B	316	2	-	0/1/6/8	-
3	CSO	D	316	3	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	322	I7F	O1-OG	-2.68	1.42	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

20 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	$\#\|Z\|>2$
5	NAG	G	1	5,2	14,14,15	0.25	0	17,19,21	0.86	1 (5%)
5	NAG	G	2	5	14,14,15	0.27	0	17,19,21	0.55	0
5	NAG	H	1	5,2	14,14,15	0.26	0	17,19,21	0.75	1 (5%)
5	NAG	H	2	5	14,14,15	0.28	0	17,19,21	0.55	0
6	NAG	I	1	6,2	14,14,15	0.28	0	17,19,21	1.07	1 (5%)
6	NAG	I	2	6	14,14,15	0.27	0	17,19,21	0.81	1 (5%)
6	BMA	I	3	6	11,11,12	0.24	0	15,15,17	0.66	0
6	MAN	I	4	6	11,11,12	0.71	0	15,15,17	1.31	2 (13%)
6	MAN	I	5	6	11,11,12	0.23	0	15,15,17	0.67	1 (6%)
6	FUC	I	6	6	10,10,11	0.28	0	14,14,16	0.37	0
5	NAG	J	1	3,5	14,14,15	0.27	0	17,19,21	0.90	1 (5%)
5	NAG	J	2	5	14,14,15	0.26	0	17,19,21	0.54	0
5	NAG	K	1	3,5	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
5	NAG	K	2	5	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
6	NAG	L	1	3,6	14,14,15	0.29	0	17,19,21	1.01	1 (5%)
6	NAG	L	2	6	14,14,15	0.26	0	17,19,21	0.78	1 (5%)
6	BMA	L	3	6	11,11,12	0.25	0	15,15,17	0.80	1 (6%)
6	MAN	L	4	6	11,11,12	0.66	0	15,15,17	1.17	2 (13%)
6	MAN	L	5	6	11,11,12	0.21	0	15,15,17	0.60	1 (6%)
6	FUC	L	6	6	10,10,11	0.28	0	14,14,16	0.51	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
5	NAG	G	1	5,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	NAG	H	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
6	NAG	I	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	0/6/23/26	0/1/1/1
6	BMA	I	3	6	-	0/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	1/1/1/1
6	MAN	I	5	6	-	0/2/19/22	0/1/1/1
6	FUC	I	6	6	-	-	0/1/1/1
5	NAG	J	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	NAG	K	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
6	NAG	L	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	0/2/19/22	0/1/1/1
6	MAN	L	4	6	-	1/2/19/22	0/1/1/1
6	MAN	L	5	6	-	0/2/19/22	0/1/1/1
6	FUC	L	6	6	-	-	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	1	NAG	O5-C1-C2	-4.10	104.81	111.29
6	I	4	MAN	C1-O5-C5	3.74	117.26	112.19
6	L	1	NAG	O5-C1-C2	-3.72	105.42	111.29
5	J	1	NAG	C1-O5-C5	3.30	116.66	112.19
5	K	1	NAG	O5-C1-C2	-3.14	106.32	111.29
6	L	4	MAN	C1-C2-C3	2.92	113.26	109.67
5	G	1	NAG	C1-O5-C5	2.89	116.10	112.19
6	I	4	MAN	C1-C2-C3	2.86	113.18	109.67
6	L	4	MAN	C1-O5-C5	2.74	115.91	112.19
5	H	1	NAG	O5-C1-C2	-2.41	107.48	111.29
6	L	2	NAG	C1-O5-C5	2.35	115.37	112.19
6	I	5	MAN	C1-O5-C5	2.32	115.34	112.19
6	I	2	NAG	C1-O5-C5	2.20	115.18	112.19
6	L	5	MAN	C1-O5-C5	2.10	115.03	112.19
6	L	3	BMA	O3-C3-C2	2.06	113.95	109.99
5	K	2	NAG	O5-C1-C2	-2.06	108.03	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

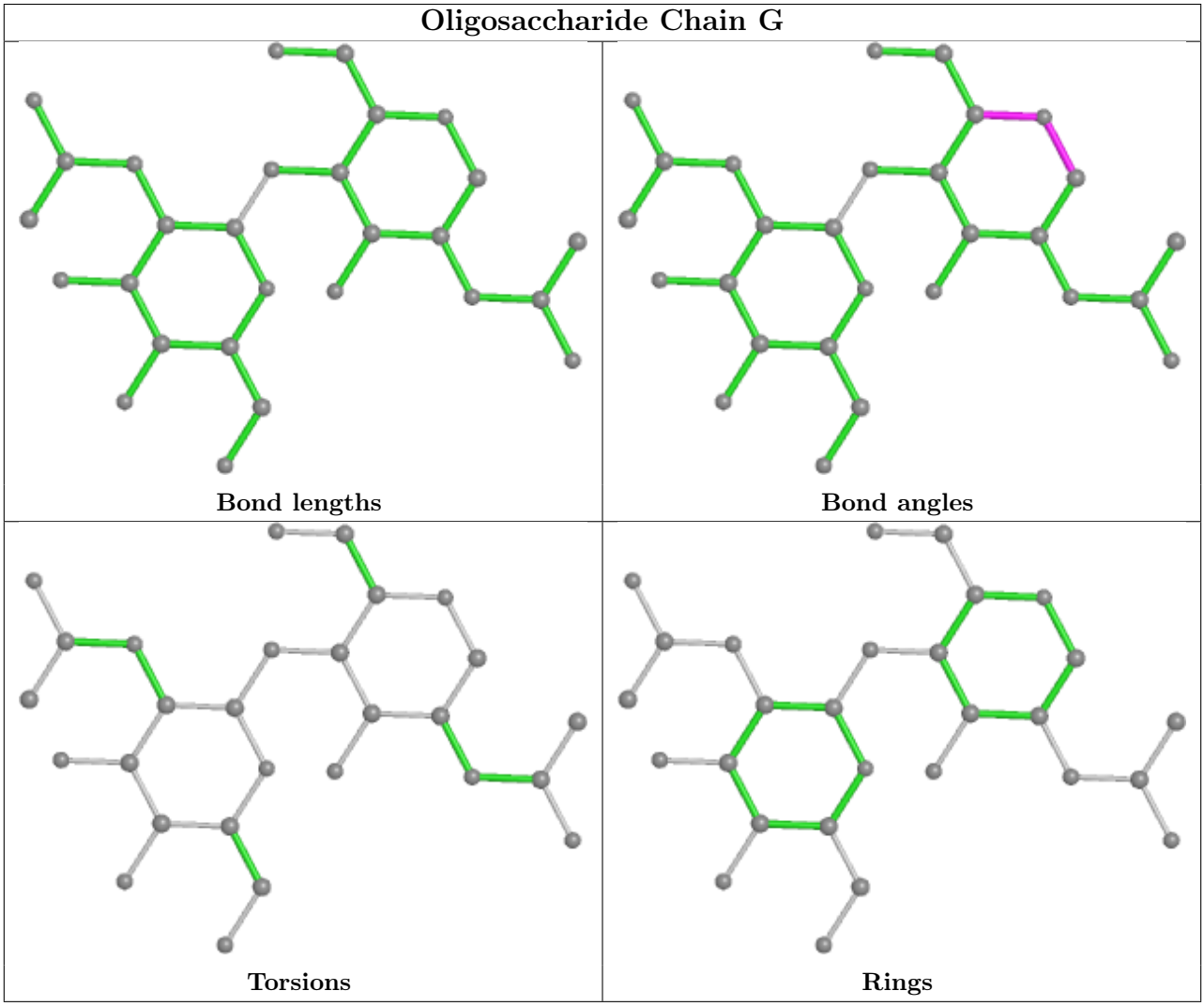
Mol	Chain	Res	Type	Atoms
5	H	2	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
6	L	4	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

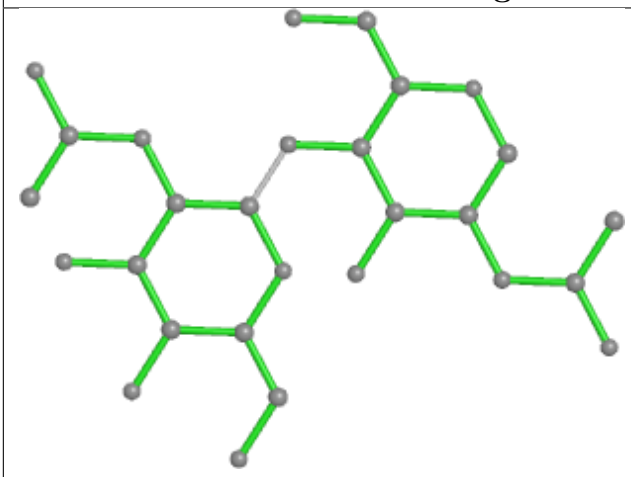
Mol	Chain	Res	Type	Atoms
6	I	4	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

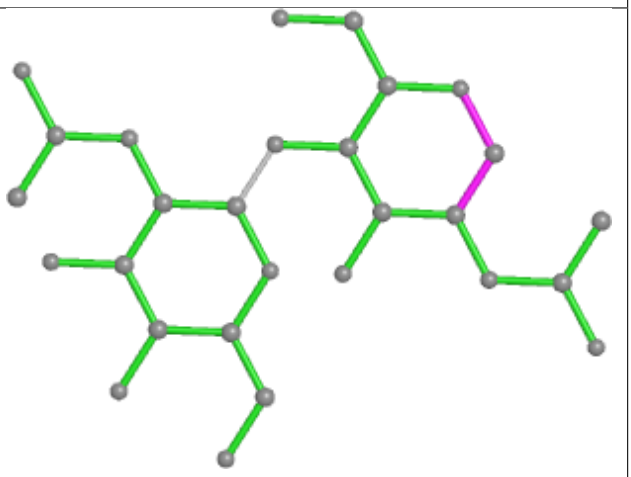
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



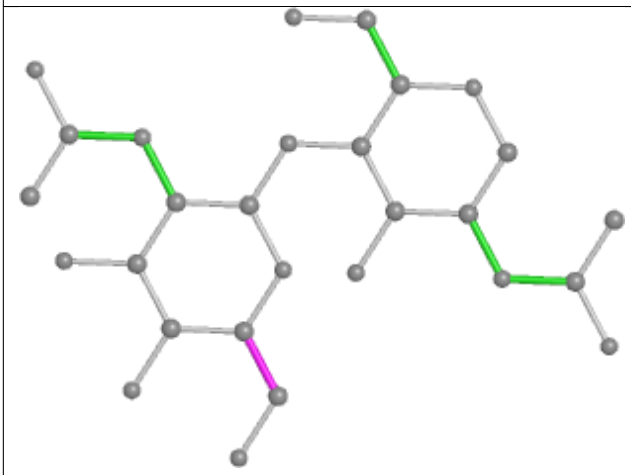
Oligosaccharide Chain H



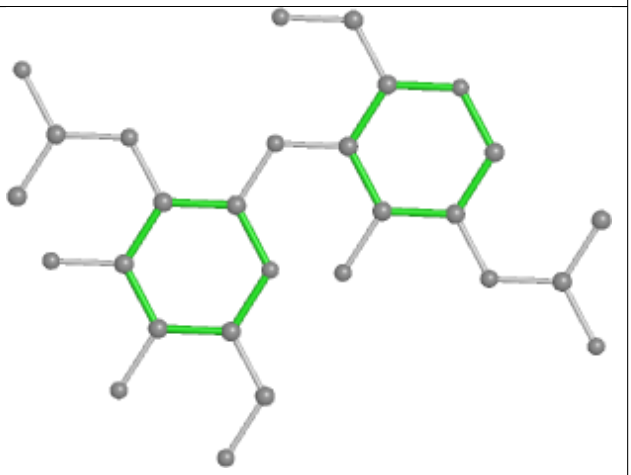
Bond lengths



Bond angles

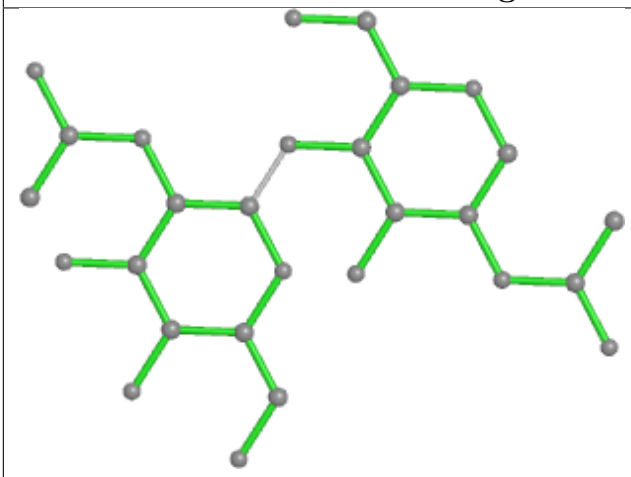


Torsions

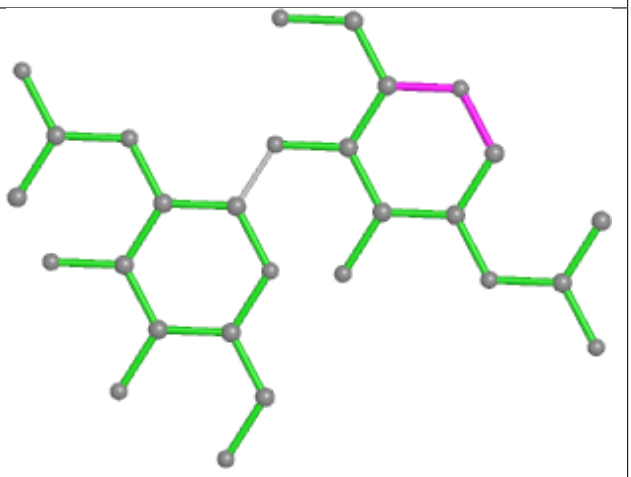


Rings

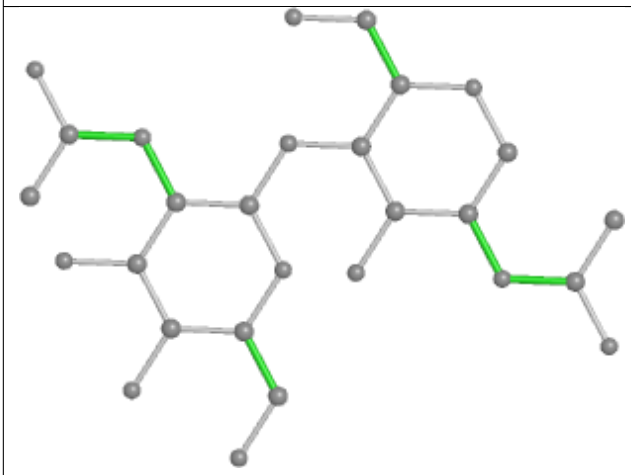
Oligosaccharide Chain J



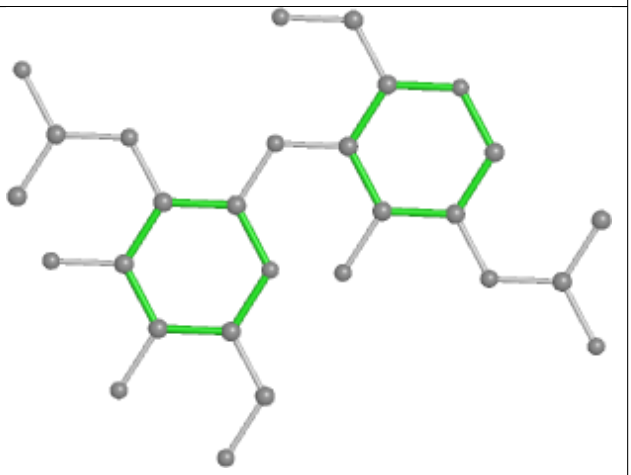
Bond lengths



Bond angles

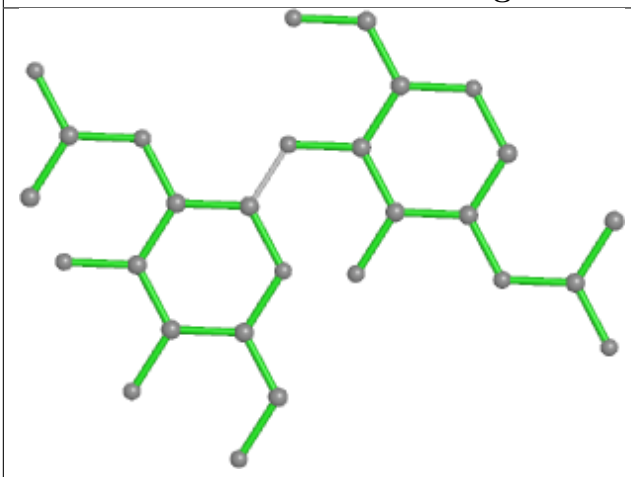


Torsions

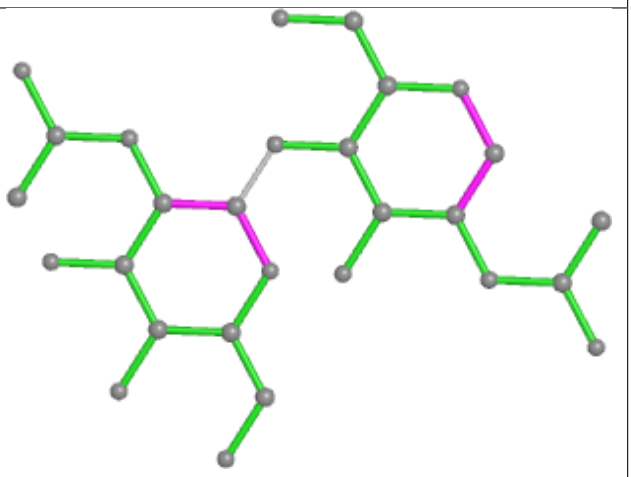


Rings

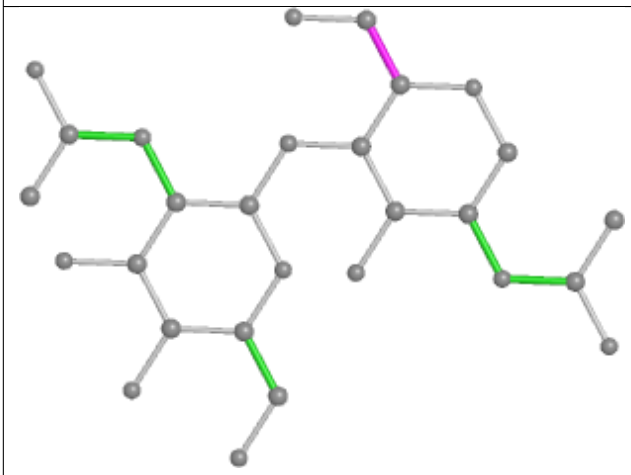
Oligosaccharide Chain K



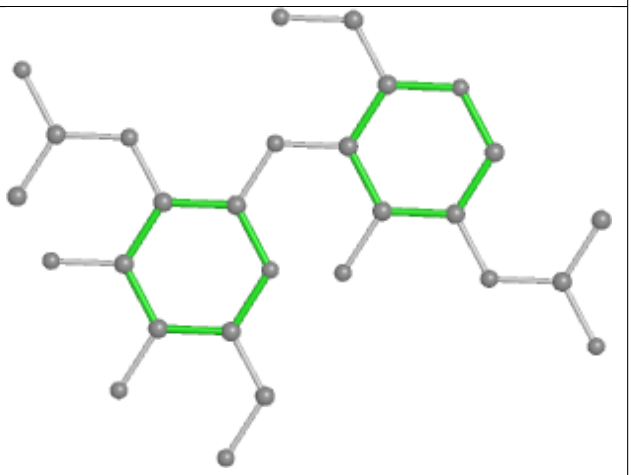
Bond lengths



Bond angles

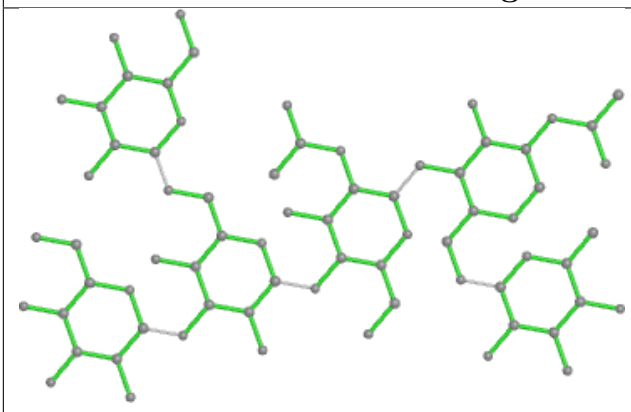


Torsions

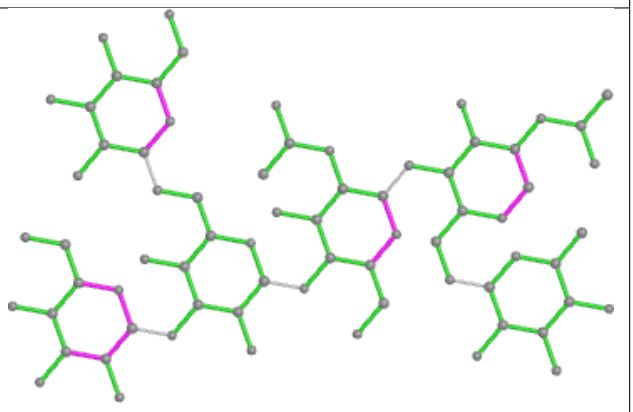


Rings

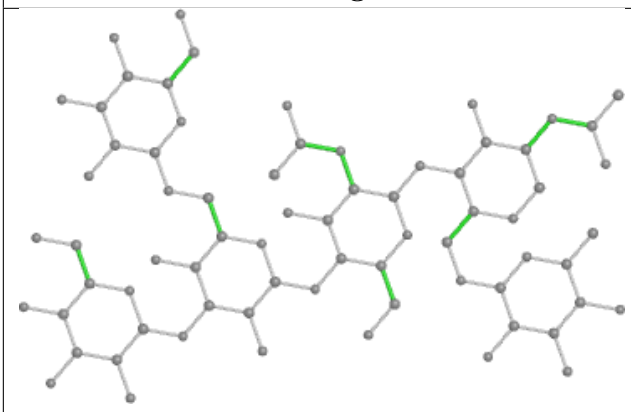
Oligosaccharide Chain I



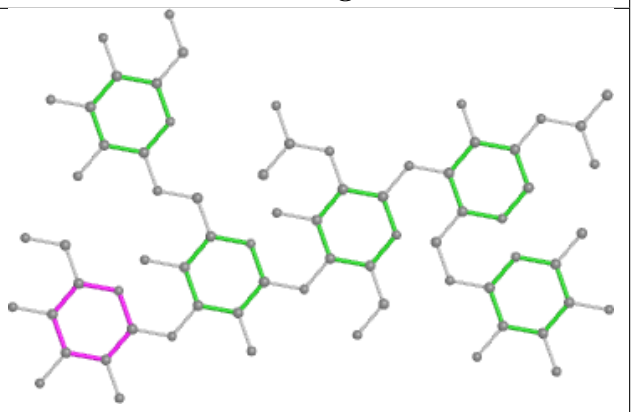
Bond lengths



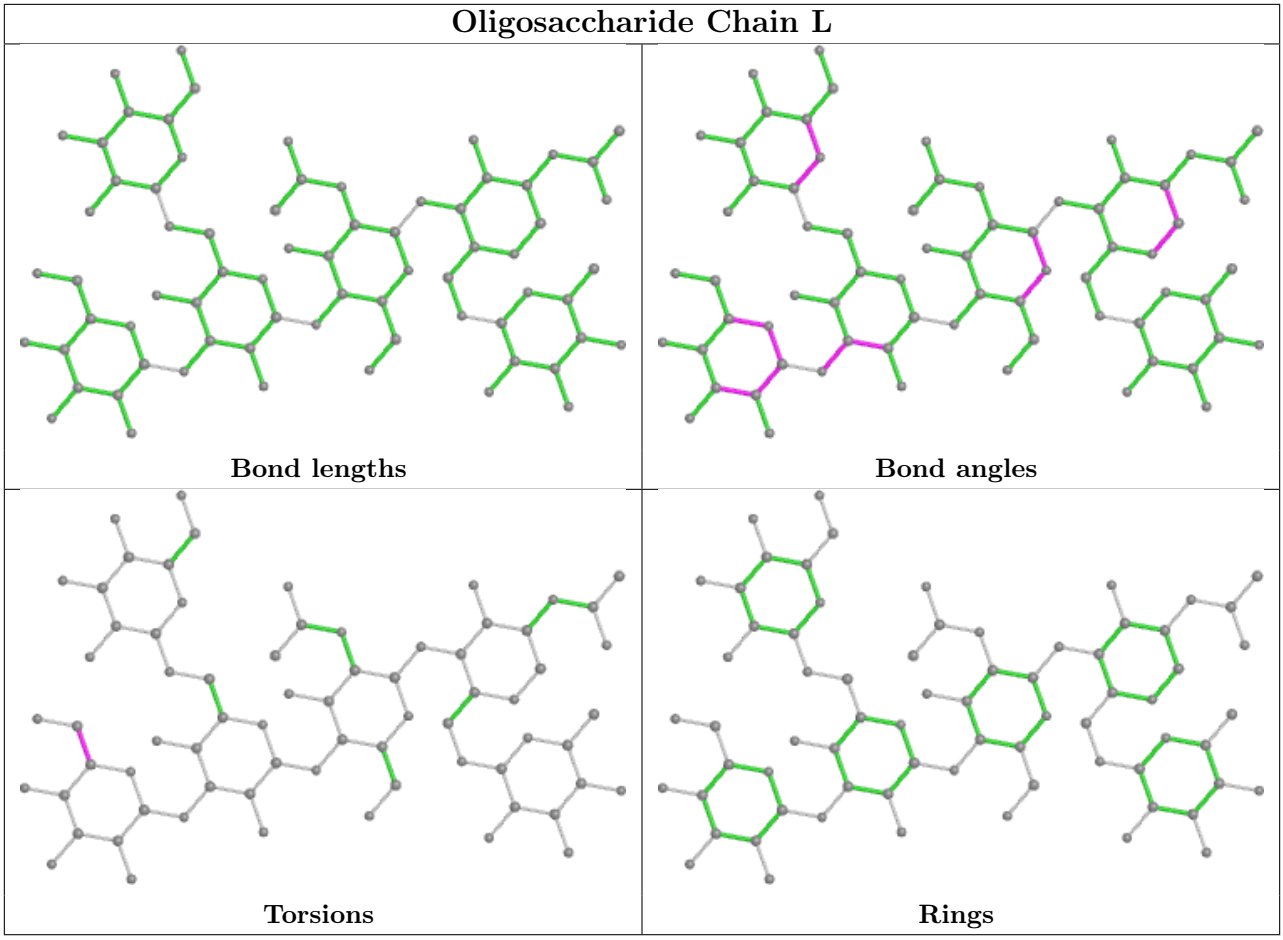
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
7	EDO	A	301	-	3,3,3	0.56	0	2,2,2	0.28	0
11	PO4	B	804	-	4,4,4	1.97	0	6,6,6	0.47	0
8	HEC	C	301	1,3	32,50,50	2.55	12 (37%)	24,82,82	2.67	8 (33%)
7	EDO	B	803	-	3,3,3	0.71	0	2,2,2	0.33	0
7	EDO	B	806	-	3,3,3	0.56	0	2,2,2	0.33	0
7	EDO	B	802	-	3,3,3	0.75	0	2,2,2	0.49	0
12	PEG	B	805	-	6,6,6	0.12	0	5,5,5	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	HEC	A	302	1,2	32,50,50	2.55	12 (37%)	24,82,82	2.49	6 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	A	301	-	-	0/1/1/1	-
8	HEC	C	301	1,3	-	4/10/54/54	-
7	EDO	B	803	-	-	1/1/1/1	-
7	EDO	B	806	-	-	0/1/1/1	-
7	EDO	B	802	-	-	0/1/1/1	-
12	PEG	B	805	-	-	3/4/4/4	-
8	HEC	A	302	1,2	-	4/10/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	302	HEC	C3C-C2C	8.02	1.49	1.40
8	C	301	HEC	C3C-C2C	7.67	1.48	1.40
8	C	301	HEC	C2B-C3B	7.07	1.48	1.40
8	A	302	HEC	C2B-C3B	6.91	1.48	1.40
8	A	302	HEC	C4B-C3B	3.99	1.50	1.43
8	C	301	HEC	C4B-C3B	3.63	1.49	1.43
8	C	301	HEC	C2A-C3A	3.57	1.48	1.37
8	A	302	HEC	C3D-C2D	3.31	1.47	1.37
8	C	301	HEC	C3D-C2D	3.22	1.47	1.37
8	A	302	HEC	C2A-C3A	3.20	1.47	1.37
8	C	301	HEC	C3C-C4C	3.11	1.48	1.43
8	C	301	HEC	C3A-C4A	3.03	1.49	1.42
8	A	302	HEC	C3C-C4C	2.79	1.48	1.43
8	A	302	HEC	C3A-C4A	2.76	1.48	1.42
8	C	301	HEC	C1B-CHB	2.73	1.48	1.41
8	C	301	HEC	C2A-C1A	2.72	1.48	1.42
8	A	302	HEC	C1C-CHC	2.65	1.48	1.41
8	C	301	HEC	C1C-CHC	2.62	1.48	1.41
8	A	302	HEC	C1B-CHB	2.51	1.48	1.41
8	A	302	HEC	C2A-C1A	2.48	1.48	1.42
8	C	301	HEC	C4D-CHA	2.41	1.47	1.41
8	A	302	HEC	C4D-CHA	2.39	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	302	HEC	C1D-CHD	2.30	1.47	1.41
8	C	301	HEC	C1D-CHD	2.20	1.47	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	301	HEC	C1D-C2D-C3D	-6.90	102.19	107.00
8	A	302	HEC	C1D-C2D-C3D	-6.65	102.37	107.00
8	C	301	HEC	CBD-CAD-C3D	-6.59	101.38	112.62
8	A	302	HEC	CBD-CAD-C3D	-5.93	102.51	112.62
8	C	301	HEC	CBA-CAA-C2A	-5.35	103.58	112.60
8	A	302	HEC	CBA-CAA-C2A	-4.63	104.80	112.60
8	C	301	HEC	C4C-C3C-C2C	-3.90	102.14	106.35
8	A	302	HEC	C4C-C3C-C2C	-3.39	102.69	106.35
8	A	302	HEC	C2B-C3B-C4B	-2.90	103.22	106.35
8	A	302	HEC	CMC-C2C-C3C	2.67	128.96	125.82
8	C	301	HEC	C2B-C3B-C4B	-2.30	103.87	106.35
8	C	301	HEC	CMB-C2B-C3B	2.29	128.51	125.82
8	C	301	HEC	CMC-C2C-C3C	2.17	128.37	125.82
8	C	301	HEC	O2A-CGA-CBA	2.01	120.48	114.03

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	B	805	PEG	O2-C3-C4-O4
12	B	805	PEG	C1-C2-O2-C3
12	B	805	PEG	O1-C1-C2-O2
8	C	301	HEC	CAD-CBD-CGD-O1D
8	A	302	HEC	CAD-CBD-CGD-O1D
8	A	302	HEC	CAD-CBD-CGD-O2D
8	C	301	HEC	CAD-CBD-CGD-O2D
8	C	301	HEC	CAA-CBA-CGA-O2A
8	C	301	HEC	CAA-CBA-CGA-O1A
8	A	302	HEC	CAA-CBA-CGA-O1A
8	A	302	HEC	CAA-CBA-CGA-O2A
7	B	803	EDO	O1-C1-C2-O2

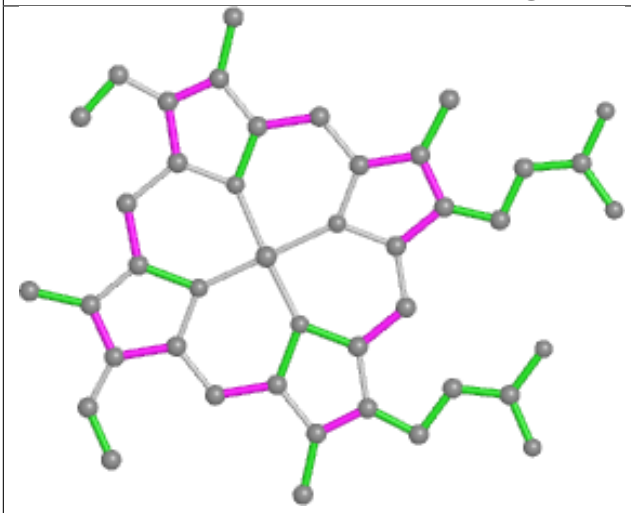
There are no ring outliers.

3 monomers are involved in 6 short contacts:

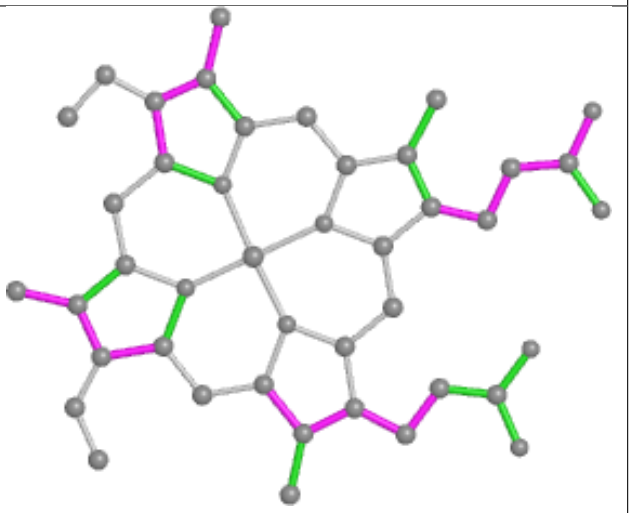
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	301	HEC	2	0
7	B	802	EDO	3	0
8	A	302	HEC	1	0

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.

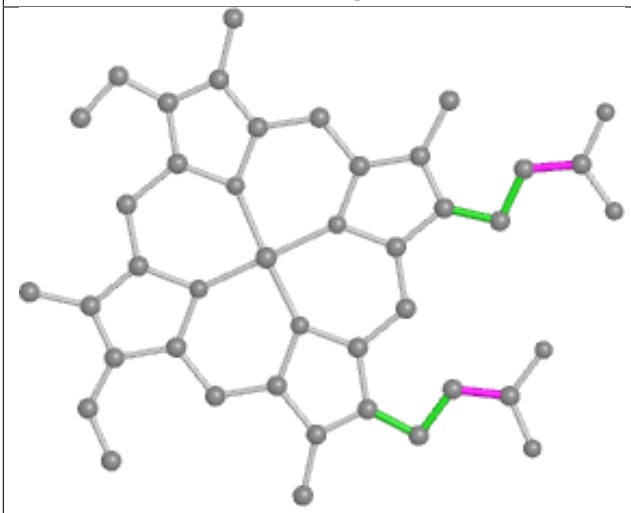
Ligand HEC C 301



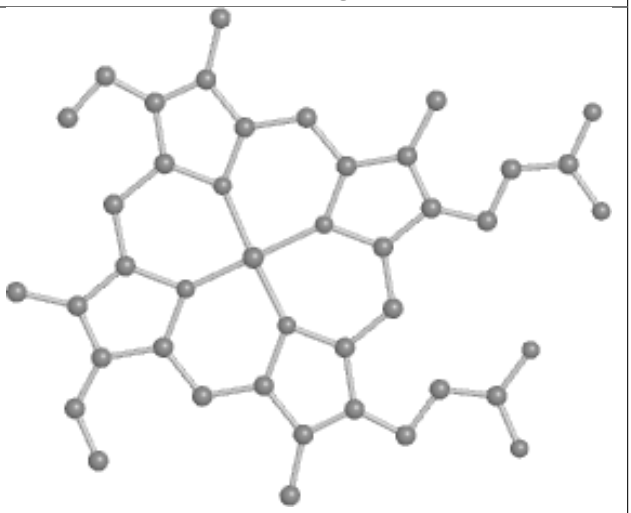
Bond lengths



Bond angles

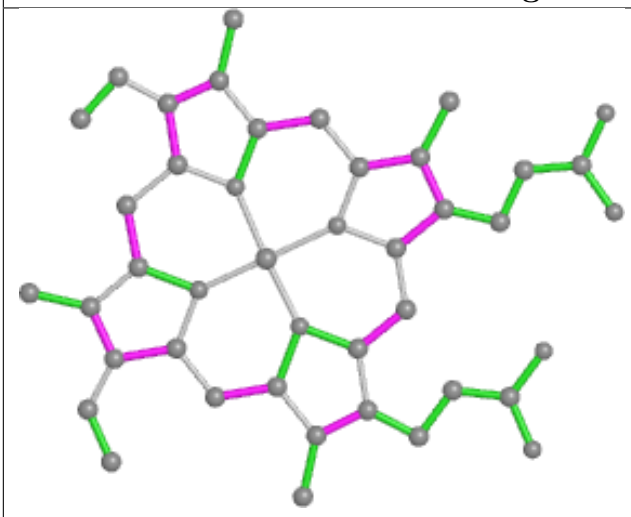


Torsions

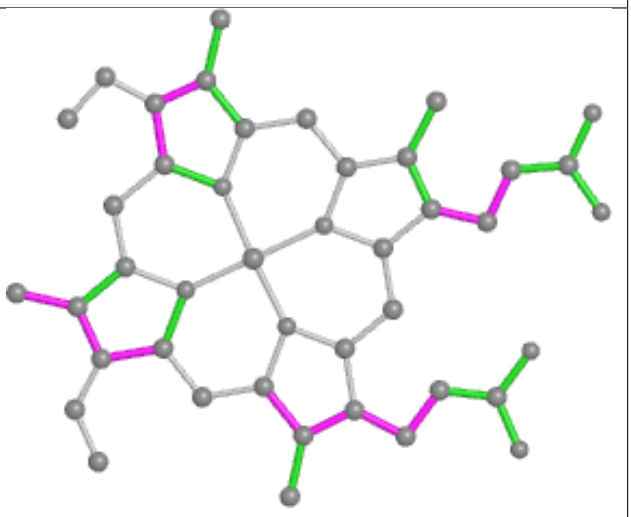


Rings

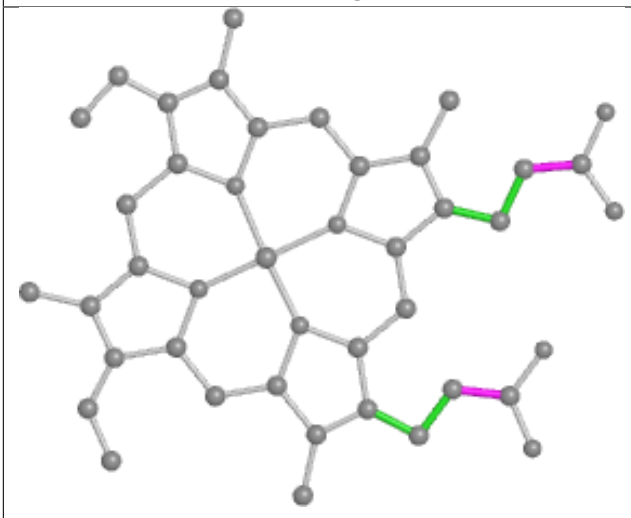
Ligand HEC A 302



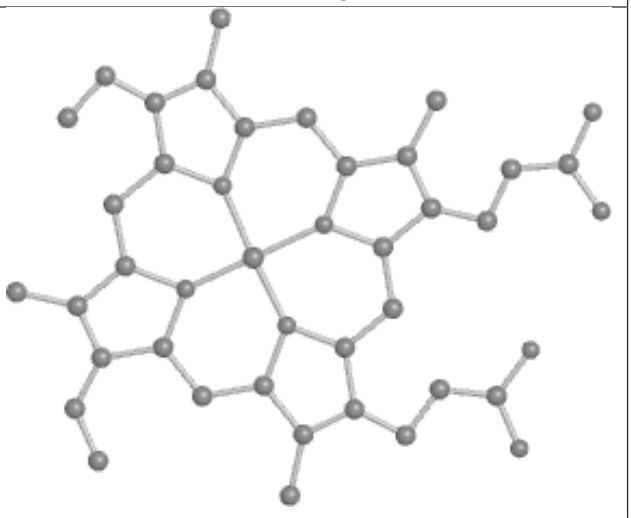
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	105/114 (92%)	-0.24	2 (1%) 66 67	21, 26, 39, 62	0
1	C	105/114 (92%)	-0.10	4 (3%) 40 41	19, 28, 45, 60	0
2	B	465/467 (99%)	-0.17	11 (2%) 59 59	17, 27, 42, 64	3 (0%)
3	D	463/467 (99%)	-0.12	9 (1%) 66 67	20, 30, 46, 63	2 (0%)
4	E	70/102 (68%)	0.62	7 (10%) 7 7	28, 40, 59, 69	0
4	F	69/102 (67%)	0.92	10 (14%) 2 2	38, 53, 69, 76	0
All	All	1277/1366 (93%)	-0.05	43 (3%) 45 46	17, 29, 53, 76	5 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	520	GLU	8.2
3	D	279	VAL	5.8
4	E	33	LYS	5.0
3	D	521	PRO	4.6
2	B	744	ALA	4.4
1	A	169	GLU	4.4
2	B	521	PRO	3.9
2	B	715	ASN	3.9
4	E	34	VAL	3.9
2	B	321	GLY	3.7
2	B	392	ARG	3.7
3	D	520	GLU	3.7
3	D	383	HIS	3.6
2	B	323	ASN	3.6
4	E	45	ASP	3.6
3	D	436	ARG	3.5
1	C	169	GLU	3.5
4	F	62	LYS	3.4
2	B	383	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	44	ASP	3.3
4	E	63	ASN	3.2
2	B	384	ASP	3.1
3	D	515	ARG	2.9
4	E	35	TYR	2.9
4	E	102	GLU	2.9
4	F	45	ASP	2.9
4	F	39	GLY	2.8
1	C	271	ALA	2.8
1	A	170	GLN	2.8
4	F	35	TYR	2.8
3	D	280	ASN	2.8
3	D	731	SER	2.8
4	F	63	ASN	2.7
3	D	384	ASP	2.7
4	F	40	LEU	2.6
4	F	46	ALA	2.4
4	F	80	GLY	2.4
1	C	270	ALA	2.4
1	C	168	PRO	2.3
2	B	480	ARG	2.1
4	E	62	LYS	2.1
4	F	93	GLN	2.0
2	B	279	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	I7F	D	322	7/8	0.84	0.13	42,44,45,46	5
2	2CO	B	316	8/9	0.94	0.09	23,27,32,33	5
3	CSO	D	316	7/8	0.96	0.09	24,27,30,30	6

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

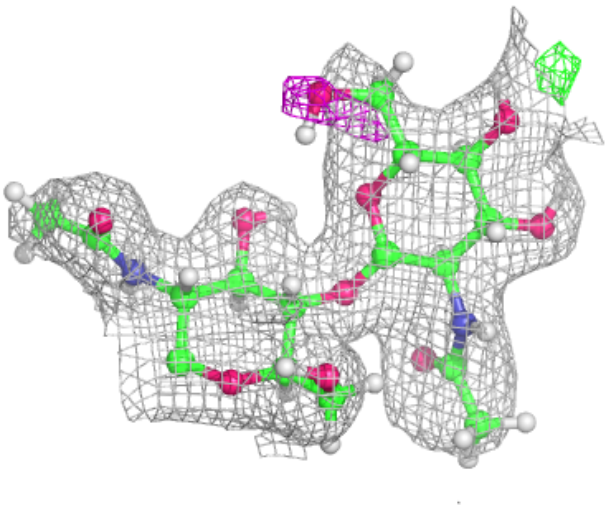
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

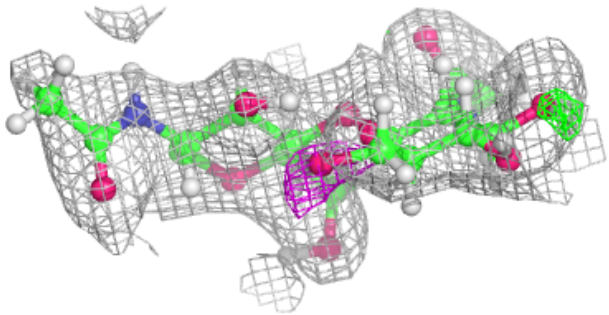
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	H	2	14/15	0.77	0.34	53,56,60,60	13
6	MAN	I	4	11/12	0.80	0.41	44,48,51,52	10
6	MAN	L	4	11/12	0.81	0.23	44,47,50,51	10
5	NAG	J	2	14/15	0.83	0.29	47,50,54,55	13
5	NAG	K	2	14/15	0.83	0.35	60,62,68,69	13
5	NAG	K	1	14/15	0.84	0.17	55,57,61,62	12
5	NAG	G	2	14/15	0.89	0.22	42,46,48,48	13
5	NAG	G	1	14/15	0.90	0.12	34,38,40,41	12
5	NAG	J	1	14/15	0.91	0.11	42,43,46,47	12
5	NAG	H	1	14/15	0.92	0.14	48,50,52,52	12
6	MAN	I	5	11/12	0.92	0.11	35,36,38,38	10
6	BMA	I	3	11/12	0.92	0.12	34,37,41,41	8
6	MAN	L	5	11/12	0.93	0.09	36,38,39,39	10
6	BMA	L	3	11/12	0.94	0.13	35,38,41,42	8
6	FUC	L	6	10/11	0.94	0.09	29,31,32,32	10
6	NAG	I	2	14/15	0.96	0.09	26,29,31,32	12
6	NAG	I	1	14/15	0.96	0.09	29,30,33,33	11
6	NAG	L	1	14/15	0.96	0.08	26,28,28,30	11
6	NAG	L	2	14/15	0.96	0.08	25,28,30,33	12
6	FUC	I	6	10/11	0.97	0.09	32,33,34,34	10

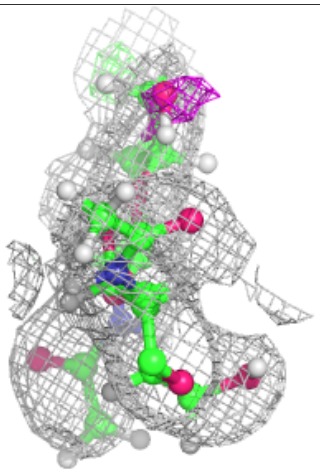
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

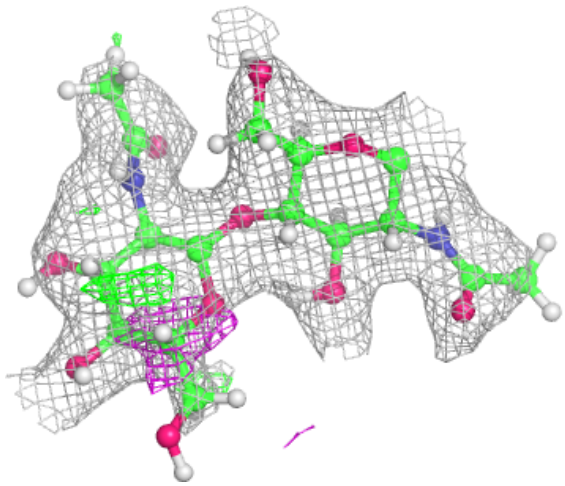


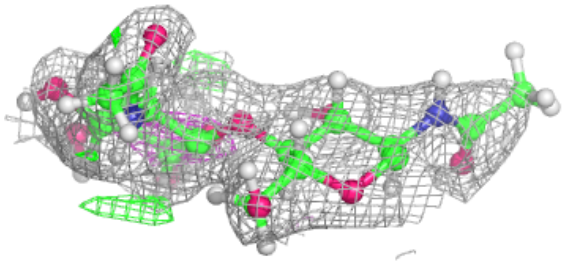


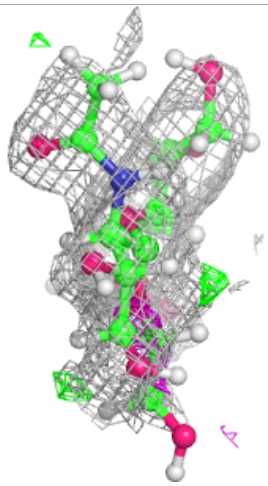


Electron density around Chain H:

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

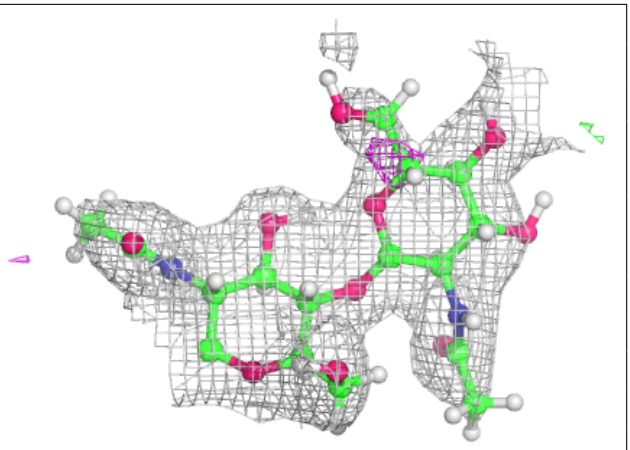


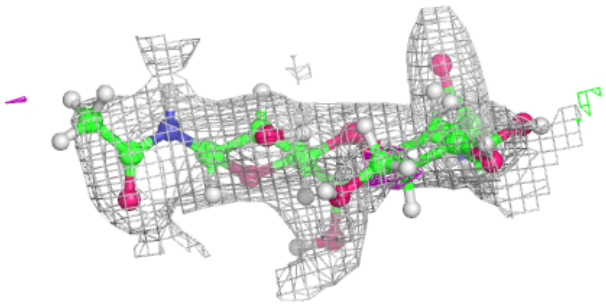


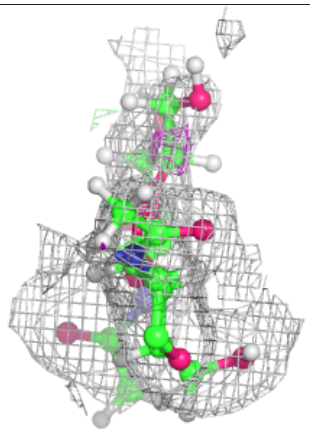


Electron density around Chain J:

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

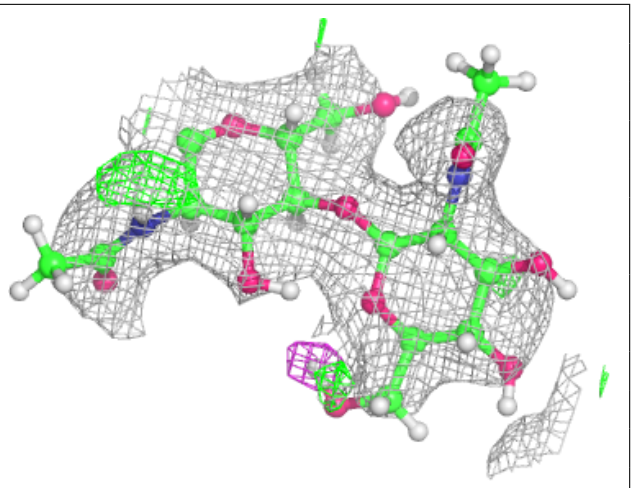


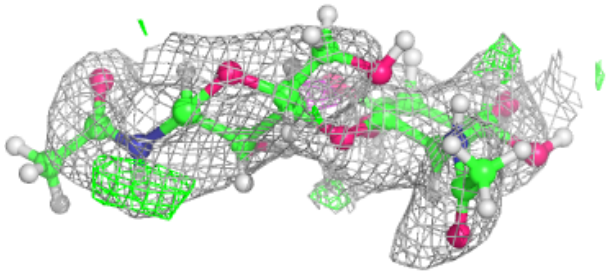


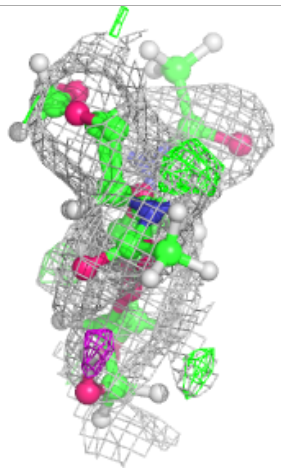


Electron density around Chain K:

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

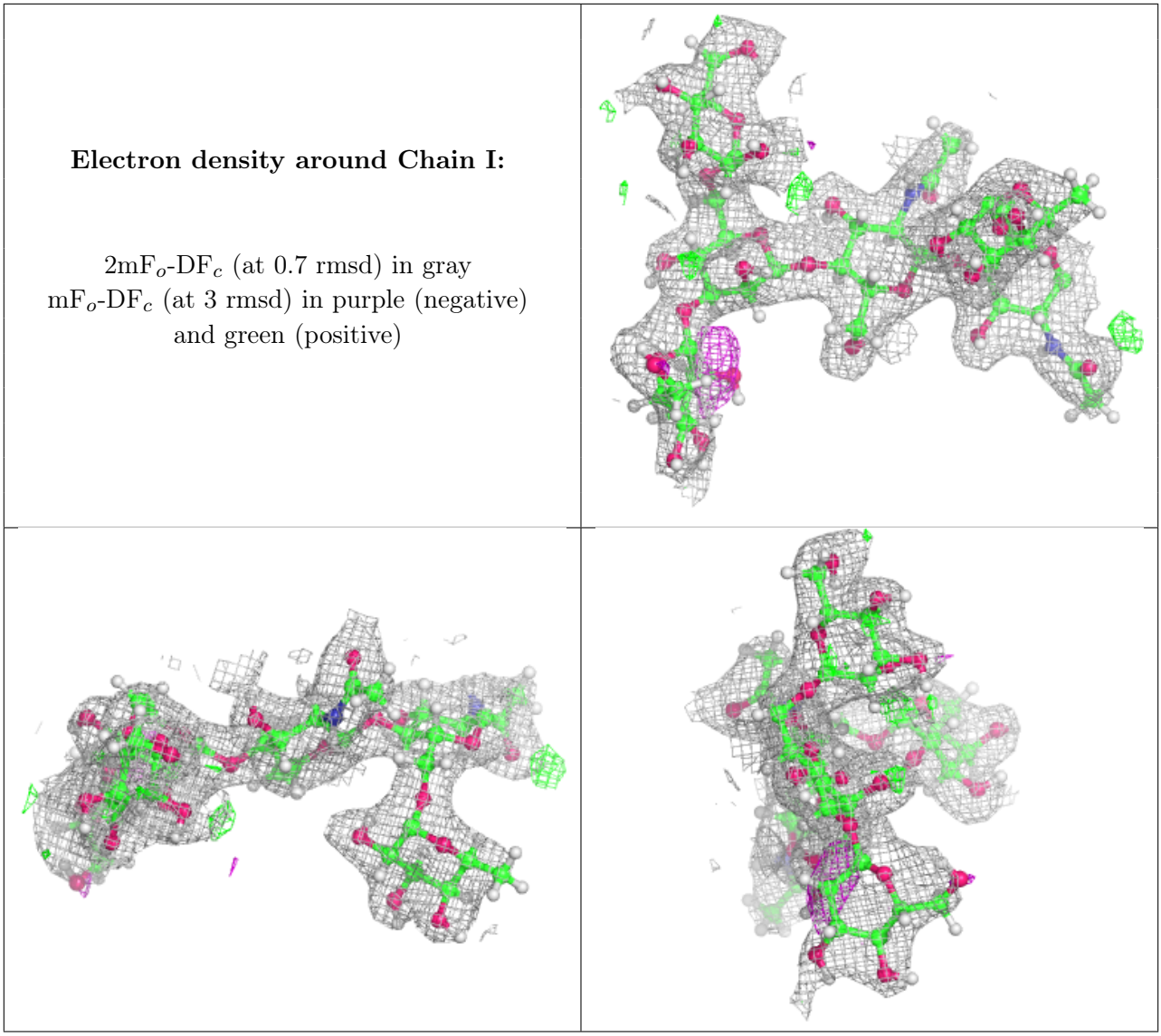






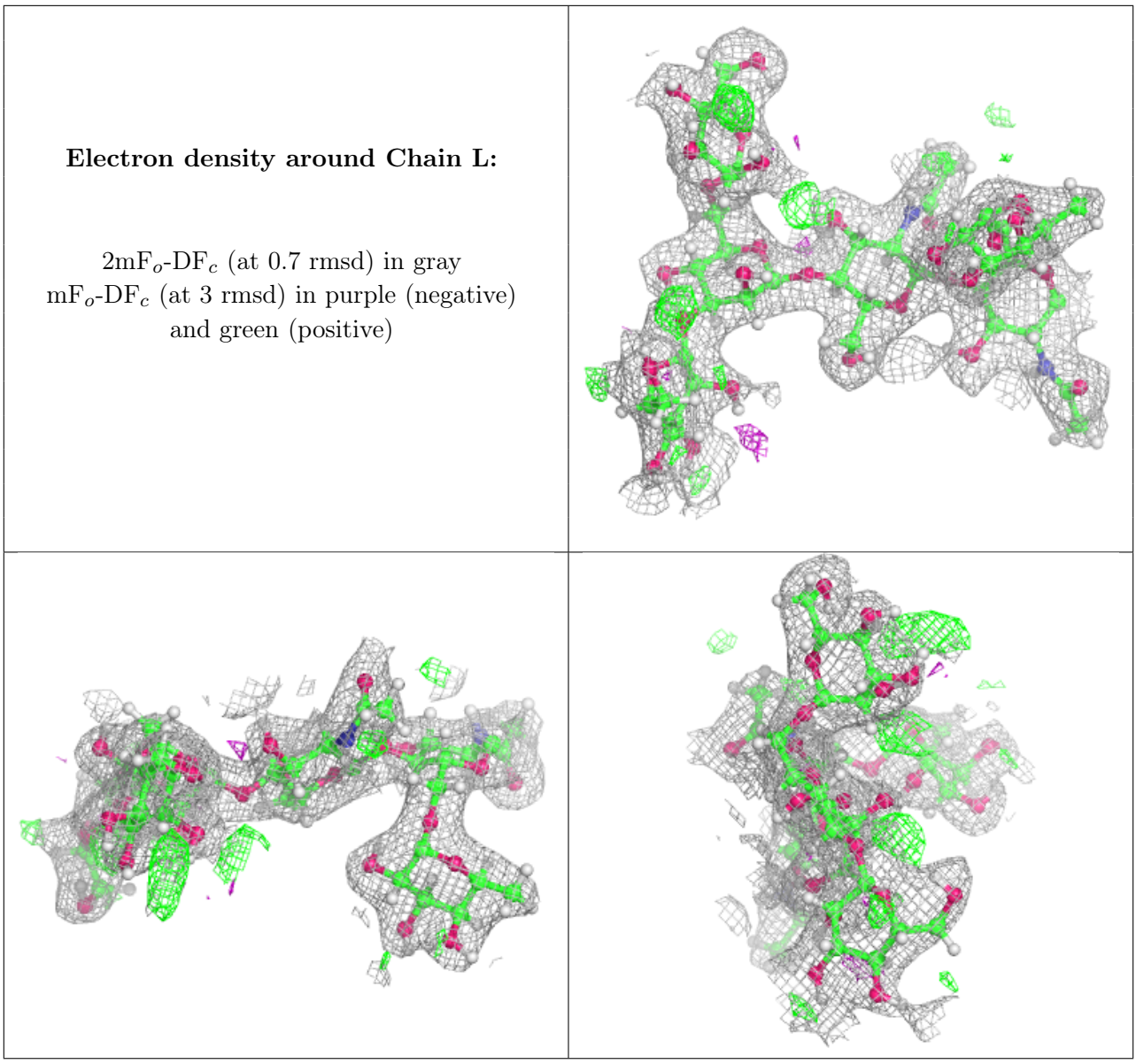
Electron density around Chain I:

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



Electron density around Chain L:

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



6.4 Ligands

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
7	EDO	B	803	4/4	0.74	0.25	40,41,42,42	6
12	PEG	B	805	7/7	0.85	0.25	48,50,52,52	10
11	PO4	B	804	5/5	0.86	0.40	76,76,76,76	0
7	EDO	B	802	4/4	0.87	0.20	39,39,41,41	6
7	EDO	B	806	4/4	0.87	0.14	43,44,46,46	6

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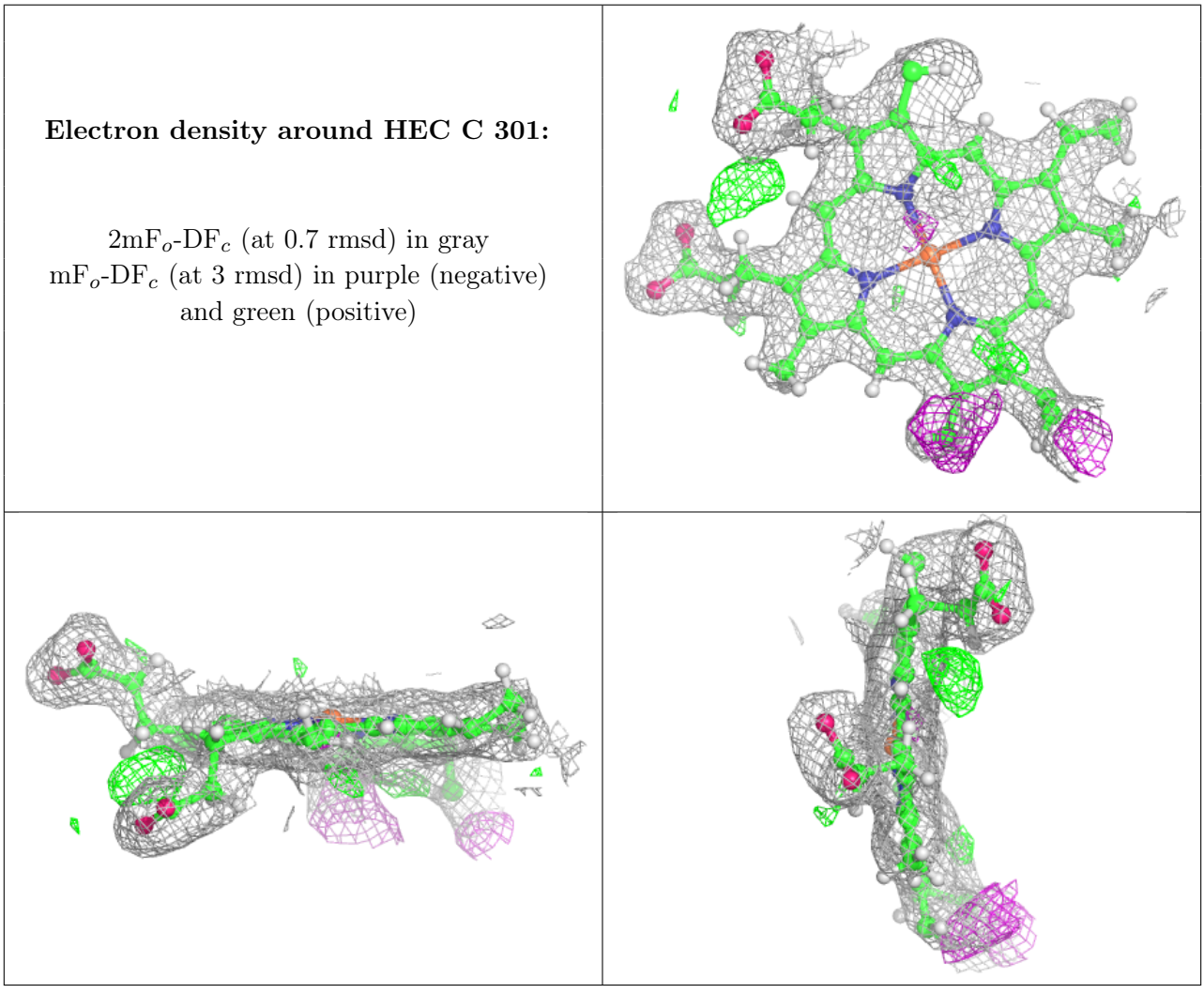
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	A	301	4/4	0.91	0.11	40,41,42,42	6
8	HEC	C	301	43/43	0.95	0.12	24,29,33,36	28
8	HEC	A	302	43/43	0.96	0.12	18,24,29,33	28
9	CL	A	303	1/1	0.99	0.05	21,21,21,21	0
10	CA	D	801	1/1	0.99	0.05	25,25,25,25	0
10	CA	B	801	1/1	1.00	0.09	26,26,26,26	0
9	CL	C	302	1/1	1.00	0.04	20,20,20,20	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.

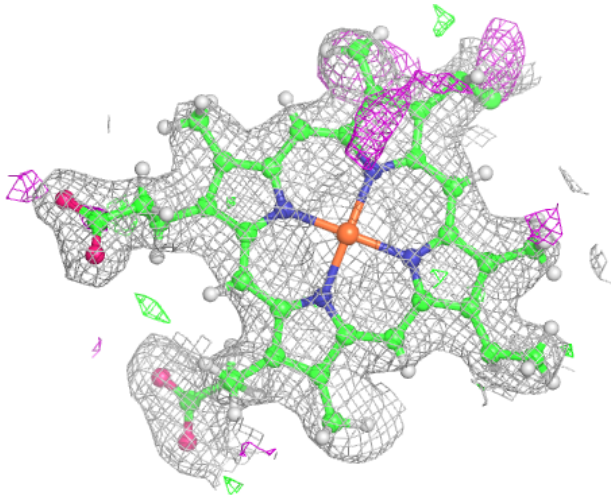
Electron density around HEC C 301:

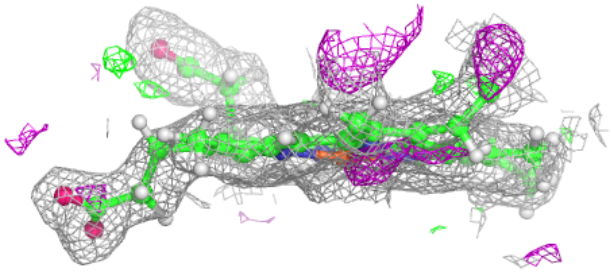
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

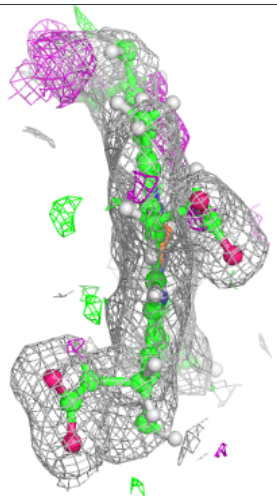


Electron density around HEC A 302:

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

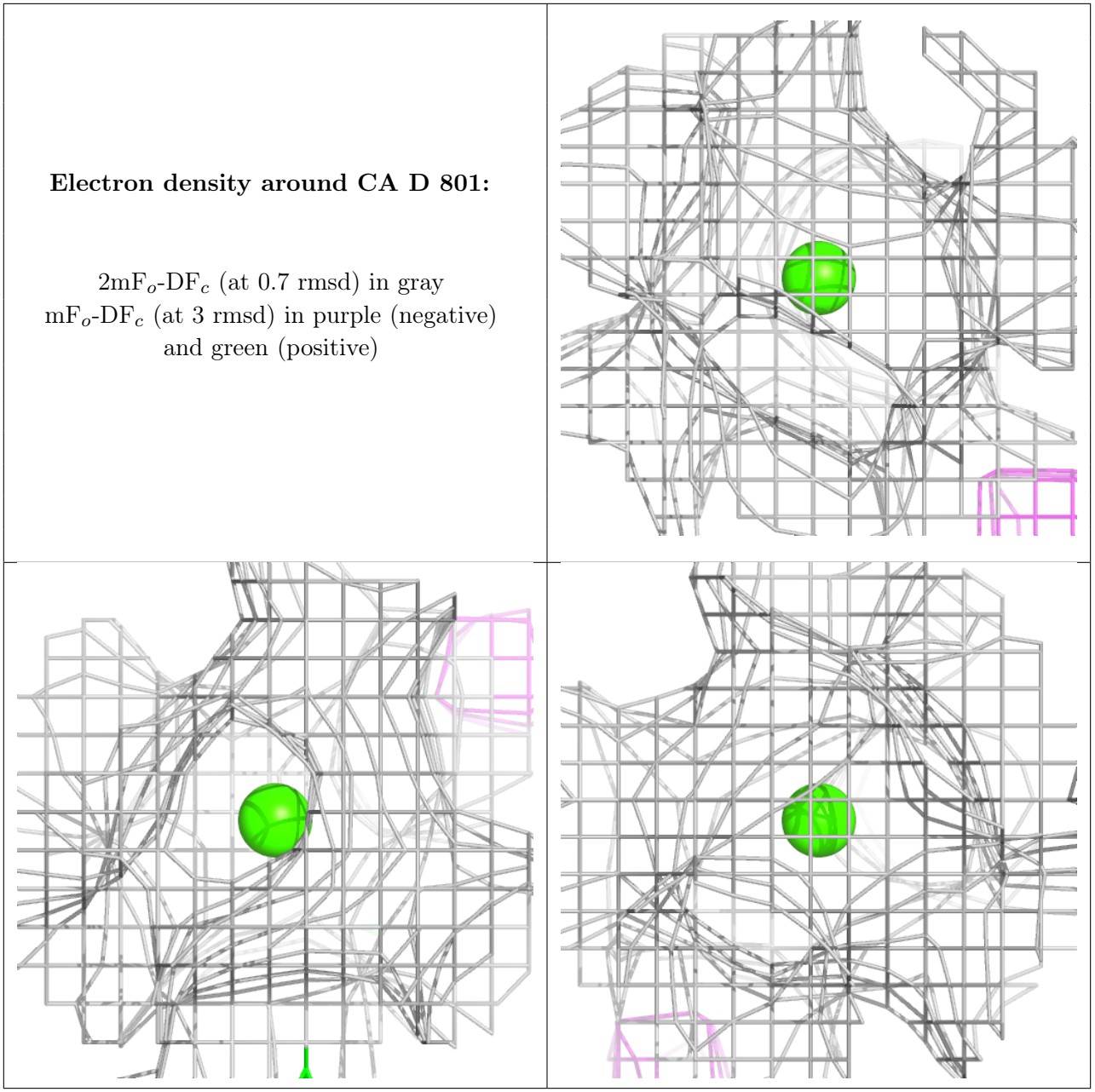






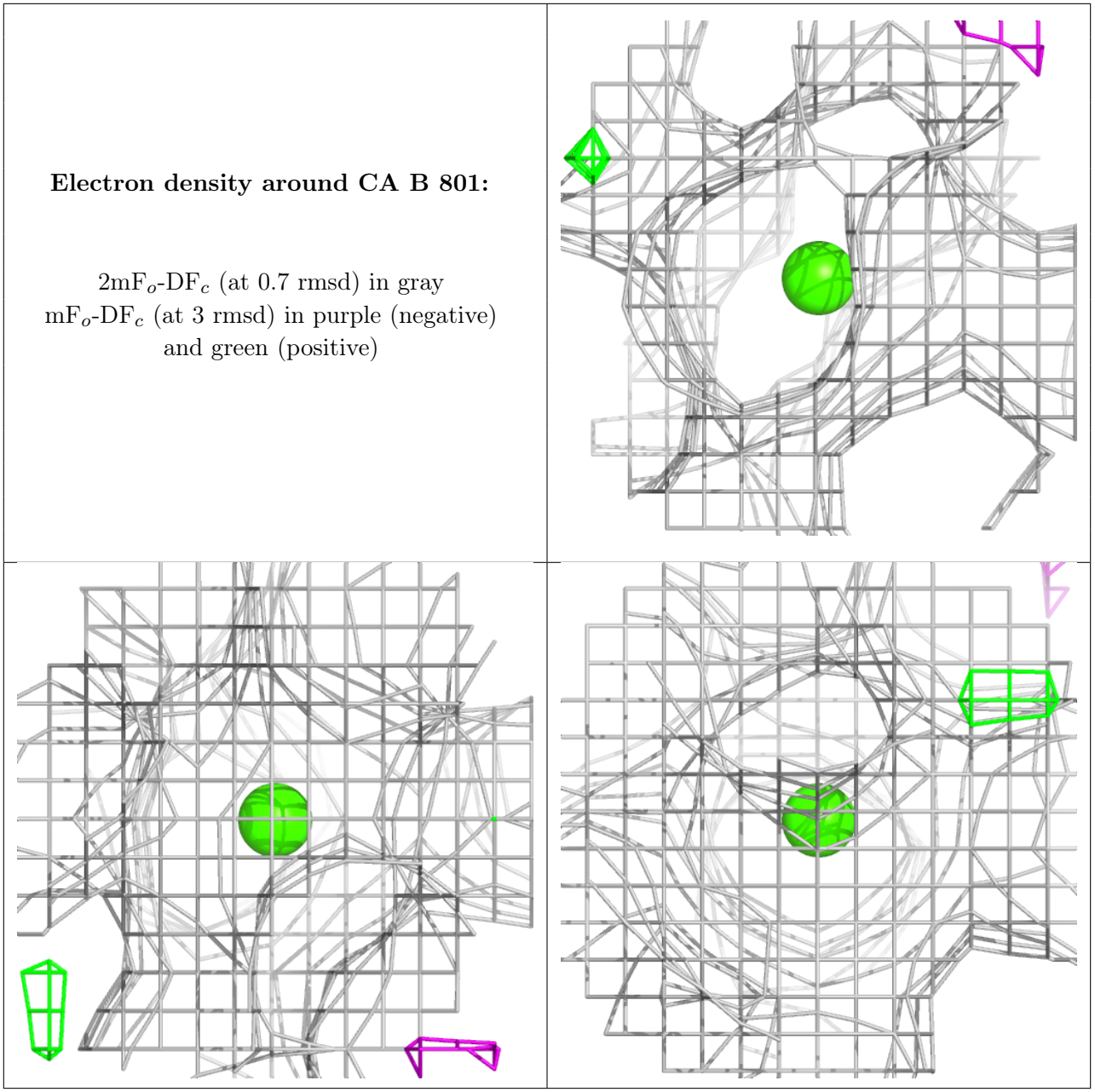
Electron density around CA D 801:

$2mF_o$-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:

$2mF_o$-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)

There are no such residues in this entry.